PROJECT INITIATION

September 13, 1967

Project Title: Interface Phenomena in Engineering Materials

Project No.: A-1024

Project Director: Dr. L. J. Scheibner

Sponsor: Air Force Office of Scientific Research

Effective: 1 September 1967

Estimated to run until: 31 August 1970

Type Agreement: F44620-63-C-0003

Amount: $350,000*

Reports: Interim Scientific Reports

Final Scientific Report

Contract Person: Mr. John E. Lintner, Contracting Officer

Air Force Office of Scientific Research

1400 Wilson Boulevard

Arlington, Virginia 22209

* $175,000, first year

$75,000, second year

$57,750, third year

Assigned to Physical Sciences Division

OPIES TO:

[ ] Project Director
[ ] Director
[ ] Associate Director
[ ] Assistant Director(s)
[ ] Division Chiefs
[ ] Branch Head
[ ] General Office Services
[ ] Engineering Design Services
[ ] Photographic Laboratory
[ ] Research Security Officer
[ ] Accounting
[ ] Purchasing
[ ] Report Section
[ ] Library

2212-66}
PROJECT TERMINATION

GEORGIA INSTITUTE OF TECHNOLOGY
Engineering Experiment Station

PROJECT TITLE: Interface Phenomena in Engineering Materials
PROJECT NO: A-1044
PROJECT DIRECTOR: Dr. E. J. Scheibner
SPONSOR: Air Force Office of Scientific Research
TERMINATION EFFECTIVE: August 31, 1972

All charges have cleared
CHARGES SHOULD CLEAR ACCOUNTING BY:

PHYSICAL SCIENCES DIVISION

COPIES TO:
Project Director
Director
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PROGRESS REPORTS NO. 1 & 2

PROJECT No. A-1044

AN INTERDISCIPLINARY RESEARCH PROGRAM ON THE INTERFACE PHENOMENA IN ENGINEERING MATERIALS

(Project THEMIS Contract F44620-68-C-0008)

15 January 1968

Sponsored by
DEPARTMENT OF THE AIR FORCE
AIRCRAFT RESEARCH

Prepared by
GEORGIA INSTITUTE OF TECHNOLOGY
ATLANTA, GEORGIA 30332
PROGRESS REPORTS NO. 1 & 2

PROJECT No. A-1044

AN INTERDISCIPLINARY RESEARCH PROGRAM ON THE INTERFACE PHENOMENA IN ENGINEERING MATERIALS

(Project THEMIS Contract F44620-68-C-0008)

15 January 1968

Sponsored by
DEPARTMENT OF THE AIR FORCE
AIR FORCE OFFICE OF SCIENTIFIC RESEARCH

Prepared by
GEORGIA INSTITUTE OF TECHNOLOGY
ATLANTA, GEORGIA 30332
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<thead>
<tr>
<th>TABLE OF CONTENTS</th>
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<td>IDENTIFICATION AND PARTICIPATION OF PERSONNEL</td>
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<td>TRIPS AND VISITS</td>
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</tr>
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<td>ABSTRACTS OF SEMINARS PRESENTED UNDER THE PROGRAM</td>
</tr>
</tbody>
</table>
INTRODUCTION

Project THEMIS (A-1044) is a comprehensive program of research, initiated in September 1967 under Contract No. F44620-68-C-0008 and sponsored by the Air Force Office of Scientific Research. The program, covering phenomena occurring at the interfaces between different materials or between different phases of the same material, is oriented toward materials of practical importance in engineering, but is intended to contribute knowledge of the phenomena at a fundamental level. It is planned to complete a critical review of interface phenomena which will provide a focus on DoD needs in specific problem areas and thereby indicate where the emphasis should be placed in the studies at the fundamental level.

The experimental and theoretical activities of the program are organized into the following independent but related sub-programs:

(1) Thermodynamics of Interfaces (A-1044-101) and (A-1044-115)
(2) Measurements of Thermodynamic Quantities (A-1044-102)
(3) Electron Interactions with Solids (A-1044-103)
(4) HEED/LEED Studies of Gas-Solid Interactions (A-1044-104)
(5) Optical Studies of Interfaces in Controlled Environments (A-1044-105)
(6) Field Emission and Field Ion Microscopy (A-1044-106)
(7) Ultrasonic Effects on Metal Processing (A-1044-107)
(8) Adhesion, Friction and Wear Studies (A-1044-108)
(9) Solidification and Machinability of Metals (A-1044-109)
(10) Surface and Diffusion Coatings (A-1044-116)

Analytical support for these primary research areas is available through the Analytical Instrumentation Laboratories of the Physical Sciences Division (A-1044-112). X-ray diffraction studies in support of these areas is available through the Diffraction Laboratories of the Physical Sciences Division.
The division's Technical Information Section is collecting existing information covering the various aspects of interface fundamentals and administrative support is being provided through the Office of Interdepartmental Programs.

Task descriptions identifying primary areas of interest and specific tasks undertaken are provided for each sub-program on a quarterly basis, and are contained in Section II, together with quarterly progress reports.

The interdisciplinary approach of the program involves faculty members, graduate students and undergraduate students in the Schools of Chemical Engineering, Physics, Mechanical Engineering, Electrical Engineering and Chemistry, together with members of the Engineering Experiment Station's Physical Sciences and High Temperature Materials Divisions. Identification and participation of personnel involved in the experimental and theoretical aspects of the program are included in Section III.

Trips and visits in connection with the program are included in Section IV.

A series of seminars has been established under the program, whereby each participating school will sponsor a seminar by a faculty member carrying on studies in a related discipline. Abstracts of seminars to date are given in the Appendix, together with papers presented for publication.
1. Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

1. As program manager, Dr. Scheibner will be responsible for coordination of the research and the supervision of certain technical and administrative tasks.

2. He will provide the necessary briefing to the administration as required.

3. He will maintain liaison with the technical monitor and other representatives in DoD laboratories in regard to the relevance of the technical program to DoD needs.

4. He will plan and organize a technical conference on interface phenomena.

2. List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>E. J. Scheibner</td>
<td>25%/12 months (partially supported by Division)</td>
</tr>
</tbody>
</table>

3. List equipment, maintenance & operating, and travel needs, giving brief justification.

None

Signature  

E. J. Scheibner  

Program Manager  

School or Dept.  

EES - PSD
1. Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

   Appropriate studies in the area of chemical thermodynamics will be undertaken when the need arises in other parts of the program.

   Primarily the contribution of Dr. Ziegler will be in reviewing the individual tasks periodically.

2. List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

   PERCENT TIME
   NAME                     PERCENT TIME
   W. T. Ziegler            Hourly as Needed

3. List equipment, maintenance & operating, and travel needs, giving brief justification.

   None

   Signature
   W. T. Ziegler

Program Manager                School or Dept.  Chemical Engineering
1. Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

Measurements will be made to determine certain surface thermodynamic parameters. In particular, the surface tension of metals will be determined by measurements of very small strain differentials resulting from exposing the cleaned surfaces of thin foils to various gases in a special ultra-high vacuum chamber.

During the First Quarter the design of the special vacuum chamber will be completed and an order will be placed. Construction will begin on the micro strain apparatus. The vibration free table needed for mounting the experiment will be built or purchased as the chamber design is finalized. Various accessory items will be collected for inclusion in the system as needed.

2. List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>B. R. Livesay</td>
<td>25%</td>
</tr>
<tr>
<td>J. Eriksson</td>
<td>15%</td>
</tr>
<tr>
<td>Graduate Student</td>
<td>50%</td>
</tr>
<tr>
<td>Machinist, Technician</td>
<td>150 hours</td>
</tr>
</tbody>
</table>

3. List equipment, maintenance & operating, and travel needs, giving brief justification.

<table>
<thead>
<tr>
<th>Equipment</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Granville-Phillips Electro Ion Pump</td>
<td>$5,500</td>
</tr>
<tr>
<td>Special Vacuum Chamber</td>
<td>4,000</td>
</tr>
<tr>
<td>Sorption Pump, Gas Delivery System</td>
<td>4,811</td>
</tr>
<tr>
<td>Residual Gas Analyzer Head</td>
<td>4,000</td>
</tr>
<tr>
<td>Vibration Free Table</td>
<td>300</td>
</tr>
<tr>
<td>Travel</td>
<td>300</td>
</tr>
<tr>
<td>M &amp; S</td>
<td>1,100</td>
</tr>
<tr>
<td>Relay Rack</td>
<td>$100</td>
</tr>
<tr>
<td>Highly Regulated D.C. Power</td>
<td>100</td>
</tr>
<tr>
<td>Supply</td>
<td>160</td>
</tr>
<tr>
<td>Gauge</td>
<td>625</td>
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<tr>
<td>Gauge Control</td>
<td></td>
</tr>
<tr>
<td>Ion Bombardment Equipment</td>
<td>400</td>
</tr>
</tbody>
</table>

Signature
B. R. Livesay
Program Manager
School or Dept. EES - PSD
Measurement of Thermodynamic Quantities

During the Fall Quarter, detail design work was accomplished on the equipment needed for the surface tension measurement. The theoretical analysis of the problem has been pursued by Dr. Eriksson, and he has completed the rough draft of a paper describing this work for publication.

The special ultra-high vacuum chamber required to house the surface tension apparatus has been designed, and an order is placed with Varian Associates. A high speed electro-ion pump was ordered from Granville-Phillips. Some preliminary experiments indicated that a special concrete slab poured into the ground and isolated from the building would be necessary for our ultimate precision. An electronic light chopping technique is being explored to minimize the effect of vibrations on the system. Details of the gas delivery system have been worked out and the orders are being placed.

A thermodynamic fundamental equation has been derived for the surface phase of a solid exposed to an adsorbing has. This equation is more general than the corresponding equation given by Gibbs in the sense that it is applicable with less restriction as to the state of strain of the solid surface. An equation has been obtained relating the surface tension to reversible cleavage work. Some new thermodynamic expressions were derived for the effect of temperature and gas pressure changes on the surface tension and on the reversible cleavage work.

Bill Livesay
Task Leader
1. Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

Measurements will be made to determine certain thermodynamic parameters. In particular, the surface thermodynamic parameters. In particular, the surface tension of metals will be determined by measurements of very small strain differentials resulting from exposing the cleaned surfaces of thin foils to various gases in a special ultra-high vacuum chamber.

During the next quarter, the construction of the various sub-assemblies making up the surface tension apparatus will continue. It was determined that a special vibration slab poured in the ground, separated from the building, is required, and this is being done. The testing and the sub-assemblies will be done as they are completed so that the entire system can be ready for mounting in the vacuum chamber when it arrives.

2. List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
<th>PERCENT TIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>B. R. Livesay</td>
<td>.25</td>
<td>.15 thru January '68</td>
</tr>
<tr>
<td>J. Eriksson</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Roger Woodward (optical detector electronics)</td>
<td>4 weeks (40 hours)</td>
<td></td>
</tr>
<tr>
<td>Grad. Stud. (Vacant)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

3. List equipment, maintenance & operating, and travel needs, giving brief justification.

A sorption pump, delivery system and gauge are required to make the system operational. M&S needs for electronics for photo cell detector, attachments to the gas delivery system, and feedthroughs for the vacuum system.

$5,000

$1,000
1. Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

   Research consists essentially of developing a means of characterizing solid surfaces with respect to structure and composition for monolayer coverages of impurities. Work during the First Quarter will be concerned with developing a high-resolution electron spectrometer and setting up a vacuum system which will contain the experiment.

2. List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>Academic Year</td>
</tr>
<tr>
<td>L. N. Tharp</td>
<td>50%</td>
</tr>
<tr>
<td>Research Engineer</td>
<td>50%</td>
</tr>
<tr>
<td>Undergraduate Student</td>
<td>25%</td>
</tr>
</tbody>
</table>

3. List equipment, maintenance & operating, and travel needs, giving brief justification.

   For M. E. Sikorski and L. N. Tharp, see the following page.


**Equipment List**

1. Bakeable, ion pumped basic vacuum system  
   (supplied with glass bell jar)  
   $14,500.00

2. Custom chamber (for adhesion and electron  
   spectroscopy measurements)  
   4,500.00

3. Accessory items
   A. Observation window (Varian - 5 1/2" diameter)  
   548.00
   B. Crystal manipulator (Varian LEED type)  
   2,135.00
   C. One linear motion feedthrough (Varian)  
   475.00
   D. Two rotary motion feedthroughs (Varian) @ $355  
   710.00
   E. Miscellaneous electrical feedthroughs  
   325.00
   F. Simple Granville-Phillips gas delivery system  
   2,000.00

4. LEED optics (Varian 3-grid) (Needed in 2nd or 3rd  
   quarter)  
   5,535.00

5. Quadrupole residual gas analyzer (with sensing  
   head)  
   13,000.00

6. Electronics and hardware for electron spectrometer
   A. High-resolution spectrometer (M&S and PSD)  
   3,500.00
   B. Miscellaneous power supplies  
   1,500.00
   C. Pulse counting circuitry  
   1,500.00
   D. X - Y plotter (Varian)  
   2,000.00
Electron Interactions with Solids

The efforts of the past quarter have been aimed at the design and construction of the high-resolution spectrometer and associated vacuum system and accessory equipment. The design of the vacuum system has been completed, and the purchase of this item awaits only the sponsor's approval.

An accessory LEED optics has been designed, the major parts have been made, and the unit is essentially ready for final assembly.

Materials are being obtained for the construction of the high-resolution spectrometer, and machine work on the first parts of this instrument will be begun during the next quarter.

L. N. Tharp
Task Leader
1. Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

Research efforts are currently aimed at the design and construction of a high-resolution electron spectrometer and supporting electronics and vacuum equipment. During the next quarter it is expected that most efforts will be concentrated on the construction of the electron monochromator, to be followed by testing of vacuum system and preliminary testing of monochromator while construction of analyzer is begun.

2. List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
<th>Academic Year</th>
<th>Summer</th>
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</thead>
<tbody>
<tr>
<td>L. N. Tharp</td>
<td>25%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>R. P. Woodward</td>
<td>50%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>K. B. Wear</td>
<td>25%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>G. W. Spann</td>
<td>50%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Shop man</td>
<td>100%</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

3. List equipment, maintenance & operating, and travel needs, giving brief justification.

Capitol equipment same as submitted with last task description except that items 1, 2, 4, and 5 should be deleted.

Additional $2,000 in M.S. required for assembling some of the electronics and to cover materials for electron spectrometer.

Signature ____________________________

L. N. Tharp

Program Manager ____________________________

School or Dept. Physical Sciences Division
The study of gas-solid interactions will be undertaken for the chemical systems considered in THEMIS. The initial stages of reactions will be investigated with low energy electron diffraction. The composition, morphology, epitaxy, and structure of thick films of reaction products will be determined by electron microprobe techniques, optical and electron microscopy, and high energy electron diffraction. Equipment will be designed so that reactions of materials in highly corrosive atmospheres can be studied under a wide range of pressures and temperatures. These procedures will be used in cooperation with other tasks within the THEMIS program.

Specific work to be done in the Second Quarter includes the design and construction of a corrosive gas handling manifold. The chemical problems of interest to THEMIS will be defined, literature survey of these specific problems will be made, and the methods of investigation outlined.

1. List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
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<tbody>
<tr>
<td></td>
<td>Academic Year</td>
<td>Summer</td>
</tr>
<tr>
<td>Gary W. Simmons</td>
<td>20%</td>
<td>20%</td>
</tr>
<tr>
<td>Robert Young</td>
<td>25%</td>
<td>100%</td>
</tr>
<tr>
<td>Graduate Student (Chemical Engineering or Metallurgy)</td>
<td>(vacant)</td>
<td></td>
</tr>
</tbody>
</table>

2. List equipment, maintenance & operating, and travel needs, giving brief justification.

1. Corrosive gas delivery system and auxiliary pumping station for LEED-HEED system (estimated cost: $4,800.00).
2. General purpose reaction chamber for gas-solid interactions (estimated cost: $5,200.00).
3. Maintenance and operation e.g., chemicals and liquid nitrogen (estimated cost: $500.00).
4. Travel to other laboratories and to professional meetings (estimated cost: $400.00).

Signature
Gary W. Simmons
Program Manager
School or Dept. EES - PSD
LEED Studies and Gas Solid Interaction

As originally planned, the first quarter was devoted entirely to the design of a general purpose reaction chamber.

G. W. Simmons
Task Leader
1. Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

The study of gas-solid interactions will be undertaken for the chemical systems considered in THEMIS. The initial stages of reactions will be investigated with low energy electron diffraction. The composition, morphology, epitaxy, and structure of thick films of reaction products will be determined by electron microprobe techniques, optical and electron microscopy, and high energy electron diffraction. Equipment will be designed so that reactions of materials in highly corrosive atmospheres can be studied under a wide range of pressures and temperatures. These procedures will be used in cooperation with other tasks within the THEMIS program.

The components for the general purpose gas-solid reaction chamber are now on order. The specific work during the next quarter will be the construction and testing of this reaction system. In anticipation of specific research in the following quarters, efforts are continuing in defining the chemical problems related to the THEMIS program. Subsequently, literature surveys of specific problems will be undertaken.

2. List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
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</thead>
<tbody>
<tr>
<td>Gary W. Simmons</td>
<td>25%</td>
</tr>
<tr>
<td>Kenneth B. Wear</td>
<td>25%</td>
</tr>
<tr>
<td>Robert L. Young</td>
<td>25%</td>
</tr>
<tr>
<td>Graduate Student</td>
<td>Vacant</td>
</tr>
<tr>
<td>Technical assistance and machinist</td>
<td>$500</td>
</tr>
</tbody>
</table>

3. List equipment, maintenance & operating, and travel needs, giving brief justification.

Materials and supplies:

- Liquid nitrogen, gases, and chemicals $200
- Sample materials including single crystals $500

Signature

Gary W. Simmons

Program Manager

School or Dept. EES - PSD
1. Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

An interface will be characterized by an optical response function such as the real and imaginary parts of the index of refraction. Measurements will be made in a controlled environment from the vacuum ultraviolet into the infrared. Particular attention will be given to the electronic structure associated with chemical bonding.

During the First Quarter, the following objectives will be accomplished:

1. complete move into new laboratory,
2. continuation of optical measurements on some thallium halides,
3. test ultra-high vacuum sample chamber, and
4. design and construct reflectivity apparatus for ultra-high vacuum chamber.

2. List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>J. R. Stevenson</td>
<td>25%</td>
</tr>
<tr>
<td>Undergraduate</td>
<td>25%</td>
</tr>
<tr>
<td>Undergraduate</td>
<td>25%</td>
</tr>
<tr>
<td>Graduate Student</td>
<td>33%</td>
</tr>
</tbody>
</table>

3. List equipment, maintenance & operating, and travel needs, giving brief justification.

<table>
<thead>
<tr>
<th>Item</th>
<th>Cost</th>
<th>Justification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vacuum U.V. arc + power supply</td>
<td>($3,450)</td>
<td>M &amp; S ($250 per month)</td>
</tr>
<tr>
<td>Residual gas analyzer</td>
<td>($10,600)</td>
<td>Travel - AFS and Air Force ($300)</td>
</tr>
<tr>
<td>Grating - vacuum U.V.</td>
<td>($1,000)</td>
<td>Cambridge</td>
</tr>
<tr>
<td>Laser source for infrared</td>
<td>($15,000)</td>
<td>Infrared grating instrument and gratings ($12,500)</td>
</tr>
</tbody>
</table>

Signature:   
James R. Stevenson  
Program Manager:  
School or Dept.:  
Physics
Optical Properties of Materials

The move from the old Physics Building to the new Physics Building was completed in September. Mr. Harry Ellis, a second year graduate student in Physics, has reassembled the vacuum ultraviolet equipment and has started taking optical reflectivity data on mixed crystals of thallium bromide and thallium chloride. Reflectivity is being measured at 20° and 70° angles of incidence between 6eV and 12eV. Preliminary data indicates a qualitative agreement with the data obtained by Hinsen on individual single crystals of these compounds. Certain structure in the reflectivity data seems shifted in energy from the structure observed in the individual single crystals. This shift in energy rather than the superposition of the reflectivity structure of the two crystal systems suggests that a new bond structure exists in the mixed crystal form which can be probed by optical measurements. A new computer program is being written for a PDP8 computer to see if this machine can satisfactorily solve the Fresnel equations for the optical constants from the reflectivity input.

Mr. Maury Zivitz will join the program in January and has already done preliminary work. Mr. Zivitz will begin an optical study of a semiconductor alloy system, Cd_{3-x}Zn_{x}As_{2}. A group of six samples have been obtained from the semiconductors branch of the U. S. Naval Research Laboratory. As these samples will require an ultra high vacuum to be certain that surface contamination is not a problem, Mr. Zivitz is currently working on a design of a crystal holder and the internal mechanical linkage between the crystal and light pipe. He will use an ultra high vacuum chamber built by Hughes Aircraft and purchased by the School of Physics for this effort.

Mr. Ron George and Mr. Jarvis Aldridge have assisted in routine operations in the laboratory as undergraduate assistants. Mr. Aldridge has investigated some polishing techniques for the Cd_{3-x}Zn_{x}As_{2} samples.

James R. Stevenson
Task Leader
Optical Studies of Interfaces in Controlled Environments

PROJECT NO. A-1044-105
DATE 12/29/67

Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

Optical reflectivity measurements will be continued on mixed crystals of the thallium halides. Measurements will be extended in energy and the reflectivity data will be used to calculate the real and imaginary parts of the index of refraction and the energy loss function. Some preliminary reflectivity data will be obtained on the Cd, Zn, As system; however, reproducible data on this system is not expected until the ultra high vacuum sample chamber is in operation—probably by the end of this quarter. Some consideration will be given to extending our ultraviolet measurements into the infrared.

List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
<th>PERCENT TIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>James R. Stevenson</td>
<td>30</td>
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</tr>
<tr>
<td>Harry Ellis (Grad. Stud.)</td>
<td>50</td>
<td>100</td>
</tr>
<tr>
<td>Maury Zivitz (Grad. Stud.)</td>
<td>50</td>
<td>100</td>
</tr>
<tr>
<td>Jarvis Aldrich (Stud. Asst.)</td>
<td>25</td>
<td>50</td>
</tr>
</tbody>
</table>

List equipment, maintenance & operating, and travel needs, giving brief justification.

- X-Y Recorder - Record reflectivity vs Angle $1200
- Vacuum Pump - Replacement pump on 2nd system $670
- Infrared Thermocouple - Increase sensitivity of infrared equipment $350


Signature James R. Stevenson
Program Manager Physics
School or Dept. Physics
The initial experiments planned for this program will deal with studies of the interfaces in two phase alloy systems. Binary systems of iron-nickel, iron-chromium and titanium-aluminum will be examined for structural characteristics in two phase and supersaturated solid solution conditions. Later possibly the iron-nickel-chromium ternary and alloys with carbon additions will be studies. These materials are important since they represent the basic components of the major high strength alloy systems. However, the development of techniques to study these materials is tedious since the background is limited on FIM/FEM studies of alloys. It is considered that a major portion of the First Quarter will be devoted to producing representative specimens and effective study techniques.

List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
<th>NAME</th>
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<tr>
<td>Robert F. Hochman</td>
<td>12 1/2% (3 months)</td>
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<tr>
<td>Bruce LeFevre</td>
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<tr>
<td>Helen Grenga</td>
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<td>Jack Sampselle</td>
<td>Hourly as needed</td>
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<tr>
<td>Panagiotis Kalofonos</td>
<td>Hourly as needed</td>
</tr>
<tr>
<td>Technical Assistance</td>
<td>40 hours</td>
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</tbody>
</table>

List equipment, maintenance & operating, and travel needs, giving brief justification.

1. Spark cutter for special machining of samples for FIM and FEM. This item is essential to the preparation of samples for study by these techniques. It will also have many ancillary uses in other portions of the overall project. Material Research - Cambridge, England $5,200.

2. M and S costs are high because of vacuum system replacements, imaging gases, liquid cooling media, etc. Dr. Ralph projects costs in excess of $150 a week for average usage of an FIM unit.

Signature
Robert F. Hochman

Program Manager
School or Dept. EES - PSD
Field Emission and Field Ion Microscopy

The work has been mainly related to the imaging characteristics of metals in preparation for examining binary iron-nickel, iron-chromium and titanium-aluminum alloys. System design to obtain the best combination of field ion microscopy and field emission microscopy has also been a major consideration. The use of a fiber optics viewing part has resulted in excellent images. Figure 1 shows a typical micrograph of a Ni₄Mo ordered structure. An excellent example of an antiphase boundary is denoted by the arrows on the photograph.

R. F. Hochman
Task Leader
Figure 1. Field Ion Micrograph of ordered Ni$_4$Mo. Arrow denote antiphase boundary.
TASK DESCRIPTION

FIELD

Field Emission and Field Ion Microscopy

PROJECT NO. A-1044-106

DATE January 29, 1968

Give a concise abstract of research under task and a summary of the specific work to performed during the next quarter.

Objective: To study interface boundaries in solid solutions and two phase alloys and determine solid surface vapor phase interaction.

Research for This Period:
1. Study the antiphase domain boundary structure in ordered Ni$_2$Mo.
2. Determine the habit plane of the rotational antiphase boundaries in ordered Ni$_2$Mo.
3. Determine the preferred (low energy) configurations of translational antiphase boundaries.
4. Determine imaging characteristics for Ti$_2$Al type structures.

List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
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<td>Bruce LeFevre</td>
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<tr>
<td>Helen Grenga</td>
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</tr>
<tr>
<td>Jack Sampselle-Student Assistant</td>
<td>Hourly as needed</td>
</tr>
<tr>
<td>Panagiotis Kalofonos - G. R. A.</td>
<td>Hourly as needed (40 hours)</td>
</tr>
</tbody>
</table>

List equipment, maintenance & operating, and travel needs, giving brief justification.

Spark cutter for special machining of samples for FIM and FEM. This item is essential to the preparation of samples for study by these techniques. It will also have many ancillary uses in other portions of the overall project.


M and S costs are high because of vacuum system replacements, imaging gases, liquid cooling media, etc. Dr. Ralph projects costs in excess of $150 a week for average usage of an FIM unit.

Signature Robert F. Hochman

Program Manager Chemical Engineering
Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

Preliminary experiments, examining the surface tension of mercury on aluminum, have shown a measurable decrease in when the aluminum plate was ultrasonically activated. This effect could produce significant advances in practical problems involving surface wetting and solid-liquid interfaces in solidification.

Experiments are planned to measure the surface energy of liquid and solid metals. Initial surface tension measurements will be made when the system is under ultrasonic activation by the sessile drop technique. Later it may be possible to coordinate studies of surface tension with Bill Livesay's experiments.

Work in this area will also be coordinated with Matt Sikorski's friction studies because of his background in ultrasonics.

List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

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<tbody>
<tr>
<td>Robert F. Hochman</td>
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<tr>
<td>J. T. Ratliff</td>
<td></td>
</tr>
<tr>
<td>Francis Toploski (Traineeship)</td>
<td></td>
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</tbody>
</table>

List equipment, maintenance & operating, and travel needs, giving brief justification.

Two special high vacuum systems, including necessary feedthrough collars, sorption pump, partial pressure analyzer glass to metal seals (to be assembled by Varian). $9,785

Special Bronson ultrasonic transducer and horn. $ 540

Signature

Robert F. Hochman

Program Manager

School or Dept. EES - PSD
Ultrasonic Effects on Surface Tension

Preliminary studies of the change of surface tension of water and mercury have been performed. A water droplet was placed on an ultrasonically activated metal horn and the characteristics of the droplet observed as a function of energy and frequency. At a frequency of 25.5 kilocycles, the bubble was observed to flatten out and wet the stainless steel surface. Once the ultrasonic energy was stopped, the water droplet assumed its original contours. Figure 1 was taken during the application of ultrasonic energy showing the flattening of the bubble.

When the frequency was decreased to 20.5 kilocycles, the water droplet was evaporated from the surface at the same energy setting. Similar effects were found with regard to increasing the energy in this same range of frequencies. However, the resonant frequency of the horn is rated at 20 kilocycles and hence more energy may be applied to the droplet at the lower frequency due to resonance. A complete analysis variation of frequency of energy is underway.

Similar experiments were initiated with mercury on a titanium tipped ultrasonic horn. Preliminary experiments do not show flattening of the drop, but rather a rapid evaporation of the mercury droplet. Further experiments varying energy and frequency are underway.

Studies have also been initiated on casting and surface tension of metal wires under ultrasonic activation.

R. F. Hochman
Task Leader
Figure 1. Photograph of water bubble during the application of ultrasonic energy.
### TASK DESCRIPTION

**TITLE**

Ultrasonic Effects on Surface Tension

**PROJECT NO.** A-1044-107

**DATE** 29 January 1968

Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

**Objective:** To determine the effect of ultrasonic energy on surface energy of solids and on solid-liquid interface during solidification.

1. Complete construction of dead weight tensile machine with attachment for ultrasonically actuating wire samples.

2. Perform preliminary tests on B.C.C., F.C.C. and H.C.P. metals. Wires of 0.005 and 0.000 mil diameter have been ordered and should be received in this quarter. Wire material—high purity—Al, Fe, Be, Ni, W, Mo, Sn, Ag and Cu.

3. Continue studies on the ultrasonic effects on casting Al, Cu and Au Cu.

4. Continue studies on liquid surface tension under ultrasonic activation. Measure change in $\gamma$ for H$_2$O, Hg and possibly Sn or Ga.

### List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

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<tr>
<th>NAME</th>
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<td>Robert F. Hochman</td>
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<td>Academic Year</td>
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<tr>
<td>Titus Ratliff</td>
<td>33%</td>
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<tr>
<td>Panagiotis Kalifonos</td>
<td>20 hours as needed</td>
<td></td>
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<tr>
<td>Francis Toploski (Traineeship)</td>
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</table>

### List equipment, maintenance & operating, and travel needs, giving brief justification.

Two special high vacuum systems, including necessary feedthrough collars, sorption pump, partial pressure analyzer glass to metal seals (to be assembled by Varian).

Special Bronson ultrasonic transducer and horn

**Signature**

Robert F. Hochman

**Program Manager**

School or Dept. Chemical Engineering
The aim of this program is to investigate those fundamental properties of materials which influence friction, adhesion and wear phenomena.

Present work started under another project is concerned with the effects of composition and ordering on the coefficient of adhesion in some solid-solution binary alloys. To date the evaluation has been completed of the copper-nickel and silver-gold systems except for the order-disorder effects in the 50/50 atomic per cent gold-silver alloy.

During the coming Quarter, adhesion studies will be made of the silver-palladium, platinum-cobalt, copper-gold and copper-zinc (8-brass) alloys. In addition, design work will start on an ultra-high vacuum chamber for friction, adhesion and wear studies (see page 24 of the Themis Proposal). Final design and manufacture of parts for the vacuum chamber will follow in the Second Quarter.

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<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
<th>PERIOD</th>
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<td>M. E. Sikorski</td>
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<td>Academic Year</td>
</tr>
<tr>
<td>S. Haas (GRA)</td>
<td>33% (3 months)</td>
<td>Summer</td>
</tr>
<tr>
<td>R. Goodman</td>
<td>Full-time for 1 week (40 hours)</td>
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</table>

M. E. Sikorski -- ASLE/ASME Conference, Chicago, October 17-19, visit to IITRI $250

Ultra-high vacuum pumping station and experiment chamber (See specifications prepared by L. N. Tharp for electron spectroscopy studies.) $500

High purity polycrystalline metal specimens (5) $500
Friction, Adhesion and Wear Studies

Work has been progressing nicely during the Fall Quarter of 1967 on the adhesion studies of binary alloy systems. A satisfactory procedure has been worked out for the encapsulation and annealing of specimens of platinum-cobalt and gold-copper alloys. Adhesion data have been obtained for the above alloys in "as-received" and disordered conditions. Ordering heat treatments and adhesion studies of ordered specimens will follow in the next quarter.

The analysis of adhesion data obtained on CuNi specimens of various alloy compositions has revealed a good correlation with the stacking fault energy (SFE) values extracted from the literature. In brief, low SFE is associated with high coefficients of adhesion and vice versa. Preliminary literature search, which has resulted in a considerable number of useful references, has shown that this type of correlation also exists for other alloy systems. In addition, it appears that the SFE is correlated with the number of electrons per atom. Thus, it should be possible to design materials with improved friction and wear characteristics by a judicious choice of impurity elements added in correct proportion. To pursue this idea further, Dr. Engel has agreed to determine the number of electrons per atom for the same alloy systems that are being used adhesion tests. Tertiary alloys should be prepared to test the validity of this apparent correlation between the number of electrons per atom (e/a) and adhesion properties. Supplementary studies involving electron spectroscopy and optical reflectivity measurements should be conducted on appropriate metal systems to elucidate the interconnections between the mechanical properties and electronic structure of metals.

The size and location of ports in the UHV friction chamber has been finalized and the design of the vacuum twist-compression apparatus is in progress.

M. E. Sikorski
Task Leader
The aim of this program is to investigate those fundamental properties of materials which influence friction, adhesion and wear phenomena.

During the last quarter the work was concerned with the effects of composition and ordering on the coefficients of adhesion in some solid-solution binary alloys. It is anticipated that during the Winter Quarter the work will be completed on the platinum-cobalt, gold-copper and copper-zinc (β-brass) alloys. The results will be correlated with the stacking-fault energies and the number of electrons per atom according to Engel's rules. Design work will proceed on ultra-high vacuum friction and adhesion apparatus. Work may also start on nickel-molybdenum and titanium-aluminum ordering alloys.

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<td>S. Haas (GRA)</td>
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<tr>
<td>R. Newsom (TA)</td>
<td>1/4 time for 3 months</td>
</tr>
<tr>
<td>K. Wear (RP)</td>
<td>1/2 time for 3 months</td>
</tr>
</tbody>
</table>

Additional flanges for the ultra-high vacuum system
High purity alloy specimens of nickel-molybdenum and aluminum-titanium
This study is concerned with the conditions at the mold-casting interface during the casting of metals. Interfacial energy and the thermal properties of both casting and mold are factors which govern the temperatures and heat transfer during solidification; therefore, these factors govern mold life and solidification rates. To determine the quantitative effect of these factors for the solidification of metals cast in metal molds is the objective of the research.

During the First Quarter, the following tasks are planned:

(a) Make a complete literature search and write a preliminary review on the current knowledge of this problem.

(b) Construct an experimental apparatus for the casting of metals and investigate the problem of temperature measurements and the use of ultrasound for detecting the conditions at the interface.
Conditions at Mold-Casting Interface During the Casting of Metals

This study, which will be concerned with the temperature and heat transfer in the casting of metals in metal molds, was initiated during the Fall Quarter. A literature survey has shown that extensive work has been done on the problem during the last two or three decades with some work dating back approximately fifty years. The literature search was approximately one-half completed and it has become apparent that some time will be required to assimilate and classify the findings.

Experimental work has been planned and equipment ordered. Initiation of the experimental program will begin as soon as equipment delivery is obtained which should be before the middle of the Winter Quarter.

J. H. Murphy
Task Leader
1. Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

This study is concerned with the conditions at the mold-casting interface during the casting of metals. Interfacial energy and the thermal properties of both casting and mold are factors which govern the temperatures and heat transfer during solidification; therefore, these factors govern mold life and solidification rates. To determine the quantitative effect of these factors for the solidification of metals cast in metal molds is the objective of the research.

During the Winter Quarter, the following tasks are planned:

(a) Continue and hopefully complete the literature survey.

(b) Complete construction of experimental apparatus, test and evaluate different types of thermocouples for use in temperature and heat transfer determination.

2. List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
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<tbody>
<tr>
<td>John H. Murphy</td>
<td>25%</td>
</tr>
<tr>
<td>Derek C. Rigby (Undergraduate)</td>
<td>Hourly as Needed</td>
</tr>
</tbody>
</table>

3. List equipment, maintenance & operating, and travel needs, giving brief justification.

(a) No travel anticipated. (b) A previous request was made for a Honeywell viscorder; an instrument is now available but the following auxiliary equipment is required: 9 galvonometers - $1,250, 2 signal conditioners - $500, rack - $220, amplifier - $400, miscellaneous potentiometers - $500.
The ultimate goal of this task is to publish a technical monograph on "interface fundamentals and their relevance to specific DoD materials problems". Near the completion of the critical review, the emphasis will be shifted to those areas or materials for which there is a high priority need for more fundamental information. The review will also establish the scientific and engineering community most directly concerned with interface problems. Interested members of this group will participate in a conference planned for the second year of the program.

First Quarter efforts will be directed towards organizing references and bibliographies on the subject into retrievable form so that the review may proceed without undue concern for information gathering details.

<table>
<thead>
<tr>
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<td>R. L. Bullock</td>
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<tr>
<td>Richard Summers</td>
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</table>

(Materials and supplies will be provided by H-700-132.)
Critical Review of Interface Fundamentals in Engineering Materials

During the First Quarter, some 400 documents were catalogued, assigned descriptors and entered into the projects' information system. A machine search from the Defense Documentation Center provided 25 documents which were subsequently ordered from DDC. Manual searches covering research for the past five years indexed in "International Aerospace Abstracts," "Scientific and Technical Aerospace Reports," and "Solid State Abstracts" have produced the balance of the documents (with the exception of RIAS reports supplied by AFOSR).

An alphabetical list of documents by title and author which were added to the system during the First Quarter was circulated to task leaders. A second list is being prepared now. Monthly acquisition lists will be distributed, if interest warrants.

R. L. Bullock
Task Leader
The ultimate goal of this task is to publish a technical monograph on "interface fundamentals and their relevance to specific DoD materials problems". Near the completion of the critical review, the emphasis will be shifted to those areas or materials for which there is a high priority need for more fundamental information. The review will also establish the scientific and engineering community most directly concerned with interface problems. Interested members of this group will participate in a conference planned for the second year of the program.

Second Quarter efforts will be directed towards evaluating the some 390 documents presently in the projects' information system for relevance to the critical review. Reference sources cover a five-year period and are now being catalogued monthly so that the collection is reasonably current.

List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

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<th>NAME</th>
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<td>Richard Summers</td>
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</table>

List equipment, maintenance & operating, and travel needs, giving brief justification.

(Materials and supplies will be provided by H-700-132.)

Signature  
R. L. Bullock  
EES - PSD
Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

The following techniques are being investigated and developed for future application on the project:

1. A combination autoradiographic-replica technique for electron microscopy.
2. Failure analysis by electron fractography.
3. Increasing electron probe microanalyzer sensitivity to surface compositions by glancing beam technique.

List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
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<tr>
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<td>J. L. Hubbard</td>
<td>30%</td>
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<tr>
<td>J. W. Johnson</td>
<td>5%</td>
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</tbody>
</table>

(This work is currently supported on E-700-245.)

List equipment, maintenance & operating, and travel needs, giving brief justification.

None

Signature
John L. Brown
Program Manager
School or Dept. EES - PSD
Analytical Studies - Electron Microscopy

The only service work furnished during this period was spectroscopic analysis of alloy samples for A-1044-108.

Preliminary work on developing a technique for examining solid-liquid interfaces in metals with the electron microscope has been done. Thin bismuth films have been prepared and thickness measurements made.

J. L. Brown
Task Leader
The development of research and analytical techniques complementary to the various phases of Proj. THEMIS.

During the next quarter the following techniques will be investigated:

1. Examination of the solid-liquid interface of low-melting alloys in the electron microscope.
2. Application of glancing beam techniques for increasing the sensitivity of the microprobe to thin surface layers.

List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

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<td>10%</td>
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<tr>
<td>J. L. Hubbard</td>
<td>5%</td>
<td>12 mos.</td>
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List equipment, maintenance & operating, and travel needs, giving brief justification.

Signature ________________________________
Program Manager John L. Brown
School or Dept. Physical Sciences Division
This project is concerned with the effect of the crystallographic properties of a metal on its casting characteristics. It is expected that for the first year or so the main concern of the project will be the determination of the relative orientation between grains, the position and Burgers vectors of dislocations and any other strain fields within the grains, the shapes of the grains, and the true contact angles between grains in the metal. The materials to be studied are aluminum and aluminum alloys. The property of greatest practical concern at the outset is susceptibility to hot shortness. The results of the studies on pure aluminum should be of interest to theoreticians since the relative interfacial energy at a solid liquid interface is measured in terms of the contact angle.

The general techniques to be used are x-ray diffraction topography, x-ray source-image distortion, and variants thereof. These will allow the crystallographic properties mentioned above to be studied in three dimensions, non-destructively, in bulk samples. These features, particularly the opportunity for determining the full three-dimensional orientation of contiguous grains, offers several obvious advantages over some other methods. The first experimental work undertaken will necessarily be a determination of the (cont.)

List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

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<tr>
<td>C. E. Wagner</td>
<td>50%</td>
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</table>

(It is expected this work will lend itself to a thesis in metallurgy. If available, during the Second Quarter it will be advisable for one graduate student to be employed approximately 50% of the time.)

List equipment, maintenance & operating, and travel needs, giving brief justification.

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<thead>
<tr>
<th>Item</th>
<th>Cost</th>
<th>Justification</th>
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<tbody>
<tr>
<td>Film and darkroom supplies</td>
<td>$100</td>
<td>No travel is expected the First Quarter, but at least one trip will probably be undertaken within the first year.</td>
</tr>
<tr>
<td>Samples</td>
<td>200</td>
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</tr>
<tr>
<td>Electron tubes and miscellaneous laboratory supplies</td>
<td>$200</td>
<td></td>
</tr>
<tr>
<td>X-ray tube (may not be needed in First Quarter)</td>
<td>800</td>
<td></td>
</tr>
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</table>
particular variations of the two techniques best suited to the study. It is expected that this will be accomplished during the first quarter of work.

In addition to the experimental work it will be necessary to do a literature search, and also to provide the personnel with a general background in the metallurgical aspects of the project.
Crystallographic Studies of Casting Phenomena

Work during the past quarter consisted of determining the orientation of some grains in a stainless steel sample to be studied by x-ray diffraction topography, putting in operating condition the x-ray generator to be used for the topographic studies and modifying the topographic camera so that section topographs could be made.

A stainless steel sample which had grains on the order of 1 mm on a side and which was on hand was selected for the initial work of determining the variations of the techniques best suited to the study.

Some time was spent correcting a malfunction (arching in the high voltage head) in the Jarrell-Ash microfocus x-ray generator. It now appears to be operating properly.

A modification of the topographic camera provides more precise positioning of a slit in the diffracted x-ray beam, and the production of high quality lead slits in precision widths down to one thousandth of an inch or less (in our shop) now allow section topographs to be made.

C. E. Wagner
Task Leader
Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

This project is concerned with the effect of the crystallographic properties of a metal on its casting characteristics. It is expected that for the first year or so the main concern of the project will be the determination of the relative orientation between grains, the position and Burgers vectors of dislocations and any other strain fields within the grains, the shapes of the grains, and the true contact angles between grains in the metal. The materials to be studied are aluminum and aluminum alloys. The property of greatest practical concern at the outset is susceptibility to hot shortness. The results of the studies on pure aluminum should be of interest to theoreticians since the relative interfacial energy at a solid liquid interface is measured in terms of the contact angle.

The general techniques to be used are x-ray diffraction topography, x-ray source image distortion, and variants thereof. These will allow the crystallographic properties mentioned above to be studied in three dimensions, non-destructively, in bulk samples. These features, particularly the opportunity for determining the full three-dimensional orientation of contiguous grains, offers several obvious advantages over some other methods.

Work during the next quarter will consist of making conventional reflection and section topographs and some reflection SLD patterns of a selected grain and its surrounding neighbors, in order to determine defect densities and strain fields in the grains.

List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

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<tr>
<th>NAME</th>
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<tbody>
<tr>
<td>C. E. Wagner</td>
<td>25%</td>
<td>Academic Year</td>
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Due to the unavailability of the microfocus generator, work during the last quarter was at the average rate of 17%. This slack will be taken up soon.

A graduate student is not necessary this quarter but it will be advisable to have one during the following quarter at approximately 50% time.

List equipment, maintenance & operating, and travel needs, giving brief justification.

No change in first-report request.

Signature       C. E. Wagner
Program Manager School or Dept. Physical Sciences
Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

The nature of an interdisciplinary research program requires an administrative unit to provide support across departmental lines with regard to planning, organizing, control, and communication.

The immediate task of this unit will be to establish any personnel status changes required for payroll purposes, to institute budget reporting procedures, to assist in expediting material and equipment requests, and to establish both formal and informal communications. The latter will include report scheduling assistance as requested, and the establishment of an internal newsletter for general information purposes.

<table>
<thead>
<tr>
<th>NAME</th>
<th>Academic Year</th>
<th>Summer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jon C. Barbour</td>
<td>50%</td>
<td>50%</td>
</tr>
<tr>
<td>Janet C. Maddox</td>
<td>100%</td>
<td>100%</td>
</tr>
</tbody>
</table>

List equipment, maintenance & operating, and travel needs, giving brief justification.

None

Signature
Jon C. Barbour
Administrative Support

The efforts during the Fall Quarter were primarily devoted to acquiring a basic understanding of the existing administrative organization. Operations concerning Procurement, Budgeting, Accounting and Contract Administration were studied. Actual administration of Project THEMIS was performed within the existing framework. Internal procedures were established as needed to operate within the framework.

Informational presentations concerning the objectives of Project THEMIS and its relationship to the Institute's objectives were presented to schools, colleges, and administrative officers of the Institute. Also, a system of reporting future work and progress has been established.

J. C. Barbour
Task Leader
Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

This task is concerned with the development of an effective system of administrative support for task leaders, school directors, and other administrative officers concerned with Project THEMIS.

Work during the Winter Quarter will be concerned with the further definition of existing operations and the establishment of a framework for the system. Special attention will be given to time-and-effort reporting and inventory control of equipment.

List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jon C. Barbour</td>
<td>50%/12 months</td>
</tr>
<tr>
<td>Clerk</td>
<td>100%/12 months</td>
</tr>
</tbody>
</table>

List equipment, maintenance & operating, and travel needs, giving brief justification.

None

Signature

Jon C. Barbour

Program Manager

School or Dept. EES - PSD
Give a concise abstract of research under task and a summary of the specific work to be performed during the next quarter.

High and low temperature data for the interaction of non-reactive gases with graphite and boron nitride will be obtained and analyzed in terms of statistical thermodynamics models in order to elucidate the nature and magnitude of the forces acting between the gas and the solid and also among the gas molecules in the presence of the solid.

During the next quarter, construction of a high precision adsorption apparatus will continue. This apparatus will be capable of covering a very broad range of gas-solid interactions from very low coverage up to the range of nucleation and multilayer formation. The apparatus is nearly completed and calibration procedures will begin immediately.

List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
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</thead>
<tbody>
<tr>
<td>Robert A. Pierotti, Assoc. Prof. Chem.</td>
<td>10% (supported by Chem. dept.)</td>
</tr>
<tr>
<td>Reginald Ramsey, Rayonier Fellow (Ph.D. candidate)</td>
<td>100%</td>
</tr>
<tr>
<td>Mr. Ramsey will require support starting the Spring Quarter at the rate of $265 per month.</td>
<td></td>
</tr>
<tr>
<td>Students on related work:</td>
<td></td>
</tr>
<tr>
<td>David Newsome, NDEA Fellow (Ph.D. candidate)</td>
<td>100%</td>
</tr>
<tr>
<td>Joseph Delay, Teaching Ass't. in Chem. (Ph.D. candidate)</td>
<td>50%</td>
</tr>
</tbody>
</table>

List equipment, maintenance & operating, and travel needs, giving brief justification.

- Personal Services: none
- Capital Outlay: $200
- Operating Expenses: 400
- Travel: none

Signature: Robert A. Pierotti
Program Manager: School or Dept.: Chemistry
This task is a literature search with the purpose of identifying technology gaps and specific research needs related to Surface and Diffusion Coatings.

Work to be performed from February 9, 1968 to March 31, 1968 will consist of the literature search definition and initiation of the literature search.

List faculty members with percentage of time on task. List graduate students & support personnel. Identify vacant positions. List graduate students doing related work but supported by fellowships, etc. Designate the task leader by an underline.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>Academic Year</td>
<td>Summer</td>
<td></td>
</tr>
<tr>
<td>Mr. J. D. Walton, Jr.</td>
<td>2</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>Dr. C. W. Gorton</td>
<td>10</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>Mr. C. A. Murphy</td>
<td>2</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>Mr. A. C. Merritt</td>
<td>25</td>
<td>25</td>
<td></td>
</tr>
</tbody>
</table>

List equipment, maintenance & operating, and travel needs, giving brief justification.

Signature

Program Manager

School or Dept. High Temperature Materials Br.
III. IDENTIFICATION AND PARTICIPATION OF PERSONNEL
Project THEMIS (A-1044)
February 1968

A. SENIOR FACULTY MEMBERS

Dr. E. J. Scheibner, Research Professor of Physics and Chief of Physical Sciences Division, EES, is the Program Manager, and is presently devoting 25% time to the program.

Dr. W. T. Ziegler, Regents Professor of Chemical Engineering, will undertake studies in the area of chemical thermodynamics as needed.

Dr. J. R. Stevenson, Associate Professor of Physics, is engaged in optical studies of interfaces in controlled environments, and is presently devoting 25% time to the program, supported in full by institutional funds through the School of Physics.

Dr. R. F. Hochman, Associate Professor of Chemical Engineering, is engaged in studies utilizing field emission and field ion microscopy, as well as studies of ultrasonic effects on surface tension. He is presently devoting 17 1/2% time to the program.

Dr. J. H. Murphy, Associate Professor of Mechanical Engineering, is studying conditions at the mold-casting interface during casting of metals, and is currently devoting 25% time to the program.

Dr. R. A. Pierotti, Associate Professor of Chemistry, joined the program in February and will be examining gas-solid interactions. Dr. Pierotti is presently devoting 10% time to the program, supported in full by institutional funds through the School of Chemistry.

J. D. Walton, Principal Research Engineer and Chief of the High Temperature Materials Division, EES, joined the program in February and will assist in investigations of surface and diffusion coatings. Mr. Walton is contributing 2% time to the program.
B. ASSOCIATE FACULTY MEMBERS

Dr. C. W. Gorton, Professor of Chemical Engineering, joined the program in February and will be investigating present technology regarding surface and diffusion coatings with members of the High Temperature Materials Division. Dr. Gorton will be contributing 10% time to the program.

B. R. Livesay, Research Physicist with the Physical Sciences Division, is studying measurements of thermodynamic quantities and is currently devoting 25% time to the program. In addition, he is pursuing a doctoral degree in Metallurgy (this participation is reflected in the Graduate Research Assistants category of the accompanying chart).

Dr. J. C. Eriksson, Postdoctoral Fellow of Physics with the Physical Sciences Division, studied measurements of thermodynamic quantities during the fall quarter and part of the winter quarter, devoting 15% time to the program. Dr. Eriksson returned to Sweden in February.

L. N. Tharp, Research Physicist with the Physical Sciences Division, is engaged in studies of electron interactions with solids, and is currently devoting 50% time to the program. He is also pursuing a doctoral degree in Physics (this participation is reflected in the Graduate Research Assistants category of the accompanying chart).

Dr. G. W. Simmons, Research Chemist with the Physical Sciences Division, is engaged in low energy electron diffraction studies of gas adsorption on solids, and is devoting 20% time to the program.

M. E. Sikorski, Senior Research Physicist with the Physical Sciences Division, is performing adhesion, friction, and wear studies and is devoting 25% time to the program. In addition, he is pursuing a doctoral degree in Metallurgy (this participation is reflected in the Graduate Research Assistants category of the accompanying chart).
B. ASSOCIATE FACULTY MEMBERS (CONTINUED)

K. B. Wear, Research Engineer with the Physical Sciences Division, is assisting in studies of electron interactions with solids, and is devoting 100% time to the program.

Dr. H. E. Grenga, Postdoctoral Fellow in Chemical Engineering, is engaged in studies utilizing field emission and field ion microscopy. She is contributing 33% time to the program.

Dr. B. G. LeFevre, Assistant Professor of Chemical Engineering, is engaged in studies utilizing field emission and field ion microscopy, and is presently contributing 12 1/2% time to the program.

R. P. Woodward, Assistant Research Engineer with the Physical Sciences Division, is assisting in the design of electronic systems for several tasks, and is presently contributing 50% time to the program. In addition, Mr. Woodward is pursuing a doctoral degree in Electrical Engineering (this participation is reflected in the Graduate Research Assistants category of the accompanying chart).

C. A. Murphy, Research Engineer with the High Temperature Materials Division, joined the program in February. Mr. Murphy is assisting in investigations concerning surface and diffusion coatings, and is contributing 2% time to the program.

C. GRADUATE RESEARCH ASSISTANTS

H. W. Ellis, Masters candidate in Physics, is assisting in the optical studies of interfaces in controlled environments.

P. Kalofonos, Ph.D. candidate in Metallurgy, is assisting in the field emission and field ion microscopy studies.

J. T. Ratliff, Ph.D. candidate in Chemical Engineering, is assisting in the studies of ultrasonic effects on surface tension.
C. GRADUATE RESEARCH ASSISTANTS (CONTINUED)

S. L. Haas, Ph.D. candidate in Mechanical Engineering, is assisting in the adhesion, friction, and wear studies. His research at the doctoral level has been under the direction of Dr. J. A. Bailey, who is maintaining close contact with the program from North Carolina State University.

M. Zivitz, Ph.D. candidate in Physics, is assisting in the optical studies of interfaces in controlled environments.

In addition, the following graduate students, receiving support from other sources, are performing studies related to our THEMIS program investigations (this indirect participation is shown in the accompanying chart):

J. D. Delay, Ph.D. candidate in Chemistry (Teaching Assistant).

D. S. Newsome, Ph.D. candidate in Chemistry (NDEA Fellow).

R. N. Ramsey, Ph.D. candidate in Chemistry (Rayonier Fellow).

D. STUDENT ASSISTANTS

R. L. Young, Senior Physics Student, is assisting in the low energy electron diffraction studies.

M. J. Aldridge, Senior Physics Student, is assisting in the optical studies of interfaces in controlled environments.

R. D. Summers, Senior Physics Student, is assisting in the critical review of interface fundamentals.

A. C. Merritt, Senior Chemical Engineering Student, is assisting in investigations concerning surface and diffusion coatings.

G. W. Spann, Senior Physics Student, is assisting in the studies of electron interactions with solids.
# Representation of Disciplines in Science and Engineering for Project Themis (A-1044)

February 1968

<table>
<thead>
<tr>
<th>Discipline</th>
<th>(A) Senior Faculty Members</th>
<th>(B) Associate Faculty Members</th>
<th>(C) Graduate Research Assistants&lt;sup&gt;1&lt;/sup&gt;</th>
<th>(D) Student Assistants</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical Engineering</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>Chemistry</td>
<td>1</td>
<td></td>
<td>3</td>
<td></td>
<td>4</td>
</tr>
<tr>
<td>Electrical Engineering</td>
<td></td>
<td></td>
<td>1</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>High Temperature Materials (E.E.S.)</td>
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<td>1</td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>Mechanical Engineering</td>
<td>1</td>
<td></td>
<td>1</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>Metallurgy (Chemical Engineering)</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td></td>
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<tr>
<td>Physical Sciences (E.E.S.)</td>
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<td>Physics</td>
<td>1</td>
<td></td>
<td>3</td>
<td>4</td>
<td>8</td>
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<tr>
<td><strong>Total</strong></td>
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<td><strong>11</strong></td>
<td><strong>12</strong></td>
<td><strong>5</strong></td>
<td><strong>35</strong></td>
</tr>
</tbody>
</table>

Notes:

<sup>1</sup>Personnel listed in other categories and pursuing advanced degrees are included under discipline in which the degree is being sought.
IV. TRIPS AND VISITS

Mr. M. E. Sikorski attended the 1967 ASLE/ASME Lubrication Conference in Chicago, October 17-19, 1967. While in Illinois he also visited Dr. John Schey at IITRI. Dr. Schey is engaged in lubrication studies as they pertain to friction, wear, and metalworking operations.

In late November 1967, Mr. Sikorski participated in a Symposium on Interdisciplinary Approach to Friction and Wear, sponsored by NASA and organized by the Southwest Research Institute in San Antonio.
V. APPENDIX
The Effect of Composition and Ordering on the Coefficient of Adhesion in Some Solid Solution Alloy Systems

by

M. E. Sikorski and J. A. Bailey*
Georgia Institute of Technology
Atlanta, Georgia

Abstract

The aim of this work was to investigate those fundamental properties of metal alloys which influence adhesion, and hence friction and wear phenomena. Since the simplest type of alloy system to study is the solid solution system the following metal alloys were chosen for this work: copper-nickel, silver-gold, silver-palladium, copper-gold, platinum-cobalt and copper-zinc (β brass). In addition to the effects of compositions the results of ordering of materials on the coefficient of adhesion were evaluated. In general, the coefficient of adhesion decreases with an increasing amount of order.

The analysis of adhesion data obtained on CuNi specimens of various alloys compositions has revealed a good correlation with the stacking fault energy (SFE) values extracted from the literature. Briefly, low SFE is associated with high coefficients of adhesion and vice versa. A literature search has shown that this type of correlation also exists for other alloy systems. In addition, the SFE appears to be correlated with the number of electrons per atom. Thus, it should be possible to design materials with improved friction and wear characteristics by a judicious choice of impurity elements added in correct proportion.

† This paper is to be published in Wear Magazine.
* Now at the School of Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, North Carolina.
General Discussion Following Dr. Tabor's and Dr. Lawless' Papers†

Recent advances in the understanding of the basic phenomena, such as the effect of crystal structure on friction, have led to the formulation of metal alloys with improved friction and wear characteristics as described by Dr. Johnson of NASA.

Figure 1 shows another example of the importance of crystal structure on adhesion. In this figure the coefficients of adhesion are given for the platinum-cobalt alloy system as a function of cobalt content. It can be seen that as the amount of cobalt is increased, the crystal structure changes and so does the adhesion coefficient. It is possible that in some cases the transition from a mild to a severe wear regime with a subsequent failure of bearings may be traceable to changes in the composition of the bearing materials under prolonged use or severe pressure and temperature conditions.

In addition to the Pt-Co system, other relatively simple binary alloys characterized by complete solid solubility have been studied for the purpose of uncovering important parameters governing adhesion and friction. For example, the copper-nickel alloys, which retain the face-centered cubic structure for all concentrations, have been slid against iron and molybdenum to study the effect of low solid solubility of copper in these elements. Similarly, gold-silver alloys have been slid against iron to evaluate the effects of low solubility of silver in iron. The experiments showed that the adhesion was low when the concentration of the immisible element in the alloy was high. In the above twist-compression tests the specimens were placed in contact under the combined action of normal and tangential forces.

† Submitted for publication in the Proceedings of the Conference on the Interdisciplinary Approach to Friction and Wear.
More recent results on copper-nickel alloys slid against themselves indicate a very interesting correlation between the coefficients of adhesion and the work-hardening coefficients, as well as stacking fault energies of these alloys. Similar work is being presently carried out on silver-gold and silver-palladium alloys in an interdisciplinary effort to relate the materials properties of these alloys to their adhesion and friction behavior.\textsuperscript{2}

1. M. E. Sikorski, V. Kleiza and J. S. Courtney-Pratt, to be published.

2. M. E. Sikorski and J. A. Bailey, to be published.
Coefficient of Adhesion Versus Percent Cobalt for Pt-Co Alloys.
Discussion of Dr. Lawless' Paper

I wish to describe briefly a combined technique for characterizing surfaces which is presently under study at the Georgia Institute of Technology. The approach taken has been to consider the energy distributions of the secondary electrons emitted from a sample in addition to the LEED patterns obtained from the surfaces. LEED can be used to investigate the elastic scattering of the low energy electrons and to get information about the structures of atomically clean single crystal surfaces or surfaces with ordered adsorbed gas layers. However, as was mentioned in Dr. Lawless' lecture, because of the dependence on periodic structures, the LEED patterns can not always be used to detect surface contamination, and no information is given concerning the nature of a contaminant. The secondary electron energy distributions, on the other hand, result from inelastic processes which do not depend in detail on the structure of an adsorbed layer or on the ordering of crystallites in the substrate. These distributions can then be used to study surface contamination. Figure 1 shows an energy distribution curve of electrons for the clean tungsten(110) surface. There are three distinct groups of electrons contributing to the features observed in the curve of Figure 1. The electrons in region I are the elastically reflected primaries. The electrons in region II are primaries which have undergone losses. Region III corresponds to the true secondaries. The small broad peaks that appear in region II and the subsidiary maxima contributing to the structure of the large secondary peak are related to the electronic properties of the material under study and to the contamination present on the surface. Studies have been made thus far of single crystal surfaces of tungsten, graphite and copper, and also aluminum and nickel. Work on additional elemental metals and alloys is contemplated using
single crystal, as well as polycrystalline specimens. It appears that the technique outlined above should be applicable to the characterization of surfaces in friction and wear-type experiments.


5. G. W. Simmons, Georgia Institute of Technology, private communication, 1967.

Figure 1. Energy Distribution Curve of Electrons for the Clean Tungsten (110) Surface.
Abstract of two-part seminar given in the School of Chemical Engineering by Dr. J. C. Eriksson, Postdoctorate Fellow in Physics with the Physical Sciences Division:

Thermodynamics of Fluid Surface Phase Systems

The fundamental thermodynamic relations for a fluid, arbitrarily chosen surface phase are deduced on the basis of general considerations. It is shown that partial surface phase quantities can be introduced in a rigorous way and that partial molar surface phase areas and volumes can be utilized for selecting a particular surface phase for study. The thermodynamic evaluation and molecular interpretation of surface tension measurements for some pure liquids and liquid mixtures is discussed.

Thermodynamics of the Solid-Gas Interface

A general thermodynamic theory of the solid-gas interface valid for physical absorption as well as chemisorption systems is presented. Some implications of the formalism are considered with special emphasis on questions related to measurements of cleavage work, surface tension of solids and surface structure transitions.

Abstract of seminar given in the School of Mechanical Engineering by Douglas Godfrey of Chevron Research Company, Richmond, California:

Boundary Lubrication and Cavitation of Oils & Hydraulic Fluids

Boundary lubrication will be discussed in terms of the lubricating films on sliding surfaces. Films are formed by physical adsorption, chemisorption, and chemical reaction. The physical properties of the films, particularly melting point, shear strength, hardness, and adhesion to the surface, are important to lubrication. Film failure mechanisms include
desorption, melting, solution, discontinuity, detachment, and rupture. This review reveals that there is no adequate theory for boundary lubrication. Also, there is a lack of knowledge of the chemical composition of films on sliding surfaces and their physical properties under conditions of high pressure, high shear rate, and high temperature.

Literature on cavitation of oils and hydraulics fluids will be reviewed briefly. Cavitation can be expected when oil suddenly experiences low pressure, such as during the rapid separation of surfaces and during pure sliding and pure rolling. A motion picture will be shown which shows cavitation between sliding, rolling, and vibrating surfaces. The paper will describe a thin film cavitation apparatus for measuring damage to metals in a hydraulic fluid subjected to ultrasonic cavitation. Typical results will be presented for ferrous and nonferrous metals subjected to cavitation of a phosphate ester.
AN INTERDISCIPLINARY RESEARCH PROGRAM ON THE INTERFACE PHENOMENA IN ENGINEERING MATERIALS

(Project THEMIS Contract F44620-68-C-0008)

A renewal proposal submitted to the

Department of the Air Force
Air Force Office of Scientific Research

by the

Georgia Institute of Technology
Atlanta, Georgia 30332

6 January 1969
Air Force Office of Scientific Research (OAR)
Department of the Air Force
Arlington, Virginia 22209

Attention: Lt. Col. Randal A. Houidobre
Chief, Solid State Sciences Division
Directorate of Physical Sciences

Subject: Contract No. F44620-68-C-0008. Project THEMIS
Renewal Proposal - Interdisciplinary Research
Program on the Interface Phenomena in Engineering Materials

Gentlemen:

The Georgia Institute of Technology desires to submit for your consideration this renewal proposal for the subject Project THEMIS contract. Attachment I of the proposal sets forth the technical and related data, Attachment II presents a special report of progress, while Attachment III covers the administrative and financial portions.

We believe that the enclosed material will give you the necessary information; however, if anything additional is desired, please let us know and we will see that it is forwarded promptly. Any matters pertaining to the scientific program may be referred to the program manager, Dr. Edwin J. Scheibner, Chief, Physical Sciences Division, Engineering Experiment Station. Contractual or administrative matters may be referred to the undersigned. The telephone number is (Area Code 404) 873-4211; the extensions are 272 and 801 respectively.

We appreciate the opportunity of submitting this proposal, and look forward to a continuation of our association with you on this research program.

Very truly yours,

Harry L. Baker, Jr.
Director

Addressee: 10 copies
Enclosures: Attachments I, II and III - 10 copies

cc: Dr. E. D. Harrison, President
Dr. W. L. Bloom, Acting Vice President, Academic Affairs
Dr. A. G. Hansen, Dean, Engineering College
Dr. V. Crawford, Dean, General College
Dr. M. W. Long, Director, Engineering Experiment Station
Dr. E. J. Scheibner, Chief, Physical Sciences Division
AN INTERDISCIPLINARY RESEARCH PROGRAM ON THE INTERFACE PHENOMENA IN ENGINEERING MATERIALS

A renewal proposal submitted to the
Air Force Office of Scientific Research
Project THEMIS Contract F44620-68-C-0008

by the

Georgia Institute of Technology
Atlanta, Georgia 30332

ENDORSEMENTS:

Edwin J. Scheibner
Program Manager

Arthur G. Hansen, Dean
Engineering College

Vernon Crawford, Dean
General College

Maurice W. Long, Director
Engineering Experiment Station

Harry L. Baker, Jr., Director
Research Administration

6 January 1969
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<td>EXHIBIT I: Budget Detail by Categories</td>
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ABSTRACT

The continuation of a comprehensive program of research, initiated under Contract No. F44620-68-C-0008 and covering phenomena occurring at the interfaces between different materials or between different phases of the same material, is proposed. In the conduct of these fundamental and applied studies emphasis is now placed on a broader definition of the interface to include portions of the phases present on either side. The objectives are: (1) to firmly establish a program of fundamental and applied studies on interfaces which along with the necessary technical support groups can lead to a coherent approach to the solution of several materials problems that are relevant to the needs of the Department of Defense; (2) to strengthen the graduate program, particularly at the Ph.D. level, in the academic departments involved by enhancing the professional background of competent faculty, by assisting in the development of specialized laboratory facilities and by providing graduate student support; (3) to provide for the coupling between faculty participants from different disciplines and between the faculty and scientific personnel of DoD laboratories by stimulating their interest in a planned series of critical review papers and by arranging joint seminars or conferences. The projected plan of research includes: (a) a continuation of the studies currently in progress; (b) the development of a general approach for relating fundamental and applied studies to each other; (c) the detailing of mechanisms for describing the fundamental basis of several problem areas; (d) the preparation of review papers for the areas of stress corrosion cracking, wear and machining; and (e) the planning for review papers in other areas.
I. TITLE: Interface Phenomena in Engineering Materials

II. SCOPE:

Interface phenomena are important in many applications of engineering materials and in the basic fabrication processes. Certain fundamental questions with respect to interface effects are common to a wide range of practical problems of direct defense interest. It was initially proposed therefore that coordinated, multidiscipline studies be conducted on several of these fundamental questions in order to provide a basis for approaching the practical problems. As a result of the first year's effort however it is evident that besides the fundamental studies emphasis should be placed on two aspects of the research which have not been explicitly identified previously. The first relates to a broader definition of the interface to include a significant region of the phases present on either side and the interrelationship between interface and bulk properties. The second relates to direction of the research towards a closer correlation of fundamental and applied studies. This approach involves the development of a mechanistic description of selected problem areas, identifying the crucial steps, and then carrying out in-depth theoretical and experimental studies as appropriate.

The objectives of the proposed research are threefold: (1) technical - to firmly establish a program of fundamental and applied studies on interfaces which along with the necessary technical support groups can lead to a coherent approach to the solution of several materials problems that are relevant to the needs of the Department of Defense; (2) academic - to strengthen the graduate program, parti-
cularly at the Ph.D. level, in the academic departments involved by enhancing the professional background of competent faculty, by assisting in the development of specialized laboratory facilities and by providing graduate student support; and (3) management - to provide for the coupling between faculty participants from different disciplines and between the faculty and scientific personnel of DoD laboratories by stimulating their interest in a planned series of critical review papers and by arranging joint seminars or conferences. Another management objective is the adaptation of Institute administrative procedures for budgeting, accounting, purchasing, personnel, etc. to the special requirements of an interdepartmental research program.
III. BACKGROUND AND SUMMARY OF PREVIOUS WORK

Many engineering materials which have desirable structural properties unfortunately are also highly susceptible to environmental factors such as chemical attack in a gaseous or liquid medium. In military applications of certain of these materials, normal stresses combined with the environmental factors can cause catastrophic failure of a critical structural member. Other materials are used in devices where physical, metallurgical, and chemical phenomena at interfaces play a vital part in performance and reliability. These devices would range from electrical contact-type devices containing brushes and slip rings to devices requiring rotating members in bearings. Devices of the latter class and the associated phenomena of friction, wear, and lubrication are of particular concern, for instance, in high-load, high-vacuum, and high-temperature applications. In processing of materials, machinability depends on similar fundamental quantities. Other areas involving interface phenomena are creep and fatigue, diffusion bonding of materials, diffusion coatings, adhesives, the solidification of materials, other types of corrosion and the fabrication and strength of composite materials.

It was recognized that a basic understanding of the properties of solid-solid, solid-liquid and solid-gaseous interfaces would be a common requisite for making significant progress with respect to all of the above engineering materials problems. Furthermore, our acquaintance with the report, Military Themes of High Scientific Merit for Oriented Basic Research, published by the U. S. Army Research Office-Durham, the project THEMIS descriptions of relevant research areas and our participation in the ARPA Coupling Program on Stress Corrosion Cracking (ARPA Order No. 878) brought to our attention the critical defense need
for more fundamental interface studies. Therefore, in our original THEMIS proposal to the Department of Defense dated 1 May 1967 we proposed to approach the basic understanding by considering certain fundamental questions on the thermodynamics of interfaces, structural and compositional aspects, reaction kinetics, and optical or electronic processes. At the same time we proposed to initiate studies which were more practically oriented such as those in solidification, machinability, and adhesion, friction and wear. The initial studies under THEMIS contract F44620-68-C-0008 were begun on 1 September 1967 and represent activities of both experimental and theoretical types by faculty members and students from several schools or divisions of the Institute. The progress of these initial studies and proposed directions in the continuation of the program were reported in our renewal proposal to the Air Force Office of Scientific Research dated 15 January 1968.

The various sub-programs, or tasks, are administered through an Office of Interdepartmental Programs which is under the direction of the program manager. Task descriptions stating briefly the progress under the task, plans for the next period, personnel, equipment and other significant information are required both quarterly and annually from the task leaders. Copies of the annual task descriptions are included in the appendix.

In the previous year's report we identified two areas where some contributions had already been made. One was Sikorski's adhesion studies on CuNi specimens of various alloy compositions in which correlation between stacking fault energies and adhesion coefficients was established. The other was the theoretical work on the thermodynamics of interfaces by Dr. Eriksson. This year we will mention two other areas of interest, the optical studies of Dr. Stevenson and the results of
a survey of surface coatings by Dr. Gorton.

The program in optical physics has been concerned with measurements of optical reflectivity on Cd-Zn-As alloy systems permitting a determination of the complex dielectric constant in studies of collective electron oscillations and inter-band transitions characteristic of these alloys. Measurements are currently being made in two vacuum ultraviolet monochromators capable of covering the wavelength spectrum from approximately 400 Angstroms to the visible region, although for the experimental arrangement used, the data obtainable have been limited by the lithium fluoride cutoff at approximately 1200 Angstroms. A third system is available which can be coupled with a low-energy electron diffraction system for making optical measurements on carefully characterized single crystal surfaces and for comparison of the complex dielectric constant with the energy loss function for slow electrons obtained from inelastic scattering measurements in the same system. A valuable extension of these experiments contemplates the use of the University of Wisconsin Storage Ring as a source of ultraviolet radiation with wavelengths down to 100 to 200 Angstroms. Arrangements are now being made to utilize this facility, and the required auxiliary equipment is under construction. The data thus made available should prove quite useful for comparison with the recent theoretical band structure calculations on the above alloy systems being made at the Naval Research Laboratory.

A detailed survey has been conducted in the area of high temperature, oxidation resistant surface and diffusion coatings to identify gaps in technology and needs for specific research. The survey consisted of a literature survey made with the use of published abstracts in related fields and a letter survey in which question-
naires were sent to a number of individuals closely associated with this broad area of research. The results of this survey have been assembled in the form of a report now in the draft stage. This report contains recommendations concerning new coatings, deposition techniques, basic data related to compounds formed in surface and diffusion coating systems, and methods of evaluation. This internal report will be expanded and finalized by initiating a more comprehensive survey of certain aspects of the surface and diffusion coating problem.

The backgrounds, experience, and interests of the members of the research team at Georgia Tech provide a strong base for advancing the important materials area of interface phenomena. The manner in which this team functions and the plans for including participation by scientific personnel of DoD laboratories are discussed in section V of this proposal. Biographical sketches on two staff members added during the year, Dr. C. W. Gorton, Professor of Chemical Engineering, and Dr. J. M. Bradford, Assistant Professor of Mechanical Engineering, are included in the appendix. Dr. Gorton has assumed the active direction of the program on surface and diffusion coatings. Dr. Bradford came to us from NASA's Langley Research Center where he was engaged in adhesion studies under ultra-high vacuum.
IV. PROJECTED PLAN OF RESEARCH

Surface or interface properties have been recognized as being important in many engineering materials areas but it has been difficult in the past to find an approach that will relate, for example, the results of fundamental surface physics studies on nearly perfect single crystals to the mechanical behavior of practical engineering materials in various environments. Thus, one of the primary aims of the proposed research under project THEMIS is to develop an approach that will lead to a connection between fundamental and applied studies on selected materials for a limited number of problem areas. The procedure will be to devise a network that will connect the research at a given stage to the nearest related stages which are perhaps more applied or more fundamental. It will be necessary in this procedure to have some mechanism in mind for each problem area. In fact, another purpose of the research will be to define or clarify mechanisms where it appears to be necessary from an examination of the literature. The value of such a network is immediately apparent in either of two ways. An investigator using one of the fundamental techniques, such as LEED, can immediately see the relevance of his research to a particular applied problem and the feedback of ideas from the applied side can suggest further fundamental studies. Or from a broader management view the development of a network itself will identify the need for certain information that might be obtained by a literature search but most likely will involve the initiation of a new research task.

The organization of the various studies (or tasks under the project) is set forth in the following chart and, by way of illustration, a typical branch of the network is traced for one aspect of the problem of stress corrosion cracking of high strength alloys.
INTERFACE PHENOMENA

CHARACTERIZATION

- Electron spectroscopy
- Work function
- Contact resistance
- Surface topology
- X-ray diffraction
- FIM-FEM
- Electron microscopy
- LEED

FUNDAMENTAL QUANTITIES

- Thermodynamic Quantities
- Electrons and Holes transport
- Band structure
- Optical properties
- Defects
- Vacancies
- Dislocations

SYSTEMS

- Electronic
- Mechanical dislocation
- Pileup
- Chemical

PROBLEM AREAS

- Stress Corrosion Cracking
- Friction, wear and lubrication
- Machining

SOLUTIONS

- Diffusion coatings
- Alloy control, e.g. ordering in surface region
- Oxides
- Fatigue and creep
- Diffusion barriers
- High-temperature oxidation
- Solidification
- Semiconductor Interfaces
1. Characterization

A detailed treatment of characterization would include a discussion of the various techniques for determining surface structure, composition, impurity concentration, strain, ordering and morphology of both single crystals and engineering materials. However, some of these techniques have been adequately described previously. Extensive use of LEED and inelastic electron scattering techniques have been made by our group in the past few years in surface physics studies of tungsten, copper, nickel, aluminum, titanium, graphite and silicon and in an investigation of the surface chemistry of the titanium-oxygen system.

Surface characterization techniques can therefore be coupled with other experiments so as to monitor the state of a surface while other physical properties are investigated. The combined optical, LEED and electron spectroscopy study of Jordan and Scheibner is a good example.

Surface characterization techniques can also be used effectively to establish reproducible conditions of surface cleanliness prior to other studies such as friction, adhesion or wear. Bradford has used work function measurements prior to adhesion studies in ultra-high vacuum to monitor surface cleanliness and Keller has examined the effect of a contaminating layer on the contact resistance between loaded metallic surfaces, the contact resistance being decreased when the surfaces were cleaned.

The nature of surface topology is obviously important in friction and wear but it also is considered an important factor in the solidification of metals from the melt.

Besides the characterization of surfaces before or during the studies men-
tioned above, one should be equally concerned about bulk material modifications as a result of thermal-mechanical treatments such as those used in the ordinary production and fabrication of materials. Simple machining, for instance, may produce a mosaic structure, microstrains or faulting in the workpiece and this modified material may then be greatly susceptible to environmental conditions. X-ray diffraction techniques are extremely useful in studies of the surface substructure since small mosaic size, stacking faults and residual strains affect x-ray diffraction peaks and quantitative measurements of these structural imperfections can be obtained from peak analysis. The same techniques can be used to examine the substructure as influenced and altered by certain surface or environmental conditions.

Field ion microscopy techniques are particularly useful for studying short range order and they therefore readily complement LEED studies of ordering near the surface and x-ray diffraction studies of long range order in the bulk.

Finally, stacking fault energies are related to the work hardening and adhesion coefficients of alloy systems \(^{10}\) and the individual dislocation type in ordered alloys is determined in part by the stacking fault energy.

2. Fundamental Quantities

Thermodynamic quantities, band structure and defects are all important in developing mechanisms for the different problem areas. It is probably not immediately clear how band structure determinations can lead to an understanding of mechanical properties. This follows however from a consideration of the tight-binding method.

Most of the work concerning the electronic structure of solids has been directed toward understanding electrical properties -- the extensive treatment of
semiconducting crystals substantiates this view. However, as Slater has pointed out, the analysis of perfect crystals with variable lattice constant permits one to determine important physical properties such as compressibility and cohesive energy, and even the elastic constants involved in uniform shear. It is his feeling that these topics, namely those involving the mechanical properties of crystals have been seriously neglected. In the case of perfect crystals, Hall\textsuperscript{12} and Slater\textsuperscript{13} have shown that equivalent bonding orbitals, similar to those used in molecules, may be constructed from the crystal wavefunctions of electrons. The crystal wavefunctions employed were linear combinations of Bloch functions constructed from atomic orbitals, a characteristic of the tight-binding method of calculation.

It has proven useful to carry out most calculations at symmetry points of the Brillouin zone, then apply an interpolation scheme\textsuperscript{14} to obtain energy eigenvalues over the whole zone. From these data one would calculate equivalent bonding orbitals for the crystal. Lye has used a technique in which optical measurements over a wide range, from the visible to well into the vacuum ultraviolet, have been combined with theoretical calculations to examine the bonding in TiC. His analysis does not employ the full bonding orbitals, but, supposedly, the principal contributions to the bonding orbitals. As a consequence, predictions are made concerning the relative importance of Ti-Ti, Ti-C, and C-C bonds to the mechanical properties of the alloy crystal. It is clear from the discussion that a more extensive understanding of bonding orbitals would be very useful in the analysis of alloys. Further, Lye\textsuperscript{16} has shown that, once the bonding structure of a given alloy is established, it is possible to make semiquantitative conjecture about the mechanical properties of similar alloys.
The various types of dislocations present in different structures and their dynamics are factors in mechanisms for mechanical effects at surface. The effect of ordering, e.g., in Ni$_3$Mn alloys,\textsuperscript{17} is to produce an equilibrium configuration of superlattice dislocations which considerably increase the strength of an alloy. Each dislocation is now composed of four bound partials, stacking faults and slip-produced antiphase boundaries. This complex arrangement is more difficult to move than a simple edge or screw dislocation so that order hardening is the result and stress concentration due to dislocation pileup near the surface is reduced.

3. Systems

In the formation of a suitable network for each problem area it is required to propose a mechanism which combines the fundamental quantities in a particular way to explain the electronic, chemical or mechanical behavior of a material. One such mechanism which is important in discussing the stress corrosion susceptibility of high strength alloys is the dislocation pileup mechanism which is active whenever there are barriers to dislocation motion, such as oxide films or discontinuous structural changes. Research in this area of dislocation-surface interactions is already in progress by Livesay and Dr. Starke, Associate Professor of Metallurgy.

4. Problem Areas

Of the possible problem areas to be investigated three have been selected for further study during the next period. These are stress corrosion cracking, wear and machining. Some idea of the fundamental factors that need to be considered in developing a mechanistic network can be obtained by referring to the following three diagrams. Other problem areas such as fatigue, solidification, high temperature oxidation and semiconductor interfaces will be considered later. It is
STRESS  
CORROSION  
CRACKING

TYPES OF CORROSION

METALLURGICAL MICROSTRUCTURE

HYDROGEN EMBRITTLEMENT

ORDERING (a) IN SURFACE LAYERS
(b) BULK
(c) EFFECT ON DISLOCATION MECHANICS

DISLOCATION MECHANICS (a) AT SURFACE (PILEUP)
(b) AT GRAIN BOUNDARIES
(c) AT PRECIPITATES, ETC.

SURFACE ENERGY (a) EFFECT ON FRACTURE
(b) CHANGES WITH CHEMICAL REACTION
(c) EFFECT ON DISLOCATIONS

STACKING FAULT ENERGY

CRYSTAL STRUCTURE AND TEXTURE

ELECTRO CHEMISTRY

ENVIRONMENT

PROTECTION AGAINST (a) DIFFUSION COATINGS
(b) SURFACE TREATMENTS
(c) ALLOY MODIFICATION
WEAR

TYPES OF WEAR

ADHESIVE
  Chemical attack,
  Stress corrosion
  cracking

CORROSIVE
  Stress corrosion
  cracking

ABRASIVE

SURFACE

FATIGUE

PHASE CHANGE
  Mild-to-severe wear regime.
  Superplastic effects - used
  in metalforming, may affect
  wear regime at high tempera-
  tures.

CRYSTAL STRUCTURE AND TEXTURE
  In general, hexagonal metals
  have low wear

ALLOYING
  Composition affects wear. Study of homogeneous alloys, solid-
  solution systems, inhomogeneous materials.

MUTUAL SOLUBILITY - SURFACE ENERGY - WETTABILTY
  BULK
    Lack of solid solubility leads to low wear.
  SURFACE
    Surface phase diagrams are not available, however,
    effects may be important.

SURFACE STRUCTURE
  Texture, amount of stored energy, dislocations

ORDERING
  Long and short range order, domain size.

ELECTRONIC STRUCTURE
  Effect of impurity additions on mechanical properties;
  possible way to design low wear materials.

STACKING FAULT ENERGY
  Alloying effects.

HARDNESS AND WORKHARDENING PROPERTIES
  Area of contact versus strength of interface (Talysurf surface
  characterization)

SURFACE COATINGS
  Diffusion, oxidation, platings

LUBRICANT EFFECTIVENESS
  Surface cleanliness and characterization
METAL MACHINING

OPERATION

TURNING

PLANING

DRILLING

TAPPING

BROUCHING

Machinability data tables

MATERIAL: Aerospace alloys - Steels (4340, H11); Titanium alloys (6Al-4V, 8Al-1Mo-1V)

EFFECT OF TOOL

GEOMETRY AND CUTTING SPEED

LUBRICATION

Chemical effects of lubricants. Surface interactions.

TOOL WEAR

Diffusion wear, analysis. Tool disintegration, microprobe analysis

CHIP FORMATION

Continuous, discontinuous, fracture, built-up edge.

FRICITION AND ADHESION

Tool rake face, tool land.

METAL DEFORMATION

Strain, strain rate and temperature distributions.

SURFACE INTEGRITY

Surface finish, structure, residual stresses. Metallography, electron microscope, X-ray.

EFFECT ON

MECHANICAL PROPERTIES

CREEP

IMPACT STRENGTH

PAGUE
planned to publish a series of review papers on the different areas in the open literature as they are completed.

5. Solutions

The possible modifications in the surface region and the preparation of surface coatings which can influence the mechanical properties at the surface are included in this phase. Solutions to some of the more important practical problems can result from applied studies in this phase. However, the fundamental basis for these applied studies will have been indicated.

In summary, the projected plan of research includes: (a) a continuation of the studies currently in progress; (b) the development of a general approach for relating fundamental and applied studies to each other; (c) the detailing of mechanisms for describing the fundamental basis of several problem areas; (d) the preparation of review papers for the areas of stress corrosion cracking, wear and machining; and (e) the planning for review papers in other areas, such as fatigue, solidification, high temperature oxidation and semiconductor interfaces.
V. IDENTIFICATION OF PERSONNEL

The research team formed at the Georgia Institute of Technology for the study of interface phenomena comprises senior faculty members from various schools and divisions, associate faculty members, graduate and undergraduate students and support personnel. The following table gives a summary of various science and engineering disciplines represented on project THEMIS as of January 1969.

As originally proposed the organization of the team was designed so that the senior faculty members would provide advice in developing the technical program of the project while at the same time being aware of, and contributing to, the individual departmental plans for achieving excellence in their graduate programs. At the present time it seems in order to view the personnel on the project THEMIS team somewhat differently, retaining however the same general objectives. There are several reasons for this. First of all, the technical programs have become well established and often the direct supervision of a specific task is not necessarily the responsibility of a senior faculty member. Secondly, by focussing on a limited number of problem areas we are in a better position for coordinated effort and the management of such an effort can best be accomplished by the program manager dealing directly with the appropriate task leaders. Thirdly, additional faculty members with broad experience are participating in the program and their participation has considerably enhanced the capability of the team. In a number of cases the academic faculty member is partially supported by institutional funds as soon as the contribution to the graduate program of the academic department is recognized. And finally, the advisory group is being expanded to include staff members from other universities or DoD laboratories as well. These additions will be particularly important for formulating and preparing the series
<table>
<thead>
<tr>
<th>Discipline</th>
<th>(A) Senior Faculty Members</th>
<th>(B) Associate Faculty Members</th>
<th>(C) Graduate Assistants</th>
<th>(D) Undergraduate Student Assistants</th>
<th>TOTAL</th>
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<tr>
<td>Chemical Engineering</td>
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<td>3</td>
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<tr>
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<tr>
<td>High Temperature Materials Division, Engineering Experiment Station</td>
<td>1</td>
<td>2</td>
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<td>4</td>
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<tr>
<td>Mechanical Engineering</td>
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<tr>
<td>Metallurgy (School of Chemical Engineering)</td>
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<td>Nuclear Engineering</td>
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<tr>
<td>Physical Sciences Division, Engineering Experiment Station</td>
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<td>6</td>
<td>3</td>
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<tr>
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<tr>
<td><strong>TOTAL</strong></td>
<td>7</td>
<td>11</td>
<td>11</td>
<td>3</td>
<td>32</td>
</tr>
</tbody>
</table>

1 Includes one postdoctoral fellow receiving support from other sources.

2 Includes one Associate Faculty Member pursuing a Ph. D. degree in Metallurgy and one Graduate Assistant receiving support from other sources.
of critical review papers.

The team is thus composed of a program manager, senior faculty members, advisory faculty members, associate faculty members, graduate and undergraduate students, and support personnel. Consideration is being given to the obtaining of additional funding for postdoctoral appointments with the project.

The following personnel have been associated with the project during the past period:

E. J. Scheibner, Research Professor of Physics and Chief of Physical Sciences Division, is the Program Manager. He was supported in part by institutional funds through the division and in part by the program.

C. W. Gorton, Professor of Chemical Engineering, is directing studies of surface and diffusion coatings through the High Temperature Materials Division. Dr. Gorton's biographical sketch is included in the appendix.

R. F. Hochman, Associate Professor of Chemical Engineering, is supervising studies utilizing field emission and field ion microscopy.

J. H. Murphy, Associate Professor of Mechanical Engineering, is studying conditions at the mold-casting interface during casting of metals and was supported in part by institutional funds through the School of Mechanical Engineering.

R. A. Pierotti, Associate Professor of Chemistry, is conducting studies on gas-solid interactions. Dr. Pierotti was supported in full by institutional funds through the School of Chemistry.

J. R. Stevenson, Associate Professor of Physics, is engaged in optical studies of interfaces in controlled environments and was supported in full by institutional funds through the School of Physics.
W. T. Ziegler, Regents Professor of Chemical Engineering, will help direct studies in the area of chemical thermodynamics.

* * *

S. H. Bomar, Research Engineer with the High Temperature Materials Division, will assist Dr. Gorton in studies on surface and diffusion coatings.

J. M. Bradford, Assistant Professor with the School of Mechanical Engineering, joins M. E. Sikorski in the studies on friction, adhesion, wear, and lubrication. He was supported in part by institutional funds through the School of Mechanical Engineering. Dr. Bradford’s biographical sketch is included in the appendix.

Helen E. Grenga, Assistant Professor with the School of Chemical Engineering, is assisting in studies utilizing field emission and field ion microscopy.

C. A. Murphy, a Senior Research Engineer with the High Temperature Materials Division, is assisting Dr. Gorton in studies on surface and diffusion coatings.

M. E. Sikorski, a Senior Research Engineer with the Physical Sciences Division, is involved in the studies on friction, adhesion, wear, and lubrication.

G. W. Simmons, Research Chemist with the Physical Sciences Division, is conducting studies of the Gas-Solid Interface.

L. N. Tharp, Research Physicist with the Physical Sciences Division, is using LEED and electron spectroscopy studies to examine electron interactions with solids.

* * *

B. R. Livesay, a candidate for the Ph. D. in Metallurgy and a Research Physicist with the Physical Sciences Division, is conducting studies on measurements of thermodynamic quantities.
R. P. Woodward, a candidate for the Ph.D. in Electrical Engineering and Assistant Research Engineer with the Physical Sciences Division, assists in LEED and electron spectroscopy studies.

J. O. Darnell, an Assistant Research Engineer with the Physical Sciences Division, is presently providing technical assistance to Dr. Simmons.

K. B. Wear, a Research Engineer with the Physical Sciences Division, is assisting both Dr. Simmons and Dr. Bradford in the design of experiments in their respective areas of interest.

* * *

Harry E. Ellis, a Ph.D. candidate in Physics, is assisting Dr. Stevenson in optical studies of interfaces in controlled environments.

Panagiotis Kalofonos, a graduate student in the School of Chemical Engineering, is assisting Dr. Hochman in field emission and field ion microscopy studies.

T. W. Kaltenberg, a graduate student in the School of Nuclear Engineering, is assisting Dr. J. H. Murphy in mold-casting studies.

A. C. Merritt, a graduate student in the School of Chemical Engineering, is assisting Dr. C. W. Gorton in his work on surface and diffusion coatings.

D. S. Newsome, a candidate for the Ph.D. degree in Chemistry, is assisting Dr. R. A. Pierotti.

R. N. Ramsey, a graduate student in the School of Chemistry, is assisting Dr. R. A. Pierotti.

B. N. Ranganathan, a graduate student in the School of Chemical Engineering, is assisting Dr. Hochman in studies utilizing field emission and field ion microscopy.
H. M. Thron, Jr., a graduate student in the School of Chemical Engineering, is assisting Dr. R. F. Hochman in field emission and field ion microscopy studies.

Maury Zivitz, a Ph.D. candidate in Physics, is assisting Dr. Stevenson in optical studies of interfaces in controlled environments.

D. M. Myers, a Senior in Industrial Management, is assisting in the collection of information for the critical review of interface phenomena.

C. T. Randall, a Senior in Chemical Engineering, is assisting Mr. Livesay in measurements of thermodynamic quantities.

J. G. Underwood, a Junior in Physics, is assisting Dr. Simmons in studies of the gas-solid interface.

* * *

In addition, the following persons contributing to the program are supported by other sources:

H. E. Thomas, a Postdoctoral Fellow in Chemistry, is assisting Dr. Pierotti in studies on interactions of gases with solids.

Joseph Delay, a Ph.D. candidate in Chemistry, is assisting Dr. Pierotti in studies on interactions of gases with solids.
VI. FACILITIES AND EQUIPMENT

The laboratories within the various schools, the High Temperature Materials Division and the Physical Sciences Division have adequate basic facilities for performing the proposed research. Moreover, with these facilities and the specialized laboratory facilities, some of which are described below, the project will be equipped with a unique combination of experimental techniques for carrying out fundamental research on many important materials problems. When this capability is augmented by that of certain other university or government laboratories associated with the project it will be realized that a new center for research in the nation's interest will have been established.

Consistent with this national goal is an Institute goal of achieving excellence in its graduate programs. Through project THEMIS it has been possible to assist in the development of specialized laboratory facilities needed in the graduate program of the various schools. Many of these are located in the academic buildings; others are located in the Physical Sciences Division laboratory building. Thus, rather than housing all the related graduate research within a single, multi-story building on campus, the center concept envisioned here includes the facilities of a "core" laboratory (the PSD building) and "satellite" laboratories in other locations on and even off the campus.

Some of the specialized laboratory facilities that are being developed are now described.

The facilities of the Surface Physics and Chemistry Laboratories of the Physical Sciences Division used primarily in the Physics program include several ultra-high vacuum systems for LEED and electron spectrsocopy studies, associated instru-
mentation for measuring work function, photoemission, Auger emission and optical reflectivity and systems for controlled chemical reaction studies. One special Varian post-acceleration LEED system includes a servo-controlled gas-handling manifold and accessories for performing simultaneous optical reflectivity and energy analysis measurements; the energy analysis measurements can be performed with improved sensitivity and resolution because of modifications made in the original system. Data acquisition and processing will soon be accomplished using an on-line special purpose computer unit now being incorporated. Another LEED system, designed particularly for surface chemistry studies, includes in addition a reaction chamber that can isolate the specimen from the main system, a corrosive gas handling manifold, auxiliary pumping by means of a mercury diffusion pump or an Electro Ion pump (titanium pump manufactured by Granville-Phillips). This system is designed to incorporate a HEED attachment which will be added at a later date. During the current year a high resolution electron spectrometer was designed and constructed. This unit is being incorporated into a third ultra-high vacuum system obtained under the contract and the necessary electronic and vacuum accessories are being assembled. Some of the items for the electronic control and programming unit are included in the budget estimate. Also available is a quadrupole residual gas analyzer, the electronics console of which is shared among a number of ultra-high vacuum systems, each providing its own sensing head.

The program in optical physics makes use of two vacuum ultraviolet monochromators located in the School of Physics and a third located in the Engineering Experiment Station. These instruments are capable of covering the wavelength spectrum from approximately 400 Angstroms to the visible region. Reflection and transmission
measurements can be made in ultrahigh vacuum at either location but these measurements are restricted to the lithium fluoride cutoff at approximately 1200 Angstroms. Utilization of a storage ring facility at the University of Wisconsin will enable us to make measurements in ultrahigh vacuum to approximately 200 Angstroms. In the infrared a Perkin-Elmer model 99 prism monochromator with sodium chloride cesium bromide and cesium iodide prisms in available in the School of Physics for measurements to approximately 40 microns wavelength. An infrared laser capability is being developed and a CO₂ laser is operational with approximately 5 watts of power at 10.6 microns.

The Micromechanics Laboratory of the Physical Sciences Division, particularly available to graduate students in Metallurgy and Mechanical Engineering, includes instrumentation for measuring mechanical properties of thin samples (to enhance surface effects) in deformation modes of bending, tension and torsion in environments ranging from corrosive liquids to ultra-high vacuum. The laboratory also includes an apparatus for friction studies in the load range of only a few dynes. An apparatus for the measurement of surface tension of metals is assembled in a specially designed ultra-high vacuum system provided under the project during the past year. The chamber is evacuated with a 1600 liter/sec Granville-Phillips Electro Ion pump and has an ultimate pressure in the 10⁻¹⁰ Torr range. Two optical ports are provided, one for observation and the other for measuring minute displacements with a laser beam. An associated gas manifold provides either of three different high purity gases in the chamber through a servo-controlled leak valve. The entire apparatus is mounted on a vibration-free table positioned on a concrete isolation slab to achieve the ultimate sensitivity in the surface tension measurements. Elongation measurements sensitive
to less than 0.1 micron have been made using the laser beam deflected by an optical lever and detected by a dual photodiode. Samples are cleaned within the chamber by various techniques including ion bombardment and provision is made for measurements at sample temperatures as high as 800°C. The chamber is also adaptable to other micromechanical measurements related to studies of dislocation interactions at well defined surfaces.

The friction, adhesion and wear studies in ultrahigh vacuum will be conducted with the help of a special system obtained under the project and due for delivery at the end of January of 1969; it will be located in the School of Mechanical Engineering. The apparatus will allow experiments to be conducted at a pressure of $10^{-11}$ Torr by the use of an oil-free pumping system consisting of a 400 liter/second Varian ion pump and a Ti sublimation pump. Provisions are also being made for cryopumping. (A cryopanel item is included in the budget estimate.) Facilities will also be provided for cleaning the surfaces by ion bombardment and electron annealing and for surface characterization using the work-function method. In the future, electrical contact resistance and Auger electron emission methods may also be incorporated into the chamber. The vacuum system allows for the use of different gases to investigate the effect of controlled environments on the friction, adhesion and wear properties of materials having well-characterized surfaces.

The metallurgical and metals processing laboratories of the School of Mechanical Engineering and the School of Chemical Engineering contain the usual heat treatment and materials testing equipment. The special facilities within the Metallurgy program of the School of Chemical Engineering include laboratories for x-ray diffraction, electron microscopy and field ion and field emission microscopy. X-ray diffuse
scattering measurements are made with a General Electric XRD-6 diffractometer equipped with a doubly-bent LiF single crystal monochromator. This equipment is automated with a step scanner and print-out unit. Electron microscopy and electron diffraction are carried out on two microscopes, one a high resolution, 125 KV electron microscope Siemens Elmiskop II installed during the past year. The combined field ion and field emission microscope which includes a gas supply system and sample temperature control has been used extensively for studies on ordered and two phase alloys.

In addition to the above facilities two other laboratories are available for support of the primary research programs. These are the Analytical Instrumentation Laboratories and the Crystal Physics Laboratories of the Physical Sciences Division. The Analytical Instrumentation Laboratories provide services in electron microscopy, optical microscopy, x-ray and electron diffraction, x-ray fluorescence, spectrographic analysis, electron microprobe analysis and scanning electron microscopy. A Cambridge Instruments Stereoscan scanning electron microscope was added during the past year. The Crystal Physics Laboratories provide facilities and experienced personnel in all aspects of x-ray and neutron diffraction and in the techniques of neutron scattering, x-ray topography, source image distortion, line profile analysis and optical crystallography.

Other facilities of the Institute such as an excellent library, central machine shop, photographic shop and electronic, nuclear and chemical laboratories are also available.
VII. TRAVEL

It is anticipated that senior staff members will visit DoD and other scientific laboratories engaged in similar work and attend appropriate scientific meetings. Advisory assistance will be provided as requested on defense problems closely related to the work under the program. The travel costs involved are included in the budget estimate.
REFERENCES

APPENDIX

A. Biographical Sketches

B. Task Descriptions
JAMES M. BRADFORD, JR., Assistant Professor of Mechanical Engineering

EDUCATION: B.S. in Mechanical Engineering (1959), Clemson University, M.A. in Physics (1964), William and Mary, Ph.D. (1968), North Carolina State University.

PRESENT DUTIES AND AREAS OF INTEREST: As Assistant Professor in the School of Mechanical Engineering he teaches courses in materials science and high vacuum technology. He is conducting research in the adhesion and friction of metals with the emphasis on defining the parameters which control the adhesion and friction and directs Ph.D. thesis research of students in Mechanical Engineering. His interests are in the areas of surface phenomena, materials research, and high vacuum technology.

EMPLOYMENT HISTORY: Employed as product engineer with Western Electric Company in 1959-1960, was a design engineer with Douglas Aircraft Company in 1960-1961, and joined NASA at Langley Field in 1961. In 1968 he joined Georgia Tech as Assistant Professor in Mechanical Engineering.

PROFESSIONAL EXPERIENCE SUMMARY: He has studied the properties of materials in low pressure environments during the last seven years. At NASA he was a member of a group studying the effect of the space environment upon space craft materials. In this group he was concerned with the changes in material properties induced by the space environment, particularly properties related to surfaces. He has conducted research in surface phenomena using ultra-high vacuum techniques. At Georgia Tech he is continuing his interests in surface phenomena with studies into adhesion and friction of metals in ultra-high vacuums.

SELECTED PUBLICATIONS:

2. "A Large Ultra High Vacuum Environmental Chamber with Liquid Helium Cooled Walls," Journal of Environmental Sciences, vol. 8, pp. 11-15, December 1965. (This paper was presented at the 1965 Technical Meeting of the Institute of Environmental Sciences, April 21-23, 1965.)
SELECTED PUBLICATIONS: (Continued)


CONTRIBUTION TO INTERFACE PHENOMENA PROGRAM:

Dr. Bradford will continue the studies in friction, adhesion, and wear begun by M. E. Sikorski. Emphasis will be placed on the study of adhesion of alloys in a vacuum.
CHARLES W. GORTON, Professor of Chemical Engineering

EDUCATION: B.S.M.E. (1950), Louisiana Polytechnic Institute; M.S.M.E (1951), Georgia Institute of Technology; Ph.D.M.E. (1953), Purdue University.

PRESENT DUTIES AND AREAS OF INTEREST: As Professor in the School of Chemical Engineering he teaches courses in transport phenomena, fluid flow, and heat transfer. He is currently directing research at the Ph.D. level in combustion, transpiration cooling, and free-convection from inclined surfaces. He is working with the High Temperature Materials Division, EES in heat transfer and stress analysis.

EMPLOYMENT HISTORY: Employed as a Research Engineer with United Aircraft, Research Department from 1953-1955. In 1955 he joined Georgia Institute of Technology as an Associate Professor of Mechanical Engineer and was promoted to Professor in 1960. In 1965 he became a Professor of Chemical Engineering. He is also presently acting as a consultant to the Oak Ridge National Laboratory.

PROFESSIONAL EXPERIENCE SUMMARY: He has studied aspects of heat transfer and combustion since he began work with United in their Analysis Section. His transfer studies have encompassed the areas of free-convection, transpiration cooling, aerodynamic heating, and ablation. At the Stations High Temperature Materials Division he has worked on hydro-cyclones, reentry heating, aerodynamic heating for low altitude supersonic flight, arc-plasma testing, and rain erosion.

SELECTED PUBLICATIONS:

SELECTED PUBLICATIONS (Continued)

SELECTED PUBLICATIONS (Continued)


CONTRIBUTION TO INTERFACE PHENOMENA PROGRAM:

Dr. Corton will supervise the continuing studies on surface and diffusion coatings, with emphasis on the use of Chemical Vapor Deposition.
PROJECT NUMBER A-1044-200

TITLE

"Program Manager"

DATE 20 September 1968

TASK DESCRIPTION

1. (a) Give a concise progress report for the last quarter (attach additional sheets if necessary) in the case of a continuing program, or if just beginning work, an abstract of research under task, and (b) a summary of the specific work to be performed during the next quarter year.

1. As program manager, Dr. Scheibner will be responsible for coordination of the research and the supervision of certain technical and administrative tasks.

2. He will provide the necessary briefing to the administration as required.

3. He will maintain liaison with the technical monitor and other representatives in DoD laboratories in regard to the relevance of the technical program to DoD needs.

4. He will plan and organize a critical review on interface phenomena.

2. List faculty members, graduate students, and support personnel, including vacant positions, with percentage of time to be spent during the next quarter, designating task leader by an underline. Identify any portion to be supported by departmental funds. List graduate students doing related work but supported by fellowships, grants, etc.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
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<tbody>
<tr>
<td>E. J. Scheibner</td>
<td>25%/12 months (partially supported by Division)</td>
</tr>
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</table>

3. List equipment, M&S estimate, and anticipated travel for next quarter with brief justification.

NONE

Program Manager__________________________ Task Leader E. J. Scheibner

School/Dept. Physical Sciences Division

Revised 3-68
TITLE
"Thermodynamics of Interfaces"

TASK DESCRIPTION

1. (a) Give a concise progress report for the last quarter (attach additional sheets if necessary) in the case of a continuing program, or if just beginning work, an abstract of research under task, and (b) a summary of the specific work to be performed during the next quarter year.

   Appropriate studies in the area of chemical thermodynamics will be undertaken when the need arises in other parts of the program.

   Primarily the contribution of Dr. Ziegler will be in reviewing the individual tasks periodically.

2. List faculty members, graduate students, and support personnel, including vacant positions, with percentage of time to be spent during the next quarter, designating task leader by an underline. Identify any portion to be supported by departmental funds. List graduate students doing related work but supported by fellowships, grants, etc.

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<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
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<tbody>
<tr>
<td>W. T. Ziegler</td>
<td>Hourly as Needed</td>
</tr>
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</table>

3. List equipment, M&S estimate, and anticipated travel for next quarter with brief justification.

   NONE

Program Manager ____________________    Task Leader ____________________
School/Dept. ____________________  W. T. Ziegler

revised 3-68
TITLE
"Measurement of Thermodynamic Quantities"

PROJECT NUMBER
A-1044-202

DATE
September 20, 1968

1. (a) Give a concise progress report for the last quarter (attach additional sheets if necessary) in the case of a continuing program, or if just beginning work, an abstract of research under task, and (b) a summary of the specific work to be performed during the next quarter year.

1. (a) During the Spring Quarter accomplishments included the following:
- Modifications to laboratory for surface tension apparatus were completed. These included additional power, water connections, lighting, floor tile and a 4' x 6' x 4' concrete vibration isolation slab.
- Arrival of vacuum chamber and pump from Varian. Improper packing of the G.P. electro-ion pump by Varian involved certain legal procedures and additional testing of pump.
- Additional vacuum components were also received and are being assembled.

During the Summer Quarter assembly and mounting of the gas handling system will be done. A special mount for the vacuum chamber and laser is also to be completed. Construction can then begin on the bakeout ovens required for UHV. Vacuum tests on the entire system should be possible in late September.

1. (b) During the Fall Quarter the entire surface apparatus should be completed and studies begun. Certain important items, however, remain to be constructed or (continued)

2. List faculty members, graduate students, and support personnel, including vacant positions, with percentage of time to be spent during the next quarter, designating task leader by an underline. Identify any portion to be supported by departmental funds. List graduate students doing related work but supported by fellowships, grants, etc.

NAME	PERCENT TIME

Academic Year	Summer

B. R. Livesay	.25	.25
C. T. Randall (Student Assistant) .30 .30
Machinist	100 hours	
J. Carr (Elec. Tech.)	75 hours

3. List equipment, M&S estimate, and anticipated travel for next quarter with brief justification.

Materials
- Components for Ion Bombardment System $400
- UHV Transducers (2) @ $300 ea. 600
- Miscellaneous Parts (S.S.E. Electronics) 300
- Materials for bakeout oven 600

Program Manager	Task Leader	B. R. Livesay

School/Dept. Physical Sciences Division

revised 3-68
1. (b) (Continued)
purchased. These include the bakeout oven system, two U.H.V. transducers, a highly regulated d.c. current power supply and components for an ion bombardment system for cleaning samples in U.H.V. The initial measurements will be made on mica and metal foils of copper. The ion-bombardment hardware will then be added.

2. (Continued)

**Equipment**

- **Highly Regulated D.C. Current Power Supply**
  - Sorrenson Model QRC 40-4A $ 315
- X-Y Recorder 2,500
- Relay Rack 130
- Poppit Valve 2,000
1. (a) Give a concise progress report for the last quarter (attach additional sheets if necessary) in the case of a continuing program, or if just beginning work, an abstract of research under task, and (b) a summary of the specific work to be performed during the next quarter year.

(a) Work during first year has consisted of design and fabrication of LEED Optics, design and purchase of ultrahigh vacuum system (now delivered), and design and partial construction of high resolution electron spectrometer.

(b) During the next year it is anticipated that spectrometer system will be completed and measurements initiated related to the use of electron scattering for characterizing surfaces.

2. List faculty members, graduate students, and support personnel, including vacant positions, with percentage of time to be spent during the next quarter, designating task leader by an underline. Identify any portion to be supported by departmental funds. List graduate students doing related work but supported by fellowships, grants, etc.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
<th>Academic Year</th>
<th>Summer</th>
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<tbody>
<tr>
<td>L. N. Tharp</td>
<td>.25</td>
<td>.25</td>
<td></td>
</tr>
<tr>
<td>R. P. Woodward</td>
<td>.50</td>
<td>.50</td>
<td></td>
</tr>
<tr>
<td>Machinist</td>
<td>1.00 for two months</td>
<td>1.00 for two months</td>
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</table>
1. (a) Give a concise progress report for the last quarter (attach additional sheets if necessary) in the case of a continuing program, or if just beginning work, an abstract of research under task, and (b) a summary of the specific work to be performed during the next quarter year.

   a. Summary of Progress: A general purpose gas-solid reaction chamber was designed, and this system is now nearly complete.

   Literature surveys have been carried out in the fields of chemisorption and stress corrosion cracking. Specific literature studies of the titanium-oxygen system have been made in conjunction with the ARPA program.

   LEED studies of titanium have resulted in a paper entitled, "Order-Disorder Phenomena in the Surface of Titanium Oxygen Solid Solutions".

   b. Plans for Coming Year: The reaction chamber will be finished, and components will be added as specific experimental needs arise.

   A number of experimental problems have evolved from the ARPA program. These experiments could be readily performed in the reaction system described above. It is suggested that one of these problems be undertaken by an advanced undergraduate or by a beginning graduate student. This plan would: (i) introduce the student to the field of surface research, (ii) support research that is already in progress, and, (iii) provide an example of the reaction chamber capabilities to other members of the THEMIS program.

2. List faculty members, graduate students, and support personnel, including vacant positions, with percentage of time to be spent during the next quarter, designating task leader by an underline. Identify any portion to be supported by departmental funds. List graduate students doing related work but supported by fellowships, grants, etc.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
<th>Academic Year</th>
<th>Summer</th>
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<tbody>
<tr>
<td>Gary W. Simmons</td>
<td>.15</td>
<td>.15</td>
<td></td>
</tr>
<tr>
<td>Ken B. Wear</td>
<td>.05</td>
<td>.05</td>
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<tr>
<td>James Darnell</td>
<td>.25</td>
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<td></td>
</tr>
<tr>
<td>Jeff Underwood</td>
<td>.10</td>
<td>.10</td>
<td></td>
</tr>
<tr>
<td>Graduate student (vacant)</td>
<td>.50</td>
<td>.50</td>
<td></td>
</tr>
<tr>
<td>Machine shop and analytical services</td>
<td>$500.00</td>
<td></td>
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</table>

   List equipment, M&S estimate, and anticipated travel for next quarter with brief justification.

   Equipment: Parts needed to complete reaction chamber $2,840.00 *

   Maintenance and Operation Costs: Liquid nitrogen, gases, chemicals, and sample materials (including single crystals) 750.00

   *for breakdown see attached sheet.

Program Manager ___________________ Task Leader G. W. Simmons

School/Dept. ___________________ Physical Sciences Division

Revised 3-68
3. (Continued)

*PARTS NEEDED TO COMPLETE REACTION SYSTEM*

<table>
<thead>
<tr>
<th>ITEM</th>
<th>ESTIMATED COST</th>
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<tbody>
<tr>
<td>1-Power supply for 8 l/s ion pump (Varian)</td>
<td>$200</td>
</tr>
<tr>
<td>3-Granville-Phillips Type C Valves @ $300</td>
<td>$900</td>
</tr>
<tr>
<td>2-Bakeable Valves (Varian) @ $420</td>
<td>$840</td>
</tr>
<tr>
<td>Vacuum connections</td>
<td>$700</td>
</tr>
<tr>
<td>Miscellaneous (bolts, Nuts, gaskets, etc.)</td>
<td>$200</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>$2,840</strong></td>
</tr>
</tbody>
</table>
1. (a) Give a concise progress report for the last quarter (attach additional sheets if necessary) in the case of a continuing program, or if just beginning work, an abstract of research under task, and (b) a summary of the specific work to be performed during the next quarter.

(a) During the past quarter Mr. Zivitz and Mr. Ellis have taken some additional optical data on Cd-Zn-As alloy systems. A revised computer program was made to reduce the reflectivity data to a determination of the complex dielectric constant. Work on an electronic analog system was initiated to facilitate the taking of reflectivity data. Component parts of the new ultra high vacuum reflectivity sample chamber have been fabricated and the sample chamber has been successfully tested to $10^{-9}$ torr range. Consideration has been given to making use of the storage ring facility at the University of Wisconsin and a visit to the facility has been arranged.

(b) Next quarter we will plan to continue our optical studies in ultra high vacuum and make the necessary modifications to allow us to use our sample chamber at the University of Wisconsin storage ring. We will initiate a program to evaluate the electroreflectance technique as a method of improving our resolution. Additional data will be taken using polarized and unpolarized radiation on the Cd-Zn-As system.

2. List faculty members, graduate students, and support personnel, including vacant positions, with percentage of time to be spent during the next quarter, designating task leader by an underline. Identify any portion to be supported by departmental funds. List graduate students doing related work but supported by fellowships, grants, etc.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
<th>SUMMER</th>
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<tbody>
<tr>
<td>James R. Stevenson</td>
<td>(.30) Supported by Physics</td>
<td>.50</td>
</tr>
<tr>
<td>Maury Zivitz</td>
<td>.50</td>
<td>.50</td>
</tr>
<tr>
<td>Harry Ellis</td>
<td>.50</td>
<td>.50</td>
</tr>
<tr>
<td>1 Student Assistant (vacant)</td>
<td>.25</td>
<td></td>
</tr>
<tr>
<td>1 Machinist</td>
<td>(.10) Supported by Physics</td>
<td>.10</td>
</tr>
<tr>
<td>1 Machinist (EES)</td>
<td>.05</td>
<td></td>
</tr>
<tr>
<td>1 Electronic Technician (EES)</td>
<td>(.05) Supported by Physics</td>
<td></td>
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<tr>
<td>1 Electronic Technician</td>
<td>(EES)</td>
<td></td>
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</table>

3. List equipment, M&S estimate, and anticipated travel for next quarter with brief justification.

Equipment: Replacement capital outlay items $350

M&S: $200-$250 per month - Such items as a Bendix channeltron detector will be necessary for use with the storage ring facility. In addition photomultipliers, optical components, electronic components, and ultra high vacuum valves must be purchased.

Travel: $1500--This includes 2 students each spending 30 days at the storage ring at $12 per diem in addition to a total of 5 individual round trips to Wisconsin. A trip to one meeting for two individuals is included.

Program Manager

Task Leader	James R. Stevenson

School/Dept. Physics

revised 3-68
1. (a) Give a concise progress report for the last quarter (attach additional sheets if necessary) in the case of a continuing program, or if just beginning work, an abstract of research under task, and (b) a summary of the specific work to be performed during the next quarter year.

(a) The major object of this program is the application of field ion microscopy and field emission microscopy to interfacial phenomena of engineering materials. Initially the work has involved technique development so the various types of interfaces in engineering alloys may be examined, i.e., grain boundaries, G.P. zones, two phase boundaries, order-disorder anti-phase boundaries, etc. This has been the primary concern of the early portion of this program. The major success to date has been achieved in the study of anti-phase and grain boundaries in Ni₃Mo. However Ti and Ti₃Al have also been examined and some success has been achieved in imaging these difficult materials. Other experiments have been initiated on iron base alloys, particularly those which represent the basic features of high strength alloy systems. Interest has also been in working with a low melting point metallic compounds to develop techniques so these materials can be examined with FIM. To date initial studies have been made on Ag₃Sn.

Two additional experimental systems have been added to our laboratory, both designed during the past year. The first is a combination field ion

(continued)

2. List faculty members, graduate students, and support personnel, including vacant positions, with percentage of time to be spent during the next quarter, designating task leader by an underline. Identify any portion to be supported by departmental funds. List graduate students doing related work but supported by fellowships, grants, etc.

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<tr>
<th>NAME</th>
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<tbody>
<tr>
<td>Dr. R. F. Hochman</td>
<td>.10</td>
<td>.10</td>
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<tr>
<td>Dr. Helen Grenga</td>
<td>.33 1/3</td>
<td>.33 1/3</td>
</tr>
<tr>
<td>Ranganathan (GRA)</td>
<td>.33 1/3</td>
<td>.33 1/3</td>
</tr>
<tr>
<td>Thron (GRA)</td>
<td>.33 1/3 (Sept., Nov.)</td>
<td>.33 1/3</td>
</tr>
<tr>
<td>Panagiotis Kalofonos (GRA)</td>
<td>.33 1/3 (start Nov. 68)</td>
<td>.33 1/3</td>
</tr>
<tr>
<td>Machinists Technicians, etc.</td>
<td>Total 200 hours @ 4.00/hour</td>
<td></td>
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</table>

3. List equipment, M&S estimate, and anticipated travel for next quarter with brief justification.

Materials & Supplies

For FIM-FEM support on the project $1,800
1. (a) (Continued)

and field emission microscope, designed by the staff with the help of Dr.
Brian Ralph, Cambridge. The other system is a small glass unit which will
be used for rapid examination and screening of samples. The latter will
greatly improve the ability of the group to effectively examine specimens
since it may be easily opened so specimens can be inserted and removed.
Those samples which show promise may be put into the more elaborate sys-
tems, those not capable of imaging can be discarded.

In addition to the laboratory work members of the staff participated
in preparation of a three day national symposium held here at Georgia Tech,
May 16, 17 and 18. Two papers were presented by the staff at this sympo-
sium. In addition another paper on field ion microscopy was presented at
the National AIChe meeting in Philadelphia, April 3, 1968.

Several interesting results have already been derived from basic studies
of interfaces and precipitation in solid solution alloys. For example Ralph's
work has proven in a number of systems that the "Coincident Lattice Theory"
actually exists in reality. This was accomplished by examination of atomic
positions across the boundary interfaces for a number of metals. The work on
grain boundaries by Muller, Ralph, and Ranganathan have shown that the width
of grain boundary in many cases may only be one to two atomic layers thick,
and in many cases it only represents the mismatch between the lattice of two
grains rather than any amorphous or discontinuous layer.

Another project of importance to engineering materials is the precipi-
tation of secondary phases from saturated solid solutions. Work by Muller
(Mo-Re alloy) and Ralph on steels have shown a great deal can be learned from
the proper application of field emission and field ion microscopy to two phase
systems, hence efforts will be directed in such studies of engineering alloys.

(b) In brief the work for this coming project year may be summarized as follows:
1) Complete the installation of the second combined field ion-field emission
microscopy system and new field ion microscopy glass screening system.
2) Continue studies of high strength alloys based on iron, nickel, cobalt
and titanium. 3) Study precipitation from two phase systems and the impor-
tant considerations of precipitation and interphase boundaries. 4) Study
order precipitation systems and the interface between the matrix and the
ordered precipitate so that more information on the strengthening mechanism
of such precipitation can be determined. 5) Evaluate in conjunction with
LEED, when possible, gas-metal surface interactions for important engineering
systems.
Justification of Program

In the precipitation or ordering in two-phase systems, certainly the width of the equilibrated phase boundaries is extremely important to the strengthening mechanisms of these systems. A study of this boundary, at least in principle, can best be determined by FIM. Although it is slow, tedious work to develop techniques for new systems in field ion microscopy, the rewards are extremely worthwhile. Over the long range this type of study will provide some of the most useful basic data in the study of alloy systems.

This year two post-graduate students will initiate work in the area of field ion-emission microscopy directly related to interface phenomena. In addition to this at least one, and possibly two papers, in field ion or field emission microscopy will be ready for publication before the end of this coming project year. One paper, a review of applications field ion and field emission microscopy, will be given in conjunction with the national fall meeting of the ASTM in Atlanta, October 4, 1968.
TASK DESCRIPTION

TITLE
"Friction, Adhesion and Wear Studies"

PROJECT NUMBER
A-1044-208

DATE
September 6, 1968

1. (a) Give a concise progress report for the last quarter (attach additional sheets if necessary) in the case of a continuing program, or if just beginning work, an abstract of research under task, and (b) a summary of the specific work to be performed during the next quarter year.

(a) The purpose of the work was to investigate those fundamental properties of metal alloys that influence adhesion and hence friction and wear phenomena. Since the simplest type of alloy system to study is the solid solution system, the following metal alloys were chosen for this work: copper-nickel, silver-gold, silver-palladium, copper-gold and platinum-cobalt. The adhesion tests were made in air by the twist-compression method. In addition to the effects of composition, those of ordering in the copper-gold and platinum-cobalt systems were also evaluated.

The results show that the adhesion of metals is affected significantly by their composition. In some instances adhesion increased with hardness in a certain range of alloy compositions, and in others the opposite was true; that is, hard metals were characterized by low adhesion coefficients. These phenomena appear to be related to the work-hardening properties of the material as was shown by the determination of work-hardening coefficients and by micro-hardness tests made on cross-sectional specimens.

(continued)

2. List faculty members, graduate students, and support personnel, including vacant positions, with percentage of time to be spent during the next quarter, designating task leader by an underline. Identify any portion to be supported by departmental funds. List graduate students doing related work but supported by fellowships, grants, etc.

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<thead>
<tr>
<th>NAME</th>
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<tbody>
<tr>
<td></td>
<td>Academic Year</td>
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<tr>
<td>J. M. Bradford</td>
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<tr>
<td>M. E. Sikorski</td>
<td>.10 (Sept., Oct.)</td>
</tr>
<tr>
<td>R. A. Newsom</td>
<td>.50 (Sept., Oct.)</td>
</tr>
<tr>
<td>K. B. Wear</td>
<td>.25</td>
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<tr>
<td>Graduate Student (vacant)</td>
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<tr>
<td>Machinist</td>
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<td>Electronics Tech.</td>
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</tbody>
</table>

3. List equipment, M&S estimate, and anticipated travel for next quarter with brief justification.

<table>
<thead>
<tr>
<th>Item</th>
<th>M&amp;S Estimate</th>
<th>Travel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Samples</td>
<td></td>
<td>Travel</td>
</tr>
<tr>
<td>Rotary feedthrough</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Screw jack</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Custom parts</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Flanges</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bellows</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bearings</td>
<td>$2,000.00</td>
<td></td>
</tr>
</tbody>
</table>

Program Manager ___________________________ Task Leader __________ J. M. Bradford

School/Dept. ___________________________ Mechanical Engineering

revised 3-68
1. (a) (Continued)

In both ordering alloy systems Cu-Au and Pt-Co it was found that adhesion was reduced with ordering and increased by disordering. In particular, the adhesion was so low for ordered specimens of 50 atomic per cent (a/o) Cu-Au, 50 a/o Pt and 10 a/o Pt Pt-Co, that it could not be measured with the twist-compression apparatus in air. It would be of interest to extend this study to a UHV apparatus in order to assess the effect of the degree of order on adhesion.

Except for some additional tests that should be made on silver-palladium systems, the experimental work has been completed. As soon as the additional results are obtained, the paper for publication in "Wear" will be completed.

(b) M. E. Sikorski: Anneal specimens of Ag-Pd alloy system and remeasure micro-hardness and adhesion values. The results obtained thus far appear to be somewhat inconsistent. This may be due to the fact that not all specimens were obtained at the same time, and therefore they may differ in mechanical history. Simultaneous homogenization treatment of all the specimens should lead to improved results.

J. M. Bradford: During the next quarter the design and fabrication of the apparatus to conduct the friction and adhesion tests in ultra-high-vacuum will be completed.

Since the vacuum system will arrive about 1 January 1969 the experimental investigations cannot begin until the winter quarter.
1. (a) Give a concise progress report for the last quarter (attach additional sheets if necessary) in the case of a continuing program, or if just beginning work, an abstract of research under task, and (b) a summary of the specific work to be performed during the next quarter year.

   (a) The initial work was directed toward a literature search with respect to the heat transfer, temperatures and solidification rates obtained in casting. A considerable amount of analytical and experimental work has been done on such problems during the last forty years. It seems that good correlations and predictions are possible when casting metal into a mold made such as sand. In this case, the interface temperature between casting and mold remains essentially constant and heat extraction rates are determined by the bulk thermal properties of the materials. When molten metals come into contact with a solid metal surface the situation is different and no systematic treatment of the conditions at the interface has been found. Heat transfer rates into metal molds are initially very high and solidification of the cast metal starts early. The existence of solidified metal next to a mold surface radically changes the heat transfer condition with the result that large variations occur during the early stages of casting. It is noted that this early stage of casting can itself be altered considerably by the application of some type of surface treatment, such as mold dressings, to the metal mold face.

   During the year, experimental work was done on casting low temperature melting (continued)

2. List faculty members, graduate students, and support personnel, including vacant positions, with percentage of time to be spent during the next quarter, designating task leader by an underline. Identify any portion to be supported by departmental funds. List graduate students doing related work but supported by fellowships, grants, etc.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
<th>Academic Year</th>
<th>Summer</th>
</tr>
</thead>
<tbody>
<tr>
<td>John H. Murphy</td>
<td>(.10) supported by M.E.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Theodor W. Kaltenberg (GRA)</td>
<td>.33 1/3</td>
<td></td>
<td>.33 1/3</td>
</tr>
<tr>
<td>Machinist</td>
<td>100 hours</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Technician</td>
<td>20 hours</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

3. List equipment, M&S estimate, and anticipated travel for next quarter year with brief justification.

   Miscellaneous supplies in the nature of thermocouples, electric wire and resistors and materials will be required at an estimated cost of $500.00.

   Travel: To attend short course on "Engineering Aspects of Solidification": (Oct. in Boston) Registration and travel--$300.00.

---

Program Manager          Task Leader John H. Murphy
School/Dept. Mechanical Engineering

Revised 3-68
1. (a) (Continued)

lead into steel molds. Surface temperatures were determined using thermo-
couples similar to ones which have been used in high speed gas flow. This
approach appears to be satisfactory but other methods of determining sur-
face temperature variation are being considered.

Preliminary investigations were made on the use of ultrasonics for detect-
ing changes in the contact between the cast metal and the mold. Although
only a limited amount of work has been done, this method appears to be
very promising as it was possible to detect changes in the contact under
some conditions.

(b) Work during the next year will be concerned with both the analytical and
experimental aspects of the project. It is desired to expand the literature
search to include a consideration of the work which has been done on
liquid metal heat transfer. A large amount of work has been done on the
use of liquid metal as a cooling agent, although this application of liquid
metals does not normally include the problem of phase change it may provide
information applicable to the initial stage of casting.

The experimental program will be continued on the investigation of the heat
transfer rates, temperatures and the formation of the air gap during the
casting of lead. It is planned to construct an analog network which will
allow the direct measurement of heat flex rates from surface temperature
measurement. The effect of surface roughness and various surface coating
will be investigated.
1. (a) Give a concise progress report for the last quarter (attach additional sheets if necessary) in the case of a continuing program, or if just beginning work, an abstract of research under task, and (b) a summary of the specific work to be performed during the next quarter year.

(a) The ultimate goal of this task is to publish a technical monograph on "interface fundamentals and their relevance to specific DoD materials problems". Near the completion of the critical review, the emphasis will be shifted to those areas or materials for which there is a high priority need for more fundamental information. The review will also establish the scientific and engineering community most directly concerned with interface problems.

(b) Second Quarter efforts will be directed towards continuing evaluation of documents presently in the projects' information system for relevance to the critical review.

2. List faculty members, graduate students, and support personnel, including vacant positions, with percentage of time to be spent during the next quarter, designating task leader by an underline. Identify any portion to be supported by departmental funds. List graduate students doing related work but supported by fellowships, grants, etc.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>R. L. Bullock</td>
<td>.10 (Supported by PSD)</td>
</tr>
<tr>
<td>Don Myers</td>
<td>60 hrs./mo.</td>
</tr>
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</table>

3. List equipment, M&S estimate, and anticipated travel for next quarter with brief justification.

Materials and supplies - $250

Program Manager 
Task Leader R. L. Bullock
School/Dept. Physical Sciences Division

revised 3-68
1. (a) Give a concise progress report for the last quarter (attach additional sheets if necessary) in the case of a continuing program, or if just beginning work, an abstract of research under task, and (b) a summary of the specific work to be performed during the next quarter year.

(a) Efforts since the beginning of the program have been directed toward establishing and maintaining budgets, procedures, and communications as needed, under the direction of the Program Manager.

(b) These efforts will continue during the coming year, with modifications as required by the nature of the program. Additionally, it is hoped that greater use can be made of the Office of Interdepartmental Programs by the administrative and academic departments in developing their ideas for improving existing systems and procedures, whether external to or connected with Project THEMIS.

2. List faculty members, graduate students, and support personnel, including vacant positions, with percentage of time to be spent during the next quarter, designating task leader by an underline. Identify any portion to be supported by departmental funds. List graduate students doing related work but supported by fellowships, grants, etc.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
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</thead>
<tbody>
<tr>
<td>Jon Barbour</td>
<td>.25 (12 months)</td>
</tr>
<tr>
<td>Sandra Young (Clerk)</td>
<td>.50 (12 months)</td>
</tr>
<tr>
<td>Technical Assistance</td>
<td>50 hours</td>
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<tr>
<td></td>
<td>(For preparation of proposals and reports)</td>
</tr>
</tbody>
</table>

3. List equipment, M&S estimate, and anticipated travel for next quarter with brief justification.

NONE

Program Manager ___________________ Task Leader ___________________ Jon Barbour

School/Dept. ___________________ Physical Sciences Division

revised 3-68
TASK DESCRIPTION

"The Interaction of Gases with Solids"

TITLE PROJECT NUMBER A-1044-215

DATE September 20, 1968

1. (a) Give a concise progress report for the last quarter (attach additional sheets if necessary) in the case of a continuing program, or if just beginning work, an abstract of research under task, and (b) a summary of the specific work to be performed during the next year.

(a) Three basis adsorption systems are under construction:
1. A very high precision volumetric system designed for studying gas-solid interactions in the very low coverage region.
2. A more or less conventional volumetric system designed to study multilayer formation.
3. A gravimetric system designed to study two-dimensional phase transitions. Systems 1 and 2 are virtually complete except for minor alterations required as we begin using the systems. The third system is in the final stage of construction and should be complete this summer. System 1 has been tested by using it as an oxygen vapor pressure thermometer. The system operated very well although we found it desirable to reconstruct and thermostat the entire gas pipette system. This has been done.

(b) During the next year, we plan to carry out the measurements of the interaction of neon, argon, krypton and xenon with boron nitride using the high precision apparatus. System 2 will be used to study the formation of multilayers of krypton on graphite and boron nitride in the temperature range 70°K to 85°K. System 3 will be completed and we will study the nature of the phase transitions of CH₃Cl, CHCl₃ and CCl₄ on both graphite and on boron nitride.

2. List faculty members, graduate students, and support personnel, including vacant positions, with percentage of time to be spent during the next year, designating task leader by an underline. Identify any portion to be supported by departmental funds. List graduate students doing related work but supported by fellowships, grants, etc.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
</tr>
</thead>
<tbody>
<tr>
<td>R. A. Pierotti</td>
<td>.10 acad. yr. (supported by Chemistry Dept.)</td>
</tr>
<tr>
<td>David Newsome (Ph.D. candidate)</td>
<td>.50</td>
</tr>
<tr>
<td>Reg N. Ramsey (Ph.D. candidate)</td>
<td>.50</td>
</tr>
</tbody>
</table>

Persons on related work receiving support from other sources

- Joseph Delay, (Teaching Ass’t) (Ph.D. candidate) .50
- Dr. H. E. Thomas, Postdoctoral Fellow 1.00 (starting Oct. 1968)

3. List equipment, M&S estimate, and anticipated travel for next year with brief justification.

- Equipment: $1,000 ($250/quarter for items over $25)
- Materials & Supplies: 1,600 ($400/quarter)
- Travel: 300

Program Manager

Task Leader R. A. Pierotti

School/Dept. Chemistry

Revised 3-68
1. (a) Give a concise progress report for the last quarter (attach additional sheets if necessary) in the case of a continuing program, or if just beginning work, an abstract of research under task, and (b) a summary of the specific work to be performed during the next quarter year.

(a) The continuation of this task from September 1968 to September 1969 will be an investigation of a specific research need in the area of surface and diffusion coatings as indicated by our survey conducted during February 1968 through August 1968. Part of the effort this year will be directed towards incorporating the results of the survey into the Critical Review for the THEMIS Program. This will also include the proposed contract with key individuals in government agencies.

A parametric experimental study for the preparation of a coating by Chemical Vapor Deposition (CVD) will be undertaken. CVD is the primary mechanism in the preparation of coatings by the pack-cementation and fluidized bed processes and is the essential mechanism in the strictly gas phase CVD process. The analysis of the data will include the consideration of gas-phase diffusion as well as deposition kinetics with the purpose of determining the pertinent variables so that the effect of changes in geometry, flow conditions, and operating conditions may be predicted. Studies of this nature should lead in the future to a more quantitative approach to full-scale coating preparation utilizing CVD.

(b) The work to be done next quarter will include a brief look at the literature to determine the particular coating system to be studied, and modifying the necessary equipment, and ordering supplies.

2. List faculty members, graduate students, and support personnel, including vacant positions, with percentage of time to be spent during the next year, designating task leader by an underline. Identify any portion to be supported by departmental funds. List graduate students doing related work but supported by fellowships, grants, etc.

<table>
<thead>
<tr>
<th>NAME</th>
<th>PERCENT TIME</th>
<th>SUMMER</th>
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<tbody>
<tr>
<td>C. W. Gorton</td>
<td>.15</td>
<td>.15</td>
</tr>
<tr>
<td>C. A. Murphy</td>
<td>.05</td>
<td>.05</td>
</tr>
<tr>
<td>S. H. Bomar</td>
<td>.05</td>
<td>.05</td>
</tr>
<tr>
<td>A. C. Merritt (GRA)</td>
<td>.50</td>
<td>-</td>
</tr>
<tr>
<td>Graduate Research Asst. (vacant)</td>
<td>-</td>
<td>.50</td>
</tr>
</tbody>
</table>

3. List equipment, M & S estimate, and anticipated travel for next quarter with brief justification.

   Equipment: (The equipment, including a CVD rig which with suitable modifications can be used in the present study is currently available at the HTMD).

   M & S: (research notebooks, Xerox copies, gases, miscellaneous tubing, valves, etc. $500

   Travel: (Primarily to discuss Critical Review with suitable Government Agencies) $500

---

Program Manager

Task Leader: C. W. Gorton

School/Dept.: High Temperature & Materials Div

Revised 3-68
SPECIAL REPORT OF PROGRESS

1. Papers presented at meetings


"Inelastic Scattering of Low Energy Electrons," by E. J. Scheibner. A Series of lectures were presented at the NATO International Summer Course on Fundamental Processes on Semiconductor Surfaces, held at the University of Ghent, Belgium, August 26 - September 6, 1968.


In addition to the above, the following seminars were presented under a quarterly seminar series established in connection with the THEMIS program:


"Thermodynamic Stability Theory, Phase Separation in Liquid and Solid Solutions, Spindal Decomposition," Ten-part series by W. T. Ziegler, Regents Professor of Chemical Engineering, School of Chemical Engineering, Summer quarter, 1968.


"Thermodynamics of the Solid-Gas Interface" by Jan C. Eriksson, Postdoctoral Fellow in Physics, Physical Sciences Division, EES, November, 1967.

2. Journal papers published or submitted for publication

Eriksson, Jan C., "Thermodynamics of Surface Phase Systems." To be published in "Surface Science."


In addition, Dr. R. F. Hochman directed the following unpublished Master of Science Thesis:

Topolski, F. J., "The Effects of Ultrasonics on the Physical and Mechanical Properties of Metals."

3. Fiscal Information

<table>
<thead>
<tr>
<th></th>
<th>Budget 1</th>
<th>Expended 2</th>
<th>Encumbered 2</th>
<th>Balance 2</th>
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<td>$97,355.98</td>
<td>$</td>
<td>$69,545.02</td>
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<tr>
<td>Overhead (57% of PS)</td>
<td>95,134</td>
<td>55,492.86</td>
<td>39,641.14</td>
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<tr>
<td>Materials and Supplies</td>
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<td>10,475.02</td>
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<tr>
<td>Equipment</td>
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<td>24,756.65</td>
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<td>Travel</td>
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<td>Computer</td>
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<td>1,680.00</td>
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<td>TOTAL</td>
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<td>$189,939.27</td>
<td>$40,778.72</td>
<td>$126,532.01</td>
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Notes:

1. Since initiation of the program.

4. Faculty and Staff Participation

<table>
<thead>
<tr>
<th></th>
<th>Actual Number of Individuals</th>
<th>Actual FTE Man-Years</th>
</tr>
</thead>
<tbody>
<tr>
<td>Senior Faculty Members</td>
<td>8</td>
<td>.903</td>
</tr>
<tr>
<td>Associate Faculty Members</td>
<td>18</td>
<td>3.930</td>
</tr>
<tr>
<td>Graduate Research Assistants</td>
<td>12</td>
<td>2.695</td>
</tr>
<tr>
<td>Undergraduate Student Assistants</td>
<td>10</td>
<td>.632</td>
</tr>
<tr>
<td>Technical Staff</td>
<td>34</td>
<td>1.862</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>82</strong></td>
<td><strong>10.022</strong></td>
</tr>
</tbody>
</table>

Notes:

1. From September 1, 1967 through November 30, 1968. Figures through December, 1968 unavailable at time of printing.

2. Includes .379 man-years supported by institutional funds.

3. Includes .020 man-years supported by institutional funds.

4. Technical staff includes all personnel, not previously listed (e.g., report reproducers, technical assistants, machinists, etc.), who have contributed to the program since its initiation.

5. Three Most Significant Technical Achievements

A. Two-Phase Alloys and Order-Disorder Transformations.

A major program related to the THEMIS effort is the study of two-phase alloys and order-disorder transformations. Impetus in the field has been provided by Dr. Brian Ralph of Cambridge University, Cambridge, England, who serves as a visiting Professor and consultant to Georgia Tech. This area has developed because of the interest of Dr. Hochman and his staff in the study of interfaces and phase transformations in applied metallurgical systems. To date, studies on alloys of nickel, titanium, iron and silver have been initiated.

B. LEED and Analysis of Inelastically Scattered Electrons.

The combined techniques of LEED and electron spectroscopy, which is the energy analysis of inelastically scattered electrons, have been developed to the extent that significant information can be expected on energy band structure at surfaces, the identification of trace impurities, and the nature of chemical bonding.
C. Thermodynamics of Gas-Solid Interfaces.

The theoretical development of the thermodynamics of gas-solid interfaces, summarized in the paper submitted by Dr. Eriksson, is a significant step in the understanding of engineering interfaces and provides a basis for further experimental studies now in progress under the THEMIS program.

6. Advisory Assistance Provided

Inquiries in regard to the program have been made by various individuals in DOD to AFOSR. Further requests for information have been directed to Georgia Tech. Technical discussions have been held with Dr. L. Jenkins, Solid State Division ORNL, Dr. T. W. Haas, Aerospace Research Labs, Wright-Patterson Air Force Base and Dr. J. O. Porteus, Naval Weapons Center, China Lake, California. In addition, participation with NRL on a stress corrosion cracking program has brought us into contact with interface problems related to this area.

A series of critical review papers on interface phenomena in selected problem areas are planned for publication in the open literature. Consultation and cooperation with various individuals in DOD laboratories in connection with these reviews should result in a close awareness of DOD needs.

7. Other Significant Developments

A. The integration of basic studies on adhesion with studies on the machinability of materials has begun with an association between M. E. Sikorski and Dr. John Bailey of N. C. State University. A new faculty member, Dr. J. Bradford, has been added to the School of Mechanical Engineering and the THEMIS program. Dr. Bradford has experience on characterization of surfaces in ultra-high vacuum and adhesion. He will strengthen the area of adhesion-machinability.

B. A Field-Ion Microscopy Symposium in Physical Metallurgy and Corrosion, held at Georgia Tech on May 15-17, 1968 was organized by Dr. R. F. Hochman of Georgia Tech and Dr. Brian Ralph of Cambridge University.

C. The Technical Information Section of the Physical Sciences Division has devoted considerable effort to the examination and cataloging of articles and other publications relating to interface phenomena. This information has been provided to the task leaders as a basis for preparing the planned critical review of interface phenomena.

D. The Office of Interdepartmental Programs has provided administrative assistance to the Program Manager and Task Leaders as dictated by the nature of the interdisciplinary program.
This proposal is made on the basis that any resulting contract will be negotiated, and that it will be an amendment to cost-reimbursement (no-fee) Contract No. F44620-68-C-0008. It is made out in the name of the GEORGIA TECH RESEARCH INSTITUTE, which is incorporated under the laws of the State of Georgia, with its business address at the Administration Building, Georgia Institute of Technology, Atlanta, Georgia 30332.

Time and Budget Estimate

Contract No. F44620-68-C-0008 currently operates on schedule calling for research to be conducted during the period 1 September 1967 through 31 August 1971, and is "step-funded" over the four year period. This renewal proposal (and the budget estimate below) is predicated on performance at the established level-of-effort for the second year ($182,250 for the period 1 September 1968-31 August 1969); an increase to full level-of-effort for the third year (increase to $189,417 for the period 1 September 1969-31 August 1970); and step-funding at the increased level through the fourth year (1 September 1970-31 August 1971) and through the addition of a fifth year (1 September 1971-31 August 1972).

A summary budget estimate and detailed estimate follow:
<table>
<thead>
<tr>
<th></th>
<th>First Year 9/1/67-8/31/68</th>
<th>Second Year 9/1/68-8/31/69</th>
<th>Third Year 9/1/69-8/31/70</th>
<th>Fourth Year 9/1/70-8/31/71</th>
<th>Fifth Year 9/1/71-8/31/72</th>
</tr>
</thead>
<tbody>
<tr>
<td>Direct Salaries and Wages</td>
<td>$101,185</td>
<td>$107,173</td>
<td>$113,459</td>
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<tr>
<td>Overhead (at 57% of DSW)</td>
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<td>57,305</td>
<td>60,718</td>
<td>64,301</td>
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<td>Retirement Benefits (at 8.5% of applicable DSW)</td>
<td>4,450</td>
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<tr>
<td>Materials and Supplies</td>
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<td>13,378</td>
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<tr>
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<td>980</td>
<td>980</td>
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<tr>
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<tr>
<td>Equipment</td>
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<td>15,000</td>
<td>10,000</td>
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<tr>
<td>TOTAL</td>
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<td>$182,250</td>
<td>$189,417</td>
<td>$198,334</td>
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<table>
<thead>
<tr>
<th></th>
<th>Already Allotted</th>
<th>Proposed Additional</th>
<th>Total</th>
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</thead>
<tbody>
<tr>
<td>First year</td>
<td>$175,000</td>
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<td>$175,000</td>
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<td>Second year</td>
<td>182,250</td>
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<td>182,250</td>
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<td>Third year</td>
<td>122,750</td>
<td>$66,667</td>
<td>189,417</td>
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<tr>
<td>Fourth year</td>
<td>65,000</td>
<td>67,222</td>
<td>132,222*</td>
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<tr>
<td>Fifth year</td>
<td>-0-</td>
<td>66,667</td>
<td>66,667**</td>
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<tr>
<td>TOTAL</td>
<td>$545,000</td>
<td>$200,556</td>
<td>$745,556</td>
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*2/3 of $198,334
**1/3 of $200,000
### Detailed Budget Estimate

<table>
<thead>
<tr>
<th></th>
<th>Third Year 9/1/69-8/31/70</th>
<th>Fourth Year 9/1/70-8/31/71</th>
<th>Fifth Year 9/1/71-8/31/72</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Direct Salaries and Wages</strong></td>
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<tr>
<td><strong>Senior Faculty Members</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dr. E. J. Scheibner, Research Professor of Physics -- Program Manager:</td>
<td>$7,138</td>
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<tr>
<td>($27,000/12 mos.) 25% time/yr.</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Dr. C. W. Gorton, Professor of Chemical Engineering</td>
<td>3,838</td>
<td>3,925</td>
<td>4,121</td>
</tr>
<tr>
<td>($24,370/12 mos.) 15% time/yr.</td>
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<tr>
<td>Dr. J. H. Murphy, Associate Professor of Mechanical Engineering</td>
<td>1,595</td>
<td>1,673</td>
<td>1,756</td>
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<td>($15,200/9 mos.) 33 1/3% time/summer</td>
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<td>Dr. R. A. Pierotti, Associate Professor of Chemistry</td>
<td>1,888</td>
<td>1,982</td>
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<td>($18,000/9 mos.) 33 1/3% time/summer</td>
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<td>Dr. J. R. Stevenson, Associate Professor of Physics</td>
<td>1,750</td>
<td>1,838</td>
<td>1,930</td>
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<tr>
<td>($20,000/12 mos.) 33 1/3% time/summer</td>
<td></td>
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<tr>
<td><strong>Advisory Faculty Members</strong></td>
<td>3,650</td>
<td>3,800</td>
<td>4,000</td>
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<tr>
<td>To provide assistance as needed, W. T. Ziegler, Regents' Professor, Chemical Engineering</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>R. F. Hochman, Associate Professor, Chemical Engineering</td>
<td></td>
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<tr>
<td>E. A. Starke, Jr., Assistant Professor, Chemical Engineering</td>
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<tr>
<td><strong>Associate Faculty Members</strong></td>
<td>28,000</td>
<td>29,400</td>
<td>30,870</td>
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<td>Research Scientists &amp; Research Engineers 7 at average $16,000/12 mos. 25% time/yr.</td>
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<td><strong>Graduate Research Assistants</strong></td>
<td>41,000</td>
<td>45,100</td>
<td>49,200</td>
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<td>50% time at average $8,200/12 mos.</td>
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<td><strong>Student Assistants</strong></td>
<td>7,176</td>
<td>7,486</td>
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<td>3 at 50% time each ($2.20/hr.)</td>
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<td></td>
<td>Third Year</td>
<td>Fourth Year</td>
<td>Fifth Year</td>
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<tr>
<td>--------------------------</td>
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<td>-------------</td>
<td>------------</td>
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<tr>
<td><strong>Other Personnel</strong>: Machinists, technical assistance, report reproducers, etc. at average $4.50/hr.</td>
<td>(1,000 hrs.)</td>
<td>(850 hrs.)</td>
<td>(700 hrs.)</td>
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<td>4,500</td>
<td>3,825</td>
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<td><strong>Professional Services</strong></td>
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<tr>
<td>For advisory assistance on related problems (e.g., machinability - Dr. J. A. Bailey, Associate Professor, Mechanical Engineering at North Carolina State University)</td>
<td>650</td>
<td>650</td>
<td>650</td>
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<td><strong>Total Direct Salaries and Wages</strong></td>
<td>$101,185</td>
<td>$107,173</td>
<td>$113,459</td>
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<td><strong>Retirement Benefits</strong></td>
<td>4,450</td>
<td>4,585</td>
<td>4,744</td>
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<tr>
<td>At 8.5% of applicable salaries (excluding Graduate and Student Assistants and Professional Services)</td>
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<tr>
<td><strong>Overhead</strong></td>
<td>57,305</td>
<td>60,718</td>
<td>64,301</td>
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<tr>
<td>At a predetermined fixed rate of 57% of Direct Salaries and Wages as established by the Navy Material Command upon advisory audit by the Defense Contract Audit Agency</td>
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<tr>
<td><strong>Materials and Supplies</strong></td>
<td>8,717</td>
<td>13,378</td>
<td>10,516</td>
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<tr>
<td>Electronics for vacuum systems, chemicals, and specimens (metal samples, crystals)</td>
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<tr>
<td><strong>Computer Time</strong></td>
<td>560</td>
<td>980</td>
<td>980</td>
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<tr>
<td>Burroughs B-5500 (Contractor-owned) at $140/hr.</td>
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<td><strong>Travel Time</strong></td>
<td>2,200</td>
<td>1,500</td>
<td>1,000</td>
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<tr>
<td>Visits to scientific meetings, DOD agencies and laboratories including advisory assistance</td>
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<tr>
<td><strong>Equipment</strong></td>
<td></td>
<td></td>
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<tr>
<td>Cryopanel</td>
<td>$800</td>
<td></td>
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<tr>
<td>Transducers and Indicators</td>
<td>2,000</td>
<td></td>
<td></td>
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<tr>
<td>Gas Inlet System</td>
<td>1,331</td>
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<tr>
<td>Gas Delivery System</td>
<td>1,878</td>
<td></td>
<td></td>
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<tr>
<td>Quadrupole</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Residual Gas Analyzer Head</td>
<td>4,600</td>
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<tr>
<td>Miscellaneous Equipment Items</td>
<td>4,391</td>
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<tr>
<td><strong>Total Annual Budget Estimates</strong></td>
<td>$189,417</td>
<td>$198,334</td>
<td>$200,000</td>
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</table>
Notes:

1. Salaries shown are actual FY 1969 rates; salaries for third, fourth and fifth years are projected.

2. Summer salaries are computed at 30% of the previous 9 month salary according to Institute policy.

3. A part of the time noted is to be supported by institutional funds.

4. Direct labor costs involved in report reproduction are included under Direct Salaries and Wages.

5. The specific items are detailed only for the third year since it is difficult to anticipate precise needs for subsequent years.

Contractual Arrangements

This proposal is made on the basis that Contract No. F44620-68-C-0008 will be amended, and that except to the extent modified by this material or by negotiation, the same terms and conditions will apply.
EXHIBIT I: Budget Detail by Categories
(for Equipment and Materials and Supplies)

Equipment:

1. The following items are needed to complete existing basic vacuum systems.
   a. Varian.* Cryopanel. To be fabricated by manufacturer to order. $800
   b. Stratham, Daytronic. 3 bakeable UHV transducers at average $375/each. 1,125
   c. Daytronic. Transducer control circuit indicators, #300D-P-71 and Type 93 input module. 875
   d. Granville-Phillips. 1 each bakeable and non-bakeable ion leak valves for gas inlet system. #202016-02-089-089 at $196/each. 392
   e. Granville-Phillips. 2 automatic pressure control valves for gas inlet system and gas delivery system. #213001-02-088-088 at $939/each. 1,878
   g. Granville-Phillips. 2 Type C valves with low torque drivers for gas delivery system. #202019-02-089-089 at $339/each. 678
   h. Varian. Quadrupole residual gas analyzer sensing head. 4,600

2. Miscellaneous equipment items
   a. Sorenson. Highly regulated DC power supply. #QRC 40-4A 315
   b. Moseley. X-Y recorder. #7030A 2,500
   c. Hewlett-Packard. DC milliammeter. #428B 600
   d. Electronics, valves, small tooling items 976

   TOTAL $15,000

*Manufacturers listed are typical, and it is understood that equal products are acceptable.
Materials and Supplies:

1. Single Crystals

Materials Research Corporation, Orangeburg, New York

Crystal categories and cost examples:

high purity poly-crystals, approximately 1/4" x 1" x 1"

<table>
<thead>
<tr>
<th>Material</th>
<th>Quantity</th>
<th>Cost per Item</th>
<th>Total Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>iron</td>
<td>6 @ $25</td>
<td>$150</td>
<td></td>
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<tr>
<td>silver</td>
<td>6 @ $15</td>
<td>90</td>
<td></td>
</tr>
<tr>
<td>nickel</td>
<td>6 @ $40</td>
<td>240</td>
<td></td>
</tr>
<tr>
<td>magnesium</td>
<td>6 @ $35</td>
<td>210</td>
<td></td>
</tr>
<tr>
<td>copper</td>
<td>6 @ $10</td>
<td>60</td>
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</tbody>
</table>

Estimated total cost $750

2. Special Alloys - custom made:

Suppliers: Hamilton Precision Metals, Lancaster, Pennsylvania
Materials Research Corporation, Orangeburg, New York

copper, silver, gold, palladium, beta brass, zinc

5 pcs. at average of $120 each

Estimated total cost $600

3. High Vacuum Components

Suppliers: Granville-Phillips Company
Varian

a. Gauges and cost examples
Varian. UHV 24 Gauge tube 200

b. Flanges and fittings and cost examples
Varian. Thermocouple feedthrough. #954-5015 105
Varian. 8-pin feedthrough. #954-5012. 2 @ $180 360
Varian. Medium current feedthrough. #954-5019 2 @ $60 120
Varian. High voltage feedthrough. #954-5007. 2 @ $50 100

Estimated total cost 685

c. Valves
Matheson. High pressure regulating valve
Model No. 2 4 @ $50 200

Estimated total cost 1,085
4. Chemicals and Gases

Liquid Nitrogen, Helium, Argon, Hydrogen, Neon, Hydrofloric Acid, Methanol, etc. 2,382

5. Electronic supplies

Replacement filaments, electronic components, solid state devices, meters, panels, etc. 1,200

6. Page charges for publications

2 articles at $350 700

7. Materials and supplies for reports (printed by contractor) 2,000

Estimated Total $8,717
Proceedings of the FIRST ANNUAL SYMPOSIUM ON INTERFACE PHENOMENA IN ENGINEERING MATERIALS

A report on research in progress related to and under Department of the Air Force THEMIS Contract F44620-68-C-0008

10 December 1969

Georgia Institute of Technology Atlanta, Georgia 30332
Proceedings of
the
FIRST ANNUAL SYMPOSIUM
ON
INTERFACE PHENOMENA IN ENGINEERING MATERIALS

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10 December 1969

Georgia Institute of Technology
Atlanta, Georgia
30332
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<td>Dr. Bruce W. Davis</td>
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<tr>
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<td>Dr. Helen Grenga and Dr. R. F. Hochman</td>
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<tr>
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*Not presented orally
FOREWORD

Since 1 September 1967 a team of faculty members, technical staff and students from several departments of Georgia Institute of Technology has been conducting research on various aspects of surface or interface phenomena. Prior to that date individual efforts had received recognition but there were few coordinated studies. With the onset in 1967 of Project THEMIS, sponsored by the Air Force Office of Scientific Research under Contract F44620-68-C-0008, it became possible to strengthen existing programs and to develop new groups in accordance with certain objectives. These objectives are to strengthen the graduate programs of the Institute which include the area of interface phenomena and to achieve a significant capability for responding to the needs of the Department of Defense in the same area.

The symposium on "Interface Phenomena in Engineering Materials" held at Georgia Tech on 10 December 1969 was organized to serve several purposes: it provided a means for reporting on all the THEMIS research and other efforts related to the scope of the THEMIS program; it gave graduate students an opportunity to participate so that they would gain experience for other similar meetings; through the presentations all participants could hear what others were doing; and through these proceedings further exchange between participants should result.

The symposium comprised four sessions whose general themes were as follows: Session I - Fundamental Science, i.e., physics and chemistry of surfaces; Session II - Oriented Basic Research, i.e., research directed towards the solution of broadly defined problems; Session III - Conceptual Studies, i.e., models or techniques; and Session IV - Application Investigations.

It is hoped that by the publication and dissemination of these symposium proceedings appropriate Department of Defense agencies, laboratories or individuals will find certain programs or groups of programs of interest to them and that they will contact us for further information.

The assistance of the Department of Defense through our AFOSR THEMIS Contract is acknowledged with thanks.

Dr. Edwin I. Scheibner
Research Professor of Physics
Program Manager
SESSION I
FUNDAMENTAL SCIENCE
CHAIRMAN
DR. A. L. BENNETT
THE LONG RANGE OBJECTIVES OF THE OPTICAL PHYSICS PROGRAM
RELATING TO PROJECT THEMIS

Dr. J. R. Stevenson

I. One of our first objectives is to develop a capability of responding quickly to new ideas. In this regard we must have two ingredients, namely the necessary technical population as well as the capital equipment required for experimentation. In regard to the technical population, Project THEMIS has encouraged us to make use of both "in-house" technical people at Georgia Tech as well as collaborative efforts with government laboratories. We hope that the collaborative effort will not be restricted to the faculty and staff at Georgia Tech with respect to the government laboratories, but also that we can build a collaborative effort which will involve postdoctoral students, graduate students and undergraduate students. Only by involving the latter three categories will we really accomplish the educational objective associated with Project THEMIS and hopefully, provide a nucleus for future collaborative efforts between the students now enrolled at Georgia Tech and government laboratories. Regarding equipment, we have available a capability of doing "vacuum ultraviolet reflectivity" measurements as well as extending our measurements into the visible region of the electromagnetic spectrum. Our capability in the infrared is somewhat limited although we do have a prism monochromator allowing us to extend our measurements to approximately 30 or 40 microns. We are attempting to build up a laser capability in which we would use the lasers as tools in making optical measurements.

II. Another objective is to remain in the forefront of programs related to "materials design". By this statement we imply that some time in the future an engineer would be able to request a material with specific parameters for a device application and that a computer could be employed to specify the conditions under which such a material could be made and used. As optical measurements serve as valuable input parameters to theoretical band structure calculations, we are hoping to provide enough experimental input that meaningful calculations can be made on alloy systems and on materials subject to some sort of stress bias. The use of alloys in materials design will certainly increase the number of permutations available as well as provide a much higher degree of flexibility in the parameters of interest. In addition the use of a material under some sort of stress will allow for the modulation of many important parameters incorporated in the band structure calculation. The modulation of band structure parameters with an externally applied pressure or externally applied electric field are well known and can certainly be utilized to produce a material of desired characteristics. A recent report in the Journal of Applied Physics has indicated the feasibility of making a mechanical bond of glass to metal in which the glass is kept at a temperature below its softening point. This particular bond is accomplished through the use of an externally applied electric field.
III. Although there are many areas of optical physics which are of value in studying interface phenomena, we plan to capitalize on our demonstrated areas of achievement while we are developing other specializations. In particular at Georgia Tech the capability exists for the characterization of a solid surface under ultrahigh vacuum conditions by making use of low energy electron diffraction as well as low energy scattering and Auger electron microscopy. The availability of optical measurements on well characterized surfaces is very limited and we will certainly strive to achieve the required instrumentation such that we can simultaneously make low energy electron measurements at the same time we are making optical reflectivity measurements. In this regard the availability of the storage ring facility at Stoughton, Wisconsin, enables us to realistically consider such an experimental arrangement. The storage ring provides us with a light source under ultrahigh vacuum conditions. In addition, we will increase the resolution of our reflectivity measurements by making use of differential techniques. In the future we plan to extend our optical measurements to other areas of the electromagnetic spectrum as well as making use of emittance, photoemission, and ellipsometry techniques.

IV. In addition to making use of new techniques we also plan to investigate new areas associated with the optical physics of materials. In particular, we have concentrated on the vacuum-solid interface but we would like to extend these measurements to the liquid-gas interface as well as the liquid-solid interface. The use of lasers to produce nonlinear surface effects is of considerable interest as is the possibility of creating new surface transport phenomena by applying field gradients as well as uniform static fields.

+Professor of Physics

The characteristic energy losses for clean titanium and chromium have been measured. Clean surfaces were prepared in situ by evaporation with pressure increases of less than $2 \times 10^{-9}$ Torr. Qualitative analysis by Auger spectroscopy indicated that the films were essentially free from contamination.

The peaks observed in the electron loss spectra that are reported in this paper have been interpreted as bulk loss, harmonics of the bulk loss, surface loss and combination of bulk and surfaces losses. The identification of surface losses was based on two criteria. The relative intensity of the surface loss should be voltage dependent, and surface loss intensity should be dependent on the presence of adsorbed gases.

Plasmon theories are directly applicable only to "free" electron metals, such as aluminum, which has received considerable theoretical and experimental attention. We have made energy loss measurements for clean and oxygen covered aluminum films in order to provide a standard for comparison with our results from titanium and chromium. Figure 1 summarizes the data obtained for aluminum. Curve (a) represents a clean surface, and (b)-(d) show the effects of increasing oxygen exposures. The bulk loss was observed at 15 eV. and the surface loss at 10 eV.; both values are in agreement with theoretical and other experimental values. Note that the intensity of the surface loss decreases with increasing oxygen exposure. No changes were observed below exposures of $6 \times 10^{-6}$ Torr-sec. Since the loss peak at 25 eV. also decreased with oxygen coverage, we have interpreted this loss to be a combination surface and bulk loss. The peak at 30 eV. is the second harmonic of the bulk loss.

The energy loss spectra for titanium is shown in Fig. 2. Curve (a) again represents a clean surface and (b)-(d) show the effects of increasing oxygen coverage. Oxygen exposures of $3 \times 10^{-7}$ Torr sec. are required to change the intensity of the surface loss. If one assumes that the same coverage is required to alter the loss intensity for both aluminum and titanium, then these results indicate that the sticking coefficient for oxygen is about 20 times that for aluminum. The bulk loss for titanium is observed at 13 eV. and the surface loss was measured at 7 eV. These values are not in agreement with theoretical values for the titanium $4s^23d^4$ valence configuration. Theoretical consideration of these measured values are now in progress. Note the improved resolution of the loss peak at 26 eV shown in curve (d). This loss has been interpreted as the second harmonic of the bulk loss. The improvement in resolution of this peak with oxygen coverage is attributed to the decrease in intensity of a combination surface and bulk loss at 20 eV.
Measurements for chromium films exhibit similar changes in peak intensity for the surface and combination losses for oxygen adsorption. The sticking probability for oxygen on chromium appears to be about the same as for titanium. The bulk loss at 10 eV and the surface loss at 8 eV do not agree with calculated values for chromium $4s^15d^2$ valence configuration.

*Supported in part by ARPA Contract No. 878.
+Research Chemist
Fig. 1. Energy Loss Spectrum for Aluminum
Fig. 2. Energy Loss Spectrum for Titanium.
THE AUGER EFFECT:

L-SERIES TRANSITION PROBABILITIES

J. D. Phillips

If an atom of any element is suddenly ionized in an inner shell, it is then in an unstable configuration. In a time of order $10^{-14} - 10^{-16}$ seconds, the resulting system will de-excite in one of two ways. First, the vacancy may be filled by an electron from an outer shell accompanied by the emission of a photon with energy determined by the Bohr frequency condition. Thus, if the initial vacancy is in the K-shell and an electron from the L-shell fills it, the photon energy is given by

$$E_p = E_K - E_L$$

where $E_p$, $E_K$, and $E_L$ are the photon, K-shell, and L-shell energies respectively.

Such a mode of de-excitation is commonly termed a radiation transition. In the second mode, the outer electron again fills the inner vacancy but an electron—rather than a photon—is emitted. No photon occurs in this de-excitation mode and this "radiationless" transition is called the Auger effect. Since the effect involves ionization of the inner levels, it is relatively insensitive to the behavior of the valence electrons. Therefore, even if the atom is chemically bound—as might be the case at a gas-solid interface—the Auger spectra from it will be essentially unchanged from that of a free atom. We see then that a knowledge of the Auger effect will enable one to better understand the nature of surface contamination by identifying the Auger spectra arising from the surface.

Unfortunately, theoretical treatment of the Auger effect is still lacking with only the K-series receiving significant attention (the series name is determined by the shell of the initial vacancy). Since the investigation of the surfaces of materials requires low energy probes, we cannot expect to obtain K-series Auger spectra in any but the lightest elements. Instead the L-series and M-series are the most important, and here the theoretical work is significant. We have, therefore, undertaken a program which will ultimately lead to theoretical predictions for the energies and intensities of L-series Auger spectra. Completion of such a program inevitably will require large amounts of computation. A synopsis of the requirements of the program describes the work in fair detail. First, we must compute the one electron wave functions for the initial and final states of the atom in question. A variation of the self-consistent field formalism will be utilized for this in order to obtain the best possible wave functions—and thereby the best possible intensity predictions. Computation of these functions—though straightforward—is a tedious and time-consuming task requiring computers for meaningful results.
Once we have attained these single particle functions, it remains to combine them in such a way that we have—as nearly as possible—an exact wave function for the system Hamiltonian. This may be done in a variety of ways but the two most common methods involve the coupling of the angular portions of the single particle functions into one angular function. This is, of course, just the coupling of the angular momenta of the various electrons in say the LS or jj schemes. Even these are generally not sufficient since most atoms require a hybrid of these two schemes—e.g., intermediate coupling. This will be included when needed in our computations. It is also anticipated that the simplest approach in the calculation of energies and transition probabilities will be insufficient in the general case. Thus it is found that the Hamiltonian has matrix elements linking states of different configurations (different principle quantum number n) which are ignored in the simplest approach. This configuration interaction will also be included in our calculations. Finally, relativistic effects become important quite rapidly and will have to be included in any comprehensive treatment of the Auger effect. At the outset, we will be concerned primarily with the L-series for titanium and may be able to ignore relativistic corrections.

Upon completion of this task in a satisfactory fashion, it would be desirable to extend the procedure to the case of solids. This would require a knowledge of the band structure for the solid in question requiring in turn the computation of the complicated band functions. Our results will, in all stages, be compared with current experimental values and used in surface contamination studies.

*Supported in part by AEC under Contract No. AT - (40-1) -2755.

+Graduate Student in Physics


INTERACTION OF THE INERT GASES WITH HEXAGONAL BORON NITRIDE

Reginald N. Ramsey and Dr. R. A. Pierotti

An adsorption virial equation of state is used in the investigation of the argon-boron nitride (hexagonal modification of boron nitride) system. The $n^{th}$ coefficient of an adsorption virial equation, derived by statistical mechanical techniques, is related to the simultaneous interaction of $n-1$ gas molecules with the adsorbent and with each other. The statistical relation for the second gas-solid virial coefficient, with a Lennard-Jones potential energy function for one gas molecule-surface interaction is used to determine the depth of the potential well and the approximate boron nitride surface area from experimental data.

A precision adsorption apparatus for making measurements on low surface area solids suitable for the virial treatment is described. The sample temperature can be controlled to ±0.001° K over the temperature range from below the normal boiling point of nitrogen to above room temperature and the gas pressure is measured with a mercury manometer from 10-760 torr with a precision of ±0.01 torr. The boron nitride surface area is estimated to be 4.98 square meters per gram from BET treatment of a 90° K isotherm and other apparatus calibration procedures are described in detail.

Other adsorption isotherms are measured in the seldom used region above the adsorbate critical temperature. For the argon-boron nitride system several isotherms are measured in the interval from 141° K to 273.15° K and for the xenon-boron nitride, neon-boron nitride, and krypton-boron nitride systems measurements are made at 273.15° K. These isotherms are interpreted to show that at least two different types of energy surface are present in the system. One surface (lower energy) is assumed to be the basal plane and the other surface (higher energy) is probably crystal edges. Due to the surprisingly large effect of the high energy surface, the isotherms were measured at too high pressures and a Henry's Law region is not observed which complicated graphical determination of the virial coefficients. For this reason the isotherm data is treated by a computer technique to determine the gas-solid virial coefficients for each isotherm. The experimental second gas-solid virial coefficients for the argon-boron nitride system with several assumptions are used to calculate the depth of the potential well for each surface. The results of this treatment are given in the table on the following page.

+Graduate Student in Chemistry
++Professor of Chemistry

1. This work is being continued by Dr. H. E. Thomas and Mr. J. Bullock.
DEPTH OF POTENTIAL WELLS FOR THE INERT GASES-HEXAGONAL BORON NITRIDE SYSTEMS

<table>
<thead>
<tr>
<th>Gas</th>
<th>High Energy Surface (°K)</th>
<th>Low Energy Surface (°K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ne</td>
<td>550</td>
<td>344</td>
</tr>
<tr>
<td>Ar</td>
<td>1670</td>
<td>981&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Kr</td>
<td>2040</td>
<td>1321&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Xe</td>
<td>2660</td>
<td>1662</td>
</tr>
</tbody>
</table>


Graphitized carbon black (P-33, 2700°) is known to be an exceptionally uniform surface. Thus, such a surface is of great interest, and many studies have been made of the interaction of the rare gases with P-33.

This work is concerned with the interaction of Kr atoms with graphitized carbon black (P-33, 2700°) in the temperature range from about 69°K to 77°K. Both sub-monolayer and multilayer work has been done, and the phenomena of two dimensional condensation has been observed. The equipment used will now be discussed briefly.

The apparatus used in these measurements is a conventional high vacuum type which measures pressures and temperatures. It is a modification of the equipment used by Pierotti and Levy. The pressure measuring system consists of a U-tube Hg manometer, a McLeod gauge, and a Granville-Phillips capacitance manometer. The U-tube manometer is used for measuring pressures of large gas doses, and for the calibration of volumes using He. The McLeod gauge is used for measuring pressures of smaller gas doses. In conjunction with the capacitance manometer, the McLeod gauge is also used for the measurement of equilibrium Kr pressures above the graphite sample. For equilibrium Kr pressures less than about 60 microns, the capacitance manometer is used as a direct pressure measuring instrument. Above this pressure the capacitance manometer is no longer linear and it serves as a null instrument.

Liquid nitrogen serves as the coolant. Temperatures are varied by bubbling He gas through the liquid nitrogen. It is found that the sample temperature can be maintained and reproduced to within about ± 0.02°K. The P-33 sample is about 0.25 g. It is spread on the bottom of a flat glass bulb. With this arrangement equilibrium times are very short.

Three sub-monolayer isotherms are shown here for Kr adsorption on P-33. The pressures are measured with a recorder in conjunction with the capacitance manometer. The recorder is used for slight scale expansion of the capacitance manometer and insures a permanent record of all isotherms.

The 69.6° isotherm seems to have a vertical discontinuity from about 8 x 10^-6 to 24 x 10^-5 moles of Kr adsorbed. This indicates that two-dimensional condensation has occurred, and that 69.6°K is below the two-dimensional critical temperature. The 75.6° isotherm has no region of vertical discontinuity. The 73.5° isotherm may have some slight vertical region in its central portion. Thus, the two dimensional critical temperature of Kr on P-33 is less than 75.6°K, but greater than 69.6°K. It seems to be right around 73.5°K.
Multilayer adsorption studies have also been made at 74.6°K and 73.4°K. Three steps can clearly be seen. These isotherms indicate a monolayer capacity of about 3.1 STP cclg for Kr adsorbed on P-33. These studies are continuing.

+Graduate Student in Chemistry
++Professor of Chemistry

In probing chemical systems, a sound practice is to examine the simplest systems and then to go to systems of increasing complexity. In adsorption these simplest systems consist of spherical atoms of the inert gases adsorbed on the uniform surface of graphitized carbon black at very low temperatures and low surface coverage. A logical step toward increasing complexity is to go to higher temperatures; then a further step could be to examine polyatomic, but symmetrical, molecules such as carbon tetrachloride, \( \text{CCl}_4 \).

James McAlpin, formerly of this lab, examined the data of Ross and Machin dealing with \( \text{CCl}_4 \) adsorption on the graphite, P-33. McAlpin fitted the Significant Structure Theory to their data at 296 K, 288 K, and 278 K and then with this information was able to predict their adsorption isotherms at the lower temperatures of 257 K, 248 K, and 231 K. However, Ross' data intermediate to these e. g. 266 K and 273 K was not predicted as precisely. The present work is that of re-examining experimental data in this intermediate range.

Some notable features of the research equipment used in these current experiments are:

(1) metal bellows valves to handle organic vapors,
(2) capacitance manometer to allow isolation of the adsorbing system,
(3) Cahn electromicrobalance to detect the weight of \( \text{CCl}_4 \) vapor adsorbed.

The Cahn balance is read to \( 2 \times 10^{-6} \) gram by means of a one millivolt Hewlett-Packard strip chart recorder.

Spectroscopic grade \( \text{CCl}_4 \) is adsorbed on the graphite, Sterling FT 2800. Data in the monolayer and Henry's Law region (1 % coverage) have been taken at 259 K, 253 K, and 271 K. Currently some difficulties in maintaining constant temperatures are being experienced.

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**Professor of Chemistry
Crystalline MgO smoke produced by burning Mg ribbon in pure oxygen is primarily cubic crystallites with (100) faces. Exposure to the atmosphere with subsequent outgassing leaves behind an imperfect surface. Adsorption isotherms indicate definite signs of adsorbate-adsorbate interaction despite residual heterogeneities. Heterogeneities are explained in terms of surface carbonate and hydroxyl groups. Isotherms on known isoenergetic substrates are compared with MgO.

+Professor of Chemistry
SURFACE TENSION OF METALS

B. R. Livesay and J. E. Kuykendall

An apparatus has been developed for the measurement of the surface tension at a solid-gas interface. It is designed to measure small sample extension changes resulting from exposure to high purity gas environments at pressures as low as $1 \times 10^{-10}$ torr. The sensitivity of the elongation detection system is sufficient for measurements of changes in surface tension at room temperature but the apparatus has the versatility required for a precision zero creep technique as well. Ultra high vacuum stress-strain measurements at various temperatures on tensile specimen are also accommodated with this apparatus.

The basic concept for the surface tension measurement technique being employed here was initially suggested to us by Dr. J. C. Eriksson. The bulk of available surface tension data on metals has been obtained either near the melting point where zero creep techniques could be used or at the melting point using the sessile drop method. Various powder techniques are employed for measurements at lower temperatures but there are obvious uncertainties involved, particularly in regard to estimates of the true surface area of a powdered sample.

A constant force is applied to a long thin specimen and the elongation is measured by means of an optical lever system. Changes in elongation are observed while admitting a desired quantity of high purity gas to react with the sample surface. Sample cleaning procedures are followed prior to the reaction after the sample is clamped in place in the U.H.V. chamber.

The device consists of what is essentially a vacuum microbalance arm. The sample is attached at one end to a clamp located just above the arm. A coil similar to that used in loud speakers is attached below the arm to the lower end of the sample clamp holder. This coil is suspended in a speaker type permanent magnet system. At the fulcrum is a taut-band arrangement with a galvanometer type coil attached to the balance arm along the pivot axis. A second magnet provides a field in the plane of this coil. A small front surface mirror for the optical level is attached to the balance arm just above the pivot axis. Forces are applied to the lower end of the sample, energizing either the speaker type coil for larger forces or the galvanometer type coil for very small forces.
The optical lever system consists of a He-Ne gas LASER to provide a small diameter collimated light beam, the mirror on the balance arm and a split beam dual photo-diode arrangement fed into a chopper amplifier to detect small displacements. Both the LASER and the photocell arrangement are located outside the chamber with the light beam passing through one of two optical ports.

The apparatus is mounted in an 18-inch diameter stainless steel ultra high vacuum chamber. At every stage the construction is of relatively massive support materials in order to minimize flexures and mechanical vibrations which in turn determine the ultimate sensitivity of the apparatus. The chamber is evacuated with a 1600 liter/sec Granville-Phillips Electro Ion Pump. A manifold attached to the chamber provides any one of or a combination of three different high purity gases in the chamber through a servo-controlled leak valve. The entire apparatus is positioned on a special platform to minimize the introduction of building vibrations to the system.

In addition to the surface tension studies it is anticipated that the course of investigation associated with dislocation at an interface will make desirable the measurement of interfacial energies. For example, a copper sample can be mounted in the device and a load applied. A film may then be evaporated on the two sides of the sample while continuously monitoring the sample elongation. The analysis of such data to evaluate the actual interfacial energy may prove to be difficult but this type of information is needed.

Research Physicist and Graduate Student in Metallurgy
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SESSION II

ORIENTED BASIC RESEARCH

CHAIRMAN

DR. S. SPONGER
A number of experiments and several theoretical treatments have demonstrated the importance of a thin surface coating on the mechanical properties of a metal. Most of the experiments have involved single-crystal samples in order to avoid the additional interpretive complications introduced by grain boundaries. The fundamental processes, however, operate within the individual grains of a polycrystalline material and therefore theoretical models and experiments applicable to surface effects on single-crystals are of great value.

Some fundamental properties of metals which are important in a consideration of the effect of surface conditions on mechanical behavior are: (a) metals are good electrical conductors, (b) most metals are highly active chemically, (c) metals are crystalline, (d) metallic bonding properties, (e) surface energy.

The elastic stress field resulting from the presence of a dislocation accounts for most important dislocation interactions with other dislocations and with such features as grain boundaries, precipitation, and surfaces. If the medium about a dislocation is considered isotropic then the resulting stress field can be expressed in terms of the components of the stress tensor. It is sufficient here to note that all the non-vanishing stress tensor components expressed in cylindrical coordinates for both screw and edge dislocations vary as $1/r$ and therefore interactions involving isolated dislocations have a long range nature.

The current state of understanding of the fundamental mechanisms involved in surface mechanics is not at all clear. One finds that the number of well defined composite metal systems on which mechanical measurements have been carried through is actually very small. Even in the best situations it has not been found possible to invoke current theoretical models to provide a quantitative description of the experimental data. The approach followed here is to employ sample configurations where the surface region occupies a significant fraction of the material but not so thin that the approximation for a semi-infinite substrates are no longer valid. Therefore single crystal substrates with thickness ranging between 3 or 4 microns and 50 microns are used with surface layers ranging between 500-1000Å. It has been necessary to develop special sample preparation techniques for this thickness range and to design and construct the special mechanical testing instrumentation.

Dislocation motion occurs in order to lower the strain energy associated with the presence of the dislocation in the crystal. Material discontinuities such as free surfaces or interfaces introduce modifications of the stress field and there is a tendency for dislocation motion to lower the strain energy.
For example, a dislocation near a free surface will tend to move towards the surface in order to relieve the strain within the crystal. However, consider two crystals connected by some sort of coherent interface where one crystal has a higher elastic modulus than the second. A dislocation near the interface but in the less stiff crystal tends to move away from the interface to minimize the portion of its strain field which extends into the stiffer crystal. Quantitative theoretical treatments of the problem of dislocations near material discontinuities are difficult and only a few simple configurations have been considered in any detail. Stress field calculations are available for both screw and edge dislocations near a planar interface between two materials having different elastic modulii. Taking into account only the stress field one would expect a dislocation in a semi-infinite substrate near a perfectly adherent surface layer will be attracted or repelled by the surface with a magnitude depending upon the relative elastic modulii of the two materials and the thickness of the surface layer.

Additional factors arise because of differential lattice constants. First there is an accommodating network of dislocations which occurs at the interface to lower the elastic strain energy associated with the misfit. A dislocation passing from the substrate into the film must therefore cut through the accommodating network. A second process concerns the difference in magnitude of a Burgers vector in the substrate crystal and the coating crystal. An accumulated displacement residual at the interface gives rise to a long range elastic stress field similar in nature to that resulting from a dislocation. Some apparently very carefully done measurements on copper single crystals electro-plated with nickel have recently been reported which showed a significantly decreased strength due to the presence of the nickel film. These results are in direct contradiction to the behavior one would predict by considering only the relative elastic modulii of the two materials. The shear modulus of nickel is listed as 1.65 times that of copper and the Young's modulus of nickel is about 7 times that of copper. The authors explain their results by proposing that the accommodating network of dislocations leads to easy activation or nucleation of additional dislocations when stress is applied to the crystal required for these measurements. A micromechanics laboratory has been constructed to make mechanical measurements on very thin samples in environments ranging from corrosive liquids to ultra high vacuum. The instrumentation in this laboratory is used for environmental mechanical property measurements for the deformation modes of simple tension, bending, torsion and fatigue in either bending or tension modes. The various precision transducers in this laboratory allow force measurements ranging from 25 pounds down to $10^{-6}$ grams and extension measurements as small as 10004. Two of the tension instruments avoid the problems associated with the nonexistence of a perfectly stiff force transducer and the comparatively large loads required to extend usual extensiometers by electromagnetically applying a desired force through a friction-free suspension system and then using nonloading extensometer arrangements.
Obtaining the desired thin single crystal copper samples involved the development of a thinning procedure since deposited films have a dislocation density which is much too high. The procedure includes the following steps: (a) A sample is spark machined from a larger single crystal with a desired orientation, (b) This sample is placed in a nuclear reactor core and radiation hardened for about a week, (c) After cooling off, thin cuts are made on the sample using a spark slicer, (d) The slices are then sparkplained to a few mils thickness, (e) The sample surfaces are made parallel with each other by mechanical polishing which does not deeply damage the crystal because of its hardened condition, (f) The sample is further thinned by electropolishing, (g) Tensile specimen shapes are generated by a photoetching technique, (h) The radiation hardening is annealed out in a high vacuum oven, (i) The desired coating is applied to the substrate.

Measurements are currently in progress using (a) no coating, (b) epitaxial evaporated nickel films, (c) epitaxial evaporated copper films, (d) thermal oxide films.

*Supported in part by ARPA under order no. 878.

+Research Physicist and Graduate Student in Metallurgy

++Associate Professor of Metallurgy
FIELD ION MICROSCOPY OF STEELS

Dr. Helen Grenga and B. N. Ranganathan

Steels have only recently been investigated by FIM (1), because of the inherent difficulties in imaging by the conventional techniques. The image is unstable in pure helium ion microscopy, and field induced corrosion of the specimen occurs if hydrogen is used as the imaging gas. These difficulties can be overcome for pure iron by using a mixture of 1% H₂ - He as the imaging gas at liquid hydrogen temperatures, the technique being known as 'hydrogen promoted imaging'. For a two phase material, however, only one phase is likely to be imaged by this technique at any given voltage (2). The resolution improved considerably for the ferrite phase as shown in figure 1. However a number of dark regions are present in the image, the origin of which is uncertain.

The intention was to study the proeutectoid ferrite - pearlitic ferrite interface and the cementite - ferrite interface in pearlite. The material studied was music wire (0.75% C and 1% Mn). Figure 2 shows a typical field ion micrograph of pearlite, the dark bands being cementite and the bright matrix ferrite. The distance between the cementite plates was found to be 500-600 Å. This result agreed very well with the spacing calculated from electron micrographs of shadowed replicas of these specimens. These platelets were considerably finer and more closely spaced than those observed by others for pearlite in plain carbon steels (3). The thickness of these cementite platelets was found to be 30-50 Å.

It is hard to say much about the proeutectoid ferrite - pearlitic ferrite interface because of the poor clarity of the images. The ferrite-cementite interface was in general of very poor clarity also. However, a number of poles were resolved in both phases, and in a few instances the poles appeared to be continuous across the cementite-ferrite interface, as shown in figure 3. Further studies should show whether this is a common feature for this particular steel. No such observation of coherency has been made in FIM studies of pearlite in plain carbon steels. Figure 4 shows a spiral structure due to a dislocation in the ferrite matrix.

*Supported in part by ARPA order no. 873.

+Assistant Professor of Metallurgy
++Graduate Student in Metallurgy

Figure 1. Hydrogen promoted image of as-received music wire.

Figure 2. Hydrogen-ion micrograph of pearlite.
Figure 3. Poles running continuously across the ferrite-cementite interface.

Figure 4. Spiral structure caused by a dislocation.
The objectives of these studies were to investigate the reaction of gases, particularly hydrogen and oxygen, with titanium and ordered Ti$_3$Al and the effect of these gases on the metallic bonding of these materials. Obtaining a clean, well-characterized surface is a necessary requirement for meaningful results on the reaction of gases with metals. Field evaporation and field ion microscopy (FIM) provide one of the few methods for doing this. A material can be cleaned by field evaporation and characterized on an atomic level by FIM.

The cleaning of a material by field evaporation, however, requires that the contamination be primarily a surface one or a thin film. That is, if the contamination is extensive at about 500Å below the surface, a clean surface will not be exposed by field evaporation. Thus far, the results of these studies, as given below, have shown that the contamination of these materials as a result of fabrication and/or electrochemical polishing techniques extends quite deeply into the material.

A number of methods were used to polish and image the specimens. Polishing methods included DC etching\(^1\) in a solution of hydrofluoric and nitric acids and \(^2\) in a solution of perchloric acid, n-butanol, and methanol. Specimens were imaged at liquid nitrogen and liquid hydrogen temperatures using the following imaging gases: helium, hydrogen, neon, helium-hydrogen mixtures, and helium-neon mixtures.

Most of these techniques gave only random spot images with no regularity or pole regions developed. Specimens etched by method 2 above and imaged in neon-helium mixtures, however, produced images in which several of the low index pole regions were observable. There was a high tendency for these specimens to fracture during field evaporation so that the image could not be developed well by the field evaporation process. Two techniques were found to relieve this high tendency to fracture:

(a) Annealing at approximately 400°C for a few minutes
(b) Etching (field evaporating) the unannealed specimen in hydrogen

Method (a) produced images with reasonably good development of some of the low index pole regions as shown in Fig. 1 for titanium and Fig. 2 for ordered Ti$_3$Al. A rather high concentration of impurities (bright spots) was still present, with titanium having the greater concentration.
Method (b) produced a marked improvement in the titanium image as shown in Fig. 3. The impurity concentration for the specimen etched in hydrogen was much lower than that for the specimen annealed prior to helium imaging. This method has not yet been tried for ordered Ti$_3$Al.

The impurities found in these specimens most likely are primarily oxygen for the following reasons:

1. the size and brightness of spots compared well with those of oxygen impurities found in other systems.

2. the polishing techniques were such that oxygen contamination might be expected, although to a smaller extent.

3. annealing the specimen might cause oxygen solution into the metal, thereby increasing the impurity concentration, while hydrogen etching should remove the oxide layer without enhancing oxygen diffusion into the metal. This would account for the lower impurity concentration obtained by hydrogen etching.

*Supported in part by the Advanced Research Projects Agency (ARPA order no. 878).

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One important observation in these initial studies was that regions with high impurity concentration were less stable than other regions with lower impurity concentration at the same applied voltage. This observation was consistent with titanium as well as Ti₃Al and implied that the bond strength in titanium and ordered Ti₃Al is decreased by the presence of these impurities.

Fig. 1  Field ion micrograph of titanium, 16 KV, 21°K, He, 1%Ne imaging gas.
Fig. 2
Field ion micrograph of Ti$_3$Al, 28kV, 21°K, He, 1%Ne imaging gas.

Fig. 3
Field ion micrograph of titanium, 15 kV, 21°K, He, 1%Ne imaging gas.
The study of ordered alloys is becoming an increasingly important part of the field of alloy development. The microstructure and the resulting physical properties of these materials is almost wholly dependent on the size, distribution, and interfacial energy of the class of interfaces known as domain boundaries. Studies are being carried out on the microstructure developed during the early stages of the ordering transformation in Ni₄Mo. The high resolution of the field ion microscope has made it quite useful in this work.

During ordering Ni₄Mo exhibits a very large age-hardening effect which is characteristic of those systems undergoing a crystal structure change. The accompanying field ion micrographs show that the transformation at 700°C is characterized by the formation of many small contiguous domains (approximately 50 Å in diameter) which are not perfectly ordered internally. Further field ion and electron microscopy studies reveal a tendency for the domain boundaries to be aligned preferentially on \{112\} planes of the cubic lattice.

Calculations are being carried out to determine the orientation dependence of the domain boundary energy and to correlate this with the observed mechanical behavior. The principal factors to consider are (a) The density of wrong bonds (Mo prefers Ni nearest neighbors) and (b) The lattice misfit resulting from the tetragonal distortion which accompanies the ordering transformation.

Assistant Professor of Metallurgy
Field ion images of Ni₄Mo in the following conditions: (a) disordered (b) fully ordered (c) partially ordered at 700°C for 40 minutes (d) further ordering at 700°C for 15 hours.
X-RAY STUDIES OF THE ORDERING PROCESS
IN A SINGLE CRYSTAL OF \( \text{Ni}_4\text{Mo} \)

Fu-Wen Ling + and Dr. E. A. Starke, Jr. ++

Disordered \( \text{Ni}_4\text{Mo} \) has been shown to exhibit a significant increase in strength during isothermal annealing below the critical temperature. The improvement in mechanical properties has been attributed to a small anti-phase domain size, the extent of order, and the internal strains produced by the tetragonality of the ordered product. In order to understand the strengthening mechanisms involved it is necessary to obtain quantitative measurements of these parameters. X-ray diffraction techniques devised by Warren offer the most promising means of reaching this end. However, due to the superposition of the Bragg reflections in the powder pattern, normal powder techniques cannot be employed. Instead, the Warren method will be applied to single crystal studies of this alloy.

The computer program written for Fourier analysis of the line profiles in a previous study will be modified for single crystal studies. In the ordered alloy the effective particle size broadening contains contributions from the true particle size, intrinsic stacking faults and antiphase domain boundaries. The observation of the particle-size broadening of the superlattice peaks in different crystallographic directions can be used to determine the type and amount of antiphase domain boundaries. For small domains the presence of the antiphase domain boundaries causes significant broadening of the superlattice reflections. Mikkola and Cohen have developed a mathematical treatment which allows separation of the three components of particle size broadening for the \( \text{Ll}_2 \) superlattice. Their approach will be employed for the development of a similar treatment for the \( \text{Ni}_4\text{Mo} \) structure. Ruedl and co-workers have shown that a single crystal of \( \text{Ni}_4\text{Mo} \) contains six different orientation relationships between the disordered and ordered lattices. In addition there are two kinds of antiphase domain boundaries, two kinds of perpendicular twins and one kind of antiparallel twin in the ordered structure. By theoretically estimating the probability of the various intrinsic stacking faults and antiphase domain boundaries the true domain size can be found.

The microstrains in the ordered \( \text{Ni}_4\text{Mo} \) crystal come from several sources: dislocations, antiphase domain boundaries, antiparallel twins and perpendicular twins. These will be determined using the Fourier analysis of Bragg reflections along different crystallographic directions, and compared with theoretical estimations made from atomic displacements.

The parameters defining antiphase domain size and internal strains will be utilized in understanding the strengthening effect produced by ordering in other studies of the mechanical properties of \( \text{Ni}_4\text{Mo} \) alloys.

*Part of this work is being supported by an Atomic Energy Commission grant on ordering strengthening; E. A. Starke, Jr. and B. G. LeFevre Co-principal Investigators.

+Graduate Student in Metallurgy
++Associate Professor of Metallurgy
DEFORMATION EFFECTS IN FCC METALS
AS STUDIED BY X-RAY DIFFRACTION

Pu-Wen Ling and Dr. E. A. Starke, Jr.

X-ray diffraction lines of cold worked materials are considerably broadened as a result of fragmentation of crystals, lattice distortion and stacking faults. Warren has shown that these various causes of broadening can be separated by a Fourier analysis of the line profiles. A computer program for this analysis has been written in Fortran IV and applied to the study of anisotropic microstrain present in the filings of various fcc metals (Al, Au, Cu, Ni, and Pd). The experimental results are consistent with the theoretical work of Ryabashapha and offer the following conclusions: The microstrain due to cold work comes from the dislocations and can be found by integration of the strain field around the dislocation. The microstrain, therefore, depends on the dislocation density and the elastic properties of the crystal. The anisotropic microstrain is a result of the nature of the deformation mechanism, the anisotropic elastic properties and the arrangement of the dislocation lines in the crystal. The last factor is of significant importance in samples which have undergone recovery, a process involving dislocation network rearrangement.

+Graduate Student in Metallurgy
++Associate Professor of Metallurgy
In the initial LEED studies of bulk titanium single crystals, difficulties were encountered in obtaining clean surfaces by ion bombardment and annealing cycles. Well developed LEED patterns were observed after extensive ion bombardment at 750°C. The Auger spectrum, on the otherhand, showed the presence of sulfur, carbon, and oxygen. The growth of single crystal epitaxial films \textit{in situ} was chosen as an alternative method of obtaining clean titanium surfaces.

MgO substrates with (111) and (110) orientations were cut with a diamond saw and mechanically polished. Samples with (110) orientations were prepared by cleavage in air. These substrates were characterized by LEED and Auger analysis before the titanium metal was evaporated. LEED patterns were observed for all three orientations after outgassing at 750°C in ultrahigh vacuum. Diffraction patterns from the (111) and (110) substrates showed the presence of polishing damage, whereas, the (100) pattern indicated a highly ordered and smooth surface. Auger spectroscopy showed the presence of carbon on all three orientations. Since even the cleaved (100) showed carbon, although to a lesser extent than the other orientations, it is suggested that the oxide surface decomposed residual hydrocarbons and carbon monoxide from the vacuum system. The carbon was effectively removed by rf-sputtering in 3-8 microns of argon.

Titanium was evaporated from a tungsten filament, which was enclosed in a liquid nitrogen cooled shield. The evaporation rate was approximately 50 Å/min., and the substrate temperature 300-400°C. The pressure during decomposition did not increase above 2 x 10^{-9} Torr. Film thickness varied from about 500-750 Å.

The samples were observed \textit{in situ} by LEED and Auger spectroscopy. The films were then stripped from the substrates and examined by transmission HREM and electron microscopy. Auger spectroscopy showed the film surfaces were essentially clean for about 30-60 minutes following the evaporation. The carbon and oxygen peaks gradually increased in intensity as the film adsorbed carbon monoxide. The results of epitaxial growth are summarized in the accompanying table.

The presence of fcc titanium was not expected since only the hcp phase for temperatures below 859°C have been reported. Since the carbide, nitride and monoxide of titanium are cubic, it is possible that these impurities could stabilize the fcc phase. The Auger spectrum, however, indicated that these elements were not initially present in the films. We have interpreted the fcc structure to be associated with a high density of stacking faults in the hcp titanium. The streaks observed in the LEED patterns have been attributed to antiphase domains, since the size of the domains are the same order of magnitude as the coherence length of the electrons. One dimensional diffraction effects are also expected from the stacking faults.

* Supported in part by the Advanced Research Projects Agency (ARPA order no. 878)
++Research Chemist
++Assistant Research Engineer
METHOD OF OBSERVATION

LEED SUBSTRATE

ELECTRON MICROSCOPY

<table>
<thead>
<tr>
<th>SUBSTRATE</th>
<th>LEED</th>
<th>HEED</th>
<th>ELECTRON MICROSCOPY</th>
</tr>
</thead>
<tbody>
<tr>
<td>(111)</td>
<td>well defined Ti(0001) surface</td>
<td>Ti(0001)//MgO(111) with Ti[110]//MgO [110]</td>
<td>no texture was observed, micrographs showed only dislocations and extinction contours</td>
</tr>
<tr>
<td></td>
<td></td>
<td>evidence of fcc(111)//MgO(111) with fcc[110]//MgO [110]</td>
<td></td>
</tr>
<tr>
<td>(100)</td>
<td>streaks parallel to [011] and [011] directions of the substrate</td>
<td>two Ti(1011) rotated 90° Ti[1012]//MgO[011] and Ti[1012]//MgO[011]</td>
<td>not yet carried out</td>
</tr>
<tr>
<td></td>
<td></td>
<td>evidence of fcc(100) with fcc[011]//fcc[011]</td>
<td></td>
</tr>
<tr>
<td>(110)</td>
<td>streaks parallel to [001] direction of the substrate</td>
<td>Ti(1011)//MgO(110) with Ti[1012]//MgO[001] and Ti[1012]//MgO[001] with Ti[1011]//MgO[001] with</td>
<td>textured with grain size on the order of 1000Å</td>
</tr>
<tr>
<td></td>
<td></td>
<td>evidence of fcc(110)//MgO(110) with fcc[001]//MgO[110]</td>
<td></td>
</tr>
</tbody>
</table>

TABLE 1. Observations on the Epitaxial Growth of Titanium Films
SESSION III
CONCEPTUAL STUDIES
CHAIRMAN
M. E. SIKORSKI
TWIST COMPRESSION TECHNIQUES IN ULTRA HIGH VACUUM

Kenneth B. Wear +

The "twist-compression" technique for making various measurements of adhesion and friction has been adapted to the ultra high vacuum environment in order to control contamination and recontamination of the mating surfaces. Ultimate pressure of $5 \times 10^{-11}$ torr requires overnight bake at 240 ° C although measurements are made at room temperature. Thrust and torque are generated outside the vacuum chamber and transmitted through the chamber wall to internal members onto which the specimens are mounted, and ball bushings and ball bearings are used to provide internal alignment and rigidity for the movable specimen holders. Because of the uncertainties of magnitude and reproducibility of friction effects in the transmission of motion, measurements of thrust and torque are carried out at the specimens.

Tensile and compressive loads as high as 1000 pounds (readable with a sensitivity of one pound) and torques up to 75 inch-pounds (readable to one inch pound) seemed adequate to planned tests. Strain gages mounted on a flexural member of 304 stainless steel seemed a promising design for the load cell. A configuration resembling a three-spoked wheel, and consisting of one piece concentric plate-in-ring joined by three identical arms, provided adequate rigidity and sensitivity as well as simultaneous thrust and torque measurement in either direction. The specimen is held in a collet which is attached to the inner disc, and this assembly is mounted by the outer ring to the thrust transmission linkage, which is keyed to prevent rotation. Dimensioning of the arms was a compromise between sensitivity and the tensile strength of 0.2% offset; happily, the combination of strength, modulus, ranges, and electronic instrument sensitivity led to dimensions compatible with available strain gages.

Foil strain gages with attached leads were selected and mounted in a full bridge; miniature terminal strips were mounted for connection of gage leads and input-output connections and all connections were made using a high temperature solder. The finished load cell was calibrated separately for thrust and torque and was nicely linear for both. Poisson's ratio produced a small amount (about 5%) of crosstalk between thrust and torque measurements. However, calibration of this effect showed it to be nicely linear for both influence of torque on thrust measurement and influence of thrust on torque measurement.

The load cell has survived four overnight bakes at 230-240 ° C without failure; in fact, sensitivity has increased slightly. No outgas products from strain gages, terminal strips, adhesive or solder from the load cell has produced a noticeable degradation of vacuum system performance. The basic pattern has been successful in this case and seems useable for far wider ranges of loads.

+Research Engineer
Torque-Thrust Load Cell
SOME APPLICATIONS OF THE TWIST COMPRESSION TECHNIQUE FOR THE
STUDY OF METAL ADHESION

M. E. Sikorski and Dr. J. A. Bailey ++

The twist compression technique for the study of metal adhesion has been found very useful in illuminating relationships between various physical and mechanical properties of metals and their tendency to stick, or adhere, upon mechanical contact. This knowledge is of great importance for the design of materials for bearing and other applications in which interaction between surfaces takes place. This includes, for example, machinability of metals, casting, diffusion bonding (which requires elevated temperatures) as well as cold and warm vacuum welding of materials, etc.

In the twist compression technique a minimum of two metal specimens are required to obtain a set of data. The conduct of an adhesion test is as follows: two cylindrically shaped specimens are mounted collinearly so that the end surfaces can be brought together under the action of a normal force. While one specimen is kept stationary, the other is rotated by a fixed number of degrees (normally 180). The magnitude of the force necessary to break the resulting bond is a measure of adhesion. The details and variations of the test procedure have been described in a number of publications in the past. All these references are given in a paper by J. A. Bailey and M. E. Sikorski entitled "The Effect of Composition and Ordering on Adhesion in Some Binary Solid Solution Alloy Systems" which is scheduled for publication in "Wear" in the near future.

The work on adhesion of metals using the twist compression technique was started at Bell Telephone Laboratories in the late fifties. All of the initial experimental results have been obtained in air, mostly on pure elemental metals. Correlations have been found between adhesion and the following properties: crystal structure, hardness, surface energy, elastic modulus, work-hardening properties, recrystallization temperature, purity and atomic size. This work included adhesion of dissimilar metals in addition to like metal pairs.

A study of the adhesion properties of simple binary alloy systems has been initiated by M. E. Sikorski at Bell Labs and continued with Dr. J. A. Bailey and his students at Georgia Tech under the THEMIS program. The solid solution systems studied were: silver-gold (Ag-Au), copper-nickel (Cu-Ni), copper-gold (Cu-Au), silver-palladium (Ag-Pd) and platinum-cobalt (Pt-Co). These studies have shown that adhesion depends on chemical composition and changes in crystal structure produced by alloying and/or atomic ordering. Details are given in the above mentioned paper.

++ Associate Professor of Mechanical Engineering (North Carolina State University)
Additional results that were presented by Sikorski at the ASM Conferences on Wear in the summer of 1969 and which are important from the point of view of prevention of adhesive wear are shown in Fig. 1. Figs. 1 (a) and (b) illustrate the effect of solid solubility on adhesion. Silver has a low solubility in iron and consequently an extremely weak adhesion was observed between iron and Ag-Au specimens containing large amounts of silver. A similar situation exists for the Cu-Ni system and iron, where the solubility of copper in iron is low. Specimens containing large amounts of copper have low adhesion to iron. Figs. 1 (c) and (d), in turn, show the effect of atomic ordering on hardness and adhesion in Cu-Au alloys. The lowest adhesion has been observed for the 50 at.% Au specimens which are hardest. Similar results were obtained for the Pt-Co system, the adhesion for the 50 at.% Co ordered specimens being so low with a normal load of up to 40 lbs. that it could not be measured with the standard twist compression apparatus designed for studies in air.

Recent data obtained in a new ultra-high vacuum apparatus using the same Pt-Co specimens showed that adhesion of hard materials can be measured readily after initial mechanical abrasion of the surfaces in vacuum. The details of the apparatus and of the experimental results are described separately by K. Wear and Dr. J. M. Bradford.

Previous work indicated that fundamental studies on adhesion properties of metals can be successfully carried out in air provided that the Knoop hardness number is less than about 300 (at a 200 gram load). However, for studies involving very hard engineering alloys such as tool steels used in metal working, or iron, titanium, cobalt or nickel-base alloys that may be needed for highly demanding mechanical wear applications, a vacuum apparatus allowing operation at pressures down to 10^-11 torr is needed. The recently built equipment is also suitable for investigations involving cermets, parts with metallized surfaces, vacuum deposited coatings, ceramic-metal composites, etc.

In summary, under project THEMIS, a number of studies on simple binary alloy systems have been completed. An UHV friction, adhesion and wear apparatus has been designed, constructed and successfully tested extending the applicability of the method to very hard materials. In the future, the work should be supplemented by a very careful characterization of surfaces using special techniques such as work-function, electron spectroscopy, and contact resistance measurements. Once the surfaces are well defined, the effect of various gaseous environments on a multitude of interface phenomena can be readily studied.

+Senior Research Physicist
Fig. 1. (a) Variation of the hardness and coefficient of adhesion with composition for the Ag-Au system (top); adhesion of iron to the same alloy specimens (bottom). (b) Variation of the hardness and coefficient of adhesion with composition for the Cu-Ni system (top); adhesion of iron to the same specimens (bottom). (c) Hardness of Cu-Au specimens as a function of condition of atomic ordering. (d) Adhesion of Cu-Au specimens as a function of atomic order.
In a previous study of the effect of composition and ordering on adhesion carried out under this project it was discovered that the adhesion coefficient of some of the ordered samples was zero. The adhesion coefficients reported by Bailey and Sikorski were measured using the twist compression technique in air. A study has been undertaken to measure the adhesion coefficients of these ordered alloys in vacuum to see if the magnitude of the adhesion coefficient in vacuum is higher than in air.

A twist compression technique apparatus was designed, built, and installed in an oil free ultra high vacuum system. The test samples were ordered 50/50 platinum cobalt which previously gave a zero adhesion coefficient in air.

In the first test series the samples were put together with a force of 100 pounds, rotated 180 degrees, and then pulled apart and the adhesion force measured. The samples are then put together and the test sequences repeated. The data is plotted in Figure 1. Each test cycle shown is an average of five individual test sequences. The average adhesion coefficient is zero initially and increases with the number of test cycles. As the oxide is worn off the contact area the clean contact junctions adhere to one another. With the exception of the adhesion coefficient at the fourth test cycle the average adhesion coefficient increases in a general trend as the number of test cycles increases. The surface is becoming cleaner as they are abraded so that the adhesion coefficient increases. The maximum adhesion coefficient is also plotted in Figure 1 and shows the same dependence upon the number of test cycles as does the average adhesion coefficient.

The samples are remachined to their original configuration and the samples again installed in the vacuum system. The test load was increased to 250 pounds and the test sequence repeated. Figure 1 shows the adhesion coefficient does not start at zero as for the 100 pound load. The average adhesion coefficient is about .04 and the maximum adhesion coefficient is about 0.1. In these tests the load is large enough to cause significant abrasion during the very first test sequence and thus the contacting surfaces are cleaned during the first test sequence.

The variation of the adhesion coefficient with the load during twisting is shown in Figure 2. The samples were remachined before this test sequence. The load during twisting was increased by 50 pounds and then the load decreased back to 50 pounds. The average adhesion coefficient increases slowly up to a load of 150 pounds and then the average and maximum adhesion coefficient increase precipitously at a 200 pound load. Since the surfaces were probably not abraded enough to give the maximum adhesion the load was then decreased to 50 pounds and is shown in the figure. The adhesion coefficient increases as the load decreases. Notice that the adhesion coefficients at the 16th cycle in Figure 1 agrees with that for the decreasing load at 100 pounds in Figure 2.
Also the adhesion coefficients in Figure 1 for 250 pound load agree with the ones at the 250 pound load in Figure 2. Data was also taken on the friction coefficient during the adhesion testing and in general there is a close correlation between friction and adhesion.

*Assistant Professor of Mechanical Engineering*

1 J. A. Bailey and M. E. Sikorski accepted for publication in Wear.
Figure 1

NUMBER OF TEST CYCLES

FIGURE 1

Figure 2

LOAD FORCE (lbf)

FIGURE 2
MODEL STUDIES OF VACUUM SINTERING TREATED AS A CREEP PROCESS

Ronald W. Umphrey++, Dr. J. M. Bradford++, and Dr. W. R. Clough+++

Initial-stage vacuum sintering of pure metals is under investigation. The sintering of a sphere-plane model under the influence of a small external load is considered to be a high-temperature creep process.

Objectives of the research include 1) determination of the dominant creep mechanism at various levels of stress, 2) location of transition stress ranges over which the dominant mechanism changes, and 3) evaluation of the effects of high vacuum by comparison with experimental results obtained by others in different atmospheres. Metals to be investigated are two of the following: copper, silver, nickel, and titanium.

Sintering is assumed to mean the consolidation of powdered metals due to the influences of time, temperature, and/or pressure. It therefore includes hot pressing, or pressure sintering. Other assumptions are that 1) driving forces for sintering are surface tension, gravity, residual stresses, and external loading, and 2) stresses at an interparticle interface due to all of the driving forces may be resolved into one "equivalent stress."

A sphere-plane model is used to eliminate many of the geometrical variables present in real sintering problems. Small external loads are applied to the model in order to raise the equivalent interface stress to values more representative of those present in real sintering processes in which particles are much smaller and much greater in number.

Specimens are formed from 1/4-inch rod and take the shape of a 1/4-inch diameter flat and a 3-mm hemispherical cap. The experimental apparatus is nearing completion and is essentially as shown in the figure. Provision is made for applying and measuring the small external loads virtually without friction, for heating the specimens with a resistive coil, and for measuring the interface electrical resistance. The latter is accomplished with a precision Kelvin double bridge and is a measure of both the extent of creep and the creep rate (i.e., the neck size and the rate of neck growth).
Under isothermal conditions, the creep rate is generally proportional to some power of the stress, i.e., \( \varepsilon \propto \sigma^n \). Determination of the exponent \( n \) can lead to conclusions about the dominant creep mechanism. For example, \( n = 1 \) indicates diffusion creep while \( n = 4.5 \) is typical of the slip controlled by dislocation climb in pure metals. An abrupt change in the stress at the sphere-plane interface and knowledge of the corresponding creep rates enables calculation of a value for \( n \) which, in turn, provides information regarding the creep mechanism.

Values of \( n \) definitely indicating the predominance of particular creep mechanisms for different stress levels are normally separated by transition values of \( n \) for intermediate stress levels. These transition stress ranges provide interesting comparisons between metals and also between different atmospheres in which otherwise similar tests are made.

Experimental work is planned to begin in January, 1970. Efforts to the present time have been in formulating the problem, extensively surveying the literature, and designing and constructing the apparatus.

*This abstract is based on a Ph.D. thesis proposal by this same title submitted by the author to the School of Mechanical Engineering, Georgia Institute of Technology.

+Graduate Student in Mechanical Engineering
++Assistant Professor of Mechanical Engineering
+++Professor of Mechanical Engineering
In metal casting, many of the important parameters of the process are dependent on the existing heat transfer rates and temperature gradients. By control of the heat flow from a casting it is possible to produce a directionally solidified structure. Directional solidification pertains to the growth of columnar grains in the direction of significant thermal gradients and this type of structure is known to produce a casting with superior mechanical properties. Temperature and temperature gradients are also important with respect to the response and life of the mold. For example, in die casting, cyclic thermal stresses in the die lead to surface deterioration with a resulting degrading of casting surface quality.

Heat transfer rates in casting are largely governed by the conditions at the casting-mold interface. This is especially true in the case of metal molds where the resistance to heat flow at the interface is often much larger than that in either the casting or the mold. Lack of knowledge of conditions at the interface prevents a realistic analytical solution to the casting problem. In the case of metal molds-metal castings, many studies have shown the complexity of the interface conditions. It seems possible to identify two stages. In the first stage, liquid metal is in contact with the mold and high mold temperatures and high heat transfer rates are obtained. It is this first stage which is of primary interest with respect to mold life and with the initial formation of the surface of the casting. In the second stage, a significant amount of casting has formed and an "air gap" exist between the casting and the mold. The second stage is of importance in governing overall solidification rates.

In this work, the first stage in the casting process is being studied. The first stage is extremely transient in nature and it appears that, under realistic casting conditions, thermal equilibrium at the interface is never reached. Very little information is available on this and apparently no attention has been given to the wetting characteristics of the liquid metal on the mold. The specific study is concerned with the initial solidification of lead-tin alloys on steel. The surface wetting of this system varies by a factor of about two with alloys ranging from pure lead up to about 65 atomic per cent tin.

Temperatures are measured in a steel plate under conditions of pouring liquid alloy onto the plate and also for submerging the plate into a liquid bath. These measurements are used to establish thermal response and heat transfer rates. Under the pouring condition, two methods have been used to
establish the time for the "air gap" formation. One is by noting the time for electrical contact between the plate and alloy to be broken, and the other is by the use of ultrasonics to establish a significant change in contact at the interface. The electrical contact method is simpler and appears to give a more positive indication; however, the ultrasonic method has proven to be feasible and additional evaluation will be carried out.

To date, a preliminary literature search has been conducted, analytical and computer methods for data reduction studied. Preliminary testing has been carried out but a systematic test program has yet to be initiated.

+Associate Professor of Mechanical Engineering


USE OF THE STORAGE RING FACILITY FOR OPTICAL MEASUREMENTS

Maury Zivitz and Dr. J. R. Stevenson

Synchrotron radiation from the electron storage ring at the PSL of the University of Wisconsin in Stoughton is nearly an ideal source for the extension into the VUV of reflection measurements obtained from discharge lamps as light sources. The radiation is stable, continuous, affords a high vacuum sample environment, and is highly polarized in the orbit plane to which most of the radiation is confined. An on-site monochromator which will better utilize the polarization than existing commercial monochromators and eliminate the need for differential pumping, is to be employed within a couple of years; and by that time, the beam currents will be on the order of 1 amp. As the radiation is incoherent, it should increase from the 1 ma level of $10^{10}$ to $10^{13}$ photons per Å-sec-mrad. This will indeed be a light source of unprecedented intensity throughout the VUV region.

The principal investigators of our group, to date, are Dr. Stevenson, Maury Zivitz, and Harry Ellis. Our visits of duration were made last April and November; each visit lasted 3 weeks. We "piggybacked" with our high-vacuum sample chamber onto either a normal incidence or a Seya-mounted monochromator to make DC reflection measurements on the semiconductor alloy system $\text{Cd}_{3-x}\text{Zn}_{x}\text{As}$.

We have scanned the end members and one mid-range member from 900 to 300 Å and have observed the gentle roll in reflection typical of semiconductors or insulators with d-bands in the region following the plasmon. The absolute value of reflection in this region is quite small, about 1%. The structure consisting of broad peaks is tentatively identified as due to d-bands as both doubly ionized atomic Zinc and Cadmium have ionization potentials of 17eV and these atomic transitions are from d-shells. For ZnIII, $(3d^{10} \rightarrow 3d^{9}4p)$; CdIII, $(4d^{10} \rightarrow 4d^{9}5p)$. The d-band of As would be well isolated from the above transitions as AsVI, $(3d^{10} \rightarrow 3d^{4}4p)$ corresponds to 54eV.

+Graduate Student in Physics
++Professor of Physics
BAND STRUCTURE INVESTIGATIONS BY MEANS OF MODULATION SPECTROSCOPY

Harry W. Ellis and Dr. J. R. Stevenson

At present our group is making measurements of the optical reflectance of the Cadmium-Zinc Arsenide alloy system over a wide range of frequency. By defining a complex reflectivity, and using a Kramers-Kronig integration to find the imaginary part, we may then calculate the complex index of refraction from Fresnel's equations, and finally obtain the complex dielectric function $\varepsilon(\omega)$.

This function is important because it is intimately connected with the electronic band structure of the material, and to the density of states within the bands. In particular, if we examine the expression for the contribution $\varepsilon^p(\omega)$ arising from interband electronic transitions, we see that $\varepsilon^p$ exhibits maxima when the incident light frequency $\omega$ corresponds to an interband energy $\hbar\omega_{\ell,k} = \hbar\omega_{\ell} - \hbar\omega_{k}$ (between bands $\ell$ and $k$) at those points in the Brillouin Zone where

$$\nabla k\omega_{\ell,k} = 0$$

Now the detection and precise location of these so-called critical points are seen to be crucial for good band structure calculations. About these points, the dielectric function reduces to

$$\varepsilon = b/\sqrt{\omega - \omega_G} + \text{Constant}$$

where $b$ is a complex number and $\hbar\omega_G$ is the band gap energy.

The location of peaks in $\varepsilon(\omega)$ is made difficult because often the constant term is much larger than the (peaked) interband contribution. If, however, a parameter $x$ existed, upon which $\varepsilon$ was dependent, we could differentiate, obtaining

$$\frac{d\varepsilon}{dx} = \frac{b}{2\sqrt{\omega - \omega_G}} \frac{d(\omega - \omega_G)}{dx},$$

da function which becomes large in the region $\omega \sim \omega_G$, and which is free of the constant term. Structure in $\varepsilon(\omega)$ becomes obvious.

One simple choice for this parameter, and the one which we propose to use, is the band gap energy $\omega_G$. (The other obvious choice, the incident frequency $\omega$ is rejected due to experimental difficulties involving source stability.) Several methods exist for introducing a small change in $\omega_G$, enabling us to measure $\varepsilon(\omega_G + \Delta \omega_G)$ and $\varepsilon(\omega_G)$. The difference in these two numbers, at a constant incident frequency $\omega$, should exhibit the properties of $d\varepsilon/dx$.

In terms of actual experimentation, the observable being measured is
reflectivity. It is shown by Seraphin and Bottka, however, that in the vicinity of \( \omega_g \), the differential of reflectivity is related to that of \( \epsilon(\omega) \) by

\[
\frac{\Delta R}{R} = \beta_r(\omega_g) \Delta \epsilon_r + \beta_i(\omega_g) \Delta \epsilon_i
\]

where the coefficients \( \beta \) depend upon \( \epsilon \), but not the differential.

The experimental procedure which has been used by Cardona and others, and which we hope to use is that of cementing our sample to a piezoelectric crystal to which a periodic electric field is applied with frequency \( \omega_0 \). This produces a strain in the sample which distorts the lattice, and thus the band structure. The measured reflected intensity then contains a steady (dc) component \( I_R \) plus a periodic (ac) component \( I_{\Delta R} \) repeated with frequency \( \omega_0 \), and produced by the change in \( \omega_0 \). The two signals can be separated and amplified, the (ac) signal being amplified by a lock-in amplifier in order to separate this small signal from the noise. The ratio of the two signals may be taken electronically, yielding directly \( \Delta R/R \). Critical points in the Brillouin zone can then be located precisely and easily, since they produce large structure on the measured quantity, \( \Delta R/R \).

+Graduate Student in Physics
++Professor of Physics
Chemical vapor deposition (CVD) is a method of plating in which the deposits are produced by heterogeneous gas-solid or gas-liquid chemical reaction at the surface of a heated substrate. The use of CVD to prepare protective coatings was developed around 1935 and is used today to produce many other coating systems. CVD is finding wide application in solving other present and future materials problems. While CVD still constitutes a highly versatile and flexible means of applying coatings of most refractory metals and non-metals, as well as preparing the pure metal itself, it is also used to produce coatings for electronic and optical applications. For example, investigations are underway to produce filters and selective reflectors in laser systems or optical slabs for IR transmission windows using CVD techniques.

The principal advantages of the CVD process are as follows: 1. The myriad of chemical reactions available make the CVD process very versatile. 2. The actual CVD mechanism is an atomistic process. That is the deposit is built on the substrate atom by atom (or molecule by molecule). It is therefore capable of providing deposits of maximum density and of closely reproducing fine detail in the substrate surface. 3. The CVD process does not require ionizable compounds in either the coating or the substrate for successful application, as for example in electrophoresis or electroplating. Thus highly insulating compounds can be deposited as readily as pure metals. 4. CVD can be carried out at moderate pressures so that high vacuum is not required.

Certain problems encountered in the processing limit the use of CVD in practical applications. Uniform coatings on large objects or complex contour surfaces are difficult to obtain because of mass transfer or temperature restrictions. And even though CVD coatings do approach theoretical density careful techniques and control are required to obtain the coatings of sufficient integrity often necessary for complete protection.

CVD was selected for study as a result of a survey begun in February 1968 of the literature and industry involved with the production or study of high temperature oxidation resistant surfaces and diffusion coatings. The literature search included literature beginning in 1963. The survey of the industry also included government and private research institutes as well as the hardware manufacturer. The survey was conducted to determine problem areas and research needs resulting from high temperature oxidation resistant coatings utilization. One recommendation resulting from this survey was that the coating process, CVD, be studied from a basic engineering approach. Knowledge of this process would also further the understanding of many other industrial coating processes, such as pack cementation, in which CVD is the primary basic coating mechanism.
The particular CVD system selected by this group for initial studies was the hydrogen reduction of silicon tetrachloride to produce a solid silicon coating on a tungsten wire. This system was selected because it is representative of those used in CVD and because the resultant coating is an important silicide used in oxidation protection for defense and industrial hardware.

The first stages in the basic engineering study of the silicon CVD system was a search of the literature to provide design criteria for fabrication of a bench scale apparatus to produce silicon coatings on tungsten wires by CVD. During the fiscal year 1968-1969 this was accomplished and a preliminary bench scale apparatus constructed. The apparatus was a simple, inexpensive glassware system consisting of a reactor chamber, a bubbler arrangement to saturate the hydrogen reactor gas with silicon tetrachloride, and the necessary support and measurement equipment. Preliminary experiments indicate that the system functions satisfactorily.

The next stage in the program will be a detailed parametric stage. This study will be undertaken to investigate the interrelationship between surfaces kinetics and the flow. Data of this type should provide information necessary to study basic problems in coating technology such as scale up in which CVD is an essential part of the coating mechanism. This study will also serve as a guide for obtaining experimental data on other reaction systems. Long range plans for the future include an investigation of the pack cementation process and eventually methods of scale up with both the CVD and pack cementation process.

+Graduate Student in Chemical Engineering

++Professor of Chemical Engineering
X-RAY STUDIES OF INTERFACE PHENOMENA

C. E. Wagner and Dr. R. A. Young

Several x-ray techniques lend themselves particularly well to studies of interface phenomena. The most outstanding are perhaps x-ray diffraction topography, precision structure refinement and the external reflection of x-rays in the vicinity of total reflection.

**X-Ray Diffraction Topography**

A number of experimental x-ray diffraction techniques have been developed by which a two-dimensional display of the microscopic defect structure of a crystal can be obtained. They are referred to as x-ray topographic techniques, or topography. Topography is thought of as a relatively new tool, but the idea originated with W. W. Berg in the 1930's.

Electron Diffraction is capable of much better resolution, but thin samples are necessary; a restriction not imposed on topography, where crystals as thick as 1 cm have been studied. Large area topographs are also possible, and no vacuum is necessary.

There are essentially six variations of the topographic technique, some which are useful for the study of crystals with up to $5 \times 10^6$ dislocation lines/cm$^2$, and some which have a sensitivity to strains as small as $10^{-5}$ to $10^{-9}$. All of the variants are capable of displaying individual lattice distortions such as dislocation lines and of determining the crystallographic direction of their fault vector.

The contrast observed in a topograph arises in most cases from one of two causes, depending upon whether the intensity observed is the peak intensity or the integrated intensity. If peak intensity is observed then the contrast is produced by a simple tilt of the lattice or a change in lattice parameter. If the integrated intensity is observed the strained regions will be seen as more intense regions because less perfect regions diffract more strongly than the ideally perfect ones.

The selectivity of the technique to fault (lattice displacement) vector is illustrated in Figure 1a and b which are integrated intensity topographs of the same quartz crystal oscillating in both cases in the same resonant mode. The direction of lattice displacement to which each topograph is sensitive is indicated by the arrows.

Observations have been made of dislocations, stacking faults, low-high angle grain boundaries, twin boundaries, magnetic domains, and precipitation and segregation of impurities. The materials so far studied by various workers include diamond, silicon, germanium, InSb, NaCl, AgCl, SiC, MgO, Al$_2$O$_3$, BeO, aluminum, copper, Fe-5%Si, calcite, quartz and ice.
The strains produced by surface films are important because of their influence on the rate of diffusion and defect generation and movement. Both qualitative and quantitative determinations of the strains produced by films deposited on single crystal substrates have been made by topographic techniques. An integrated intensity topograph of a quartz crystal with aluminum electrodes evaporated in a keyhole pattern on both surfaces is shown in Figure 2. The strain generated over the entire film-crystal interface, as well as the strain at the film boundary, can be seen as variations of intensity. Numerous surface scratches also produce some of the observed intensity variations. The location and Burgers vector of dislocations generated at diffusion interfaces in semiconductor materials have also been observed as have micro-cracks and the onset of fatigue in other materials.

Applications to interface phenomena include any studies where strains or the generation or change of microscopic defects is anticipated to be significant, and where the material of interest (or some similar material) can be obtained with a large grain size. Friction and wear phenomena, for example, might be studied by (1) observing the approximate densities and Burgers vectors of dislocations generated by or changed by frictional forces, both at the surface and within the bulk, and (2) by determining the spatial extent of scratches and the magnitude of the associated strain fields in the various crystallographic directions. Or, the influence of substrate strains on the perfection of epitaxial films could be studied by observing substrate strains and the strains in the epitaxial layer. A related study would be the quantitative determination of the effect of polarization, amplitude and frequency of ultrasonic standing waves in a substrate on the nucleation and growth of surface films. Recent preliminary investigations have shown substrate oscillation to exhibit the same influence on film perfection as that of a higher substrate temperature.

Precision Structure Refinement

The x-ray diffraction precision structure refinement techniques have progressed to the point that very small changes in atomic position can be meaningfully determined. One such study is being carried on here at Georgia Tech on the mineral apatite with one avenue of investigation being the determination of the atomic-scale mechanism of diffusion.

To better understand the formation and interaction of a surface film with its substrate, an understanding of the atomic-scale mechanism of diffusion is necessary for both strained and unstrained lattices. The bulk diffusion coefficients and activation energies for single crystals are relatively easily determined and offer an opportunity for testing of atomic-scale diffusion theories, once the crystal structural locations and motions of the diffusing atoms in the host structure have been determined.

A quantitative knowledge of the influence of both inhomogeneous and homogeneous strains on diffusion phenomena would allow diffusion characteristics to be calculated, for example, for models other than the simple single crystal, irrespective of whether the strain is produced by a dislocation or by a thermal gradient.
Two series of experiments would be necessary: (i) a precision x-ray structure refinement of a crystal with a high concentration of diffusant, undertaken in order to determine the location of the diffusing atoms and to determine the reaction of the host structure (in terms of detailed atomic positions and thermal vibrations - perhaps reflecting bonding influences) to these atoms, and (ii) an x-ray topographic study of the effects of homogeneous strains (produced by ultrasonic standing waves) on the parameters, such as temperature, influencing diffusion.

X-Ray External Reflection

A technique particularly suited to the study of surfaces is that of the external reflection of x-rays near the total reflection region. The surface may be that of a homogeneous material, a homogeneous solid into which some material has been diffused, or a deposited thin film of either the same or different composition as the substrate. The technique can determine the absolute electron density and variations in it. As a consequence one can determine film thicknesses from 20\(\AA\) to several thousand \(\AA\), models for electron density as a function of depth, and surface roughness and other discontinuities in electron density such as voids or clusters of material with a density different from the average. Several papers have been published by workers in the field illustrating the usefulness of the technique in the above areas. For example, the depth of oxidation of a copper sample was deduced to be 150\(\AA\) on the basis of the model of electron density as a function of depth. Another study showed the density of copper films thicker than about 300\(\AA\) to be the same as the bulk density. The possibility of observing localized detachment (or lack of adherence) of a film from a substrate is one pertinent to adherence studies.
Fig. 1 Integrated intensity topographs of an SL-cut quartz crystal frequency control device resonating at its fundamental frequency of 455 kHz (a) 01.1 reflection (b) 21.0 reflection. Diffraction vectors are as shown. Intensity contrast is produced only by the component of lattice displacement that is parallel to the diffraction vector.
Fig. 2. Integrated intensity topograph of a quartz crystal with evaporated thin-film aluminum electrodes. Strain under the entire plated area as well as at the film edges is seen as variation of intensity.
SESSION IV

APPLICATION INVESTIGATIONS

CHAIRMAN

DR. L. N. THARP
This year's effort has been devoted to developing the Auger technique into a workable spectroscopy. Therefore the principal results are of a practical nature rather than theoretical. As a result of our efforts a new program is being negotiated with NASA under the title "Development of Improved Analytical Techniques to Control Surface Contamination of Semiconductor Materials During Device Processing and Correlation of Detected Impurities with Device Parameters."

Considerable time has been spent with manufacturers of semiconductor devices and with other workers investigating the use of Auger spectroscopy as a tool for improved understanding and manufacturing techniques of semiconductor devices. As a result of this survey of the state-of-the-art, the following goals and problem areas have been defined.

Goals:

**Improved manufacturing techniques.** Contamination present at the surface of a semiconductor wafer has been generally recognized as having a profound influence on the electrical properties of the device\(^1\). Dust and chemicals remain on the wafer surface even after cleaning steps\(^2\). Control and identification of these contaminants is one future use of Auger spectroscopy.

**Improved performance and reliability.** Of particular interest here are those factors which cause a gradual long-term degradation of a device in service and which cause secondary breakdown of the collector junction. The problem of "walk-away" - a change in junction breakdown voltage in time - will be investigated in the above mentioned NASA program. The influence of contaminants on oxide quality and threshold voltage of MOS devices has already been established\(^3\).

**Improved understanding of transistor operation.** The behavior of oxides is profoundly influenced by contaminants. An improved understanding of MOS devices should result from correlation of contaminants with electrical parameters. Another area which is now being actively pursued is the correlation of contaminants and noise phenomena - particularly \(1/f\) or "excess" noise which dominates in the spectral region below 1000 Hz. Both "slow states" and "popcorn" noise\(^4\) are probably related to contamination.
Effect of electron beam. The electron beam incident on the sample can perturb the surface in at least two ways. Thermal heating of the sample can be caused by the electron beam. Beam current can be varied on our apparatus from less than one microampere to about 100 microamps. The upper limit on beam voltage is 3kV. Thus 300 milliwatts of power can be dissipated on the sample. The thermal resistance of our sample/sample holder combinations varies from about 1mW/°C to 10 mW/°C. Thus, a local temperature rise of 30° C to 300° C can be expected on the surface. This temperature rise can cause contaminants to react or evaporate from the surface. Another possibility is chemical desorption caused by the energetic electron beam. Our new electron gun and regulated power supply will operate from 400 V to 3000 V and over a current range from 1 microamp to 100 microamps, thus minimizing the possibility of surface damage.

Sensitivity. Sensitivity of the Auger technique is such that common surface contaminants of semiconductor wafers can be easily detected. Interestingly enough, it is difficult to see common doping levels, these being one part in a million by volume, while it is possible to see surface contamination, with a one part in a hundred sensitivity on the surface.

Our greatest effort this year has been in understanding the sensitivity limitations of the Auger method. We are presently at the theoretical limit of our present apparatus - about 0.01 monolayers for most common materials - but hopefully this limit will be lowered at least an order of magnitude in the coming year. The present energy analyzer is a three grid retarding field type. The detector collects all electrons more energetic than the retarding voltage. This may be compared with a "velocity analyzer" which passes only those electrons within $\Delta E$ of the desired energy. Shot noise is the limiting factor with a retarding field analyzer. This noise is proportional to the square root of the mean current collected and the system bandwidth. This relationship shows that one should operate with as high a beam current as possible, since $A_{\text{mean}}$ current should be proportional to incident beam current, but shot noise is proportional to the square root of beam current. Measurements with a ten microamp gun indicate that shot noise is the dominant and limiting factor in measurement sensitivity. A velocity analyzer is being designed to remove this limiting factor. A reduction of $10^4$ in mean current striking the detector would reduce shot noise by $10^2$. 
Additional work has been done to better define the effect of differentiation on measurement sensitivity. The result of this effort is that differentiation is most useful when one is not limited by shot noise.

**Spatial resolution.** Spatial resolution of the beam, i.e., beam width, is not of importance in studying bulk samples but does become important when studying partially completed transistors. Since the surface of the device has widely varying resistivity and may have regions covered with an insulating oxide, it is necessary to have a beam of the order of 1000Å to avoid charging problems. A field emitter tip source in the electron gun enables this problem to be solved.

+Assistant Research Engineer and Graduate Student in Electrical Engineering
++Research Physicist


The aging in the resonance frequency of quartz crystals has been a major problem in the use of quartz resonators for frequency control applications. Improvements in stability have been made in the past by continued step-wise refinements in processing and fabrication techniques. Progress has now reached the stage where there is considerable difficulty in the identification of the effects that are responsible for crystal aging. The frequency stability should ultimately be restricted by the intrinsic properties of the quartz. This ultimate cannot be realized until all of the extrinsic contributions to aging can be first identified and then minimized.

The recent development of Auger spectroscopy has made it possible to detect and to identify surface impurities in concentrations as low as $10^{-13}$ atoms/cm$^2$. This technique can be readily used to monitor the purity of the interfaces in each step of resonator fabrication. We have initially investigated the surfaces of quartz samples that were prepared and processed according to procedures for resonator fabrication. The purpose of this paper is to describe these initial results, and to emphasize the potential for using Auger spectroscopy to monitor the various steps of fabrication.

Surface analysis was made for two separate samples. The first sample was cleaned in an ultrasonic chromic acid bath, and several microns were etched from the second sample with ammonium hydrogen fluoride. The samples were mounted on a tantalum heater and placed in an ultrahigh vacuum system for observations. Auger spectra were measured for the samples after the vacuum system bakeout of $250^\circ$ C and an initial outgassing of the specimens at $350^\circ$ C in ultrahigh vacuum. Although there were considerable differences in surface preparation, the surface analysis for the two samples was essentially the same. Auger analysis showed the presence of carbon contamination for both samples. It is unlikely that this impurity originated from the cleaning procedures. We have attributed the source of carbon to the oxidation of carbon monoxide and the decomposition of adsorbed hydrocarbons during system bakeout and sample outgassing. Similar results were observed for MgO surfaces that were used in another study.

Since the treatment of the samples in this preliminary investigation did not differ appreciably from the actual fabrication procedures, it is suggested that a layer of carbon exists between the quartz and metal electrode. It is possible at present only to speculate about the effects of this carbon impurity on the aging characteristics of the resonator. These initial observations demonstrate one of the techniques available for identifying potential contributions to frequency changes in quartz resonators.

+Research Chemist
++Research Engineer
SURVEY OF OXIDATION RESISTANT COATINGS

A. C. Merritt and Dr. C. W. Gorton ++

The present study was a brief literature survey and a preliminary survey of the defense or space oriented industry in the specific area of high temperature, oxidation resistant surface and diffusion coatings. These surveys were conducted to identify technology gaps and to determine research needs.

Programs related to material reliability and durability have evolved with the development of hardware associated with space and missile programs. These programs indicate high temperature oxidation resistant coatings as a possible solution to the perpetual problem of a system's inability to function properly in the extreme environments encountered on a typical mission.

The literature survey was conducted by a search of the abstracts found in Chemical Abstracts, STAR, and the abstract files of the High Temperature Materials Division library. Key papers, summaries, and reports indicated by the literature search were read beginning with 1963. The survey of private and government facilities involved with high temperature, oxidation resistant coatings was accomplished by means of a questionnaire. Analysis of this survey resulted in specific research recommendations. These recommendations were categorized as follows:

A. New Coating and/or New Coating Concepts
B. Deposition Techniques
C. Basic Data
D. Evaluation Methods

These recommendations and a bibliography obtained in the literature search provided the basis for a preliminary report on the subject of surface and diffusion coatings which was completed August 1969. The report "A Survey of the Literature and Industry Involved with High Temperature Oxidation Resistant Surface and Diffusion Coatings" is available on request.

In conclusion this report pointed out specific research topics in the general area of surface and diffusion coatings for protecting surfaces from oxidation. Precise delineation of unique problems was not possible due to the limited nature of the survey undertaken.
A more comprehensive survey including a wider coverage of industrial and government research organizations and a more detailed questionnaire is not expected to provide a large amount of additional information, and therefore is not recommended. Rather, visits to key organizations, particularly government laboratories, and/or a more intensive review of the literature on selected topics uncovered by the survey should be initiated.

*Graduate Student in Chemical Engineering

**Professor of Chemical Engineering
An apparatus has been developed in the Micromechanics Laboratory for the measurement of small frictional forces. It operates at normal loads ranging from 1.0 mg up to about 200 mg and measures frictional forces from about 300 mg down to less than 0.01 mg. The operation of the instrument is completely automatic during a measurement and the response of the system is fast enough for details of the stick-slip process to be clearly displayed on an x-y plotter.

Prior to this time the apparatus has been employed almost exclusively for the measurement of friction between various textile fibers. In fact, the initial motive for the device was for an investigation of the friction between individual cotton fibers obtained from various sources and at different stages of textile processing. In these cases the fibers were treated as crossed cylinder pairs. However, a series of measurements involving metals as fine wires and with a stylus on thin metal platelets demonstrates that the application of this device to the wide range of sliding metal contact problems should be fruitful. The apparatus is currently being modified to operate with the friction pairs in a liquid. The system concept could be applied to the development of a similar device for operation in ultra high vacuum by using vacuum consistent construction techniques and materials.

A servo balance system is employed to measure the small friction forces. A small d'Arsonval galvanometer of the type used in portable potentiometers was adapted to provide a counterforce to the force of friction. This was done by attaching one member of the friction pair to the galvanometer needle. The frictional force acts normal to the axis of the needle producing a torque about the axis of rotation of the galvanometer.

A collimated beam of light is directed so that it strikes the galvanometer mirror and reflects on to a dual photodevice. With no mechanical torque applied to the galvanometer, the system is adjusted so that the light spot is equally distributed on the two sides of the photodiode. A small mechanical torque applied to the galvanometer coil will deflect the light beam so that the spot is more on one side of the dual photodiode than the other. The output of the photodevice is connected to the input of a high gain differential amplifier system. The servo loop is then closed by connecting the output of the differential amplifier to the galvanometer coil terminals so that the polarity of the coil current produces an electromagnetic torque always in opposition to and having the same magnitude as the applied mechanical torque. One therefore has an automatically balancing system from which the frictional force is displayed on an x-y recorder by simply recording the current through the galvanometer coil.
Loading of the friction pair is accomplished with a simple mechanism constructed from the movement of a standard indicating meter. The basic movement is removed from the meter housing and a light metal arm is attached to the coil frame. A second member of the friction pair is mounted at the end of arm so that a current in the coil results in a force pressing one member of the friction pair against the other. The normal force applicator is mounted on a horizontal linear slide stage driven by a small meter to generate the relative motion between friction pairs. The output of the amplifier is also electronically integrated to provide a time average of the friction force.

As a textile engineering tool, the apparatus has been used in investigations involving both the effect of process treatments and of characteristics intrinsic to the fiber. The frictional behavior has been measured as a function of such conditions as fiber tension, normal force, traversing speed and direction, humidity and various physical features such as shape and crimp. One of the more interesting features we have observed for a diamond stylus riding on metal films is the load required to begin breaking through a thin oxide film on the samples at loads of a few dynes. Such measurements have been completed with scanning electron micrographs of the friction tracks.

In the future we anticipate new application of this instrument concept to problems associated with such areas as lubrication, correlations between electrical contact resistance and friction and wear, sliding contact friction and wear in various corrosive environments (ranging from liquids to gases to ultra high vacuum) and to studies of the various metallurgical factors which determine friction and wear in bearing and contact materials.

*Supported in part by the Department of Agriculture (SURDD) Grant No. 12-14-100-7661 (72).
+Research Physicist
COMPATIBILITY OF MATERIALS IN MEDICAL ENVIRONMENTS

Dr. R. F. Hochman

Over the past several years, studies have been made in simulated and actual medical environments of implanted metals and alloys and the surrounding biological tissue to determine their compatibility as medical implant materials. Of the presently used orthopedic materials, 316 L stainless steel and the chromium cobalt alloy generally called vitallium or Zimalloy have been found to produce the least trauma in the biological environment. In addition, studies have been performed both on titanium and the titanium-6 aluminum-4 vanadium alloy showing their compatibility to be excellent for medical implant use. These studies include examination of clinical specimens which have been implanted in patients for quite some time; surface studies have shown little loss of metal or attack of the metal surfaces; there have been no reported patient rejection of the material; and, examination of the surrounding tissues by microprobe and other microchemical analyses have shown a minimal metal loss at the interface. Based primarily on these considerations, a recommended practice has been accepted by the American Society for Testing in Materials F-4 Committee on Medical Implant Materials. A great deal of evaluation and study of the Ti 6-4 alloy in clinical environments will now be performed.

In other areas of study on orthopedic devices, fractures have been of minimal number. In most cases, those that failed have been in implants which are intended for short-term assistance to bone healing and are restricted in size by the finite area of application. It is unique to note that both of the normally used materials have shown the least indication of corrosion fatigue in medical environments; hence, this is another major reason for their excellent stability in these applications. Studies of the fracture surfaces of those implants that have failed have yielded a tremendous amount of information indicating the major cause of implant failure to be due to fatigue rather than an environment effects producing corrosion or stress corrosion.

Presently, studies of surface finish and its effect on the medical implant environment are underway using both electrochemical-polarization studies combined with studies of the surrounding tissue. Preliminary results show that small variations in the surface finish have little effect but major changes can produce noticeable differences.

Most of the information here has been published in detail in several professional society proceedings.

+Professor of Metallurgy
Our activities have been directed towards the study of the mechanism of the lubrication of highly loaded, thin film, time unsteady contacts such as those often referred to as elastohydrodynamic contacts. Examples of these can be found in the lubrication of cams, gears, ball or roller bearings. In these situations the lubricant is subjected to very high pressures (up to 500,000 PSI), high shear rates (up to $10^6$ sec$^{-1}$), shear stresses (up to 10 dynes/cm$^2$) for very short times (average time in conjunctive region $10^{-5}$ sec).

Our approach to this area has been three pronged. It has involved the measurement of lubricant rheology in viscometric flow, the study of lubricant reaction in simulated contact experiments and lastly the analytical modeling of the lubricant rheology by employing an integral constitutive equation and measured properties to predict the behavior of the material in a simulated contact. In all the work several common materials are employed. These are all thoroughly characterized and consist of hydrocarbons, bulk polymers, polymer solutions in hydrocarbons and some synthetic fluids.

Each of the activities are briefly described below followed by a list of the pertinent publications. It perhaps should be noted that all of the equipment mentioned is currently available in our laboratories.

I. Measurement of Lubricant Rheology.

a. High Pressure Shear Stress Dependence of Lubricant Viscosity.

The high pressure capillary viscometer is capable of subjecting the fluid to pressures up to 100,000 psi and simultaneously varying the shear stress from 300 to $1.2 \times 10^5$ dyn/cm$^2$. Viscosities ranging from 1.0 to 100,000 centipoises can be measured and the fluid temperature can be controlled in the range from -50 to 450 deg F. The system accuracy was verified up to 80,000 psi by measuring the low shear viscosity of bis-2-ethyl hexyl sebacate which had been previously examined. The agreement was within two percent.

The equipment is also capable of evaluating the elastic energy stored in the fluid based on the recoverable shear strain concept. No corrections are made for viscous heating and the major source of error is related to reading the primary signals from the recorder.
To date approximately 25 fluids have been investigated in this device.

b. Shear Dependent Relaxation Time.

A parallel plate rheometer has been constructed and employed to measure the relaxation time of eight polymer and polymer containing materials as a function of relaxation time at atmospheric pressure and 100°F. The shear rate range was from $10^2$ to $5 \times 10^4$ sec$^{-1}$ and the relaxation times observed were from 4 to $10^{-5}$ sec. The relaxation time was found to be a strong function of shear. The log relaxation time was inversely proportional to the log shear rate. The equipment requires only a few cc sample.

II. Simulated Contact Studies.

a. Traction and Film Thickness Studies in Elastohydrodynamic Contacts.

This work was an experimental investigation of the elastohydrodynamic problem. The investigation was limited to a study of nominal point contacts in pure sliding motion. The profile of the lubricant film separating the bearing surfaces was determined during a transient of the normal load. During this transient the Hertzian contact stresses were increased from zero to a maximum of 150,000 lbf/in$^2$ in approximately 45 milli-seconds. The sliding velocities used in this study were varied from 13.7 to 92.1 inches per second. The resulting mean shear rate, however, was typically $10^7$ reciprocal seconds. Both pure and polymer-blended naphthenic and paraffinic oils, in addition to several synthetic fluids, were studied.

On the basis of the film thickness profiles that were obtained for the polymer-blended oils, it was concluded that the ambient value of viscosity often used in theoretical considerations does not characterize the behavior of the system. It was also found that the rapid application of the normal load had a negligible effect on the film thickness profile. During this investigation the contact traction was also measured. Under the conditions investigated the traction values appear to be primarily a function of the sliding velocity. Large variations in fluid composition and inlet viscosity had little influence on the tractive force. It was also found that rapid application of the normal load had a negligible effect on the traction.


The squeeze-film bearing is currently being studied to determine the effect of lubricant viscoelasticity on bearing performance. From theoretical considerations, viscoelastic effects will only be significant in unsteady (dynamic) loading conditions, if at all, and the squeeze film is characteristic of all unsteady lubrication. The inherent simplicity of the apparatus will enable viscoelastic effects to be clearly isolated.
Load, pressure profile, film thickness and velocity of approach are measured and compared for Newtonian control fluids and viscoelastic fluids. Rheological properties of the lubricants have been previously measured. The experimental results will be compared to analytical predictions.

III. Analytical Studies of Viscoelastic Effects in Lubrication.

An analytical technique has been developed in which experimental data on non-Newtonian fluids in viscometric flows can be used to predict behavior in the more complex flows of lubrication conditions. A continuum mechanical approach with integral constitutive equations is used. The numerical finite difference method enables more complex flows to be analyzed than were previously possible. The technique predicts an increase of load carrying capacity in lubrication under certain conditions, consistent with some prior experimental work. The analytical method will be thoroughly tested in conjunction with the afore-mentioned squeeze film study.

IV. Pertinent Publications.


Sanborn, D. M. and Winer, W. O., "Fluid Rheological Effects in Sliding Elasto-hydrodynamic Point Contacts with Transient Loading: I-Film Thickness (To Be Published).

Sanborn, D. M. and Winer, W. O., "Fluid Rheological Effects in Sliding Elasto-hydrodynamic Point Contacts with Transient Loading: II Traction" (To Be Published).


Tichy, J. A. and Winer, W. O., "Inertial Considerations in Parallel Circular Squeeze-Film Bearings" (To Be Published).

+Associate Professor of Mechanical Engineering
++Assistant Professor of Mechanical Engineering
+++Instructor and Research Associate in Mechanical Engineering
AFOSR-TR-72-2029

FINAL SCIENTIFIC REPORT

INTERFACE PHENOMENA IN ENGINEERING MATERIALS

by

Edwin J. Scheibner

This research was supported by the Air Force Office of Scientific Research (AFSC) under Contract F44620-68-C-0008 (Project THEMIS)

Georgia Institute of Technology
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I. ABSTRACT

The purpose of the research studies under Project THEMIS (Contract F44620-68-C-0008) was to examine in a fundamental manner various phenomena occurring at interfaces between different materials or between different phases of the same material, including the gas-solid interface. Of particular importance was the fact that these studies were to be directed towards an understanding of the influence of interfacial conditions on the behavior of materials in engineering applications. A multi-task, multi-discipline effort provided a broad research program which included: fundamental surface science, e.g., adsorption and surface thermodynamics; the development of surface analytical techniques, e.g., improved Auger electron spectroscopy and micromechanical techniques; engineering applications, e.g., friction and wear, and semiconductor process studies; and detailed investigations of fabrication methods, e.g., chemical vapor deposition and sintering.

Project THEMIS was a program of the Department of Defense having two specific objectives: 1) the development of basic knowledge at new centers of excellence for use in solving future defense problems; and 2) the strengthening of the graduate program of educational institutions. The material summarized in this report indicates how these objectives were achieved at the Georgia Institute of Technology.
II. SUMMARY OF RESEARCH

1. Introduction and Research Goals

Many engineering materials which have desirable structural properties unfortunately are also highly susceptible to environmental factors such as chemical attack in a gaseous or liquid medium. In military applications of certain of these materials, normal stresses combined with the environmental factors can cause catastrophic failure of a critical structural member. Other materials are used in device applications where physical, metallurgical, and chemical phenomena at interfaces play a vital role in performance and reliability. The research performed under Project THEMIS (Contract F44620-68-C-0008) was directed towards a fundamental understanding of these and other problems related to the influence of interfacial conditions on the behavior of engineering materials.

Project THEMIS was initiated by the Department of Defense (DoD) in 1967 as a national program designed to develop new centers of excellence capable of contributing basic knowledge for use in solving future defense problems. Its concept provided for program-oriented research in which it was possible to achieve at a single institution a coordinated multi-task, multi-discipline team effort directed towards a specific area of science or engineering. Consistent with this objective was the recognition that the program should contribute to the strengthening of the graduate program in accordance with the long range educational goals of the institution. Another objective of THEMIS was the establishment of closer relationships between university scientists or engineers and the DoD laboratory scientists and engineers who are regularly concerned with the analysis of long-term military problems and missions.

The Department of Defense had identified eight relevant research areas suitable for THEMIS support; one of these was materials science and engineering. At Georgia Tech we recognized the importance of interface phenomena in a number of practical problems in the materials area and therefore proposed on 1 May 1967 to establish an interdisciplinary research program on "Interface Phenomena in Engineering Materials," building upon our existing strengths and interests.

The research studies under our THEMIS program were initiated on 1 September 1967 and were continued until 31 August 1972 with a reduced
effort during the last two years. Twelve independent but related tasks comprised the total research effort. Titles of these tasks, the task leaders, and a statement of the research goals are as follows:

Thermodynamics of Interfaces  (J.C. Eriksson)

To develop, from previous studies on the thermodynamics of surface phases in fluid systems, a general thermodynamic theory to include both physical adsorption and chemisorption.

Measurement of Thermodynamic Quantities  (B.R. Livesay)

To measure the surface tension of solid interfaces and the changes in it that may be due to the adsorption of various gases.

Electron Interactions With Solids  (L.N. Tharp)

To develop means of characterizing solid surfaces with respect to structure and composition for sub-monolayer coverages of impurities.

LEED Studies of Gas-Solid Interactions  (G.W. Simmons)

To study gas-solid interactions for specific chemical systems of interest to other tasks in the program, by low energy electron diffraction (LEED) and related techniques.

Optical Studies of Interfaces in Controlled Environments  (J.R. Stevenson)

To characterize the dielectric properties of an interface region experimentally by investigating the complex index of refraction in a frequency interval (near infrared into vacuum ultraviolet) where the interface is highly absorbing.

Field Emission and Field-Ion Microscopy  (R.F. Hochman and H.E. Grenga)

To apply field emission and field-ion microscopy to the study of the structure and surface characteristics of solid surfaces and interfaces of engineering materials.

Ultrasonic Effects on Metal Processing: Surface Tension  (R.F. Hochman)

To determine the effect of ultrasonic energy on the surface energy of solids and on the solid-liquid interface during solidification.

Adhesion, Friction and Wear Studies  (M.E. Sikorski)

To investigate those fundamental properties of materials which influence adhesion, friction and wear phenomena.
Machinability of Metals (J.A. Bailey)
To study the forces at the chip-tool interface during machining operations and the effects of lubricants containing chlorine, bromine, iodine or fluorine on the reduction of frictional forces.

Solidification of Metals (J.A. Murphy)
To study the conditions at the liquid-solid interface during the casting of metals into metal molds.

Gas-Solid Interactions (R.A. Pierotti)
To obtain high and low temperature data for the interaction of non-reactive gases with graphite and boron nitride and then to analyze these data in terms of statistical thermodynamics models to elucidate the nature and magnitude of the forces acting between the gas and the solid, and among gas molecules in the presence of the solid.

Surface and Diffusion Coatings (C.W. Gorton)
To identify technology gaps and specific research problems related to surface and diffusion coatings and to undertake a parametric experimental study for the preparation of a particular coating using chemical vapor deposition.
2. Review of Achievements

In this section the research performed under the various tasks of the program is briefly reviewed, changes in emphasis are mentioned, and appropriate references in the published literature are noted.

a) Thermodynamics of Interfaces

In previous studies of the thermodynamics of plane surface phase systems, Eriksson stressed the importance of a surface phase of non-zero thickness. Thermodynamic components could have, in this region, values that may be considerably different from their bulk values. This approach is more realistic than the use of the Gibbs "dividing surface" where such "surface excesses" are located, in earlier formulations of surface thermodynamics. The systems considered previously by Eriksson were fluid surface phase systems. In this research the general thermodynamic concepts were extended to the solid-gas interface. In the paper a fundamental equation is derived for the surface phase of a solid exposed to an adsorbing gas and measurements of dimensional changes upon adsorption, heats of adsorption and surface structure transitions are discussed on the basis of the formalism.

b) Measurement of Thermodynamic Quantities

The macroscopic quantity of particular importance in the thermodynamics of surface phases is the surface tension, $\gamma$. While this quantity can readily be determined for fluid surface systems, for solid surfaces there are relatively few experimental studies, except for metals close to the melting point. Several investigators, however, have studied dimensional changes of porous solids which occur at gas adsorption. These studies are discussed by Eriksson. Porous solids have surfaces which are relatively undefined with respect to structure and composition and, therefore, fundamental information on surface tension and localized adsorption is difficult to extract from the results. On the other hand the surfaces of thin foil samples can be cleaned and characterized. When subjected to a constant stress such samples will experience a change in the state of strain if the surface tension is altered by gas adsorption. Measurements of the dimensional changes by optical lever or interferometer techniques should be made as a function of gas pressure and sample temperature. In this research task equipment was designed and constructed for performing such measurements.

Before undertaking studies of dimensional changes on gas adsorption it was considered essential that studies be made of the mechanical properties,
i.e., stress vs strain, of thin foils and the effects of changing interfacial energies by depositing various films on the foil samples. Techniques were developed for preparing thin single crystal tensile specimens and for measuring their mechanical properties. In his doctoral dissertation B. R. Livesay interpreted the results in terms of dislocation interactions with the interface. Research under this task was continued by B. R. Livesay and E. A. Starke, Jr. under Air Force Grant No. AFOSR-71-2064 on "Effects of Interface Phenomena on Mechanical Behavior of Metals."

c) Electron Interactions with Solids

Under this task several improvements were made in the experimental techniques for using Auger electron spectroscopy in the characterization of surfaces. For example, one experimental system assembled consisted of a large bell-jar type ultra-high vacuum system equipped with a turbomolecular pump-ion pump combination, a spherical retarding field electron energy analyzer for generating the Auger spectra and a special multiple sample turret assembly for sequentially analyzing several samples inserted at the same time. This system was particularly useful in studies of semiconductor device processing (supported by NASA under Contract No. NAS 8-25667) and in studies of quartz crystal resonators.

Another study of Auger spectroscopy applied to semiconductor surface problems is being completed by R. P. Woodward for a Ph.D. dissertation in the School of Electrical Engineering. Improvements in this work include the use of a high current density electron gun, the analysis of sample current to determine optimum conditions for avoiding charging and other artifacts that confuse the interpretation of Auger spectra, and the calibration of Auger electron intensities for different angles of incidence of the primary electron beam. This work also elucidates the mechanisms of carbon contamination and removal on silicon and silicon dioxide surfaces.

d) LEED Studies of Gas-Solid Interactions

A general purpose gas-solid reaction chamber was built into a conventional ultra-high vacuum LEED system for studying materials in highly corrosive atmospheres under a wide range of pressures and temperatures. In initial investigations with this system low energy electron diffraction (LEED) was used to study the surface structures of titanium single crystals that accompany reactions at the solid-gas interface and Auger electron spectroscopy was used to identify the elemental composition of the surfaces studied. Order-disorder phenomena at the surface of $\alpha$-titanium-oxygen solid
solutions was observed for various oxygen pressures and correlated with published experimental data on bulk specimens. Because of the difficulties encountered in keeping the titanium samples oxygen free during preparation of the surfaces an apparatus was constructed for depositing thin films in situ. Studies were then made of aluminum, titanium, vanadium and chromium films by Auger electron spectroscopy and by the analysis of characteristic energy losses in the inelastic electron spectrum. The titanium work was partially supported by the Advanced Research Projects Agency under Contract No. Nonr-991(15) with the Naval Research Laboratory.

The 3d transition metals were also studied theoretically by Phillips who investigated the LMM Auger transition probabilities and energies in titanium, vanadium, chromium, zirconium, niobium and molybdenum.

**e) Optical Studies of Interfaces in Controlled Environments**

The dielectric properties of a material are usually characterized by a frequency-dependent response function in the form of a complex dielectric constant, a complex conductivity, or a complex index of refraction. The frequency interval in which a dielectric response function is changing rapidly is indicative of an absorption process taking place in the material. Whenever the absorption is very strong, the high attenuation of the electromagnetic disturbance makes the reflected radiation characteristic of the dielectric properties of the interface between the transparent incident medium and the highly absorbing reflecting medium.

In the research of this task optical reflectivity studies were made of the semiconductor alloy system Cd$_x$Zn$_{3-x}$As$_2$ in the frequency interval from the near infrared into the vacuum ultraviolet. The semiconductor specimens were obtained from the Semiconductors Branch of the U.S. Naval Research Laboratory where theoretical calculations of band structure were being performed. The vacuum ultraviolet reflectivity data were obtained at the University of Wisconsin using the synchrotron radiation from the storage ring. Samples were maintained in an ultra high vacuum chamber and Auger spectroscopy was used to analyze the extent of surface contamination.

Research under this task was continued under Air Force Grant No. AFOSR-70-1892.

**f) Field Emission and Field-Ion Microscopy**

Initially the work under this task involved the development of techniques for examining the various types of interfaces occurring in engineering alloys, i.e., grain boundaries, G.P. zones, two phase boundaries,
order-disorder anti-phase boundaries, etc. Field ion microscopy studies of ordered Ni$_4$Mo and the fine structure in alloy steels were made.\textsuperscript{16,17} Titanium and Ti$_3$Al were also examined although it was difficult to image these materials.\textsuperscript{18}

Research under this task was continued under NSF Grant GK-26487.

g) Ultrasonic Effects on Metal Processing: Surface Tension

Preliminary experiments were made during the first year on the surface tension of mercury on aluminum. Using the sessile drop technique a measurable decrease in surface tension was observed when the aluminum plate was ultrasonically activated. While the effects of ultrasonic excitation could have important consequences in problems involving solid-liquid interfaces, e.g. solidification, we were unable to provide sufficient concentration of effort to obtain definitive results. The research under this task was therefore discontinued.

h) Adhesion, Friction and Wear Studies

A twist compression bonding technique\textsuperscript{19} was used to determine the coefficient of adhesion in air for alloys of a variety of compositions from the solid-solution systems Cu-Au, Cu-Ni, Au-Ag, Ag-Pd and Pt-Co. It was shown\textsuperscript{20} that the coefficient of adhesion depends on chemical composition as well as by changes in the crystal structure produced by atomic ordering.

When the twist compression technique in air is used to investigate the adhesion of hard metals (Knoop hardness greater than about 400), it is found that the adhesion coefficients are rather small. An apparatus was constructed for performing twist compression studies under ultra high vacuum conditions and results were obtained for an ordered platinum-cobalt alloy.\textsuperscript{21} Using the same apparatus a study was made of the adhesion between high purity copper specimens in vacuum and compared with measurements in air.\textsuperscript{22}

A simple modification within the ultra-high vacuum system used for adhesion studies allowed a study to be made of the initial stage of vacuum sintering of pure metals, considered to be a high-temperature creep process.\textsuperscript{23}

Finally, an instrument was developed for measuring frictional forces of small magnitude ranging from below 0.01 dyne to about 50 dyne.\textsuperscript{24} The apparatus was used extensively in friction studies of fine wire samples and of individual textile fibers under U.S. Department of Agriculture Grant No. 12-14-100-7661(72). The approach should be particularly valuable in studying the behavior of sliding contacts.
i) **Machinability of Metals**
Work under this task was not initiated due to the resignation of Dr. John A. Bailey to accept a position with North Carolina State University at Raleigh, North Carolina.

j) **Solidification of Metals**
In metal casting many of the important parameters of the process are dependent on the existing heat transfer rates and temperature gradients. Factors which govern heat transfer rates and temperatures, such as, interfacial energies and thermal properties of the casting and mold, also determine the mold life and solidification rates. It was the purpose of this task to obtain quantitative information on these factors for the solidification of metals cast into metal molds.

Two stages of the casting process can be identified. In the first stage, liquid metal is in contact with the mold and high mold temperatures and high heat transfer rates are obtained. It is this first stage which is of primary interest with respect to mold life and with the initial formation of the surface of the casting. In the second stage, a significant amount of casting has formed and an "air gap" exists between the casting and the mold. This stage is of importance in governing overall solidification rates.

In this task the first stage was studied for the initial solidification of lead-tin alloys on steel. In order to measure the thermal response and heat transfer rates, transient temperatures in the steel plate were measured when the liquid alloy was poured onto the plate and when the plate was submerged into a liquid bath. Second stage measurements were concentrated on the time for the "air gap" formation. Two methods were used. An electrical contact method was simpler and appeared to give a more positive indication; however, an ultrasonic pulse echo method proved to be feasible also.

Further work beyond these preliminary studies was discontinued as the task leader was transferred to another unit of Georgia Tech.

k) **Gas-Solid Interactions**
Initial efforts under this task involved the construction and calibration of a high precision adsorption apparatus for a broad range of gas-solid interaction studies. In addition, a conventional volumetric system to study multilayer formation and a gravimetric system to study two-dimensional phase transitions were constructed. Measurements of the interaction of neon, argon, krypton and xenon with boron nitride were made using the
During the remainder of the program a statistical thermodynamical treatment for heterogeneous surfaces was developed, and studies were made of monolayer and high coverage adsorption of krypton on graphite, and monolayer coverage of krypton on \((1,1,1)\) copper. \(^{26,27}\)

The subject of physical adsorption was extensively reviewed by Pierotti and Thomas. \(^{28}\) Pierotti also published discussions on the virial expansion treatment in physical adsorption \(^{29}\) and on second and third order interactions of benzene with graphite. \(^{30}\)

1) **Surface and Diffusion Coatings**

In the first year of this task a literature survey and a preliminary survey of the defense or space oriented industry in the specific area of high temperature, oxidation resistant surface and diffusion coatings were made. \(^{31}\) These surveys were conducted to identify technology gaps and to determine research needs.

The literature survey was conducted by a search of the abstracts found in Chemical Abstracts, STAR, and the abstract files of the High Temperature Materials Division of the Engineering Experiment Station of Georgia Tech. Key papers, summaries, and reports were read beginning with the year 1963. The survey of private and government facilities involved with high temperature, oxidation resistant coatings was accomplished by means of a questionnaire.

Analysis of the surveys resulted in research recommendations in the categories of new coating and/or new coating concepts, deposition techniques, basic data, and evaluation methods. One specific recommendation was that the coating process, chemical vapor deposition (CVD), be studied from a basic engineering approach. Knowledge of this process would also further the understanding of many other industrial coating processes, such as pack cementation, in which CVD is the primary coating mechanism.

Initial experimental CVD studies were made of the hydrogen reduction of silicon tetrachloride to produce a solid silicon coating on a tungsten wire followed by a detailed parametric study of the process. The parameters included wire temperature, hydrogen flow rate, silicon tetrachloride partial pressure, and total stream pressure. \(^{32}\)

3. **Scientific Significance**

Individually each task under the program has made a contribution to the fundamental knowledge of surfaces or interfaces. However, the real
The significance of the research is the collective nature of the knowledge generated. By the multi-task, multi-discipline approach it should now be feasible to tackle, within the Institute, significant practical problems related to interface phenomena in engineering materials.

Project THEMIS had two basic objectives: the strengthening of the graduate program at the institution and the generation of basic knowledge for solving future defense problems. The participation of faculty and students from several schools and divisions, the development of specialized laboratories in these units, the publication of papers and theses, and the stimulation of cooperative research were accomplishments towards the first objective. The focussing of basic knowledge on defense problems was difficult because of the lack of a formal mechanism for coupling with federal laboratories. It is suggested that in the future consideration be given to assigning direct responsibility to appropriate laboratories for achieving the required coupling with universities.

It is also of significance to note that during the course of the program two major professional meetings were attracted to the campus, the 45th National Colloid Symposium of the Division of Colloid and Surface Chemistry, American Chemical Society, in 1971 and the Symposium on Field Ion Microscopy in Physical Metallurgy and Corrosion in 1968. And in 1972 a new interdepartmental Masters program in Surface Science and Technology involving members of the THEMIS team was initiated.
REFERENCES

13. J.D. Phillips, Ph.D. Dissertation, School of Physics, Georgia Institute of Technology, August 1972.
17. B.N. Ranganathan, Ph.D. Dissertation, School of Chemical Engineering, Georgia Institute of Technology, March 1972.


32. A.C. Merritt, Ph.D. Dissertation, School of Chemical Engineering, Georgia Institute of Technology, June 1973.
The following scientific reports or papers are anticipated for publication:

J.R. Stevenson, H.W. Ellis and R.J. Bartlett, "Reflectivity of Cd$_x$Zn$_{3-x}$As$_2$ Semiconductor Alloy Systems," in Conference Digest, 3rd International Conference on Vacuum Ultraviolet Physics, held in Tokyo, Japan (1971).


B.R. Livesay and E.A. Starke, Jr., "Interaction of Dislocations with Interfaces," accepted for publication by Acta Metallurgica.


In addition, publications are expected to result from the Ph.D. theses of J.L. Carden and J.D. Phillips.
IV. PROFESSIONAL PERSONNEL

The following professional personnel participated in the research under Project THEMIS:

Edwin J. Scheibner, Research Professor of Physics, Program Manager
Waldemar T. Ziegler, Regents Professor of Chemical Engineering
Charles W. Gorton, Professor of Chemical Engineering
Robert F. Hochman, Professor of Chemical Engineering (Metallurgy)
Robert A. Pierotti, Professor of Chemistry
James R. Stevenson, Professor of Physics
Raymond K. Hart, Principal Research Scientist
John A. Bailey, Associate Professor of Mechanical Engineering
John A. Murphy, Associate Professor of Mechanical Engineering
Edgar A. Starke, Jr., Associate Professor of Chemical Engineering (Metallurgy)
Helen E. Grenga, Assistant Professor of Chemical Engineering (Metallurgy)
James M. Bradford, Assistant Professor of Mechanical Engineering
L. Neal Tharp, Senior Research Scientist
Mathew E. Sikorski, Senior Research Scientist
Billy R. Livesay, Research Scientist
Gary W. Simmons, Research Chemist
Roger P. Woodward, Research Engineer
Jan C. Eriksson, Post-Doctoral Fellow
V. DISSERTATIONS

The following dissertations resulted from full or partial support by Project THEMIS:


"The Adsorption of Krypton on the (1,1,1)Face of Copper," John L. Carden, Jr., Ph.D. (Chemistry), Spring Quarter 1972.


VI. INTERACTION WITH INDIVIDUALS OR ORGANIZATIONS

Members of our research group have interacted with numerous individuals and organizations through visits, scientific meetings, consultations and other sponsored programs. Some of these are tabulated below.

Individuals

Dr. L.H. Jenkins, Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tenn.

Dr. W. Pillinger, Savannah River Laboratory, Aiken, South Carolina

Dr. T.W. Haas, Aerospace Research Laboratories, Wright-Patterson Air Force Base, Ohio

J.M. Blasingame, Avionics Branch, Wright-Patterson Air Force Base, Ohio

Dr. J.O. Porteus, Naval Weapons Center, China Lake, California

Dr. John J. Burke, U.S. Army Materials and Mechanics Research Center, Watertown, Mass.

Dr. Fred Leonard, U.S. Army Medical Biomechanical Research Laboratory, Walter Reed Army Medical Center, Washington, D.C.

Institutions

U.S. Naval Research Laboratory, Metallurgy Branch and Semiconductor Branch

NASA Marshall Space Flight Center, Huntsville, Alabama (Astrionics and Materials)

Lehigh University, Bethlehem, Pa.

N.C. State University, Raleigh, North Carolina

Ohio State University, Columbus, Ohio

Batelle Memorial Institute, Columbus, Ohio

Westinghouse Research Laboratories, Pittsburgh, Pa.

Varian Associates, Palo Alto, California

Bell Telephone Laboratories, Murray Hill, New Jersey
Meetings

45th National Colloid Symposium held at Georgia Tech in June 1971

Symposium on Field Ion Microscopy in Physical Metallurgy and Corrosion
held at Georgia Tech in May 1968

Member of staff attended the Tri-Service Meeting on Corrosion of
Military Equipment at Annapolis, Maryland, November 19-20, 1969

Dr. E. J. Scheibner presented a series of invited lectures on "Inelastic
Scattering of Low Energy Electrons" at the NATO International
Summer Course on Fundamental Processes on Semiconductor
Surfaces held at the University of Ghent, Belgium, August 26--
September 6, 1968

Other Sponsored Programs

ARPA Program on "Stress Corrosion Cracking" with Naval Research
Laboratory, Lehigh University, Carnegie-Mellon University
and the Boeing Company (Contract No. Nonr-991(15).

NASA Program on "Development of Microcircuits for Space Applications"
(Contract No. NAS 8-25667).

AEC Program on "Surface Properties of Magnetic Materials"
(Contract No. AT-(40-1)-2755)
VII. PATENTABLE INVENTIONS

There were no patentable inventions resulting from the sponsored research under this contract.
The purpose of the research was to examine in a fundamental manner various phenomena occurring at interfaces between different materials, including the gas-solid interface, and their influence on the behavior of materials in engineering applications. A broad research program included fundamental surface science, e.g., adsorption and surface thermodynamics; the development of surface analytical techniques, e.g., Auger electron spectroscopy and micromechanical techniques; applications, e.g., friction and wear, and semiconductor process studies; and fabrication methods, e.g., chemical vapor deposition and sintering.
### 14. KEY WORDS

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