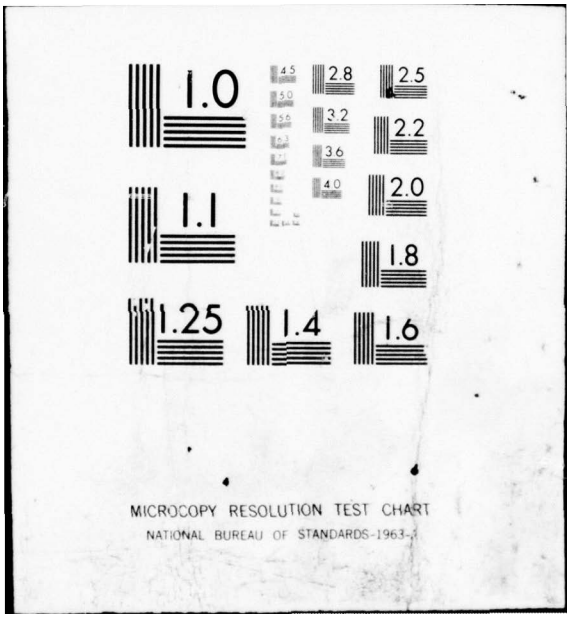
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Special Reports

INDIRECTLY FUNDED RESEARCH AND EXPLORATORY DEVELOPMENT AT THE APPLIED PHYSICS LABORATORY

FISCAL YEAR 197T AND 1977

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Special Reports

INDIRECTLY FUNDED RESEARCH AND EXPLORATORY DEVELOPMENT AT THE APPLIED PHYSICS LABORATORY

FISCAL YEAR 197T AND 1977

R. W. HART, Editor

THE JOHNS HOPKINS UNIVERSITY ■ APPLIED PHYSICS LABORATORY
Johns Hopkins Road, Laurel, Maryland 20810
Operating under Contract N00024-78-C-5384 with the Department of the Navy

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ABSTRACT

This report summarizes the Indirectly Funded Research and Exploratory Development activities of The Johns Hopkins University Applied Physics Laboratory during the transition quarter (1 October - 31 December 1976) and fiscal year 1977 (1 January - 31 December 1977).

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CONTENTS

The Indirectly Funded Research and Development Program 9

THE RESEARCH CENTER

Introduction 11

Applied Mathematics 12

Applied Mathematics 12

Atomic, Molecular, and Electronic Physics . . . 17

Mass Spectrometry of Transient Chemical Species 18
Localized Corrosion in Aluminum 23
Valance-Bond Studies of Molecular and Solid-State Systems 26

Chemical Physics 33

Molecular Structure and Chemical Reactivity 34
Molecular Energy Transfer 39
Kinetic and Collision Theory 43

Excitation Mechanisms 47

Chemical Laser Studies 47

Microwave Physics 51

Molecular Photophysics 51

Photoacoustic Spectroscopy 52
Molecular Structure and Photochemistry of Free Radicals 56

Spectroscopy of Electron-Donor-Acceptor Molecules 61

Quantum Electronics 66

Investigations in Quantum Electronics . . . 67

Solid-State Physics 75

Electronic Properties of Controlled Impurities in Amorphous Boron Films 76
Quantitative Secondary-Ion Mass Spectrometry Employing a Sputtering Ion Source . . . 79
Optical Properties of Semiconductors . . . 83
Polycrystalline Silicon Solar Cells . . . 87

Theoretical Problems 91

Wave Propagation and Scattering 92

Rough Surface Scattering 92
Laser Intensity Correlation Spectroscopy of Macromolecules 95

Fluid Mechanics 97

Internal Flow 98
Hydromagnetism 100

Bioengineering 103

Visual Signal Analysis 103
Membrane Transport 105
Pain Physiology 107

LABORATORY-WIDE
RESEARCH AND EXPLORATORY DEVELOPMENT

Introduction 111

Air Traffic Safety and Control 112

Biomedical Engineering 119

Intracranial Pressure Sensor 119
Arterial Hemodynamics and Pulsatile Flow 120

Community Annual Storage Energy System . . . 122

Electromagnetic Conductivity Survey System . . . 125

Feasibility Demonstration, Automated Maintenance Support Tool 128

Magsat-II 133

Optical Altimeter for the Surface Effect Ship Wave Profiling System 142

Passive Height Finder 145

Power Plant Waste Heat Utilization 147

Radiation Hazard Study 157

Salt Drift Deposition Studies 160

Speech Synthesis 163

Space Research and Technology 166

Reflection of Solar Electrons from the Magnetosphere 167
New Satellite Instrumentation 168
Solar Particle Propagation, Low-Energy Nucleon Spectra, and Z-Rich Solar Particle Events 170

PUBLICATIONS

Research Center Publications 173

Research Center Papers Accepted for Publication 181

Exploratory Development Publications 183

THE JOHNS HOPKINS UNIVERSITY
APPLIED PHYSICS LABORATORY
LAUREL, MARYLAND

THE INDIRECTLY FUNDED RESEARCH AND DEVELOPMENT PROGRAM

The Applied Physics Laboratory of The Johns Hopkins University is devoted to research and development tasks in the national interest for agencies of the government. The principal supporting agency is the Navy. Most tasks for which the Laboratory is funded require commitment to prescribed performance requirements and completion dates and, therefore, commit the Laboratory to the use of state-of-the-art technology. These tasks typically cannot provide the means of maintaining and developing capabilities in frontier areas of science and technology or of exploring innovative approaches to the solution of existing or foreseeable problems. Indirectly Funded Research and Development (IR&D) is a primary and efficient way for the Laboratory to maintain its value to the nation through independent research.

The central objective of the IR&D Program remains that of enhancing the present and future vigor of the Laboratory through

1. The provision of current, in-depth understanding in fields important to the Laboratory's applied tasks,

2. The origination and exploration of innovative approaches to the solution of national problems, and

3. The provision of a window into science to cultivate the effectiveness of the Laboratory as an organization primarily devoted to engineering research and development.

The IR&D Program has two major subdivisions: (a) basic research, carried out primarily in the Research Center of the Laboratory and (b) applied research (exploratory development) carried out on a Laboratory-wide basis in the various Departments and Divisions.

Since the support of national defense objectives remains the principal task of the Laboratory, the IR&D Program is mainly concerned with Navy and DoD-related problem areas. However, at the level of basic research, military and civilian problem areas overlap. Moreover, with the encouragement of the Secretary of Defense and the Secretary of the Navy, the Laboratory also works on urgent

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problems for other agencies, comprising typically 15 to 20% of its total effort. Such agencies include the National Aeronautics and Space Administration (NASA), the National Institutes of Health (NIH), the Department of Energy (DOE), the Department of Transportation (DOT), the Department of Commerce, the Department of the Interior, the Veterans Administration (VA), and the State of Maryland.

THE RESEARCH CENTER

INTRODUCTION

The central purpose of the Research Center is to serve the Laboratory as a window on science, thus providing in-depth understanding in fields important to the Laboratory's applied tasks.

The Research Center is staffed by a total of 60 scientists and supporting personnel; the level of Indirectly Funded Research and Development support for the current reporting period comprises about 50% of the total effort. It is the IR&D Program that provides the long-term continuity necessary to in-depth research. The remaining portion of the Research Center's program is devoted to investigation of and consultation with the Laboratory's explanatory and engineering development, test and evaluation tasks, and basic and applied research projects funded by agencies external to the Laboratory.

The Research Center disseminates information to the Laboratory through internal seminars and reports and to the general scientific community through participation in regional, national, and international meetings, workshops, and symposia, and by the publication of results in scientific journals.

During the period covered by this report, 80 papers appeared in print and 19 others were accepted for publication, most of which were made possible either entirely or in part by the IR&D Program. It is not possible to describe the many results in detail in a concise report such as this; the following articles can only convey an impression and an overview.

APPLIED MATHEMATICS

The Applied Mathematics Group at present consists of five senior mathematicians specializing in areas of analysis supporting Laboratory programs. During the present reporting period, approximately 20% of the work of the group was supported by the IR&D Program. Progress is described in detail in five publications that appeared during this time and in two manuscripts that have been accepted for publication. Particularly noteworthy is Dr. Vincent Sigillito's monograph (103 pages), one of a series in mathematics published by Pitman Press, London. Other items of note include the following: Dr. D. W. Fox, Supervisor of the group, completed his term as William S. Parsons Visiting Professor in the Department of Mathematical Sciences at The Johns Hopkins University; Dr. L. W. Ehrlich was elected to the Board of Directors of SIGNUM of the Association for Computing Machinery; Dr. Sigillito was appointed to membership on the Laboratory's Principal Professional Staff; and Dr. J. C. W. Rogers joined the group.

APPLIED MATHEMATICS

Two areas in applied mathematics continue under study in this period: (a) the development and application of a priori inequalities in elliptic and parabolic partial differential equations and (b) numerical approximation of solutions of certain partial differential equations that arise in fluid flows. Each has intrinsic interest and potentially wide areas of applicability to computational approximation of solutions to partial differential equations that arise in Navy problems. The new results have been mainly in areas of application: the use of finite-difference marching techniques to calculate the stream functions in equations governing the flow of thick fluids, computational techniques for applying a priori estimates to finding approximate solutions of elliptic equations on rectangular regions, and the use of a priori estimates in the bounding of eigenvalues of elliptic equations.

Problem

Navy research requirements specify the need for the investigation of numerical and combinatorial methods of computation and their applications, including a wide variety of areas of mechanics and hydrodynamics (Naval Research Requirements, ONRINST 3910.2, January 1977, R014-01, -02, -03, pp. 7-8).

Many of the problems fundamental to technological progress in areas of interest to the Navy are formulated as boundary value problems of partial differential operators or involve the

eigenvalues of these operators. It is well known that obtaining exact solutions of such problems is usually not possible, and so recourse must be made to approximation techniques. The most widely used technique for approximating boundary value problems is that of finite differences and more recently finite elements. Other techniques include Galerkin methods, spectral methods, and the method of a priori inequalities. Each method has its own area of usefulness and applicability; in fact, no one method comes close to being applicable in all problems. Thus numerical analysts are constantly working to improve the known methods and to develop new ones.

Our continuing work on numerical methods using finite differences in fluid flow problems now includes a study of the equations for viscous fluid behavior through constriction in a tube. Results are applicable to flows of thick fluids, and the techniques can be used directly to study lee waves in flows across barriers (e.g., ridges in the ocean bottom) since the shapes of the regions are similar. The method involves mathematically mapping the region under consideration onto a rectangle, either conformally or numerically, and applying highly developed finite-difference techniques.

Objective

The long-range aims are to develop the methods into a reliable tool for a wide variety of similar problems and to obtain estimates of the accuracy of the techniques.

Approach

The region is first mapped onto a rectangle to simplify the boundary shape. This naturally complicates the equations. The mapping can be conformal if the boundary shape fits a known mapping. Otherwise, a numerical map can be generated. Our methods concentrate on numerically solving the resulting complicated difference equations rapidly.

Results

We have developed a technique to solve the stream function equation faster than earlier approaches. In essence, it is a marching technique, which is occasionally restarted to control stability. The approximate solution of the vorticity equation is also currently under investigation. The marching technique has

been described in detail in Ref. 1, and three papers (Refs. 2, 3, and 4) appeared in 1977 on our earlier fluid flow work. Another report is in preparation describing the complete problem and methods of solution. Further, a lecture entitled "Applications of Linear Systems to Fluid Problems" was presented at the Applied Matrix Computation Seminar at The Johns Hopkins University in August 1977.

The method of explicit a priori inequalities is relatively unexploited but has two distinct advantages: (a) it is the only widely applicable method for which error bounds can always be computed, and (b), of those methods that use trial functions to construct the approximation, it is one of only two (the other being least squares) that does not require the trial functions to satisfy either the boundary conditions or the differential equation.

One of the objectives of this research has been completed, i.e., the mathematical derivation of the a priori estimates applicable to the three classical boundary value problems for elliptic and parabolic equations. The second part of the project, the construction of computer programs that allow the user to calculate approximate solutions to a wide variety of problems, has only recently been undertaken.

The main approach can be summarized briefly: If we wish to approximate the solution u, which satisfies the differential equation $Au = f$ and the boundary condition $Bu = g$, where f and g are given, we need an a priori inequality of the form

$$|| v || \leq F_1(Av) + F_2(Bv)$$

where $|| \cdot ||$ is a norm and F_1 and F_2 are functionals. The inequality is to hold for all functions v in a class that includes u (typically the only restriction on functions in the class are smoothness restrictions).

Now we put $v = u - \Sigma a_k \phi_k$ in the inequality to get

$$|| u - \Sigma a_k \phi_k || \leq F_1[A(u - \Sigma a_k \phi_k)] + F_2[B(u - \Sigma a_k \phi_k)], \quad (1)$$

where the ϕ_k = 1,2,..., is a sequence of approximations for u. If the ϕ_k can be systematically chosen to make the right side of Eq. 1 small, the ϕ_k will closely approximate u, and Eq. 1 will give an estimate of the error in the approximation.

Efforts in this reporting period were concentrated on producing computer software that allows one to compute approximate solutions using the a priori inequalities. The philosophy underlying this effort is ease of use. That is, the user need supply only the differential equation through its coefficients, the prescribed forcing functions for the differential equation, and the boundary conditions and parameters that define the region.

Clearly, even though the inequalities are quite generally applicable, writing software to handle the general case will be a long and laborious task. Therefore only the simplest task was attempted in this period, namely, linear second-order constant coefficient elliptic partial differential equations on rectangular regions. All three of the classical boundary value problems were treated: Dirichlet, Neumann, and Robin. The initial program uses powers of the coordinate variables as trial functions, but later versions will use Legendre and Chebyshev polynomials and trigonometric functions. More general regions will then be added, which will probably require the incorporation of special mapping techniques. Finally, the problem of nonconstant coefficients will be approached. An exactly parallel program for second-order parabolic equations will logically follow.

Reference 5, a monograph treating the entire area of explicit a priori inequalities and their applications, appeared during the reporting period, while Ref. 6 gives an explicit a priori inequality for the diffusion operator with Neumann boundary conditions. Reference 7 is also of interest.

In recent years, a method has been developed based on a priori inequalities of calculating upper and lower bounds on eigenvalues of a wide class of partial differential operators. The method is of interest since the trial functions used in the approximation do not need to satisfy any boundary conditions. This desirable feature is a direct consequence of the central role played by a priori inequalities in the procedure.

The method was first described in Ref. 8 where it was used to compute bounds on eigenvalues of fixed rhombical membranes. The method was further described in a presentation at Cornell University (Ref. 9). A further paper (Ref. 10) has been submitted for publication. In it, our method has been adapted to calculate the fundamental Dirichlet eigenvalue for rectangles; these eigenvalues are themselves constants needed in an explicit a priori inequality for Poisson's equation with Dirichlet boundary conditions.

Principal Investigators: Dr. D. W. Fox (Supervisor), Dr. L. W. Ehrlich, Dr. J. R. Kuttler, and Dr. V. G. Sigillito, senior mathematicians of the Applied Mathematics Group; Dr. M. H. Friedman (Supervisor) and Dr. V. O'Brien of the Theoretical Problems Group; and Dr. A. Elcrat. Dr. Elcrat is with the Department of Mathematics, Wichita State University, and is not funded by the IR&D Program.

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2. L. W. Ehrlich and M. H. Friedman, "Steady Convective Diffusion in a Bifurcation," IEEE Trans. Biomed. Eng., Vol. BME-24, No. 1, Jan 1977, pp. 12-18.

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6. J. R. Kuttler and V. G. Sigillito, "Explicit L_2 Inequalities for Parabolic and Pseudoparabolic Equations with Neumann Boundary Conditions" (accepted for publication, Int. J. Math. Math. Phys.).

7. A. Elcrat and V. G. Sigillito, "Coercivity for a Third Order Pseudoparabolic Operator with Applications to Semilinear Equations," J. Math. Anal. Appl., Vol. 61, No. 3, Dec 1977, pp. 841-849.

8. J. R. Kuttler and V. G. Sigillito, "Bounding Eigenvalues of Elliptic Operators" (accepted for publication, SIAM J. Math. Anal.).

9. V. G. Sigillito, "Bounds for eigenvalues of elliptic operators," Applied Mathematics Colloquium, Dept. of Mathematics, Cornell University, 1 Apr 1977.

10. J. R. Kuttler, "Dirichlet Eigenvalues" (submitted, SIAM J. Math. Anal.).

ATOMIC, MOLECULAR, AND ELECTRONIC PHYSICS

Work in atomic, molecular, and electronic physics in the Research Center is carried out by a group of six investigators who are roughly two-thirds supported through the IR&D Program. Their general objective is improved understanding of interactions among atoms, molecules, and electrons, and of radiation in selected areas of present and potential importance to the Laboratory and DoD.

The areas include lasers, computers, propellants, energy storage and conversion, and materials performance. Significant progress has been made during the present reporting period in

1. Mass spectrometry of transient chemical species,
2. Localized corrosion, and
3. Valence bond studies of molecular and solid state systems (in collaboration with the Microwave Physics Group of the Research Center).

The work is outlined in the following articles and is described in detail in nine articles published during the present period and in three manuscripts now in press. In addition to these publications, the following papers in electronic physics were published in the fiscal reporting period:

1. A. N. Jette, "The ab initio Calculation of the Spin-Rotational Coupling in the Metastable $C^3\Pi_u(1s,2p)$ State of Molecular Hydrogen," J. Chem. Phys., Vol. 65, No. 10, Nov 1976, pp. 4325-4327.
2. F. J. Adrian and V. A. Bowers, "ESR Spectrum of XeCl in Argon at 4.2K," J. Chem. Phys., Vol. 65, No. 10, Nov 1976, pp. 4316-4318.
3. B. H. Nall, "Use of a Hot Wire Anemometer as a Particle Velocity Detector in Standing Sound Waves," Rev. Sci. Instrum., Vol. 48, No. 4, Apr 1977, pp. 449-453.

MASS SPECTROMETRY OF TRANSIENT CHEMICAL SPECIES

Energetics and mechanisms of reaction were investigated in three definitive mass spectrometric studies. The heat of formation of the highly endothermic compound diimide (N_2H_2), a subject of considerable thermodynamic interest, was determined with new accuracy. The proton affinity of N_2, an important anchor point in the ladder of the relative proton affinities, was determined on an absolute scale from ionization studies of trans-diimide. Results are in good agreement with a theoretical calculation and with values derived from recent experiments on the proton affinity of CO_2. The production of highly vibrationally excited molecules in crossed molecular beam reaction was directly observed by measuring changes in ionization energy. For HF produced in F atom reactions, the ionization energy shifts were correlated with the total amount of energy available for populating the vibrational levels.

The characterization of the energy states of molecules and of energy-transfer mechanisms in their reactions is of great importance in understanding the structure, stability, and chemical reactivity of materials critical to current and future DoD requirements. As noted, for example, in Naval Research Requirements ONRINST 3910.2, January 1977 (R011-03, R013-05, R024-02), research is required on the mechanisms and kinetics of the formation of materials, degradation and energy-transfer processes, chemical reaction dynamics, electron collision processes, and the storage, release, and use of energy contained in fuels, propellants, and explosives.

Considerable attention has been focused recently on the chemical, spectroscopic, structural, and thermodynamic properties of the first member of the azo compounds, diimide (N_2H_2). This short-lived, highly endothermic compound was originally discovered at APL some twenty years ago (Ref. 1). Diimide is known to be an important intermediate in many chemical reactions. It has been shown theoretically that, of the three possible isomeric forms of diimide, the trans-diimide isomer has the lowest energy and thus represents the stable form of the molecule. However, theoretical calculations on the heat of formation of diimide have not been satisfactory, and values for this needed parameter in thermochemistry show a wide scatter, ranging from 10 to 70 k cal/mole, with the most recent treatments yielding values in the range of 45 to 66 k cal/mole. There have been few direct measurements on the experimental side. In a very recent experimental study (Ref. 2), a value was derived for the heat of formation of diimide, $\Delta H_f(N_2H_2) = 36 \pm 2$ k cal/mole, that was substantially lower than the value, $\Delta H_f(N_2H_2) = 48.7 \pm 5$ k cal/mole, obtained in our original paper identifying this molecule (Ref. 1). This prompted us to reinvestigate the energetics of diimide (Ref. 3).

The method essentially involves measuring the appearance potential of the $N_2H_2^+$ ion from hydrazine, $AP(N_2H_2^+)$, and the ionization potential of N_2H_2, $IP(N_2H_2)$, and combining them in a relationship of the form

$$\Delta H_f(N_2H_2) = AP(N_2H_2^+) - IP(N_2H_2) + \Delta H_f(N_2H_4), \qquad (1)$$

where $\Delta H_f(N_2H_2)$, the heat of formation of hydrazine, is a known thermochemical quantity. The major uncertainty in using Eq. 1 is that the fragments in the dissociative ionization reaction $N_2H_4 + e \rightarrow N_2H_2^+ + H_2 + 2e$ used to determine $AP(N_2H_2^+)$ might possess excess energy.

The diimide was prepared by subjecting anhydrous hydrazine to a low-power 5-MHz electrodeless electrical discharge. After passing through a dry ice trap to remove hydrazine and higher hydronitrogen compounds, the discharge products were sampled with our modulated molecular beam mass spectrometer. Figure 1 plots the ion intensities of $N_2H_2^+$ from N_2H_2 and $N_2H_2^+$ from N_2H_4 after deconvolution to remove the effects of thermal energy spread in the electron beam. The measured ionization potential of N_2H_2, $IP(N_2H_2) = 9.65 \pm 0.08$ eV, is in good agreement with the most recent photoelectron spectroscopic value, 9.59 eV (Ref. 4). The appearance potential of $N_2H_2^+$ from N_2H_4 is $AP(N_2H_2^+) = 10.75 \pm 0.08$ eV. These values lead to values for the heat of formation of diimide at 0 K, $\Delta H^o_{fo}(N_2H_2) = 52.4 \pm 2$ k cal/mole and the heat of formation at 298 K, $\Delta H^o_{f298}(N_2H_2) = 50.7 \pm 2$ k cal/mole. The value 50.7 ± 2 k cal/mole is in remarkably good agreement with the results of our earlier work, 48.7 ± 5 k cal/mole. This energy assignment was confirmed by additional studies in Ref. 3 involving the ionizing reaction $N_2H_4 + e \rightarrow N_2H_2^+ + 2H + 2e$.

Proton transfer reactions represent an important class of ion-molecule reactions that are usually very fast and have numerous chemical applications, including many occurring in the atmosphere. The relative values of the proton affinities of a large number of molecules have been determined by a variety of techniques (the proton affinity of a molecule, X, is the enthalpy change at 298 K for the process $XH^+ \rightarrow X + H^+$). By careful choice of reactions it is

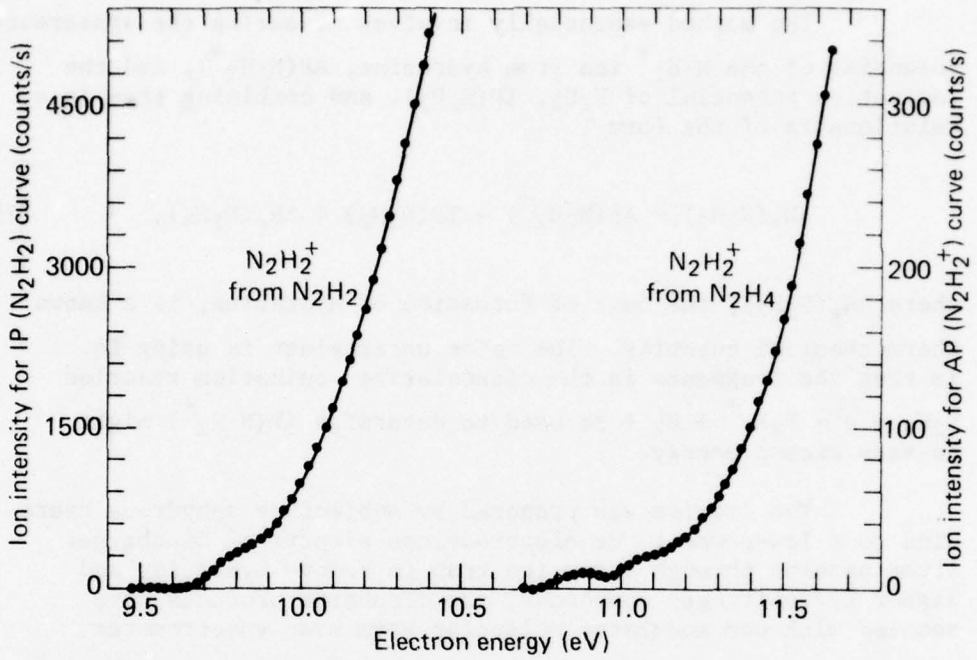


Fig. 1 Initial Portions of the Ionization Curve for N_2H_2 and the Appearance Potential Curve for $N_2H_2^+$ from N_2H_4. The electron energy scale has been standardized using argon, IP(Ar) = 15.76 eV.

possible to construct a ladder of proton affinity differences linking a series of molecules to produce a relative proton affinity scale. Although they are very difficult to measure, absolute values of proton affinities are needed to anchor the proton affinity ladder to tie-points to obtain an absolute reference scale, as well as to provide essential cross-checks.

The proton affinity of N_2, which has been the subject of several investigations, can be determined from ionization studies of trans-diimide (N_2H_2) in the reaction

$$N_2H_2 + e \rightarrow N_2H^+ + H + 2e \qquad (2)$$

if the heat of formation of N_2H_2 is known (Ref. 5). Having determined the heat of formation of N_2H_2 in the work described earlier, the only required input (other than known constants) was the measurement of the appearance potential of the N_2H^+ ion, $AP(N_2H^+)$, in Reaction 2. An appearance potential curve for N_2H^+ from N_2H_2 is shown in Fig. 2. The appearance potential of N_2H^+ from this curve

is 10.89 eV. The average of several independent measurements over a period of months gave the value of $AP(N_2H^+)$ = 10.89 ± 0.08 eV. This appearance potential combined with the heat of formation of N_2H_2 leads to a proton affinity of N_2, $PA(N_2)$ = 4.93 ± 0.11 eV (Ref. 5). The value is in good agreement with a theoretical calculation and with values derived from two recent experiments on $PA(CO_2)$, using data on the difference $PA(CO_2) - P(N_2)$ to link them together.

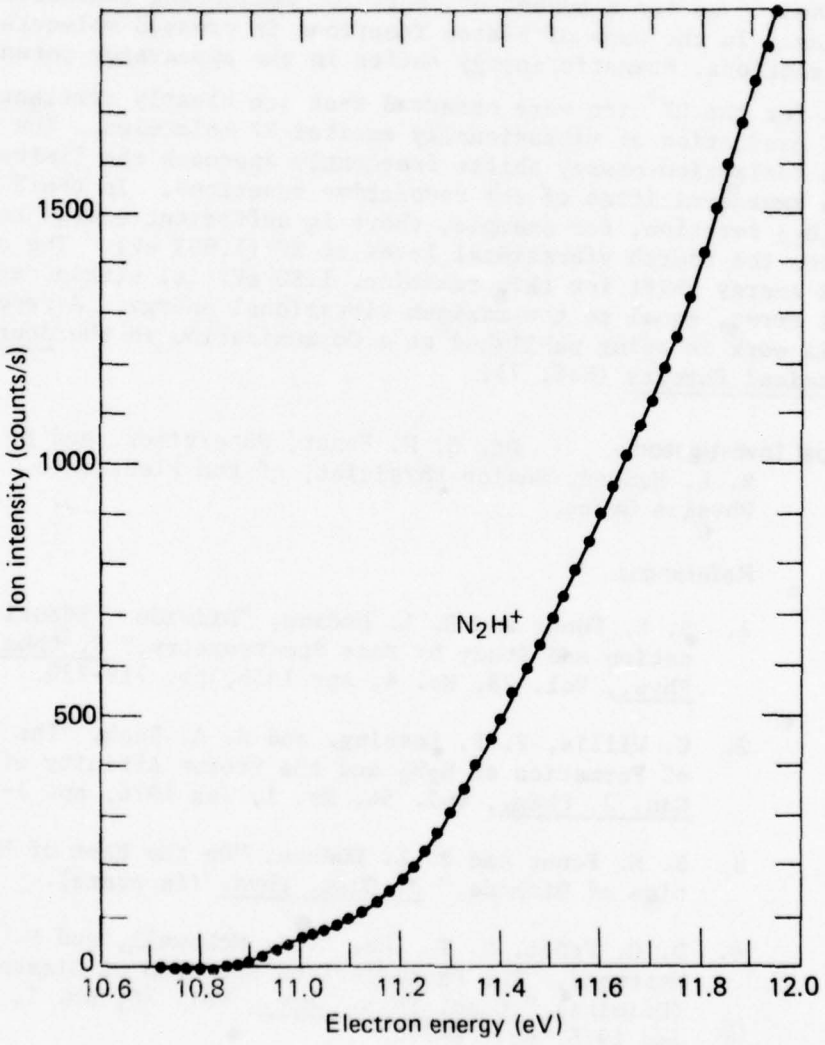


Fig. 2 Appearance Potential Curve for N_2H^+ from N_2H_2. The electron energy scale has been standardized using argon, IP(Ar) = 15.76 eV.

Mass spectrometric detection of excited state molecules can, in principle, be accomplished in two ways: (a) observing a decrease in the electron energy required for ionization, or (b) observing an increase in the proportion of fragmentation ion peaks produced by electron impact. Very recently, experiments using the second approach were reported (Ref. 6) using vibrationally excited HF, where fragmentation was shown to be approximately a linear function of the HF mean vibrational quantum number.

The ionization energy approach (the first method) has been used by us for a number of years for monitoring excitation energies. In the case of F-atom reactions in crossed molecular beam reactions, dramatic energy shifts in the appearance potential curves for the HF^+ ion were observed that are clearly attributable to the production of vibrationally excited HF molecules. The observed ionization energy shifts frequently approach the limits set by the exothermicities of the respective reactions. In the F + iso-C_4H_{10} reaction, for example, there is sufficient energy to populate the fourth vibrational level of HF (1.893 eV). The observed energy shift for this reaction, 1.80 eV, is, within experimental error, equal to the maximum vibrational energy. A report on this work is being published as a Communication in the Journal of Chemical Physics (Ref. 7).

Principal Investigators: Dr. S. N. Foner, Supervisor, and Mr. R. L. Hudson, Senior Physicist, of the Electronic Physics Group.

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LOCALIZED CORROSION IN ALUMINUM

Various types of localized corrosion processes are thought to begin by similar mechanisms. Recently an unknown step in the pitting corrosion of aluminum has been discovered in our laboratory. The passivating oxide on aluminum has been observed to blister and break prior to the onset of pitting corrosion.

The cost of corrosion in the United States has been estimated to be $30 billion annually (Ref. 1). As much as 90% of this loss has been associated with localized corrosion processes such as stress corrosion, cracking, pitting, fatigue, and crevice corrosion (Ref. 2). Because localized corrosion processes play a deleterious role militarily, DoD continues to be a major sponsor of corrosion research*, and the need for corrosion research is widely recognized (e.g., ONRINST 3910.2, January 1977, R022-18, p. 13). The objective of our research is to identify the basic mechanisms involved in the initiation phase of localized corrosion processes in metals. Currently, the effort is directed toward understanding pitting corrosion in high purity aluminum. Other types of localized corrosion are thought to have similar initiation mechanisms. even though the eventual gross manifestations of each type have distinct characteristics (Ref. 2).

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* For example, Ref. 1 describes basic corrosion research interests of the U.S. Army, and the Navy and Air Force support similar corrosion studies. Reference 2 is the proceedings of a conference supported in part by the Office of Naval Research and the Air Force Office of Scientific Research.

The experimental approach has been to use electrochemical methods coupled with light and scanning electron microscopy (Refs. 3 and 4). A typical experimental configuration was similar to that shown schematically in Fig. 1. A light microscope was focused on the aluminum electrode to observe any visible phenomena. The potential of the electrode was controlled while recording the current flowing through the specimen. After the electrochemical measurements and microscopic observations were made, the specimen was examined in a scanning electron microscope (SEM) that included spatial chemical analysis in areas of interest with an energy-dispersive x-ray analyzer.

An interesting phenomenon was observed for the first time under the following conditions. A constant potential above that necessary for pitting was maintained on the aluminum electrode in chloride solution. The electrode had an oxide of 80 nm

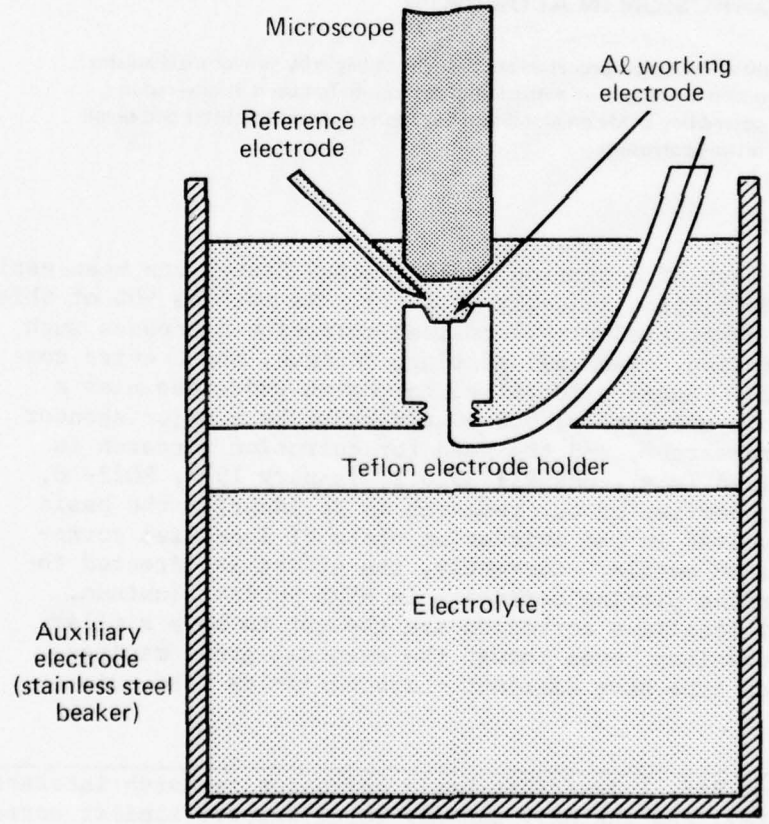


Fig. 1 Experimental Configuration for Corrosion Studies

grown on it. A potential pulse of about 1 μs duration was superimposed on this constant potential. Within a few seconds, blisters were observed growing in the oxide film on the aluminum. Eventually the blisters broke, at which time pitting corrosion began. Blisters also formed when the maintained potential was stepped from a value below the pitting potential to about 2 V higher. A typical unbroken blister is shown in Fig. 2. Blisters generally have a circular shape although their morphology can be influenced by grain boundaries and other topographical features. The light-colored ring around the blister periphery contains much larger amounts of chloride than is either inside the blister, where it is occasionally detectable, or outside the blister, where it is usually not detectable. A more detailed, though still preliminary, description has been published (Ref. 3).

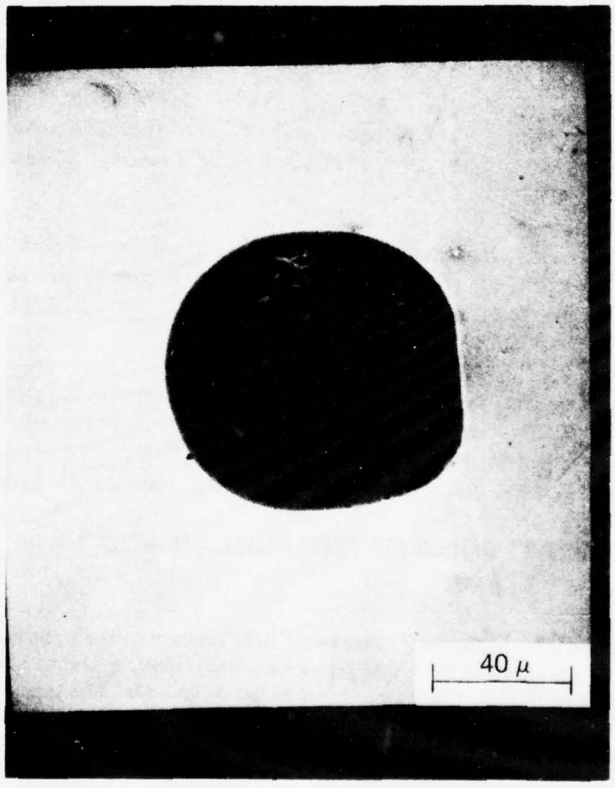


Fig. 2 Typical Unbroken Blister in the Aluminum Oxide Film

The significance of blister formation is that it is a demonstrable precursor of pitting corrosion under the described conditions. As such, it is a step in an initiation mechanism. Many relevant questions remain to be answ ed before the full significance of the blistering phenomenon can be appreciated. A demonstration of generality to other types of localized corrosion processes would be very important. Its discovery is significant because it provides a helpful insight into a complex problem.

Principal Investigators: Dr. C. B. Bargeron, senior physicist, and Mr. R. B. Givens, engineering assistant, of the Electronic Physics Group.

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VALENCE-BOND STUDIES OF MOLECULAR AND SOLID-STATE SYSTEMS

A semiempirical theory based on the valence-bond (VB) method of theoretical chemistry has been applied to the study of the noble gas monohalide molecules and to the elucidation of the structure of the H-center defect in alkali halide crystals. The theory has been found to successfully account for the electron nuclear hyperfine structure (hfs) interactions in these systems. Comparison of theoretical and experimental hfs constants yields estimates of the interatomic spacings and charge distributions.

A detailed understanding of the structure of solid-state and molecular systems on the atomic scale has led to important technological advancements in many areas, such as lasers, computers, and solid-state electronic devices. In particular, interest in the rare gas monohalide molecules has been high not only because these molecules violate the classical principle of the inertness of closed shell systems, but also because there exists the possibility of constructing powerful, partially tunable, ultraviolet (UV) lasers based on light emission from an excited state. The need for research to develop basic knowledge of electronic materials and phenomena in general and improved laser sources in particular is recognized, e.g., in Naval Research Requirements ONRINST 3910.2, R021-02, p. 10, and R011-07, p. 3. The study of defect centers in the alkali halides is important because there is a possibility that their anisotropic optical absorption properties can be exploited as memory devices in computer applications. The H-center is one of the many defects that are created by irradiation of ionic crystals at low temperatures by gamma or x rays.

Electron-Nuclear Hyperfine Structure

The noble gas monohalide work (Refs. 1 through 3) is a further refinement and extension of the preliminary study presented in the previous IR&D report (Ref. 4). Briefly a spin-correlated function (Ref. 5) is constructed of the form

$$\Psi = N(^2\Sigma^+)\left[\chi\alpha\Phi(N\ldots X) + \sqrt{1-\chi^2}\,\alpha\Phi(N^+\ldots X^-)\right] ,$$

where N and X denote the noble gas and halogen, respectively, and α is the antisymmetrization operator. The antisymmetrization and the effects of interatomic electron correlation on open shell states are the major contributors to the isotropic hfs. Interatomic correlation is treated by a perturbation theory calculation of the van der Waals polarization of X by N in the VB structure $\Phi(N\ldots X)$ and the coloumb polarization of N^+ by X^- in $\Phi(N^+\ldots X^-)$. It is also important to consider both valence and inner shell s electrons and to include intra-atomic correlation. The latter is treated by using neutral atom orbitals for N and X in $\Phi(N\ldots X)$ and cation and anion orbitals for N^+ and X^-, respectively, in $\Phi(N^+\ldots X^-)$. Relativistic corrections were incorporated into the computation for both the isotropic a and anisotropic $B_{||}$ hfs coupling constants for the heavier Xe and Kr nuclei.

The results for XeF, KrF, and XeCl are compared with the experimental results in Table 1. The experimental hfs coupling constants were corrected for orbital contributions resulting from spin-orbit mixing of ground and excited states. The internuclear distances and charge distribution parameters appearing in the table give the closest overall agreement between the experimental and theoretical hfs coupling constants, and their values are consistent with the relative sizes and electronegativities of the constituent atoms in these molecules.

Table 1

Comparison of Computed Hyperfine Constants of the Noble Gas with Experimental Values

Molecule	R a_0	χ	Nucleus	$a^{(Th)}$ (MHz)	$a^{(Exp)}$ (MHz)	$B_{\|\|}^{(Th)}$ (MHz)	$B_{\|\|}^{(Exp)}$ (MHz)
XeF	4.70	0.80	^{129}Xe	1340	1330	1227	1290
			F	509	523	2125	2126
KrF	4.00	0.98	F	552	549	2925	3093
XeCl	6.50	0.955	^{129}Xe	270	265	425	424
			^{35}Cl	37	37	260	305

H-Center Defect in Alkali Halide Crystals

The model for the intrinsic H-center in KCl and KBr (Fig. 1) is an interstitial halogen atom (A) that forms a molecular bond with a lattice halogen (B) so that the molecule (AB) has its axis in a <110> direction. As indicated by the electron spin resonance (ESR) data, there exists substantial molecular binding with the two adjacent ligand halogen ions (C,D) colinear with this molecular axis; that is, the unpaired electron or hole spends a small fraction of its time on the two ligand halogen ions. In LiF, this <110> oriented center is stabilized by a Na^+ impurity ion and is strictly speaking an extrinsic $H_A(Na^+)$ center.

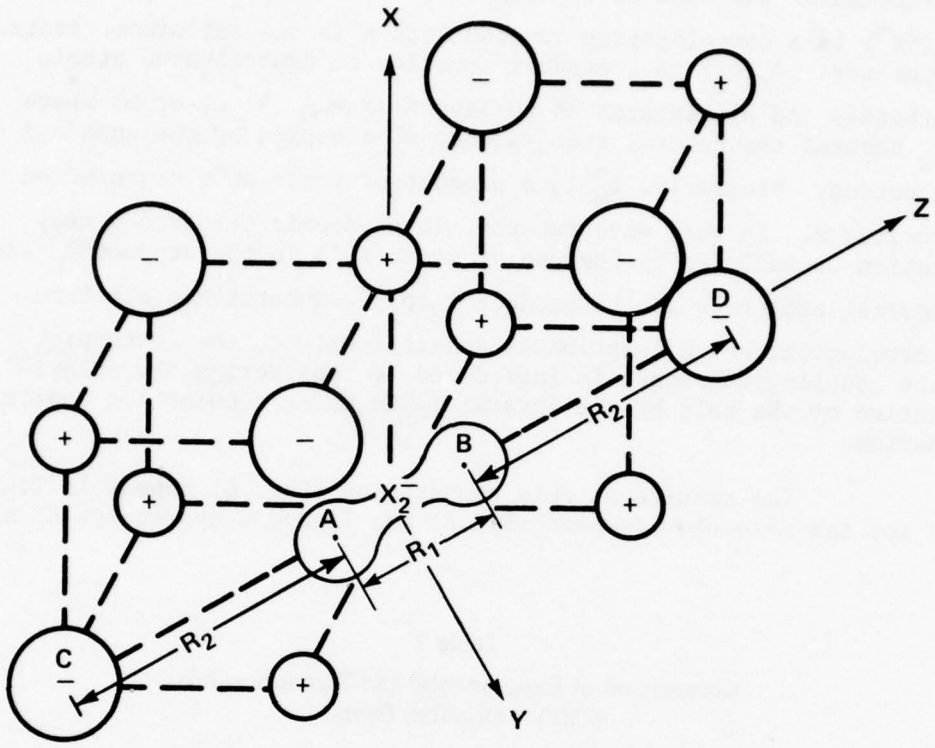


Fig. 1 The <100> Oriented H-Center

The VB wave function used to compute the hfs for the H-center is

$$\Psi = N(^2\Sigma^+)\left\{\varepsilon\left[\alpha\Phi_A(p_z)\Phi_B^-\Phi_C^-\Phi_D^- + \alpha\Phi_A^-\Phi_B(p_z)\Phi_C^-\Phi_D^-\right]\right.$$
$$\left. + \sqrt{1-\varepsilon^2}\left[\alpha\Phi_A^-\Phi_B^-\Phi_C(p_z)\Phi_D^- + \alpha\Phi_A^-\Phi_B^-\Phi_C^-\Phi_D(p_z)\right]\right\} .$$

An interstitial halogen atom A forms a X_2^- molecule ion with one of the halogen ions of the perfect crystal B with small covalent binding to the ligand ions C and D. The weight factor ε is of the order unity, so that the hole or unpaired electron is primarily localized on the halogen cores A and B but spends a small

fraction of the time on the ligand ions C and D. As before, $N(^2\Sigma^+)$ is a normalization constant and α is the antisymmetrization operator. $\Phi_N(p_z)$ is a product function of neutral-atom atomic orbitals (AO's) centered on nucleus N (N = A, B, C, or D) where p_z denotes the neutral atom valance AO occupied by the unpaired electron. Similarly, Φ_M^- is a product of ionic AO's centered on nucleus M. In this wave functon, intra-atomic electron correlation is included by the use of ionic AO's in the product Φ_M^- and neutral atom AO's in the product $\Phi_N(p_z)$. Interatomic electron correlation, which contributes significantly to the isotropic hfs coupling constant, is introduced by considering the polarization of the hole by the crystal field using a point ion approximation.

The results of this computation (Ref. 6) appear in Table 2 for the molecular (superscript A) and ligand (superscript C) hfs

Table 2

Comparison of Experimental and Theoretical hfc
<100> Oriented Center

	KCl ^{35}Cl		KBr ^{81}Br		LiF[H_A(Na+)] ^{19}F	
	Theory	Experiment	Theory	Experiment	Theory	Experiment
$a^{(A)}$	129	129	532	538	744	744
$a^{(C)}$	6	12	45	56	127	130
$B_{\|\|}^{(A)}$	171	177	830	894	1722	1959
$B_{\|\|}^{(C)}$	8.5	8.7	52	111	125	121
ε	0.990		0.985		0.985	
R_1 H	0.244		0.268		0.176	

Note: All hfc are in MHz and the internuclear distances R are in nm.

coupling constants. The internuclear distances and weight factors ε were chosen to best reproduce the experimental molecular coupling constants. The experimental isotropic ($a^{(A)}$) and anisotropic ($B_{||}^{(A)}$) coupling constants were corrected for the orbital contribution arising from the spin-orbit interaction. This was not done for the ligand coupling constants $a^{(C)}$ and $B_{||}^{(C)}$, since the correction is expected to be small for these nuclei. The agreement between theory and experiment is quite encouraging considering the approximate nature of the theory and the rather imprecise knowledge of the experimental ligand hfs coupling constants for KBr and LiF.

Principal Investigators: Dr. A. N. Jette, senior physicist in the Electronic Physics Group, and Dr. F. J. Adrian, Supervisor of the Microwave Physics Group.

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CHEMICAL PHYSICS

The Chemical Physics Group of the Research Center consists of six senior scientists whose objective is to carry out research in borderline areas between physics and chemistry appropriate to the Laboratory. Approximately 50% of the work of the group was funded by the Chemical Physics IR&D Program.

During the present reporting period, a total of 29 scientists, both APL personnel and others, participated directly in the group's IR&D program. Of the APL participants, six are currently in the Chemical Physics Group, two are retired, and seven are members of other Laboratory groups. Nineteen scientific papers were published, and six were accepted for publication. In addition to the APL personnel, authors include 14 investigators from nine other institutions in this country, England, and West Germany. (Non-APL participants were not funded by the IR&D Program.)

The past year was marked by the retirement of Dr. A. A. Westenberg after a distinguished 25-year career at the Applied Physics Laboratory, including 15 years as the supervisor of the Chemical Physics Group. He was a specialist in the high-temperature physical chemistry of gases, reaction kinetics, transport properties, combustion, flames, and air pollution chemistry. He had been awarded the Professional Achievement Award of the D. C. Engineering Council in 1964, the Combustion Institute Silver Medal in 1966, and the Hillebrand Prize of the Chemical Society of Washington in 1967. During his tenure at the Laboratory, Dr. Westenberg laid a solid foundation in the many areas of his research endeavors.

The new supervisor of the Chemical Physics Group is Dr. D. M. Silver, who is a specialist in theoretical chemistry, molecular physics, chemical reaction phenomena, mathematical analysis, and computer applications. Near the end of the year, Dr. R. M. Fristrom, who is Chief Scientist of the Laboratory's Fire Research Program, returned to the Research Center part-time to conduct basic research on combustion and flames. Dr. L. Monchick spent a month at the Max-Planck Institut in Munich where he was invited to work on interstellar gas-phase kinetic problems.

MOLECULAR STRUCTURE AND CHEMICAL REACTIVITY

The electronic structure of atoms and molecules plays a dominant role in chemical reactivities. Since chemical reactions pervade the fields of combustion, propulsion, air pollution, chemical synthesis, fuel production, and other energy-related phenomena, a detailed understanding of these processes is important for future DoD and civilian applications. Current results include the development of perturbative methods for the calculation of molecular energies, the measurement of rate constants for several atom-molecule reactions, and the design and construction of an apparatus for studying flame reactions as high throughput chemical reactors.

Problem

Chemical combustion is the main source of propulsion energy for the Navy's ships, aircraft, and weapons. Research is necessary to identify and assess the physical and chemical aspects of storage, release, and use of the energy of fuels, explosives, and propellants (Naval Research Requirements ONRINST 3910.2, January 1977, RO24-02, p. 16). In addition, an important possibility is the production and use of fuels that might be of interest for shipboard production for special purposes. The quantitative characterization of flames is of particular concern. Combustion and flame research is also relevant to fires and the prevention of fires in ships and aircraft.

Flames are an area of gas-phase chemistry that offers a unique reaction medium combining high temperature and high radical concentrations. This is especially true in the primary reaction zone where radical concentration may exceed equilibrium values by as much as a thousandfold. Reaction rates are rapid under flame conditions so that very high throughputs are possible with small reactors (as an example, a burner 1 m^2 has a possible throughput of the order of 100 tons per 8-hour day). These desirable properties have been utilized in a few industrial processes; two instances are the production of lampblack from methane and the production of rutile (TiO_2) by burning $TiCl_4$ in O_2. One flame system offering attractive possibilities that could be exploited in the production of chemicals and fuels is the hydrogen-rich hydrogen/oxygen flame. Since such flames are well understood and characterized, we plan to use them as high concentration free-radical baths to examine reactions at high temperatures. At low pressures, these flames produce as much as

20% free H atoms at 1000 K; therefore they should be useful for rapid organic reductions and hydride production and may provide a useful medium for the hydrogenation of coal and the cracking of crude oil without catalysts.

The direct study of atom and radical reactions in simple well-known flame environments allows the derivation of chemical kinetic information under thermal conditions that are difficult to obtain by other techniques, and also allows the deduction of mechanisms of combustion in more complex systems. Thus this research is concerned with the in situ study of the kinetics of elementary atom molecule reactions, flame reactions, and the chemistry of flame interactions with particles and other injected materials.

The molecular mechanisms responsible for observed reaction rates and properties are dependent on the electronic structures of the reactant, the intermediate, and the product chemical species. Thus, to complement the experimental chemical kinetics measurements on elementary reactions and flames, theoretical studies are directed toward the elucidation of the structures and reactivities of atoms, molecules, and free radicals. Eventually, the synthesis of experiment and theory is expected to lead to a broad understanding of the relationship between molecular structures and chemical reactivities.

Objective

The goal of the program is to understand chemical reactivities on the basis of their underlying molecular structures and mechanisms. In particular, these insights are to be exploited in the design and operation of flame reactions. A further objective is to measure the rates of various elementary chemical reactions that are relevant to combustion and atmospheric chemistry.

Approach

A quantitative description of the electronic structure of atomic and molecular species is obtained through quantum mechanical calculations using the techniques of many-body perturbation theory. Application of these methods to chemical reactions entails the calculation of the interspecies interaction potential from which information regarding the reaction mechanism can be extracted. The measurement of elementary gas-phase atom-molecule reactions is accomplished using a flash-photolysis resonance-fluorescence apparatus. The interactions of low-pressure hydrogen-rich flames with gases, droplets, and particles are examined by sampling the flame gases and particulates by

mass spectrometry, resonance-fluorescence spectrometry, scanning electron microscopy, and elemental analysis.

Progress

The application of many-body perturbation theory to the electronic structure of molecules (Ref. 1) has proceeded in stages through the development of numerical recursive procedures (Ref. 2), algebraic approximations (Ref. 3), and invariant Padé approximants (Ref. 4). Subsequently, the feasibility of the perturbative approach has been assessed through very accurate calculation of the ground-state energy of a series of diatomic fluorides (Ref. 5) and of closed-shell first- and second-row diatomic hydrides (Ref. 6). The importance of taking full account of three- and four-body interactions between electrons is demonstrated in a study of the nitrogen molecule (Ref. 7). A comparison of the perturbative method with the variational method of configuration interaction for the carbon monoxide molecule (Ref. 8) shows that the convergence of the perturbative series through third order is satisfactory. The influence of many-body effects on modified potentials is illustrated using hydrogen fluoride (Ref. 9). Calculations on water (Ref. 10) indicate that the analytical representation of the perturbative wave function strongly influences properties such as energy, bond distance, bond angle, and bending force constant. The use of polynomial basis functions has led to a new radial limit for the helium atom energy (Ref. 11).

Computer algorithms have been designed and implemented for general application of the perturbative method to the electronic structure of atoms and molecules (Refs. 12 and 13). Extension of the perturbative approach to chemical reactions has begun by examining the interaction potentials between closed shell atoms and molecules (Ref. 14). In related theoretical studies, reactions between hydrogen molecules have been examined using quasi-classical dynamical scattering techniques (Ref. 15).

Rate constants were determined at room temperature for the reactions of oxygen atoms with vinyl chloride and for the chemiluminescent reaction of oxygen atoms with ethylene (Ref. 16) using the flash-photolysis resonance-fluorescence technique. Further, room temperature rate constants were measured for the reaction of chlorine atoms with ammonia and for the reaction of hydrogen atoms with CF_3Br (Ref. 17). Modification of the apparatus to heat and cool the reactor has permitted the extension of these measurements over a temperature range of 200 to 500 K. With this expanded range, the apparatus has now been used to measure the previously unknown temperature dependence of the rate constant for the reaction H + CF_3Br, which is of interest in flame inhibition.

An apparatus has been designed and is currently being assembled for the study of hydrogen/oxygen flames (Ref. 18). At the present time, a low pressure burner has been assembled for test, and a particle injection system has been devised to allow periodic introduction of particles along the flame axis. Analysis will be by mass spectrometry and a C-H-X combustion train. An approximate analysis system has been devised that will allow characterization of the gas samples without requiring complete identification of the complex products.

Principal Investigators: D. M. Silver, A. A. Westenberg, R. M. Fristrom, C. Grunfelder, N. DeHaas, S. Favin, R. A. Farrell, C. H. Hoshall, H. J. Silverstone, D. P. Carroll, R. J. Bartlett, N. J. Brown, S. Wilson, K. H. Eberius, K. H. Hoyermann, and R. H. Gg. Wagner. Dr. Silver is currently Supervisor of the Chemical Physics Group. Dr. Westenberg was Supervisor of the Chemical Physics Group until his retirement in June 1977. Dr. Fristrom is a senior chemist, Mr. Grunfelder was an associate engineer until his retirement, Mr. deHaas is a senior physicist, and Mr. Favin is a senior programmer in the Chemical Physics Group. Dr. Farrell is Supervisor of the Theoretical Problems Group, and Mr. Hoshall is a senior engineer in a non-Research Center group of the Laboratory. Dr. Silverstone is professor of chemistry and Mr.Carroll is a graduate student at The Johns Hopkins University; Dr. Bartlett is at Battelle Memorial Institute, Columbus; Dr. Brown is at the University of California, Berkeley; Dr. Wilson is at the Science Research Council, Daresbury Laboratory, England; Dr. Eberius is at DFVLR, Institut für Reaktionskinetik, Stuttgart, West Germany; and Dr. Hoyermann and Prof. Dr. Wagner are at the Institut für Physikalische Chemie der Universität Göttingen, West Germany. None of the non-APL colleagues were funded by the IR&D Program.

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MOLECULAR ENERGY TRANSFER

Research in molecular energy transfer is directed toward an understanding of the mechanisms of energy transfer taking place during molecular collisions. In particular, the deactivation of molecular oxygen from its singlet excited state is investigated in various gases and liquid solvents. The research has a bearing on many important problem areas because of the pervasiveness of singlet excited oxygen in chemical processes in the earth's atmosphere. Current work involved measuring the effect of ozone in deactivating laser-excited oxygen.

Problem

The Navy's future capabilities in communications, ranging, missile guidance, surveillance, navigation, and weaponry require a diverse program for the development of advanced applications in radiation, optics, and lasers, including the interaction of a radiation field with the material environment (Naval Research Requirements ONRINST 3910.2, January 1977, RO11-07, p. 3). Thus, it is important to examine the energy transfer and relaxation processes that occur in laser-excited molecular species such as oxygen.

The existence of a long-lived metastable singlet excited-state oxygen molecule was confirmed by measurements of atmospheric absorption and emission in the 1930's. Its importance in biochemical processes was also discovered during that period. During the past ten years, particularly the past five, a substantial literature has developed calling attention to the importance of this molecule in such widely ranging areas as atmospheric chemistry (ozone), high-altitude spectroscopy (night glow and, more recently, auroral occurrences), biochemistry (oxidation of amino acids and proteins), physical chemistry (various oxidation processes and also physical quenching), biological research (damage to microorganisms), and a number of others. However, relatively little work has been undertaken in the area of physics or chemical physics directed toward the elucidation of the fundamental deactivation mechanisms.

Optical radiation of oxygen at 1.064μ generated by a Nd:YAG laser produces direct excitation to the singlet excited state. Since such radiation corresponds almost exactly to one of the absorption wavelengths of atmospheric oxygen, the properties of singlet excited oxygen become important for understanding the factors limiting atmospheric laser transmission. The Nd:YAG laser is currently used by the military for optical tracking, ranging, and communication through the atmosphere. Since earth-satellite laser communication involves transmission through the ozone layer as well as the ultraviolet (UV) irradiated region directly above, where relatively large amounts of photoexcited singlet oxygen are known to exist, determination of its interaction with ozone is of concern. Laboratory measurements using singlet oxygen generated by microwave discharge have shown ozone to be an anomalously efficient quencher. Since the excitation energy of the singlet oxygen is close to the energy required to dissociate O from O_2, it is thought that such reaction might possibly lead to O generation, an event of obvious importance in atmospheric chemical processes. Also important are phenomena associated with deactivation of singlet oxygen in an aqueous environment.

Objective

The long-range goal of this program is to elucidate the mechanism of interaction of laser-excited singlet molecular oxygen with differing environments, particularly those likely to be involved in military laser systems. Both the gas and liquid phases must be considered; the short-range goal is to determine the quenching rate of laser-excited oxygen in various solvents, particularly water and heavy water. A further objective is to investigate the effect on quenching rates of adding to the solvent such impurities as mineral salts, various compounds known to quench either physically or chemically, and substances of biological interest.

Approach

The system for experimental measurement of deactivation times involves as the main component a commercially available Korad Q-switched Nd:YAG laser that typically radiates a pulse of 20 ns duration with a total pulse energy of 0.025 J. The laser pulse excites dissolved oxygen in approximately one-hundredth the time for collisional deactivation in distilled water. The laser irradiation wavelength is 1.064μ, exciting the oxygen to the first vibrational level of the $^1\Delta_g$ state. After the rapid deactivation of this vibrational energy, the most probable following transition is a collisional deactivation to the ground electronic state. In addition, a weak radiative deactivation occurs at a wavelength of 1.27μ. This fluorescence is spectrally separated from the exciting wavelength, permitting isolation by means of appropriate optical filtering. This fluorescence signal is enhanced against detector and electronic noise by signal averaging. Since the radiative transitions are weak, the controlling deactivation process is collisional, and thus the magnitude of the fluorescence signal at any time subsequent to the pulsed laser excitation may be used to monitor the instantaneous density of excited oxygen molecules. Determining the decay constants for the deactivation process from the rate of fluorescence decay may be accomplished automatically, using available electronic instrumentation. A Biomation 8100 transient recorder coupled into a Nicolet 1070 averager is used to process the output of a germanium photodiode optical detector, with the output of the 1070 interfaced to the central computer. A Quanta-Ray DCR 100 Q-switched Nd:YAG laser has been acquired recently for future experiments. The laser provides pulse energies ten times larger than that of the Korad unit, as well as permitting operation at higher pulse repetition rates. Calculations based on data obtained to date indicate that, with this increase in average input power, it should be possible to detect fluorescence in a fully oxygenated distilled water sample.

Progress

Because of its importance for understanding atmospheric chemical processes, a series of experiments was directed toward a measurement of the effect of O_3 in deactivating laser-excited O_2. In these experiments, a chopped CW laser beam was used as the exciting source. Of particular importance was the variation of quenching rate with increasing O_3 (Ref. 1).

Collisional deactivation times of laser-excited $O_2(^1\Delta_g)$ oxygen were determined in the gas phase (typical pressures being on the order of 70 atm) and also for oxygen dissolved in a Freon 113 solvent. However, attempts to detect $O_2(^1\Delta_g)$ fluorescence generated by laser irradiation of oxygen dissolved in distilled water proved fruitless. This result was not entirely unexpected since the pulse energy output of the "vintage" Korad laser system being used was relatively low. Another problem was that of achieving saturation of the level of dissolved oxygen. This is because oxygen is not readily soluble in water and diffusion times are quite long.

A series of experiments was devoted to a determination of the time required to reach saturation, utilizing the fact that the UV absorption (220 to 230 nm) of distilled water is greatly increased by the presence of a small amount of dissolved oxygen. In these experiments, a single oxygenation chamber was used. The chamber was of the same design as one used earlier in water sterilization investigations, but modified to accommodate a Teflon-coated magnetic stirring bar that was externally activated by a magnetic driver. Results of the subsequent UV absorption measurements indicate that approximately 30 min was required to reach 100% of saturation. This shows clearly the inadequacies of the method used earlier in coliform inactivation research, which simply amounted to shaking the sample vigorously by hand for a minute or so. Quantitative comparison of the two methods showed that the manual method produced a dissolved oxygen level of only 30% of saturation. This discovery makes it clear that to insure maximum levels of dissolved O_2, magnetic stirring (or an equally effective means) must be used. A difficulty immediately presented itself in the form of insufficient space for the fluorescence cell. The problem was solved by developing a water oxygenation transfer system in which an external cell containing a magnetic stirrer is used as an oxygenation chamber. The hydraulic head existing in the vortex generated by the rapidly rotating stirring bar is then used to circulate the oxygenated water sample through the fluorescence cell. Measurements using a system of this type showed the equilibrium-dissolved oxygen levels in the two cells to be the same.

In related work, the consideration of energy transfer between optically excited surface layers and the adjacent gas phase was used to determine optimal design parameters for a photoacoustic spectroscopy cell (Ref. 2). One of the direct applications of such a cell is in the study of semiconductor materials useful in photoelectrolysis.

Principal Investigators: J. G. Parker, R. Von Briesen, L. C. Aamodt, and J. C. Murphy. Dr. Parker is a senior physicist and Mr. Von Briesen was an associate engineer in the Chemical Physics Group. Dr. Aamodt and Dr. Murphy are senior physicists in the Microwave Physics Group.

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KINETIC AND COLLISION THEORY

Work in kinetic and collision theory examines effects of internal structure on collision-related phenomena in fluids. These theoretical studies build the foundation for improved lasers, new exploitations of chemical reaction dynamics, and more realistic descriptions of fluid flow. Current results include analyses of pressure broadening and gas kinetic cross sections, development of a kinetic theory of quantum state diffusion, and a solution to the problem of chemically induced, dynamic electron polarization.

Problem

Research in scattering, cross sections, and statistical mechanics for atoms and molecules provides information needed for the design and evaluation of the effectiveness of naval systems that depend on fluid flows, plasma, and laser phenomena (Naval Research Requirements ONRINST 3910.2, January 1977, RO11-09, p. 4). Collision cross sections pervade the physics of fluids and radiation transfer. For instance, the equations of fluid flow require transport cross sections as basic inputs. Similarly,

theories of laser operation require line-broadening cross sections. To advance these applications, it is necessary to develop a means of estimating the required cross sections corresponding to various physical situations. Although this can be done fairly accurately for gases composed of noble gas atoms, the situation is much less satisfactory in the case of polyatomic gases. Collisions of polyatomic molecules are several orders of magnitude more difficult to calculate and describe than collisions of systems with no internal degrees of freedom. The main difficulties encountered with polyatomic systems are their rotational motion and intermolecular forces, which generally depend on the relative orientations of the molecules. As a result, the motion must be followed in four or five dimensions rather than the one-dimensional motion describing collisions in noble gases. Hence, this research is aimed at developing the theoretical expertise for handling complicated molecular collision problems.

Objective

The goal of the program is to assess the predictive ability and practicability of various methods for calculating molecular collision cross sections and to generalize and solve key problems in gas transport theory.

Approach

The strategy adopted is to perform highly accurate quantum mechanical calculations on several simple systems in order to (a) correlate the final cross sections with molecular forces and properties, thus assessing predictive ability, and (b) compare the results with more approximate calculation methods and theories, thus assessing the practicability of the approximations.

Progress

During the present period, quantum mechanical calculations have been performed on the dynamics and corresponding cross sections of several atom-diatom (He-HCl and He-CO) collisions as described in Refs. 1 through 5. Integral and differential scattering cross sections of molecules in a given rotational state of principal quantum number j but with random orientation are commonly used in molecular beam experiments to investigate molecular forces. In these studies (Ref. 3), it has been found that an orientation-averaged potential is insufficient to approximate the experimental results but that an approximation, called the coupled states (CS) method, is satisfactory. The CS method assumes that the component of rotational angular momentum about the axis connecting the two centers of mass stays fixed during the collision. The equivalent approximation in celestial mechanics

is the neglect of the Coriolis forces. The CS method is likewise highly successful (Refs. 2 and 3) for other properties, such as transport properties and line broadening, that also do not depend on initial and final orientation.

Start-selected cross sections having a dependence on the relative orientation of colliding species are now being measured. An initial study (Ref. 4) found that the CS method was somewhat unsatisfactory for these collisions; further studies have been initiated to assess other approximations. Along these lines, a calculation of the low temperature transport properties of H_2 has been initiated with an ab initio potential energy surface (Ref. 6).

A generalized kinetic theory (Refs. 7 and 8) has been developed for the diffusion of individual excited states of molecules in gases not too rarefied. Although this has some importance for the transport of energy in a gas at high temperatures, it would be most relevant to gases inhomogeneously excited by other means as, for instance, by a high-power laser. In a parallel development (Ref. 9), sound dispersion at low frequency has been calculated for a quasi-Lorentz gas (also known as a Rayleigh gas), which is most appropriate for the description of a dusty gas where the dust particles are much smaller than the mean free path. It is shown that slight modifications of well-known extrapolation formulae would reproduce the sound dispersion of dusty gases where the particles were much larger in size. In related work, a vector model and an asymptotic solution have been proposed for the problem of chemically induced dynamic electron polarization (Refs. 10 and 11).

Principal Investigators: L. Monchick, F. J. Adrian, L. W. Hunter, L. A. Viehland, E. A. Mason, T. H. Stevens, S. Green, R. Goldflam, and D. J. Kouri. Dr. Monchick is a senior chemist in the Chemical Physics Group. Dr. Adrian is Supervisor of the Microwave Physics Group. Dr. Hunter is a senior chemist in a Laboratory group outside the Research Center and is not funded by the IR&D Program. Prof. Viehland, Prof. Mason, and Mr. Stevens are at Brown University, Providence, RI,; Dr. Green is at Columbia University and NASA Institute for Space Studies, New York; and Dr. Goldflam and Prof. Kouri are at the University of Houston. The non-APL colleagues were not funded by the IR&D Program.

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EXCITATION MECHANISMS

The Excitation Mechanisms Group (REM) was founded shortly after the discovery of the laser and retains as a general charter the study of the dynamics of excited atoms and molecules. The group consists of four senior and two associate scientists and one technician. During 1977, only a fraction of one senior scientist was supported by IR&D funds; the remainder were supported directly by task assignments. Dr. R. E. Walker, the Group Supervisor, was assigned to the SSBN Security Program, with Mr. B. F. Hochheimer acting as supervisor in his absence. A total of nine research papers in organic dye fluorescence, retinal physiology, holography, and chemical kinetics were published during this period.

CHEMICAL LASER STUDIES

A novel APL/JHU concept for a high-pressure chemical laser is to provide volumetric ignition by radiant heating of a thermally decomposable powdered catalyst in a premixed fuel-oxidizer mixture. Appropriate catalysts might be NaN_3 or AgF_2 which could yield Na or F atoms as free radical chain carriers. The behavior of these specific materials when exposed to intense CO_2 laser irradiation has been examined. Radiative decomposition of AgF_2 has been shown to initiate combustion in premixed NF_3-H_2 mixtures. The NF_3-H_2 reaction produced spontaneous emission from vibrationally excited HF product molecules, and, although lasing has not been attempted, the fundamental concept of radiative ignition was demonstrated. Experiments with NaN_3 were not successful because this material proved to be essentially transparent to CO_2 laser radiation. A paper for publication on these research results is now in progress.

Problem

Although laser technology has matured immensely since the first laser demonstration, there is a continuing DoD interest in laser-related physics (see Naval Research Requirements RO11-03 and RO11-07, ONRINST 3910.2).

High-power lasers have been considered for a variety of DoD applications; and these interests have fostered remarkable developments in gas-dynamic, electric-discharge, and chemical lasers in recent years. Chemical lasers have several unique features that make them attractive candidates for high-power applications, but practical difficulties encountered in current technology trends do not allow their potential to be fully exploited. However, there is an attractive alternate approach.

Conventional combustion-driven, continuous-wave (CW) chemical lasers, such as HF/DF devices, operate at a rather low cavity pressure (typically 10 Torr). The low-pressure operation is a result of a compromise between the time required for the gaseous reactants to mix and chemical kinetics. Extensive work on the design of supersonic nozzles has been conducted in order to improve the mixing and elevate the operating pressure, but with only moderate success. In low cavity-pressure devices that are operated at altitudes below approximately 10 km, supersonic diffusers are unable to achieve full atmospheric pressure recovery. Additional pumping is therefore required that decreases the overall efficiency and increases the size and weight of the system. If operation at a higher cavity pressure could be achieved simply, these aerothermodynamic problems could be reduced.

A possible method to achieve high-pressure operation is to disperse a thermally decomposable powdered catalyst in a premixed fuel-oxidizer mixture. This gas-particulate mixture must remain stable until the catalyst particles are decomposed by radiant heating to yield the necessary free-radical chain carriers. After the reaction is externally initiated, some of the laser output might be apportioned to provide the continuing radiant heating. Essentially volumetric decomposition could be achieved, thereby eliminating the usual mixing problems, and high-pressure operation with atmospheric pressure recovery should then be possible. The system could operate at near room temperature with a simple nozzle and diffuser.

Although simplified calculations indicate that this chemical laser concept may offer exceptional potential, there are many areas of uncertainty. Most center around the practical problems of selecting the appropriate catalyst (i.e., the physics of the decomposition process) and the stability of the fuel-oxidizer catalyst mixture. The present study has addressed some of these important issues.

Objective

The objective of this study was limited to demonstrating that selected solid catalysts could be radiatively decomposed and initiate chain reactions in selected chemical lasing mixtures.

Approach

Although simple analytical modeling reveals the importance of the catalyst particle size and optical and thermal properties on system performance, the uncertainty of the decomposition process dictates that the first efforts should center around simple demonstration experiments involving radiative decomposition and combustion initiation. The adopted technique

used either a CW or pulsed CO_2 laser as a radiant energy source to illuminate granular or pressed catalyst samples contained in a controlled atmosphere. The decomposition process was monitored with a sensitive manometer and a mass spectrometer. When necessary, infrared absorption (or reflectance) measurements of selected catalyst samples were obtained.

Progress

The first material chosen for study was sodium azide, NaN_3, which decomposes to Na and N_2. The Na atoms then react with F_2 to form the F atoms that are required in the usual HF or DF chemical lasers. Since high-power CO_2 lasers are readily available, it was intended to decompose the NaN_3 using 10.6 μm radiation from a low-peak-power shuttered CW CO_2 laser or a high-peak-power pulsed CO_2 laser. However, because of the rather low absorption coefficient of NaN_3 at 10.6 μm and the unfavorable enthalpy of the overall decomposition, the decomposition achieved was not sufficient to warrant further investigation of chemical reaction initiation.

Alternative materials were then examined for favorable optical properties and decomposition products. Selected examples appear in Table 1. AgF_2 was chosen for additional work on the basis of a large absorption coefficient and the possibility of producing F atoms directly from the decomposition. Experiments showed that, at room temperature, mixtures of AgF_2 in F_2-H_2-O_2 and NF_3-H_2 were sufficiently stable for use in the high-pressure laser.

Table 1

Substances with Absorption Bands Overlapping the Output of the Major Chemical Lasers

HF (2.8-3.2 μm)	DF (3.8-4.1 μm)	CO (5-5.7 μm)	CO_2 (10.6 μm)
AgF_2	HCOONa	NaN_3	Na_2SO_3
Na_2O		$(COONa)_2$	$KMnO_4$
Na_2O_2		HCOONa	Na_2O_2
NH_4BF_4			NH_4BF_4

Irradiation experiments of stationary samples of AgF_2 pellets (powder that was pressed at 75 tons) and loose AgF_2 powder in vacuum using the shuttered CW CO_2 laser have shown the decomposition threshold to be ≤ 40 J/cm^2. (Decomposition was correlated with the pressure rise that occurred during the irradiation.) The temporal profile of the pressure was a very rapid increase followed by a slower decrease to an equilibrium pressure. If the AgF_2 decomposes according to the following reaction,

$$AgF_2(c) \xrightarrow{h\nu} AgF(c) + F(g),$$

then the pressure rise is due to F atom production, and the pressure decrease is presumably due to the rapid recombination or reaction of F atoms on the wall. Although the time constant (0.5 s) of the pressure gauge was too slow to measure the pressure maximum accurately, a lower limit of 0.3 Torr/J (3×10^{-7} mole/J) was determined for the decomposition efficiency.

Because of the high reactivity of F atoms, no direct methods of measuring the F atom concentration were feasible in the present apparatus. However, indirect methods, based on the amount of H_2 that reacted during irradiation and the mass loss due to decomposition, indicated that F atoms were produced in reasonable concentrations. Experiments were then conducted to initiate chain reactions involving H_2-F_2 and H_2-NF_3 by irradiating AgF_2 with a CO_2 laser. Although the H_2-F_2 system is not stable by itself (O_2 must be added), the results using AgF_2 initiation could be easily compared to the results from flashlamp initiation, which has been extensively studied. The AgF_2 initiation was found to be comparable to the flashlamp initiation. The NF_3-H_2 system is very attractive since the gases are easily handled and the mixture is quite stable. Reactions have been successfully initiated for a variety of conditions and, more importantly, spontaneous emission from vibrationally excited HF molecules has been observed. Thus, experiments on AgF_2 radiative decomposition, mixture stability, reaction initiation, and HF spontaneous emission have demonstrated some of the necessary conditions for the feasibility of this high-pressure laser concept.

Principal Investigators: R. C. Benson and R. Somers. Dr. Benson is a chemist in the Excitation Mechanism Group.

MICROWAVE PHYSICS

The Microwave Physics Group of the Research Center consists of five senior scientists and one associate engineer; about 60% of its support came from the IR&D Program during the present reporting period. The group carries on a continuing program to develop basic understanding of fundamental relationships between the structure of matter and its interaction with electromagnetic radiation to support future innovation. Such knowledge is important in many areas, including lasers, electromagnetic detectors, information processing systems, and energy conversion.

Research continues to be focused on three areas:

1. Photoacoustic spectroscopy and radiometry,
2. Molecular structure and photochemistry of free radicals, and
3. Spectroscopy of porphyrin electron-donor-acceptor molecules.

Progress in these areas is outlined below and described in more detail in eight publications and in four manuscripts that were accepted for publication during the present period. An overview of recent porphyrin spectroscopy work was published in the APL Technical Digest. Results were also described in presentations to several meetings of professional societies, including a series of four invited lectures on chemically induced magnetic polarization by Dr. F. J. Adrian (Supervisor of the Microwave Physics Group) at the NATO Advanced Study Institute (Sogesto, Urbino, Italy, April 1977). Dr. Adrian continues to serve as an associate editor of The Journal of Chemical Physics.

MOLECULAR PHOTOPHYSICS

Current work is principally concerned with two topics, photoacoustic spectroscopy and molecular structure and photochemistry of free radicals. The goal is to advance the state of knowledge of chemical and physical systems that have promise either as new radiation sources or as radiation detectors and processors. A corollary objective is the achievement of expertise in various spectroscopic techniques and the related molecular structure theory required to interpret the resulting spectra, and the utilization of this knowledge in support of other activities.

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PHOTOACOUSTIC SPECTROSCOPY

Photoacoustic spectroscopy (PAS) has recently emerged as a new form of absorption spectroscopy that offers unique advantages, particularly with respect to opaque materials. Experimental and theoretical results have been obtained and published for nonradiative transitions in a luminescent system (ruby), an investigation involving the first successful use of PAS at low temperatures. A new instrument (the photothermophone) that provides quantitative determination of the radiant energy being absorbed was also developed and patented.

Problem

Applications of electromagnetic radiation and lasers require research on the production, transmission, and detection of electromagnetic radiation at wavelengths ranging from the microwave to the ultraviolet regions (see, for example, Naval Research Requirements ONRINST 3910.2, January 1977, RO11-07, p. 3). Also, there is a strong need for research into the relations between molecular structure and electromagnetic properties (RO21-02, p. 10). Most previous advances in the generation, detection, and utilization of electromagnetic radiation, such as microwave sources, masers and lasers, and semiconducting detectors, have resulted from the skillful utilization of unique electromagnetic properties of certain material systems. Further, highly important benefits of this research are the development both of new spectroscopic techniques for studying molecular structure and of theoretical principles for interpreting spectroscopic data. These methods are valuable for investigating various materials (semiconductors, polymers, etc.) and chemical processes (combustion, corrosion, novel reactions leading to synthesis of unique materials, etc.) of importance in Naval technology (RO22-08, p. 13).

Objective

The principal objectives of this work are

1. Specific demonstration that PAS methods can be used to determine the energies and transition rates for photochemical processes;

2. Extension of PAS methods to low-temperature operation, including the liquid helium range;

3. Extension of PAS methods to very short, high-intensity pulsed-laser applications in which characteristic rates associated with faster relaxation processes can be studied; and

4. Continuation of current efforts to increase the sensitivity of the existing PAS spectrometer and to develop analytical formulations of the time-dependent PAS signals in terms of basic transition rates characteristic of the systems under investigation.

A longer term objective, which depends to some extent on the short-term goal, is the application of PAS methods to investigate photocatalytic reactions on transition metal oxides and certain metallorganics. This effort will include both gas-phase and liquid-phase reactions.

Approach

PAS is a new and rapidly developing field of research in which electromagnetic radiation is detected when the sample heats, with a consequent increased pressure in a gas in thermal contact with the sample. As typically used, the radiation source is modulated, producing a fluctuating pressure (i.e., acoustic) wave in the gas. It is believed that the method will be very useful in the investigation of a variety of important problems in defense technology, including semiconductors and especially thin films, amorphous materials, catalysts, and surface corrosion, particularly in strongly absorbing or strongly scattering samples for which conventional absorption or reflection spectroscopy is difficult. A particularly useful aspect of PAS is that, because its signal depends on the fraction of absorbed light converted to heat by nonradiative processes, these nonradiative processes can be studied directly. Also, we can study metastable states and photo-induced chemical reaction processes that temporarily store part of the absorbed energy before converting it to heat, by observing the PAS signal as a function of the frequency at which the optical source is modulated.

For investigation of photochemical transitions in competition with thermalization, the general procedure now under development makes use of the fact that the time-dependent response of a system with multiple transition rates generates phase shifts in the frequency domain when continuous-wave (CW) modulation is used and delays in the time domain when pulse modulation is used. In both cases, the amplitude of the component associated with a particular phase or time shift is related to the energy lost from the thermalization path by the presence of the secondary reaction path. Hence measurement of these parameters on the metal oxide and organic systems under study will be the primary method of investigation. Such a procedure will include a significant materials preparation component, using thin-film reactive

sputtering, pyrolytic decomposition, vapor transport, and other methods to prepare appropriate samples.

Progress

During the past year, we have made a substantial effort to construct a comprehensive analysis of the PAS signal generation process and to validate this analysis experimentally. This procedure was carried out both for CW excitation and short-time excitation. The results obtained in this analysis appear in Refs. 1 and 2. Since the PAS process is complicated, depending upon (a) the photoprocesses in the sample, (b) thermal energy transfer within the sample, (c) energy transfer to the cell gas, and (d) the thermal and acoustical properties of the gas, much of the earlier work relied on an intuitive interpretation of the PAS process. The development described in Ref. 1 was an effort to make PAS more quantitative by relating the PAS signal response to the thermal and acoustic properties of cell constituents including the transfer gas, the sample holder (substrate), and cell materials. The results obtained provided the desired quantitative expression for the PAS signal intensity as a function of cell parameters. The expression was confirmed experimentally. The results also indicated the range of cell parameters over which the assumption that the signal is proportional to the optical absorption coefficient is valid. They quantified the phenomenon of PAS saturation, indicating that this phenomenon occurs when the thermal diffusion length is less than the optical absorption length. This development also indicated that, in PAS cells longer than the thermal diffusion length of the cell gas, the PAS signal was inversely proportional to modulation frequency, and that the frequency dependence had both a cell and a sample contribution.

In Ref. 2, a similar development was made for PAS in the time regime. The expermental results obtained in this study used a photothermophone (discussed below) to simulate electrically an optically produced signal. This allowed the PAS cell response to these pulses. The development provided a basis for the use of pulsed PAS which appeared to have application in studying the lifetime of metastable states and contributed to the practical application of PAS by deriving a series of Laplace response functions that could be used to determine the effect of various contributors (such as sample thermal properties and gas properties) to the PAS signal. These experimental results indicated the desirability of replacing the microphone, which has been the acoustic detector commonly used in PAS cells, with a detector that does not require a low-frequency air leak. Work was begun to find such a replacement by using optical interferometer techniques.

The photothermophone mentioned above was developed, experimentally tested, and patented. Use of this device, which is described in Ref. 3, allows a quantified determination of the optical energy being absorbed from the PAS light source. It may be used as a photoacoustic radiometer and as a calibrator of a PAS cell. (Previously most PAS measurements have been reported in relative terms only.) The principle utilized in the photothermophone is that a thin, optically absorbing, and electrically conducting surface will give the same response to energy received through optical absorption as through electrical generation. The electrical energy created can be easily measured, thereby allowing a determination of the optical energy that gives the same PAS signal. This measurement is independent of PAS cell properties, which are often difficult or time consuming to determine.

Another major result obtained this year was an experimental and theoretical investigation of nonradiative transitions in a luminescent system. This work was the first such attempt using PAS methods (Ref. 4). The effort also involved the first successful use of low-temperature PAS (77 K). PAS was applicable to this type of experiment since it directly detects nonradiative transitions in luminescent samples. Thus, when the absorbed optical energy was separated into radiative and nonradiative components, PAS was able to detect the nonradiative component independent of the radiative (luminescent) component. Ruby powder was used in these experiments. Ruby has two dominant absorption bands that can be utilized to pump the various metastable bands in the ruby system. In samples having small Cr^{3+} ion concentrations, the pumped energy returns dominantly through radiation. Consequently, the nonradiative component of the absorbed energy and the measured PAS signal is small. As the Cr^{3+} concentration is increased, nonradiative transition becomes more important until, for heavily doped ruby, luminescence has been completely quenched, all absorbed energy is heat producing, and the PAS signal is large. Intermediate concentrations give results between these two extremes. Measurement of the PAS signal as a function of chromium concentration allowed determination of the luminescence quenching rate, which in turn allowed a determination of the radiative relaxation rates as a function of concentration. It placed bounds on the magnitudes of nonradiative transition rates directly to the ground state of the system. The technique should be applicable to other luminescent materials. It provides the possibility of directly studying nonradiative transitions that previously had to be inferred from luminescent data.

Principal Investigators: J. C. Murphy and L. C. Aamodt, senior physicists in the Microwave Physics Group, and J. G. Parker, senior physicist in the Chemical Physics Group.

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MOLECULAR STRUCTURE AND PHOTOCHEMISTRY OF FREE RADICALS

With respect to free radical structure, a valence-bond theory was used to interpret the electron-nuclear hyperfine interactions in the noble gas monohalides XeF, KrF, and XeCl in terms of their bond distances and charge distributions. The results were submitted for publication. Important theoretical refinements were developed in the field of chemically induced magnetic polarization that led to an improved model that clarifies the processes.

Problem

Naval research requirements outline the need for basic research in atomic and molecular processes and recognize specifically that knowledge is necessary for the application of processes involving the interaction of radiation with matter, including electron and nuclear magnetic resonance, to contribute to the design and operation of improved Navy systems in many planning categories (cf. Naval Research Requirements ONRINST 3910.2, January 1977, R011-03, R011-07, and R021-02).

This project seeks improved understanding of the interactions between electromagnetic radiation and matter in terms of the molecular structure and chemical reactivity of specific material systems. Such knowledge is important in many areas, including lasers, electromagnetic detectors, information

processing systems, and advanced spectroscopic techniques for investigating a variety of problems such as combustion, corrosion, and the energy level structure of semiconductive devices. During the past year, significant new results were obtained concerning the molecular structure of the noble gas monohalides (Ref. 1), which are the emitting species in ultraviolet (UV) excimer lasers, and the theory of chemically induced magnetic polarization, which is an important new method for investigating photochemical reactions.

Objective

Current goals of the free radical research program (to some extent a cooperative effort between the Microwave Physics Group and the Electronic Physics Group) are the following:

1. Improved understanding of the molecular structure and photochemistry of the noble gas monohalides and related molecules;

2. Advancement of knowledge of a number of highly exothermic free radical reactions, particularly those involving halogen atoms, which have potential importance in laser systems; and

3. Continued application of the theory of chemically induced magnetic polarization in free radicals to the elucidation of the dynamics of very rapid free radical reactions.

Approach

Free radicals are highly reactive molecules that are produced when normal molecules rupture at one or more chemical bonds during the course of a chemical reaction. They usually have only a brief existence before recombining to yield reaction products; however, they can be isolated for detailed study by being trapped in an inert matrix at very low temperatures (matrix isolation). These molecular fragments are involved in the dynamics of many important chemical reactions such as combustion, polymerization, or atmospheric photochemistry. Furthermore, as highly energetic species with a complex energy level structure, free radicals have a number of other important properties. One of these is emission from an excited electronic doublet state to the ground state, uncomplicated by the presence of a lower lying triplet state that often reduces the emission from excited singlet states of normal molecules. Such emission from the noble gas monohalides is currently utilized in high-power UV lasers, and there are a number of other free radicals with laser potential.

The experimental part of the investigation uses the technique of matrix isolation, in which the free radical product(s) of a reaction are immobilized as guests in an inert gas matrix at 4 K. The trapped radicals are readily investigated by a number of spectroscopic techniques. An especially convenient and powerful method is electron spin resonance (ESR) spectroscopy, which observes transitions between energy levels determined by the interaction between the magnetic moment of the unpaired electron associated with the broken bond of the radical and an external magnetic field. A recent example of this technique is the production and detection by ESR of xenon monochloride, which demonstrated that this molecule has a bound ground state (Ref. 2). In this work, XeCl was produced by UV photolysis of a 98% Ar: 1% Xe:1% Cl_2 matrix at 4 K, the solid state reaction being

$$Cl_2 \xrightarrow{h\nu} 2\ CL\cdot; \quad Cl\cdot + Xe \longrightarrow XeCl:$$

In addition to identifying and providing an estimate of the concentration of a given radical, ESR determines several important molecular parameters including the electron magnetic moment and the magnetic hyperfine interactions between the electron and the magnetic nuclei within the radical. Using molecular structure theory, these parameters can be interpreted to yield detailed information about the molecular structure of the radical. The application of this process to the noble gas monohalides is described in more detail in the Progress section of this article.

Chemically induced magnetic polarization results from the spin-selective nature of various chemical reactions involving free radicals (for example, radicals can combine by forming an electron pair bond only if the spins of the electrons on the individual radicals are mutually antiparallel). This spin selectivity, combined with the interconversion of reactive and unreactive spin states by variety of magnetic interactions involving the electron spins, leads to a nonequilibrium population of certain nuclear spin states of the products and reactants, and of the electron spin states of the free radical intermediates. Our investigation of this phenomenon involves solving the time-dependent Schrodinger equation so as to determine the extent and rate of both the spin selection processes and the interconversion of reactive and unreactive radical pair spin states by different types of magnetic interactions accompanying various free radical reactions. This information enables interpretation of the magnetic polarizations developed during radical reactions, which polarizations are readily measured by ESR and nuclear magnetic resonance spectroscopy, in terms of the dynamics and rate of the radical reaction.

Progress

Work on interpreting the electron-nuclear hyperfine interactions of the noble gas monohalides XeF, KrF, and XeCl in terms of the bond distance and charge distribution of these molecules was completed, and the results have been submitted for publication (Ref. 1). This investigation, carried out in collaboration with Dr. A. N. Jette of the Electronic Physics Group, is summarized in the report of that group elsewhere in this document.

Comprehensive review articles on the radical pair mechanism of chemically induced magnetic polarization (Ref. 3) and the triplet mechanism of chemically induced nuclear spin polarization (Ref. 4) were prepared in conjunction with a series of lectures at a NATO advanced Study Institute on Chemically Induced Magnetic Polarization. The radical pair mechanism involves the combined effects of electron spin selection rules for the chemical reactivity of a pair of radicals and the magnetic mixing of the reactive and unreactive spin states. The triplet mechanism involves electron spin selective intersystem crossing from a photoexcited singlet state of a molecule to yield an electron-spin-polarized triplet state that reacts to yield a pair of polarized free radicals. The electron spin polarization of the radicals is then partially transferred to the nuclei by the electron-nuclear magnetic interactions. Although most polarizations are due to the radical pair mechanism, the triplet mechanism is a substantial, if not dominant, contributor to the polarization in the photochemical reactions of carbonyl compounds. A number of the theoretical predictions resulting from the APL studies of the triplet mechanism have recently been confirmed by groups at Queen's University, Kingston, Canada, and Bell Laboratories.

Collaboration with Dr. L. Monchick of the Chemical Physics Group has produced several important refinements to the radical-pair mechanism of chemically induced electron polarization (Ref. 5). A clear model of the process resulted from showing that the evolution of the electron spin state of a radical pair can be described as the rotation of a three-dimensional vector representation of the spin state, where the rotation rate and axis are determined by the magnetic interactions within the radicals and the electron-spin-dependent valence (i.e., chemical bonding) interaction between the radicals. Also, an analytic solution has been obtained for the stochastic-Liouville equations for the electron polarization, which equations are obtained by combining the vector equation for the temporal evolution of the radical-pair electron spin with a diffusion term describing the spatial evolution of the pair. The system of three coupled differential equations that results from the stochastic-Liouville model can be transformed into a single integral equation

for the electron spin polarization component. For slow mixing of the electron spin states, which is the usual case, the kernel of the integral equation is positive-definite, symmetric, and compact. It therefore has a complete set of eigenfunctions, which happen to be zero-order Bessel functions; the integral equation may be solved by expanding in these eigenfunctions. The solution for the usual case of a strong, exponentially decaying exchange interaction, $J(r) = J_0 e^{-\lambda r}$, is

$$\text{Polarization} = \frac{\pi}{2\lambda} \left[\frac{J_0}{J_0}\right] \sqrt{\frac{a}{D}} ,$$

where a is the magnetic interaction that mixes the spin states, and D is the diffusion constant. This result agrees well with previous numerical calculations by other workers. Furthermore, it appears likely that the technique will be useful in other problems (such as magnetic polarization) where a coherent mixing of molecular energy levels is modulated by diffusion or some other incoherent process.

Principal Investigators: F. J. Adrian, Supervisor of the Microwave Physics Group; A. N. Jette, senior physicist in the Electronic Physics Group; and L. Monchick, senior physicist in the Chemical Physics Group.

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SPECTROSCOPY OF ELECTRON-DONOR-ACCEPTOR MOLECULES

The spectroscopy of electron-donor-acceptor molecules is concerned with the investigation of highly conjugated molecules in pure forms and when complexed with electron-donating or electron-accepting species. These molecular systems often have special properties associated with the presence of low-lying, readily accessible, excited electronic states in which the electron charge distribution is markedly different from the ground state. Such properties make these molecular types potentially useful in applications as laser materials, electronic and electro-optical materials, and catalysts. Recent work has focused on the class of porphyrin compounds that are used in biological systems for energy transport and conversion. Work during the past year has yielded new information on the effects of solvents and host matrix on the optical transition probabilities of these species.

Problem

Applications of radiation, optics, and lasers require basic research in the production, transmission, and detection of visible, ultraviolet, and infrared radiation (Naval Research Requirements ONRINST 3910.2, January 1977, RO11-07, p. 3, and RO11-03, p.3).

Highly conjugated organic molecules are of particular interest because they contain delocalized electrons that are easily excited to higher energy states by optical, electrical, or chemical stimuli. These electrons are primarily responsible for the optical, electronic, electro-optical, and chemical properties of such molecules. Of primary interest in our work are the changes that occur in the electronic and vibrational states of the molecules as a result of such external stimuli. The changes are relevant to a basic understanding and utilization of the molecular, physical, and chemical properties of interest.

Because the excited states of highly conjugated molecules occur in the visible and near-ultraviolet regions of the spectrum, optical molecular spectroscopy is used as the primary experimental

technique in these studies. Spectroscopy, the observation of the absorption of electromagnetic radiation with consequent molecular excitation and the emission of radiation accompanying molecular deexcitation, is an especially powerful experimental method for investigating the aforementioned structural perturbations. Usually spectroscopy is used in conjunction with efforts to describe the system and its properties in terms of a theoretical model based on quantum mechanical principles. Spectroscopic data facilitate constructing the model by suggesting which features must be included and which features can be neglected in what would otherwise be an intractably complex model, and by determining the important molecular parameters whose calculation from first principles would be very difficult if not impossible.

Porphyrin compounds are the molecular species of current interest because of their wide range of chemical and physical properties relevant to DoD research requirements. Various compounds in this class exhibit luminescence, semiconduction, photoconduction, or paramagnetism. Some exhibit catalytic activity or are photosensitizers. Because of their special properties, porphyrins occur as important constituents in natural chemical and physical systems.* In addition to their importance in complex chemical systems, they are of interest in this project because their diversity of structure and of chemical and physical properties makes them attractive as model compounds for studies correlating quantum mechanical descriptions with chemical and physical functions.

Objective

Our objective is to advance the state of understanding chemical, physical, and molecular functions by studying perturbations in molecular structure that occur as a result of interaction with other chemical species or physical forces. The immediate goal is to test and improve current theoretical models of free porphyrin compounds by experimental spectroscopic studies of por-

* Chlorophyll and heme are notable examples. Chlorophyll, a reduced magnesium porphyrin, is the primary photosensitizing agent in the photosynthesis process. Heme, an iron porphyrin, is the chemical group in hemoglobin that carries oxygen, while the heme group in certain cytochromes is the principal catalyst in the respiratory cycle in animals.

phins, the parent compounds of the general class of porphyrins. These studies are conducted with "isolated" porphins in a suitable host matrix (Ref. 1). A longer term goal is to study these same porphin species complexed with chemical ligands that are believed to be involved in biologically active forms of porphyrins. The changes in the observed spectra for the complexed species will be related to the interactions between the attacking chemical ligands and the porphin molecules.

Approach

Optical spectroscopy and electron spin resonance (ESR) are the experimental methods used in this project. Because the molecules studied are not easily vaporized, they require a liquid solvent or a solid host matrix. The host, however, can cause loss of spectral information in the guest molecule of interest because of excessive spectral line broadening. We have largely eliminated this effect by using crystalline host materials and making spectral observations at low sample temperature (4.2 K). This allows transitions between the ground and excited electronic and vibrational states to be resolved. The absorption spectra provide the excited electronic and vibrational energy levels, while the luminescence spectra yield the electronic ground-state vibrational levels.

The guest molecules often reside in different types of sites in the host lattice. This causes problems in interpretation of the spectra of the guest molecules because molecules in different types of sites yield different spectra. To eliminate such confusion, techniques involving high resolution selective excitation of fluorescence are used to record the spectra from a single type of site. This way fluorescence spectra from a single type of site are recorded by exciting a single absorption line. The corresponding absorption spectra are obtained by recording the excitation spectra of a single fluorescence line. A tunable dye laser is used as an excitation source for the observations (Ref. 2).

ESR is used to obtain information on the electronic ground-state magnetic parameters for those molecules that exhibit paramagnetism. The parameters are typically the magnetic g factor, hyperfine structure constants, and superhyperfine structure constants. The superhyperfine constants are due to interactions between the paramagnetic metal ion in the center of the porphyrin and the neighboring nitrogen atoms. Often these magnetic parameters are anisotropic. In such cases, information about the orientation of the guest molecules in a host crystal can be obtained (Refs. 3-5).

Progress

During the past year, a study of the optical spectra of free-base porphin doped into crystalline anthracene was completed (Ref. 6). Free-base porphin differs from other porphins in that it contains two hydrogen atoms in its center instead of a metal ion. There are two electronic states, denoted by Q_x and Q_y, in the spectral region studied. The relative strengths of the transitions from the ground state to these two states were of particular interest in this work. Previous spectral observations of free-base porphin in solution indicate that the Q_y transition is stronger than the Q_x. These spectra, however, consisted only of broad components. The spectra in the present study consisted of broad continua and sharp components (called quasi-lines). The broad component in the region of Q_y was stronger than that in the region of Q_x, in agreement with previous work. Conversely, in the quasi-line spectra, Q_x was stronger than the feature identified as Q_y. Simple arguments based upon vibronic borrowing in the cyclic polyene model of porphin indicate that the quasi-line spectra are appropriate for assessing the relative transition strengths for free porphin molecules, while the strengths of the broad components are due to the interactions of the lattice or solvent. Thus, in the context of this model, Q_x is stronger than Q_y for a free porphin molecule, which is the case addressed by most quantum theoretical treatments.

Principal Investigators: J. Bohandy and B. F. Kim, senior physicists in the Microwave Physics Group.

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QUANTUM ELECTRONICS

The Quantum Electronics Group of the Research Center is comprised of five investigators and is supported by the IR&D Program at a level of approximately 50%. The program is devoted to fundamental investigations in the areas of high-pressure gas lasers, chemical lasers, the quantum physics of solids, organic semiconductors, amorphous magnetic solids, and photoelectrolysis. Lasers, electro-optics, and quantum electronics comprise a growing technological area which is being actively investigated to assess its impact and applications. The laser research is directed toward understanding laser excitation mechanisms, which is required to develop new laser sources and improve existing lasers. The research in solid-state physics provides detailed knowledge of the electronic, optical, magnetic, and structural properties of new organic and magnetic materials of technological significance. Finally, an important practical alternative to photovoltaic solar energy using semiconductor p-n junction solar cells may be realized through utilization of photoactivated semiconductor-electrolyte interface devices.

During the present year, significant results have been obtained in understanding the plasma chemistry of high-pressure gas lasers and its effects on high-power laser performance. Continued progress has been made in the ongoing effort to develop organic solids with useful electronic properties, and in developing new materials for solar energy conversion. The results summarized in this report have been described in detail in 15 publications or presentations. During part of this reporting period, Dr. Kishin Moorjani began his appointment as William S. Parsons Visiting Professor in the Department of Physics at The Johns Hopkins University for the academic year 1977-1978. Dr. Theodore O. Poehler, Supervisor of the Quantum Electronics Group, continued his position as University Lecturer in the Department of Electrical Engineering at Johns Hopkins. He also served as a member of the Steering Committee for re-establishing the School of Engineering at Johns Hopkins.

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INVESTIGATIONS IN QUANTUM ELECTRONICS

New gas laser results include a definitive treatment of the effect of fast electrical excitation pulses on the distribution of electrons in a hydrogen cyanide (HCN) laser (Ref. 1), an evaluation of the utility of low ionization potential additives in high-pressure CO_2 lasers, experimental studies of the effect of high repetition rate operation on high-pressure CO_2 lasers (Ref. 2), and determination of the gain and power spectrum of DF and DF-CO_2 waveguide lasers (Ref. 3). Results of physical experiments on organic semiconductors include a new magnetic insulator of a type not previously encountered among organics (Ref. 4), elucidation of the nature of tetrathiafulvalenium-tetracyano-quino-dimethanide (TTF-TCNQ) below its metal-insulator transition temperature (Refs. 5, 6, and 7), and high-resolution conductivity measurements that provide new insight into the nature of phase transitions in several organic conductors. New mixed-transition metal oxide semiconductors have been prepared whose spectral response in semiconductor-electrolyte interface devices for solar energy conversion is well matched to the solar spectrum (Ref. 9). The stability criterion for the existence of various magnetic phases in disordered solids has been established, and the effects of disorder on thermodynamic variables have been investigated (Refs. 10 and 11).

Problem

Applications of radiation, optics, and lasers require research on the production, transmission, and detection of visible, ultraviolet, and infrared radiation (Naval Research Requirements ONRINST 3910.2, January 1977, RO11-02, RO11-03, and RO11-09). Development and improvement of new laser sources with special emphasis on wavelength range, tunability, efficiency, and frequency stability are supportive of specific Naval applications. The Navy's future capabilities in communications, ranging, missile guidance, surveillance, navigation, and weaponry require a diverse program for the development of advanced applications in radiation, optics, and lasers.

Research is required in solid-state physics for continued improvement of materials and a clearer understanding of physical effects in solids that are basic to compact and reliable electronic, magnetic, optical, and thermal devices (Naval Research Requirements ONRINST 3910.2, RO11-02, RO13-09, RO22, and RO22-06). Aspects requiring study include electronic structure, electron transport, electronic and magnetic excitations, lattice dynamics, optical properties, magnetism, critical phenomena, and crystal perfection. Naval equipment and systems are being projected into increasingly severe operational environments, which impose increasingly stringent requirements for improved materials with properties not now available. Information is required on the development of new

monomers for incorporation into polymeric materials that can provide part of the basis for chemical nonmetallic materials.

Gas lasers now available provide radiation extending over a wide spectrum and are capable of use in a wide range of diverse applications, such as short wavelength radars and radar stimulation, isotope separation, the study of high-temperature gases, and communications. The performance of gas lasers, however, depends critically on the effect of the excitation mechanism, whether electrical or chemical, on the lasing gas. Various aspects of the interaction between excitation and laser emission are studied as part of a continuing program in support of Naval requirements for production, transmission, and detection of radiation as well as development of advanced applications.

The amount of electrical energy that can be deposited in a lasing gas and the rate at which the cycle can be repeated are generally limited by the formation of arcs in the gas. The reasons for the arc formation have not been clearly established; several suggested possibilities include the buildup of impurities produced by decomposition of CO_2, thermal loading of the gas, localized thermal instabilities, inhomogeneous preionization of the gas, negative ion formation, and acoustic effects. An understanding of the details of the CO_2 laser plasma chemistry both with and without additives becomes important in this problem; several diagnostic approaches are being used in its resolution. Aspects of this research are also directly supported by the Naval Sea Systems Command.

The research involving organic conductors, amorphous magnetic materials, and semiconductor-electrolyte solar energy conversion is in support of Naval requirements for improved materials and the attainment of a clear understanding of physical effects in solids of interest for advanced applications (Naval Research Requirements ONRINST 3910.2, RO22, RO22-06, RO11-02). The organic conductor research is a continuing effort in conjunction with The Johns Hopkins University. It has concentrated on the synthesis of new organic compounds, measurements of their physical properties, and interpretation of the measurements with the ultimate goal of gaining an understanding of these unique materials.

The photo-assisted electrolysis research is a new endeavor. Photo-assisted electrolysis is an alternate approach to solar cells as a means of utilizing solar energy and is based

on photoeffects at a semiconductor-electrolyte interface. Early experiments with a TiO_2-Pt electrode pair immersed in various electrolytes have been extended to using $Ti_{(1-x)}V_xO_2$ electrodes whose response is better matched to the solar spectrum.

Novel magnetic structures, recently discovered in amorphous solids, have raised fundamental questions concerning magnetism in disordered solids and have already led to new materials with potential applications in magnetic devices due to their high permeability and low coercivity. A typical example of a disordered magnetic system is an amorphous binary alloy, $a\text{-}(TM)_xM_{1-x}$, containing x% of transition metal (TM) atoms (TM = Fe, Co, Ni) and (1-x)% of one or more metalloid (M) atoms (M = B, Si, P). However, before the full potential of these materials can be realized, questions concerning their structural stability and the effects of disorder on the electronic structure of the alloys and on the magnetic interactions must be answered.

Objective

The general objective of the work is to investigate excitation, deexcitation, and emission from atoms and molecules with particular emphasis on processes occurring in lasers. Equally important are studies of the interaction of laser radiation with matter, quantum detection, and the application of lasers and laser techniques to other research and development areas. Immediate goals of the research are directed toward plasma, chemical, and kinetic processes in CO_2 chemical and in diatomic excimer laser systems as related to rate and scalability of the devices.

The goal of the solid-state research is to develop new materials of technological significance and achieve detailed knowledge of their electronic, transport, optical magnetic, and structural properties. Important chemical, electronic, and structural features of organic conducting materials are being explored to ascertain the principal criteria for synthesis of stable organic metals. The immediate objective of the semiconductor-electrolyte studies is to fabricate materials from previously unavailable mixed TM oxides with suitable energy band gaps for useful solar energy conversion.

The goal of the theoretical investigation is to uncover the disorder-induced effects on the static and dynamic magnetic properties of real amorphous solids. Eventually such a study should answer problems concerning the effects of structural disorder on magnetic interaction and therefore on thermodynamic behavior and the stability of various magnetic phases.

Approach

The laser programs are fundamentally experimental investigations of plasma, chemical, and kinetic processes in high-pressure laser devices combined with computer modeling of the time evolution of the laser species.

Experiments have been made on a small transverse discharge CO_2 laser using two independently controlled excitation pulses, spaced 0 to 100 ms apart, together with either an intense spark preionizer or a weaker wire preionizer. The experiment has been instrumented to measure temporal dependence of visible emission; electron density; high-speed discharge photography; wavelength, gain, and power of infrared emission lines; gas current density; and plasma microwave emission (Ref. 11).

The solid-state investigations of organic materials and semiconductor-electrolytes combine synthesis and growth of new materials with programs of physical measurements to characterize the important properties of the materials in combination with theoretical interpretations of these results.

A theoretical model has been constructed to describe the magnetic phenomena in structurally and chemically disordered solids. The structural disorder is simulated by incorporating fluctuations in the exchange interactions, and the model is self-consistently solved within the Bethe-Peierls-Weiss approximation. With appropriate modifications, the model can accommodate site-diluted, bond-diluted, or bond-disordered magnetic systems.

Progress

Most recently, work has been concerned with (a) extending high-pressure chemical laser concepts to compact waveguide lasers; (b) the effect of short electrical excitation pulses on the distribution of electrons in a low-pressure HCN laser and the resulting effect on the optical properties of the laser cavity; (c) the use of low ionization potential additives in a high-pressure CO_2 laser as a means to improve laser performance; and (d) a study of causes of the reduction in the output of high-pressure CO_2 lasers operating at high repetition rates.

The HCN laser work clearly demonstrated that the generally accepted explanations for the delay between excitation

and laser emission and for the spiked output were not correct. The laser gain and the optical properties of the laser cavity are closely tied to each other, to the initial distribution of electrons, and to the radial dynamics of the laser plasma (Ref. 1).

The preliminary results on high-pressure CO_2 lasers indicate that the normal glow discharge forms into a filamentary discharge within a few ns near the peak of the excitation current. The time development of the filaments is a function of the intensity and uniformity of the preionization, the repetition rate, and the presence of additives. As the repetition rate is increased, secondary emission from the cathode increases, leading to the formation of a single arc. This occurrence, together with the facts that the laser emission remains constant and the gain remains high at high repetition rates, indicates the instability is not due to general heating of the gas but to local heating at the cathode (Ref. 2).

TTF-TCNQ crystals of sufficient magnetic purity have been prepared so that only one electron paramagnetic resonance (EPR) signal is visible, and no Curie susceptibility is detectable down to 4.2 K. Below the 38 K phase transition, the magnetic susceptibility obtained by integrating the EPR signal is the sum of two activated components, one with $E_{act} \sim 100$ K $\rightarrow E_{act} \sim 8.6$ meV and the other with $E_{act} \sim 10$ K $\rightarrow E_{act} \sim 0.86$ meV, which are precisely the activation energies for the low-field DC conductivity. Apparent differences between the activation energies for conduction and magnetism result from the difference in preexponential factors. These results imply that the important excitations in both experiments are simple single particles rather than phase solitons or spin waves. Further, we have measured the nonohmic current-voltage characteristics of semiconducting TTF-TCNQ using pulsed techniques to eliminate lattice heating effects. We find that the entire family of I-V curves from 4.2 to 38 K and from V = 0 to field saturation are quantitatively described with a one-parameter fit by simple hot-electron theory adapted to a small gap, nearly one-dimensional semiconductor, and that phase solitons need not be involved.

In amorphous solids, the model has been applied mainly to a solid in which positive and negative exchange interactions, in varying concentration, are distributed at random on a lattice. When positive (negative) interactions dominate, the conventional ferromagnetic (antiferromagnetic) phases result below the Curie (Néel) temperature. However, in the presence of competing posi-

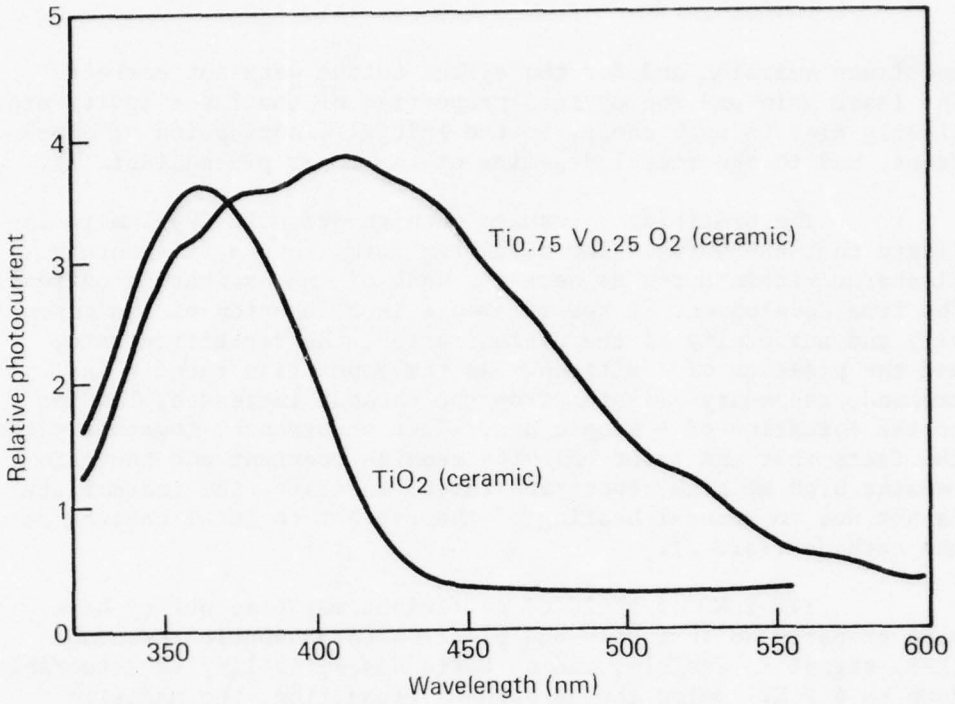


Fig. 1 Photoresponse of TiO_2 - VO_2 Alloy

tive and negative interactions, the present model predicts a concentration range in which the spin glass phase emerges at low temperature. The complete phase diagram has been obtained in the limit of large numbers of nearest neighbors. An attempt is under way to obtain a similar diagram without the above limiting restriction.

In the current investigations of semiconducting oxides for energy conversion and electrochemical applications, mixed phase alloys of several TM oxides have shown promising results, particularly $Ti_{(1-x)}\ V_x O_2$, using both single-crystal and ceramic specimens. In experiments on these materials, the optical absorption spectrum and the peak in the photoelectrolysis (PE) spectrum shift continuously as a function of x, the fractional V concentration. For $x \sim 0.25$, the edge of the PE spectrum is shifted approximately 1 eV from that found in TiO_2 and lies at 2.2 eV, close to the value needed for efficient solar energy utilization (Fig. 1). In the preliminary experiments, no measurement of the absolute PE conversion efficiency has yet been made, but the PE effect is observed to be of the same magnitude in single-crystal $Ti_{(1-x)}V_x O_2$

specimens we have used as in equal TiO_2 specimens. Furthermore, while no long-term studies of the stability of the material have yet been made, rapid photoetching is not observed.

Principal Investigators: R. Turner, T. O. Poehler, A. N. Bloch, D. O. Cowan, K. Moorjani, and S. K. Ghatak. Dr. Poehler is Supervisor of the Quantum Electronics Group. Professors Bloch and Cowan are members of the Chemistry Department of The Johns Hopkins University, and S. K. Ghatak is a faculty member of the Free University of Berlin. None of the non-APL colleagues were funded by the IR&D Program.

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4. M. E. Hawley, T. O. Poehler, T. F. Carruthers, A. N. Bloch, and D. O. Cowan, "Magnetic and Electrical Behavior of New Organic Charge Transfer Salt" (in press).

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8. A. N. Bloch, T. O. Poehler, and D. O. Cowan, "Chemical Trends in Organic Conductors: Stabilization of the Nearly One-Dimensional Metallic State," Organic Conductors and Semiconductors, T. Pal, G. Bruner, A. Janossy, and J. Solzom (eds.), Springer-Verlag, Berlin, 1977, pp. 317-348.

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11. S. K. Ghatak and K. Moorjani, "Equivalence Between the Edwards-Andersen and Luttinger Models of Spin Glass," Solid State Commun., Vol. 23, Aug 1977, pp. 399-400.

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13. K. Moorjani and C. Feldman, "Amorphous Boron Films," Chap. 5, Boron and Refractory Borides, V. I. Matkovich (ed.), Springer-Verlag, Berlin, 1977, pp. 581-596.

14. K. Moorjani and S. K. Ghatak, "Bond Diluted Heisenberg Ferromagnetic," Bull. Am. Phys. Soc., Vol. 22, 1977, p. 265.

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SOLID-STATE PHYSICS

The Solid-State Physics research group of the Research Center is concerned with both fundamental and applied aspects of noncrystalline and polycrystalline inorganic solids; it is about 80% supported by the IR&D Program. Activities in 1977 encompassed basic studies on (a) amorphous boron and (b) the energy distribution of secondary ions generated by ion beam sputtering. More applied studies include (c) the use of optical techniques for the evaluation of semiconductor solar cells and (d) the practical and important problem of developing thin-film techniques for forming inexpensive silicon solar cells. These four projects, which are interrelated and support one another, will be described in this section.

Studies om amorphous boron films emphasized the effect of carbon and hydrogen in the atomic matrix. While the introduction of both carbon and hydrogen brings about an increase in the resistivity of amorphous boron, they appear to occupy different positions in the boron icosahedral framework. This information is important to future applications of amorphous boron. Secondary-ion mass spectrometry (SIMS) analysis continues to be an essential tool in examining films and surfaces. Fundamental studies of ion production by sputtering have led to the improved analysis of solids. Optical techniques for the evaluation of physical properties of solids was expanded to include minority carrier mean free path in silicon solar cells. Infrared absorption techniques have proved invaluable in examining carbon and hydrogen impurities in amorphous boron. Significant results in polycrystalline silicon solar cell studies include the successful application of a bottom conducting electrode (TiB_2) on an insulating substrate and the evaluation of grain size versus solar cell efficiency that provides a guide to the grain size requirements of silicon polycrystalline solar cells.

During the period, six papers were published, one paper was accepted for publication, a chapter was written for a book, and seven presentations were given by the members of the group.

THE JOHNS HOPKINS UNIVERSITY
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ELECTRONIC PROPERTIES OF CONTROLLED IMPURITIES IN AMORPHOUS BORON FILMS

Understanding how the electronic properties of amorphous semiconductors can be changed by the addition of controlled impurities has great potential for extending the applications of these materials to practical devices. The investigation of elemental boron, the first semiconductor in the periodic table, is particularly useful in determining how the unique properties of this material can be utilized. The study of the roles of carbon and hydrogen in determining the electronic and optical properties of amorphous boron thin films has led to a model to explain the changes in charge transport due to these impurities. It is hoped that this will lead to additional device applications.

Problem

The introduction of controlled impurities into amorphous semiconductors in an attempt to change their electronic properties has been a goal of workers in this field for many years. Until the relatively recent work at APL on carbon in boron and on hydrogenated silicon elsewhere, it was believed that amorphous semiconductors could not be "doped." It was felt that the amorphous matrix could always accommodate a large number of impurities without changing its electronic properties, and most experiments seemed to substantiate this view. However, the work at the Laboratory has shown that amorphous boron thin films are sensitive to small amounts of carbon and hydrogen introduced during deposition, and that the electronic properties of these films could be predictably changed with the incorporation of controlled amounts of these impurities.

The work this year has focused on how the unique properties of amorphous boron films enable carbon and hydrogen to affect the electronic properties of the films. This work is relevant to problem areas R011-02, Solid State Physics, R021-02, Physical Electronics, and R021-03, Electronic Components, as listed in Naval Research Requirements ONRINST 3910.2, January 1977. In particular, the present study is relevant to radiation resistance and charge transport phenomena in advanced electronic materials. The work is also pertinent to Air Force Planning Guide HQAFSC TR 76-01, May 1976, subarea 7.8, dealing with devices that

"function in a space or weapon generated radiation environment." Thin films, amorphous semiconductors, and polycrystalline silicon in contrast to single crystals play an important role in hardening electronic devices and circuits.

Objective

The goal has been to develop a model to explain how carbon and hydrogen change the electronic properties of amorphous boron films and to explore how the effects could be applied to practical devices.

Approach

The investigation has been centered on depositing a large number of samples under various deposition conditions and with various amounts of impurities. The samples are then examined for changes in their electronic and optical properties. Films were made by electron beam deposition from three different configurations: (a) boron source only, (b) boron and carbon from separate sources, and (c) a boron source in the presence of a gas (such as hydrogen). The films were deposited on various types of substrates and were between 0.2 and 1.5 μm thick. The composition of the films was determined by secondary-ion mass spectrometry (SIMS) and infrared absorption measurements. Electronic properties investigated included DC and AC conductivity, conductivity versus temperature, thermopower, and photoconductivity. The transmission and reflection of certain films were measured in the 0.63 to 0.86 μm wavelength range to determine changes in the optical constants of the films.

Progress

The results show that films containing only hydrogen also show an increase of resistivity with increasing hydrogen content (Fig. 1) in contrast to previously reported results (Ref. 1). The optical absorption was found to decrease with increasing hydrogen content. No nonlinearities were found in low-temperature conductivity measurements on layered samples. In conjunction with the earlier electron spin resonance data, which showed a decrease in spin density with increasing hydrogen (but not carbon) content, these results lead to a model for amorphous boron that shows a high density of localized levels in the energy gap. The density of localized levels near the band edges seems to be reduced by the hydrogen. The carbon and hydrogen appear to bond to the icosahedral atom groups of the boron in different manners; the carbon must replace intericosahedral bonds whereas the hydrogen must accommodate dangling bonds on the icosahedra themselves. Both of these processes tend to localize valence electrons and thus decrease the carrier mobility in the films.

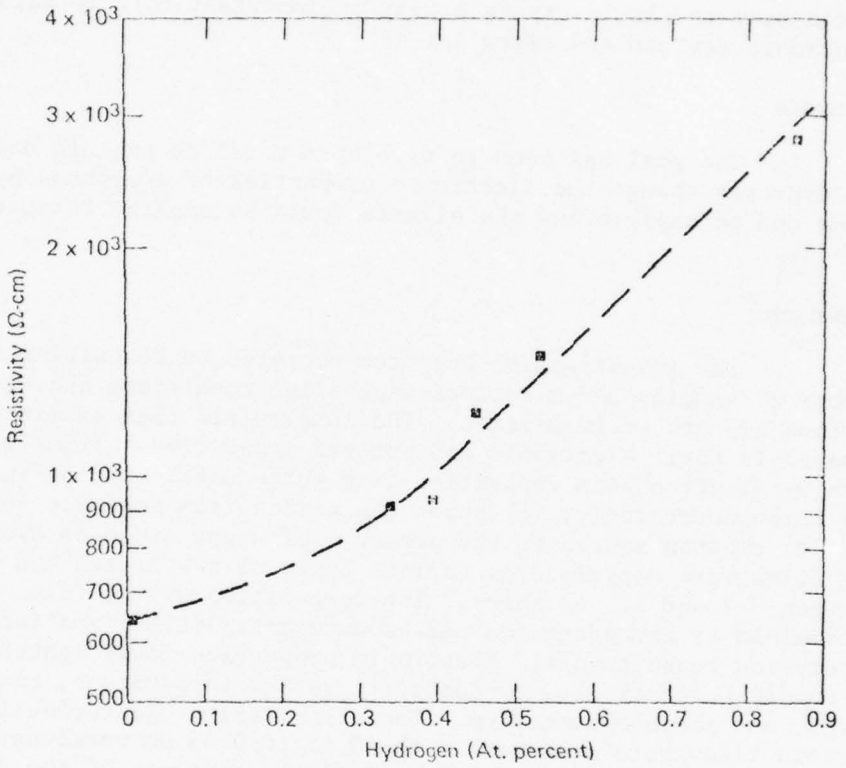


Fig. 1 Resistivity versus Hydrogen Content in Vacuum-Deposited Amorphous Boron Film

Principal Investigators: G. Turner, C. Feldman, and F. G. Satkiewicz. Dr. Feldman is Supervisor and Dr. Satkiewicz is a senior chemist in the Solid-State Physics Group. Mr. Turner is a doctorate student at The Johns Hopkins University.

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2. K. Moorjani and C. Feldman, "Amorphous Boron Films," Chap. 5, Boron and Refractory Borides, V. I. Matkovich (ed.), Springer-Verlag, Berlin, 1977, pp. 581-596.

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QUANTITATIVE SECONDARY-ION MASS SPECTROMETRY EMPLOYING A SPUTTERING ION SOURCE

Secondary-ion mass spectrometry (SIMS) employing a sputtering ion source has become increasingly important in the analysis of solids. The full effectiveness of this method is hindered, however, by the incomplete understanding of ion production, the inability to predict absolute ion yields, and the differences inherent in the various mass spectrometers in use. To overcome these limitations, the sputtering behavior of different classes of materials must be examined. In the current effort, several glasses and metals were studied.

Problem

Quantitative analysis of solids by SIMS relies on the use of ion yield factors to convert intensities into atomic concentrations. Reliable data are difficult to obtain due to the sensitivity of yield to bonding in the solid, the influence of residual gas on the electrical state of the surface, and differences in instrumental parameters such as secondary-ion extraction conditions and energy bandwidths. Naval Research Requirements (ONRINST 3910.2, January 1977, R011-02) recognizes the need for increased understanding with respect to semiconductors and interfaces. SIMS work is also relevant to Special Materials and Techniques, R022-06, in its study of surface phenomena and corrosion, as well as R013-05, Analytical Chemistry, in which new and improved analytical techniques are sought.

Objective

A method for correlating ion yield data from various SIMS instruments is being sought. It is virtually impossible for one laboratory to acquire reliable yield factors to use in all analyses; therefore, a way must be discovered to account for differences in data so that each laboratory can contribute to a general pool of information.

Approach

One of the fundamental problems to resolve in understanding ion production by sputtering is the differences in initial secondary-ion energy distribution (SIED) curves for various species. The Laboratory's GCA IMS-101B mass spectrometer can obtain these curves and provide relative ion yields that accurately reflect the sputtering process (for a given set of primary beam characteristics) independent of the spectrometer used. This capability is inherent in the design of the double-focusing spectrometer that has a variable energy window. An energy distribution curve is obtained by varying the target potential, with the acceleration voltage kept constant, in a range of 0 to 500 eV. This range includes over 95% of the ions formed at primary voltages up to 15 KeV. The secondary-ion optics adjustments were carefully studied to obviate anomalies in extraction.

Progress

Sputtering of Glasses. Glasses are a class of solids with many advantages for studies of ion production (see Refs. 1 and 2). Many elements can be uniformly dispersed in an amorphous matrix; furthermore, work function differences for elements in a specified glass do not arise. In addition, one is not worried about sputtering rate differences or other sputtering artifacts. Several glasses obtained from the National Bureau of Standards were examined. They contain known amounts of additives such as Ti, Mn, Fe, Co, Cu, and Zr as well as the more common elements O, Mg, Al, Si, Ca, and B. A typical set of distribution curves from the glass designated K-309 is shown in Fig. 1. A strong linear correlation between the partitioning of the primary energy and the first ionization potential of the element was observed.

The relative ion yields for the elements in the glass for any interval of energy studied can be obtained from the distribution curves. An example is shown in Table 1 for the experimental ranges 0 to 500 eV, 0 to 100 eV, and 225 to 275 eV; the latter two are typical bandwidths of different mass spectrometers. The results show the need for having the full distributions to make data from different instruments generally useful.

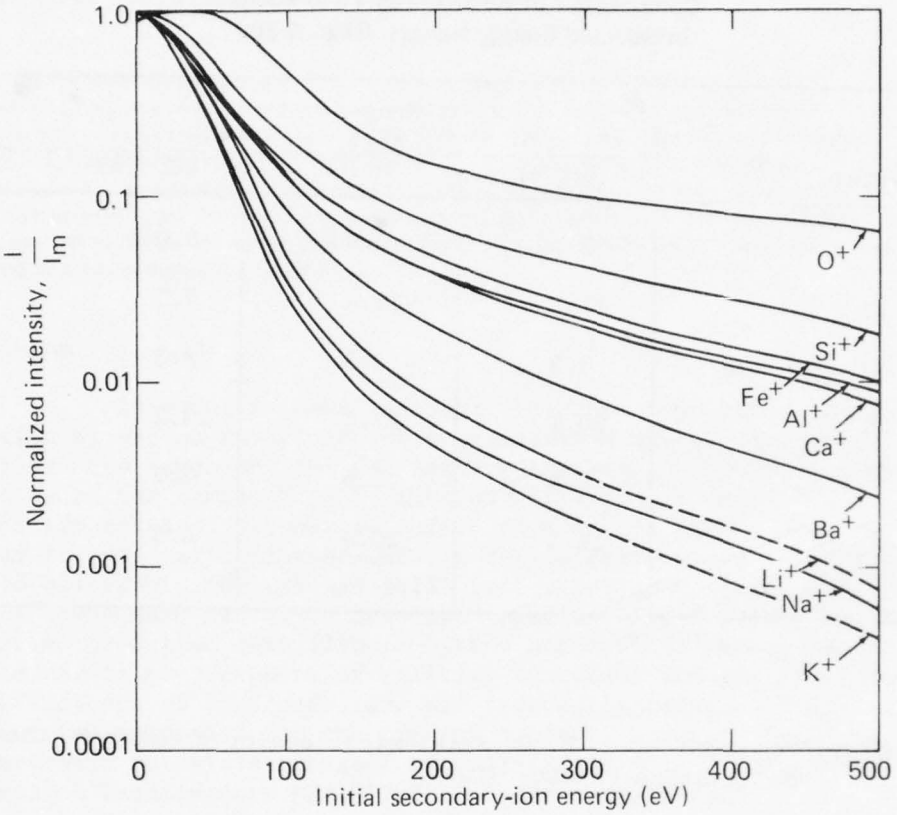


Fig. 1 Secondary-Ion Energy Distribution Curves from Sputtering of K-309 Glass with a Defocused Beam of 10 keV Ar^+.

Sputtering of Metals. SIED curves were obtained from sputtering the following elements with 10 KeV Ar^+: Mg, Al, Si, Mn, Fe, Ni, Co, Cu, Mo, Ag, and Ta. For these experiments, the energy bandwidth was reduced from $\sim$ 50 eV to $\sim$ 5 eV, resulting in histograms with better resolution at lower energies. The effect of primary flux and background oxygen on the partitioning of the primary energy was studied. The varied behavior of the sputtering yield in the presence of oxygen indicates that, even for the sputtering of elements, great care is needed to define a set of relative ion yield factors. A positive aspect of this complexity is the prospect of identifying changes in bonding with concentration of a particular element in a matrix through variations in the SIED curves.

Table 1

Comparisons of Relative Ion Yield Factors
in Selected Energy Ranges, Glass K-309

Element	Range (eV)		
	0-500	0-100	225-275
O	0.041	0.035	0.051
Al	11.1	12.4	7.3
Si	3.3	3.3	3.3
Ca	20.1	22.4	13.2
Fe	2.4	2.6	1.7
Ba	16.4	20.3	6.5

Principal Investigator: F. G. Satkiewicz, senior chemist in the Solid-State Physics Group.

Publications and Presentations

1. F. G. Satkiewicz, "Sputter-Ion Source Mass Spectrometry of Several Glasses," seminar presented at the National Bureau of Standards, 9 Mar 1977.

2. F. G. Satkiewicz, "Relative Yields of Positive Ions Sputtered from Several Glasses," Proceedings of the 25th Annual Conference of the American Society for Mass Spectrometry and Allied Topics, Washington, DC, 29 May 1977, pp. 312-314.

amorphous boron films. Similar techniques were used to continue the study of the kinetics of the amorphous-to-crystalline transformation in silicon films. Apparatus was constructed to measure the total solar efficiency and spectral quantum efficiency of photovoltaic devices. The minority carrier diffusion lengths were determined by a technique derived from the surface photovoltage method of measuring minority carrier diffusion lengths in bulk semiconductors.

Progress

Work on infrared absorption bands in carbon and hydrogen-doped amorphous boron films was reported in Physica Status Solidi (Ref. 1). The technique is now being used for routine evaluation of hydrogen and carbon content in boron films.

Experimental photovoltaic devices have been evaluated for solar conversion efficiency and spectral response using a newly constructed solar simulator. Analysis of the data is most useful in indicating future advances in cell fabrication. Figure 1 shows

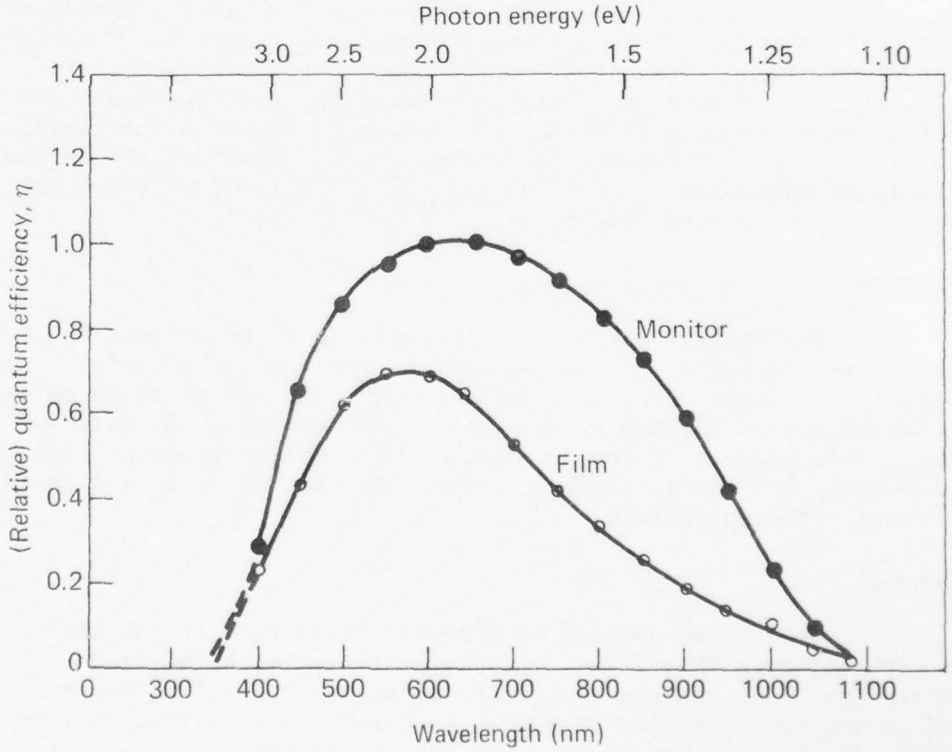


Fig. 1 Spectral Quantum Efficiency of Silicon Film and Companion Monitor (Si 165B)

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OPTICAL PROPERTIES OF SEMICONDUCTORS

Optical methods are being used for characterizing, evaluating, and understanding the electronic behavior of vacuum-deposited semiconductor films. Procedures have been perfected for measuring the hydrogen and carbon content in amorphous boron films using infrared absorption spectroscopy. The degree of crystallinity of partially disordered (amorphous) silicon and germanium films can now be accurately assessed by optical transmission spectroscopy. Methods have been developed for measuring the total solar efficiency, spectral response, and minority carrier diffusion lengths in photovoltaic diodes fabricated by vacuum-deposition techniques.

Problem

In order to make rational decisions concerning the fabrication by vacuum deposition of semiconductor electronic devices, methods are necessary for delineating the basic electronic properties of the semiconductor films and layers. It is important to identify critical parameters and to develop techniques that will lead to systematic improvements in device performance. Since thin-film electronic devices are still in the research stage, measurement techniques had to be developed specifically for the investigation of deposited thin films. Optics and optical processes are relevant to many aspects of military functions and the absorption coefficients of semiconductors are frequently required information. The prime relevancy for the present project, however, falls in the electronic materials category of RO21-22 and RO11-02 of the Naval Research Requirements ONRINST 3910.2 (January 1977).

Objective

The overall purpose of this work is to understand the electronic properties of semiconductors as revealed by their optical properties. The goal is to provide a complete characterization of semiconducting films, layers, and devices. In particular, this project is complementary to the Polycrystalline Silicon Solar Cells project (described in the following article) and shares the same broad objectives.

Approach

Well-known optical techniques are adapted to the study of semiconductor thin films. The identification of infrared absorption bands and the semiquantitative analysis of hydrogen and carbon concentration in amorphous boron, as described in last year's report, was continued. Optical transmission and reflection spectroscopy in the visible and near infrared were used to study the wavelength dependence of the complex refractive index of doped

a plot of the spectral response of a typical thin-film polycrystalline solar cell. The spectral response is obtained by comparison with the response of a standard silicon cell calibrated by the NASA/DOE solar cell project.

The minority carrier diffusion length is a convenient single parameter for characterizing qualitatively the spectral conversion efficiency of a solar cell: long diffusion lengths indicate high relative photovoltaic response to long wavelength light and vice versa. For thin-film devices, it is important to know the minority carrier diffusion lengths, which can then be compared with dimensionally compatible parameters such as film thickness and grain size.

In shallow junction devices, such as the thin-film photodiodes being investigated here, the junction serves as the detector of the "surface photovoltage" produced at the depletion region within the device rather than at the true surface, as in the conventional surface photovoltage method. The photocurrent resulting from illumination of a shallow junction photodiode may be considered proportional to the excess minority carrier density in the bulk of the photodiode. It can be shown that under these circumstances

$$I_p = K'J \left\{ [\alpha(\lambda)]^{-1} + L_n \right\}, \qquad (1)$$

where I_p is the incident photo-flux density, J the photocurrent density, $\alpha(\lambda)$ the bulk absorption coefficient, L_n the minority carrier diffusion length, and K′ a constant. If J is held constant for various values of wavelength λ, Eq. 1 becomes for each value of λ

$$I_p = K \left(\alpha^{-1} + L_n\right), \qquad (2)$$

with K a constant and α a function of λ.

A plot of the relative photo-flux density as a function of $\alpha^{-1}(\lambda)$, according to Eq. 2, should yield a straight line that, extrapolated to zero intensity, gives a negative intercept equal to L_n.

In general, L_n has been found to be of the same order as the grain diameter up to several times the grain diameter. L_n is always more closely correlated with grain size than with film thickness. The grains are longer than their mean diameters, so that L_n seems to correlate most closely with the columnar dimension of the grain, although this number is not accurately known. Figure

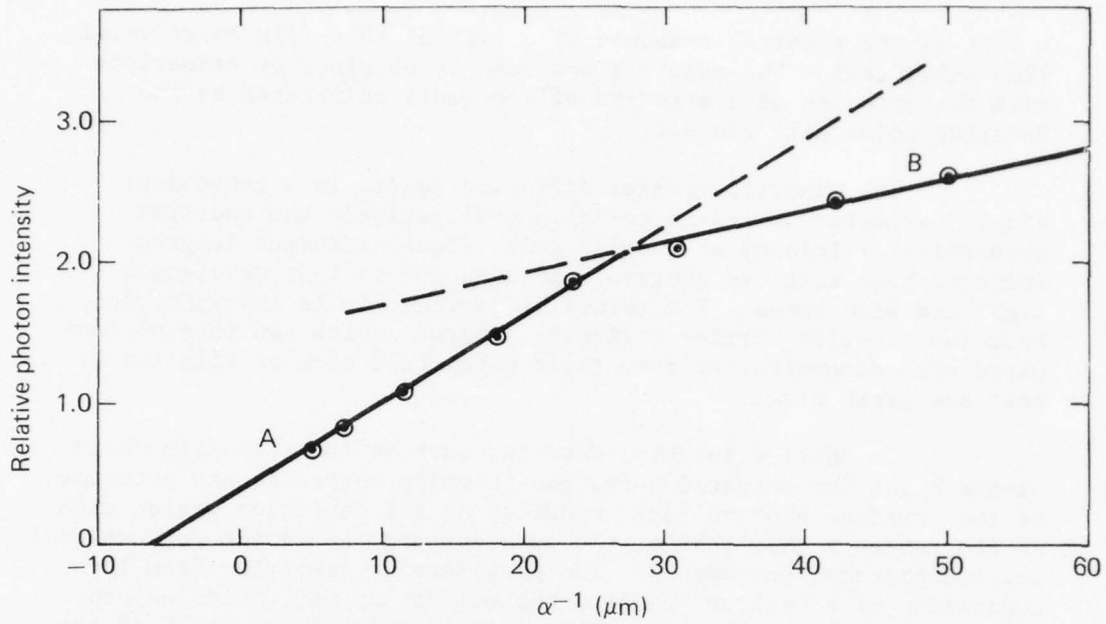


Fig. 2 Measurement of Minority Carrier Diffusion Length, L_n. The value of L_n is the horizontal intercept at α^{-1} −6.2 μm. The "crossing point" corresponds to the film thickness (29 μm), as explained in the text.

2 shows a plot of I_p versus α^{-1} (Eq. 2). This is for a test device (S_i 155B) having a Si layer ∿30 μm thick and with ∿5 μm diameter grains. L_n is equal to 6.5 μm, the negative horizontal intercept. The crossing point of the two linear fits to the shorter (A) and longer (B) wavelength data points occurs at α^{-1} = 29 μm, which is very close to the film thickness. The long wavelength data are not really linear (although the three points in Fig. 2 appear to be so), and no significance can be attached to the corresponding intercept. However, the failure of the short wavelength data to be linear beyond α^{-1} corresponding to the film thickness is because no carriers can be produced at a distance from the junction greater than the thickness of the film. This work was presented in part at the Nineteenth Electronic Materials Conference in July 1977 (Ref. 2).

Principal Investigators: C. Feldman, Supervisor, and N. A. Blum, senior physicist, of the Solid-State Physics Group.

Publications and Presentations

1. N. A. Blum, C. Feldman, and F. G. Satkiewicz, "Infrared Absorption of Amorphous Boron Films Containing Carbon and Hydrogen," Phys. Status Solidi A, Vol. 41, Jun 1977, pp. 481-486.

2. C. Feldman, N. A. Blum, H. K. Charles, Jr., and F. G. Satkiewicz, "Evaporated Polycrystalline Silicon Films for Photovoltaic Applications - Grain Size Effects," presented at the 19th Electronic Materials Conference, Ithaca, NY, Jul 1977. Also published in the J. Electron. Mater., Vol. 7, 1978, p. 309.

POLYCRYSTALLINE SILICON SOLAR CELLS

Experimental research on problems associated with the fabrication of efficient, low-cost polycrystalline silicon solar cells is being conducted. The problems include vacuum deposition, film interface interactions, grain size effects, and substrate interactions. Complete solar cells are formed and evaluated. Considerable progress has been made toward achieving the knowledge necessary to eventually mass produce solar cells by an automated vacuum deposition process.

Problem

The necessity for low-cost efficient solar cells to meet some of the future civilian and military energy requirements has been stated on many occasions by the Departments of Energy and of Defense. Of all the semiconducting materials being considered for solar cells, silicon has been used most successfully for practical applications. The technology associated with silicon is well-known: doping, junction formation, oxidation, surface protection, and lead attachment are well-established techniques. Furthermore, silicon is abundant on earth. The requirement for large arrays of solar cells, covering many square miles, necessitates the examination of techniques for depositing silicon that could easily be adapted to mass production. The practical goal of developing processes to manufacture inexpensive solar cells is relevant to requirements of the Department of Energy. Solar powered equipment has also been included in the Army's battlefield requirements. Furthermore, the study of polycrystalline silicon is relevant to Naval Research Requirements, ONRINST 3910.2, January 1977, on Electronic Components, RO31-03, and Physical Electronics, RO21-02.

Objective

The primary goal is the development of vacuum-deposited silicon solar cells with 10% conversion efficiency. Interim goals are: (a) the achievement of large crystallite growth, (b) the selection of bottom electrodes that will not interact with silicon, (c) the doping of films to form p-n junctions in the vacuum chamber, and (d) total solar cell fabrication by vacuum deposition. It is considered that this project will require four to five years to complete at the present level of effort. The project is part of a more inclusive effort dealing with the use of polycrystalline silicon films in thin-film electronics. The major effort this year, however, has been in the photovoltaic properties of p-n junctions.

Approach

The vacuum-deposition technique of forming solar cells would be eminently amenable to large-scale automated production. Electrode and antireflecting coatings are already being applied to commercial silicon single-crystal cells by vacuum deposition. Scaling up to large area films from a laboratory system would be largely a geometrical consideration. Moreover, a vacuum-deposition production unit in outer space is a distinct possibility. It is the purpose of this study to examine experimentally those processes that would fit into a vacuum production facility. The detailed physics and chemistry of crystallite growth, silicon-substrate and silicon-electrode interactions, impurity diffusion in films, doping processes, and a host of other problems must be worked out. The formation of practical, active, semiconducting devices in vacuum-deposited silicon has yet to be achieved; however, the goal fully warrants an effort even larger than that presently being conducted in the Laboratory. As far as is known, our work represents the only study of all vacuum-deposited polycrystalline solar cells in the country.

Progress

The nature of the program demands that problems be attacked in parallel rather than sequentially. Thus, work in crystallite growth, back-conducting electrodes, junction formation, and complete sample processing is being carried out. Complete cells were formed by (a) double diffusion from the front surface, (b) diffusion from the front and back surfaces, and (c) diffusion from the front surface on p-type deposited material. Secondary-ion mass spectrometry (SIMS) and scanning electron microscope (SEM) analyses were used extensively throughout the study. Progress was made during the present period in the following specific areas:

1. Cells were successfully fabricated using metal boride (TiB_2) electrodes formed between the substrate and the silicon layer from the diffusion couple: boron/titanium/(substrate). The TiB_2 was formed in the vacuum system during the outgassing stage of silicon deposition. The performance of the TiB_2 electrode appears to depend critically on the relative thickness of the titanium and boron layers. SIMS analysis was used extensively as a guide during processing. The work represents the first time an electrode was successfully formed under a high-temperature silicon vacuum-deposited layer.

2. Solar cells were formed from the layered system, silicon/boron/sapphire, in which gas-phase phosphorus diffusion and solid-phase back diffusion from the boron were carried out. These layered cells yielded efficiencies comparable to those obtained in the double-diffusion devices (approximately 2%).

3. Solar cells were formed by double diffusion from the front surface on special glass and alumina as well as on sapphire. Since all substrates yield approximately the same efficiency at the processing temperature required for the glass (900°C), this study indicates that inexpensive substrates may indeed be used for silicon solar cells.

4. The effect of grain size on solar cell properties has been examined using a series of samples having 0.3 to 5 μm grain diameters. Curves of diffusion length, cell efficiency, open-circuit voltage, and short-circuit current versus grain size were obtained. Linear extrapolation of the data indicates that grain diameters of approximately 30 μm would yield cells with a 10% efficiency. The grain lengths perpendicular to the substrate would be equal to or greater than 30 μm.

5. Details of the crystallite growth process shown by SEM photographs of film cross sections have aided the progress of growing large grains in silicon from small seeds on the substrate. Important information on the increase of grain size with an increase in film thickness was obtained.

Principal Investigators: C. Feldman, F. G. Satkiewicz, H. K. Charles, Jr., and N. A. Blum. Dr. Feldman is Supervisor, Dr. Satkiewicz is a senior chemist, and Dr. Blum is a senior physicist in the Solid-State Physics Group. Dr. Charles is a senior engineer in the Microelectronics Group of the Engineering Facilities Division.

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2. C. Feldman, H. K. Charles, Jr., F. G. Satkiewicz, and N. A. Blum, "Vacuum Deposited Polycrystalline Silicon Solar Cells," 12th IEEE Photovoltaic Specialist Conference, Baton Rouge, LA, 15 Nov 1976, p. 100. Also published in Conference Proceedings, IEEE, 1976.

3. C. Feldman, N. A. Blum, H. K. Charles, Jr., and F. G. Satkiewicz, "Evaporated Polycrystalline Silicon Film for Photovoltaic Applications - Grain Size Effects," 19th Electronic Materials Conference, Ithaca, NY, 29 Jun 1977. Also published in J. Electron. Mater., Vol. 7, 1978, p. 309.

4. C. Feldman, F. G. Satkiewicz, and H. K. Charles, Jr., "Evaluation of Vacuum Deposited Silicon Films and Junctions for Solar Cell Application," Proceedings of the National Workshop on Low-Cost Polycrystalline Silicon Solar Cells, C. Chu, ed., Southern Methodist University, Dallas, TX, Dec 1976, pp. 267-291.

THEORETICAL PROBLEMS

The Theoretical Problems Group consists of five senior physicists and one senior mathematician who employ mathematical models to describe physical phenomena. The group does research in three general areas: wave propagation and scattering, fluid mechanics, and biomedical engineering. Approximately 50% of the group's efforts was supported by IR&D funds; the remainder was supported by grants and contracts from the Public Health Services, the Army, the National Bureau of Standards, and the National Fire Prevention and Control Administration.

These studies are reported in 11 journal articles that appeared during this reporting period and in five manuscripts that have been submitted for publication. They describe in detail the development and use of mathematical models to gain insight into a variety of physical phenomena of interest to the Laboratory. In particular, during the current reporting period we have: analyzed the scattering of scalar waves by model rough surfaces; determined model size distributions that provide useful characterizations of very-low-density lipoprotein polydispersity; developed conformal transformation techniques to treat pulsatile hydrodynamic flows and simulated forced convection; calculated the hydromagnetic field induced by the interaction between acoustic motions and an ambient magnetic field in an electrically conducting medium; used signal processing techniques to analyze electroretinographs; developed a novel membrane transport cell that permits the simultaneous measurement of various transport coefficients; and found a group of nerve fibers that could be responsible for the increased magnitude of pain evoked by heat stimulation following a first degree burn. Each of these projects is described in more detail in the following articles.

Several personnel changes occurred during this period. Dr. R. A. Farrell became Supervisor of the group in September 1977, succeeding Dr. M. H. Friedman who left the Research Center to become Deputy Director of Biomedical Programs for the Laboratory. R. A. Meyer transferred with Dr. Friedman as a special advisor in the Biomedical Program Office. Dr. D. M. Silver left the group to become Assistant Supervisor of the Chemical Physics Group in January 1977 and Supervisor of that group in July 1977. Dr. E. P. Gray transferred to a position in the Research Center Office. Dr. R. H. Andreo, a Ph.D. graduate of the University of Syracuse, joined the group in November. Other items of note include the following: Dr. V. O'Brien served on the National Research Council Evaluation Panel for Research Associateship Programs (Engineering) and Review Board and on the National Science Foundation Panel for Engineering Mechanics, and Dr. Farrell served on an advisory panel for the Aging Institute of the National Institutes of Health.

WAVE PROPAGATION AND SCATTERING

Two projects were conducted in the area of wave propagation and scattering. A stochastic variational principle formed the basis for a theoretical description of the scattering of waves by statistically rough surfaces. Many of the mathematical techniques needed for that investigation are similar to those that we had developed earlier in our studies of corneal transparency (funded in part by NIH). The second project used the light-scattering technique of intensity correlation spectroscopy (ICS) to characterize the very-low-density lipoprotein component of blood.

ROUGH SURFACE SCATTERING

A stochastic variational principle was used to improve the first-order perturbational approximation to scattering from a model random rough surface. Multiple scattering was identified as the cause of a discrepancy between the variational and perturbational results.

Problem

The propagation, scattering, and absorption of electromagnetic waves provide potential tools for characterizing various media, such as the ocean's surface, chaff particles, aerosols, and bubbles. The Navy's need for research on electromagnetic radiation and propagation is clearly spelled out on page 10 of the Naval Research Requirements ONRINST 3910.2, RO21-01. Except for the most idealized situations, analytical treatments of these problems remain approximate. For example, we recently extended the variational approximation technique to the class of stochastic scattering problems. It is essential that the efficacy and tractability of such approximations be tested. Thus, during the present reporting period, the variational technique was tested by applying it to scattering from the model random rough surface.

Objective

The long-range objective in this area is better understanding of wave scattering from random rough surfaces or from volumes of random scatterers that could lead to improved design and utilization of naval systems such as radar, sonar, altimeters, and radiowave communication links.

Approach

During this reporting period, we demonstrated the tractability of a recently developed stochastic variational principle by applying it to a model rough surface. The model selected is the classical one of hemicylindrical corrugations on a conducting plane. An exact solution was obtained for a special case of this model surface that was used to test the efficacy of the variational approach.

Progress

The stochastic variational principle (Ref. 1) was used to improve the first-order perturbation approximation to the mean absolute-squared scattered field amplitude for a plane polarized wave incident on a conducting plane corrugated by a random array of many raised hemicylindrical bosses (Refs. 2, 3, and 4). The perturbation method is only valid when the boss radius is small relative to the wavelength of the incident beam. The variational method extends the range of validity to include radii comparable to a wavelength. However, there are significant differences between the perturbational and variational results even in the limit of small (i.e., Rayleigh) scatterers. In order to gain insight into this discrepancy, the simple case of two Rayleigh bosses was investigated (Ref. 5), since the exact (as well as the variational and perturbational) solutions could be obtained. The exact and variational results are in essential agreement; both differ from the perturbation result in a manner analogous to the many-boss case (cf., Fig. 1). Analysis showed that this discrepancy was due to the fact that the variational method accounts to a significant degree for multiple scattering, whereas the first-order perturbation method does not.

Principal Investigators: R. A. Farrell, E. P. Gray, R. W. Hart, and J. A. Krill. Dr. Farrell is Supervisor of the Theoretical Problems Group. Dr. Gray is a Senior Physicist who transferred from the Theoretical Problems Group to the Research Center Office in September 1977. Dr. Hart is Chairman of the Research Center. Mr. Krill is an electrical engineer in the F2A Group of the Fleet Systems Department.

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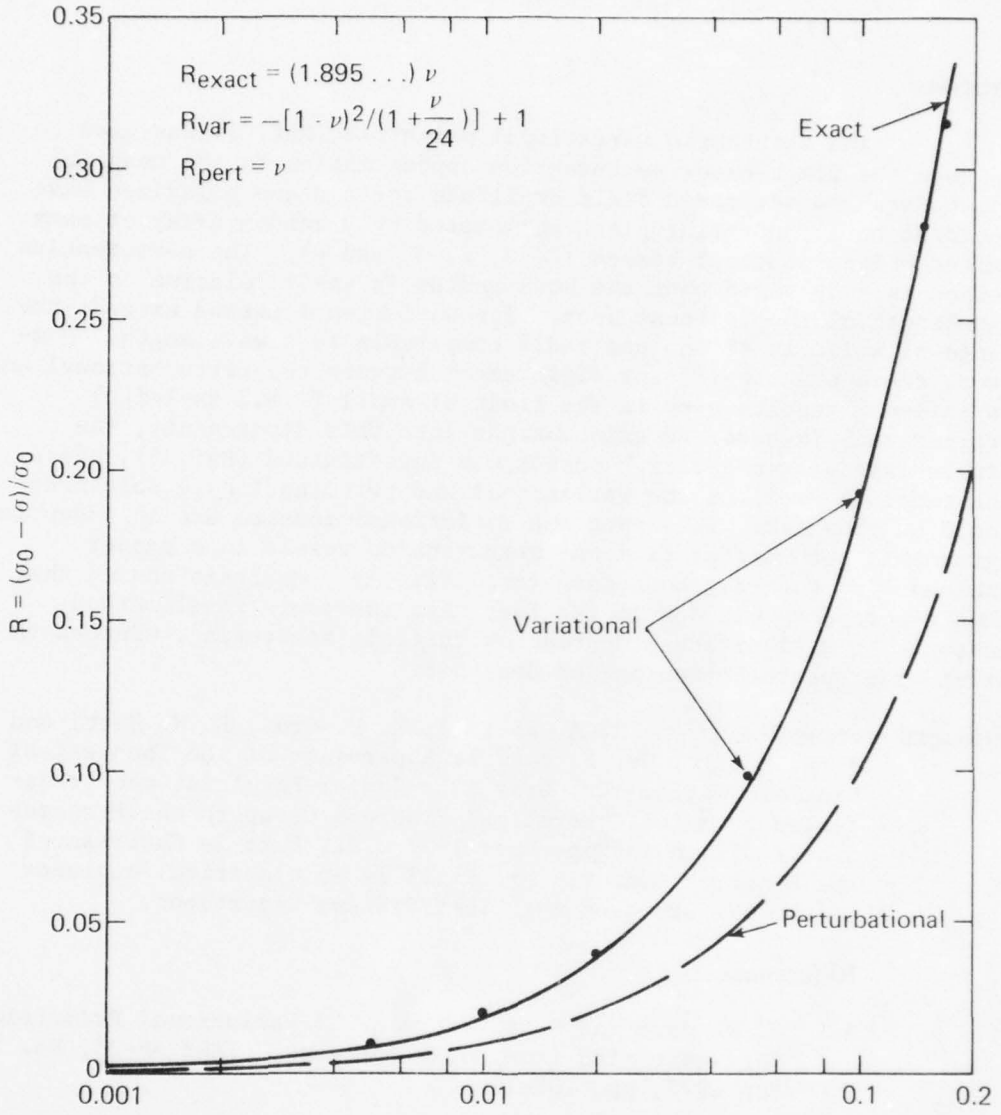


Fig. 1 Correlation in the Positions of the Nonoverlapping Hemicylinders Causes the Scattering Cross Section, σ, to Differ from σ_0, the Value for an Assembly of Overlapping Hemicylinders. Here, we have plotted the exact value of this difference (normalized by σ_0) as a function of the area fraction of the plane covered by the corrugations. The perturbational and variational approximations to this normalized difference are given by the dashed curve and the • , respectively. Although the results are for the two-hemicylinder case, a similar discrepancy between the variational and perturbational approximations is found for the N-cylinder case.

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LASER INTENSITY CORRELATION SPECTROSCOPY OF MACROMOLECULES

This study demonstrates that only certain of the standard model size distributions are suitable for describing the sizes of very-low-density lipoproteins and that comparisons of the normalized variance of the distribution of diffusion coefficients predicted by these models with those measured by intensity correlation spectroscopy (ICS) provide a useful test of the model's applicability.

Problem

Serum lipoproteins are of considerable biological interest because they play a major role in the transport and metabolism of lipids and are implicated in the development of atherosclerosis. Thus, they have relevance to Naval Research Requirements in Biochemistry (ONRINST 3910.2, January 1977, RO41-06). There is evidence that the sizes of the low- or very-low-density lipoproteins (LDL and VLDL) may provide an early indication of a propensity towards hyperlipoproteinemia. The specific problem is to determine how the sizes of LDL and VLDL differ among carefully chosen members of families having classical Type II or Type IV hyperlipoproteinemia, among normals in these families, and among normals in the general population.

Objective

The objective during the present reporting period was to find suitable model size distributions to describe VLDL and to relate the parameters of these distributions to quantities that can be determined from ICS data.

Approach

In examining lipoproteins using ICS, molecular diffusion coefficients, and therefore particle sizes, are determined from the autocorrelation functions of the time-dependent intensity fluctuations in the light scattered from the particles as they diffuse in solution. The autocorrelation function is analyzed by an expansion technique in which the coefficients, called cumulants, are related to general properties of sample polydispersity (Ref. 1). We extend this general use of cumulants by relating them to the parameters of specific model size distributions (Refs. 2, 3, and 4).

Results

Our early studies, reported previously, showed that Gaussian and rectangular size distributions failed to describe VLDL. These studies suggested that skewed, bell-shaped distributions would provide the best description of VLDL polydispersity.

We chose four mathematically tractable distributions of this form for analysis. Three of these, the Pearson V, a Schulz distribution of radii, and a Schulz distribution of molecular weight, are defined for diameters in the range $0 < d < \infty$. The Pearson III distribution is defined with a lower limit cut-off on possible diameter, i.e., for diameters $\beta \leq d < \infty$.

We found that the Pearson III (with $\beta = 28.0$ nm), the Pearson V, and the Schulz radii distributions are useful to describe VLDL size. As illustrated in Fig. 1, these distributions

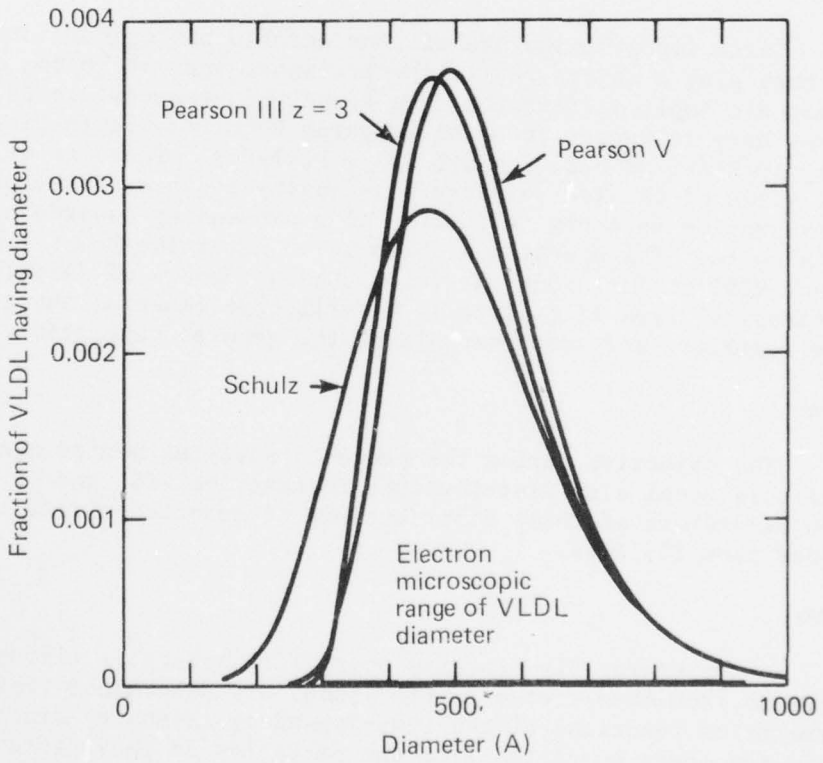
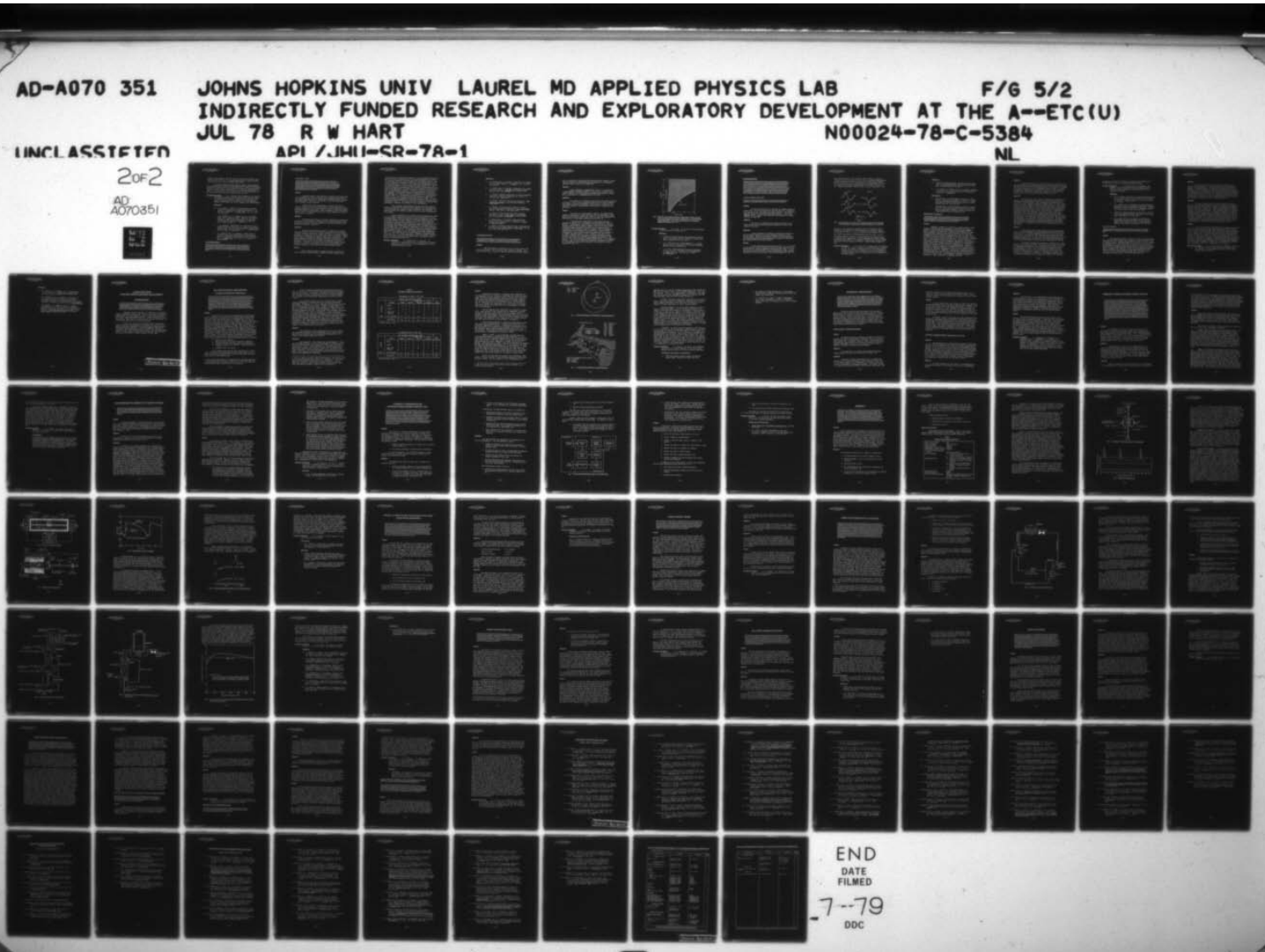


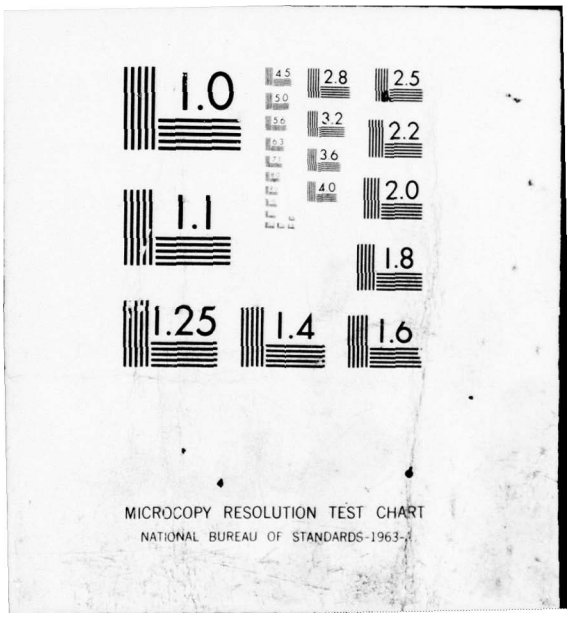
Fig. 1 The Experimentally Determined Size Distributions for VLDL. The expected range of VLDL sizes based on electron microscopic examinations is shown on the baseline.

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compare very favorably with the reported electron microscopic size range of VLDL (Ref. 4). The Schulz distribution of particle molecular weight is not useful to characterize VLDL.

A second important result was the explicit demonstration that the normalized variance of the generalized diffusion coefficient distribution has distinct upper bounds for each of these size distributions, as well as for the Gaussian and rectangular distributions (Ref. 4). This property can be used to rule out a distribution, as in the case of the rectangular distribution for VLDL.

Principal Investigators: R. L. McCally and S. Margolis. Mr. McCally is a senior physicist with the Theoretical Problems Group. Dr. Margolis is Professor of Medicine and Associate Professor of Physiological Chemistry at the Johns Hopkins Medical Institutions and is not funded by the IR&D Program.

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FLUID MECHANICS

Analytical and numerical techniques are developed to obtain a better understanding of two internal flow problems: fluid flow in a constricted tube and heat conduction in force convection. In another study, a hydromagnetic field induced by the interaction between acoustic motions and an ambient magnetic field in a conducting medium was analyzed.

INTERNAL FLOW

The simulation of pulsatile flow through tubes with constrictions revealed time-dependent regions of high tangential-shearing stress upstream of the throat and recirculation regions downstream. Recirculation is important in determining the locations of pressure taps in flow-metering devices and may also be involved in the development of atherosclerosis in human arteries. The calculations of duct forced-heat convection allowed the determination of the optimum length of internal fins to produce the greatest enhancement of heat conductance.

Problem

Advanced analytic and numerical techniques for solving the most fundamental equations governing fluid motion are pertinent to many Naval problems, such as hydrodynamics (ONRINST 3910.2, RO23-01) and aeromechanics (RO23-02). Currently, we are concentrating on flows through internal passages.

Arterial pulsatile hemodynamics exemplify the type of internal laminar flow systems investigated, illustrating both basic methods and application to cardiovascular disease, especially atherosclerosis (RO41-01, physiology). Heat transfer by forced convection, another aspect of internal viscous flow, can be important in lubrication and wear analysis.

Objective

The general objective is to obtain theoretical descriptions of various fluid mechanical phenomena in all three-dimensional time-dependent generality from the fundamental continuum equations with appropriate boundary conditions.

Approach

Although the governing equations of momentum and energy transport are well known, the nonlinear properties of the equations (or their boundary conditions) require tailoring the solution method, analytical or numerical, to the particular class of problems. During this period, two-dimensional laminar flows were investigated. Conformal mapping of obdurate geometries followed by numerical time-marching solution allows us to handle time-dependent nonlinear solutions. Although the general forced convection problem is also nonlinear, we have so far studied only the far-downstream fully developed asymptotic limit where the equations become linear.

Progress

We are making progress on general methods to handle unsteady separating laminar flows to higher Reynolds numbers and in

more arbitrary two-dimensional domains. We had previously shown the ability to model pulsatile flows, of arbitrary periodic flux wave, in branching geometries with straight flat boundaries (Ref 1). Now we can handle many axisymmetric internal flow problems with curvilinear boundaries by using an exact conformal transformation to map the physical domain to a more convenient computational one. The fluid's governing streamfunction and vorticity equations become somewhat more complicated, but satisfying the condition of viscous nonslip at the boundary is easier. A number of separating solutions for pulsatile flow through constricted passages were carried out. The technique is useful for models of atherosclerotic occlusions in arteries (Ref. 2). Preliminary calculations up to a mean Reynolds number of about 10^2 revealed interesting regions of high local shearing stress and separated recirculation regions (Ref. 3), both of which have been mentioned as causative factors in atherosclerotic development (Ref. 4). The technique can be applied to orifice flow metering to establish the effects of flow unsteadiness.

The conformal transformation method, which has proved so helpful for inviscid irrotational flow problems, is just beginning to be exploited for viscous or other rotational flow problems. It should be useful for density stratified flow or other inhomogeneous flow fields.

Forced convection is of interest for increasing heat transfer for energy conservation as well as in the lubrication or wear of moving parts. (Also we noted that theory developed in heat transfer can be applied to mass transport in biology problems as well, by analogy of mass and heat transfer (Ref. 5).) Some empirical evidence had indicated extended surfaces consisting of internal fins can increase the average heat conductance from a straight duct of hot flowing fluid. Our numerical simulation of the fully developed thermal field has shown fins may either decrease or increase overall heat conductance (Ref. 6). We determined the optimum lengths of double fins in prismatic ducts for maximum conductance enhancement (Ref. 7). Note that before the scalar transport calculations can be carried out, it is first necessary to find the complete velocity field. Our duct velocity field computational techniques include those for unsteady flow (Ref. 8).

Principal Investigators: V. O'Brien and L. W. Ehrlich. Dr. O'Brien is a senior physicist in the Theoretical Problems Group and Dr. Ehrlich is a senior mathematician in the Applied Mathematics Group.

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HYDROMAGNETISM

A survey of oceanic hydromagnetism was completed and a new hydromagnetic effect ("sonomagnetism") was calculated. This effect involves the interaction between acoustic motions and an ambient magnetic field in an electrically conducting medium.

Problem

Many hydromagnetic phenomena occur in an environment like the ocean; however, only a few have been studied in detail. The effects arise from a variety of natural and/or body-related motions

of the electrically conducting fluid across ambient magnetic fields. They are relevant to Naval Research Requirements in oceanography (ONRINST 3910.2, January 1977, R031-03).

Objective

While finishing a comprehensive survey of the multitude of hydromagnetic phenomena possible in the ocean, we undertook an indepth analysis of the heretofore overlooked hydromagnetic signal that is generated by a submerged source of sound.

Approach

The studies are theoretical and proceed from basic physical principles. This course recommends itself, both to gauge reliably the numerous possible hydromagnetic effects and to calculate from reasonable physical approximations those effects of apparent significance.

Progress

The survey of oceano-magnetic effects, including simple numerical estimators of their size and extent as discussed in more detail in the previous IR&D report (Ref. 1), has been completed for publication in the present reporting period (Ref. 2).

A new phenomenon identified in that survey has been analyzed in detail, viz. "sonomagnetic pseudoradiation" (Ref. 3). Briefly, a hydromagnetic field induced by the interaction between acoustic motions and an ambient magnetic field in an electrically conducting medium propagates with the sound radiation and is transmitted into adjacent sound-free regions. This sonomagnetic pseudoradiation was analyzed for an arbitrary acoustic source submerged in a semi-infinite conducting medium in the presence of a constant applied magnetic field. Explicit reduction of the solution integrals was illustrated by presenting approximations for both near-field and far-field sonomagnetism external to the medium in the case of ambient magnetic field normal to the semispace surface. The far field exhibits sonomagnetic pseudowaves radiated to considerable distances by high-power, low-frequency acoustic sources (cf. Fig. 1).

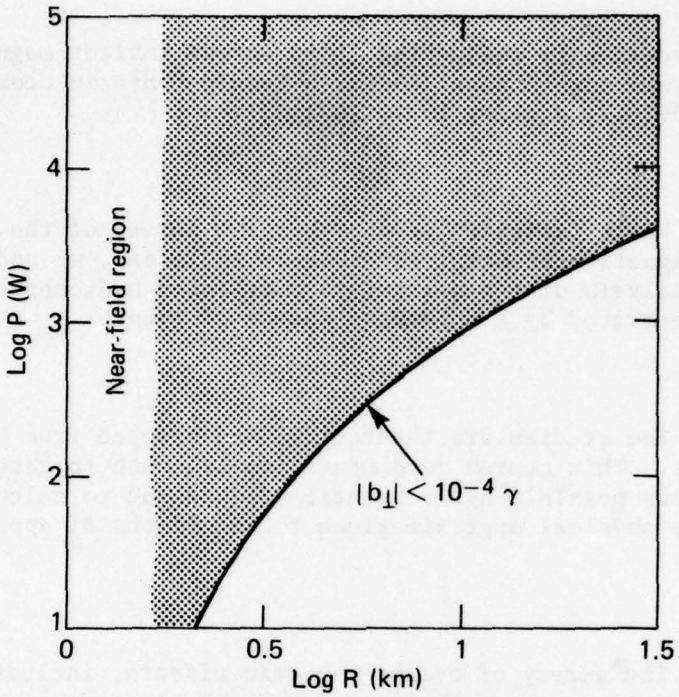


Fig. 1 Power (P) versus Range (R) Domain (shaded region) in which the Near-Surface Sonomagnetic Pseudowave Amplitude due to a Vertical Acoustic Dipole Submerged in a Polar Ocean and Radiating at 1 Hz Exceeds a Magnetometer Sensitivity of $10^{-4}\ \gamma$.

Principal Investigator: J. F. Bird. Dr. Bird is a senior physicist in the Theoretical Problems Group.

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BIOENGINEERING

Although most of the bioengineering research carried out in the Theoretical Problems Group is funded by grants and contracts from the National Institutes of Health and the Army, some bioengineering work is supported by IR&D funds. During this reporting period, three projects were in the latter category: analysis of the signal processing involved in human vision, an investigation into the effects that membrane structure has on solute transport, and an experimental study of how controlled pain stimuli are encoded into neural signals. The techniques developed in these projects are valuable in nonbiological fields as well. For example, membrane transport is important to desalination devices, and signal processing is a vital element in detection and decision procedures.

VISUAL SIGNAL ANALYSIS

Analysis of the retinal signals associated with certain suprafusion stimuli discloses two components, one correlated with brain signals, the other with specific retinal cells.

Problem

We are concerned with the analysis of complex signals in human vision, which are perhaps the most impressive in complexity and function of any information-processing system. The problem is directly relevant to Naval Research Requirements in physiology (ONRINST 3910.2, January 1977, R041-01) and indirectly to others (R021-05 and R014-08).

Objective

Our aim is to understand the sensory function of the visual system and the data-processing operations by which this function is served.

Approach

A novel technique of transient stimulation developed at APL has proven useful in eliciting elemental responses of the visual system. Theoretical analysis supported by psychophysical and electrophysiological experimentation is applied to interpret the evoked sensory and neural signals.

Progress

In the penultimate reporting period (Ref. 1), we reported on the analysis of brain signals induced by abrupt changes in the periodicity of rapidly intermittent (suprafusion) light. An analysis has now been completed of electroretinographic (ERG) signals associated with such suprafusion period-jump stimulation (Ref. 2).

The suprafusion ERG's were predicted theoretically to behave as elemental retinal responses; this has been confirmed experimentally. The ERG waveforms are quite complex, but a theoretical analysis was able to reduce all the data collected (38 waveforms) into just two significant elements, represented by the Green's functions (or "impulse responses") shown in Fig. 1 as $G_L(t)$ and $G_R(t)$. The

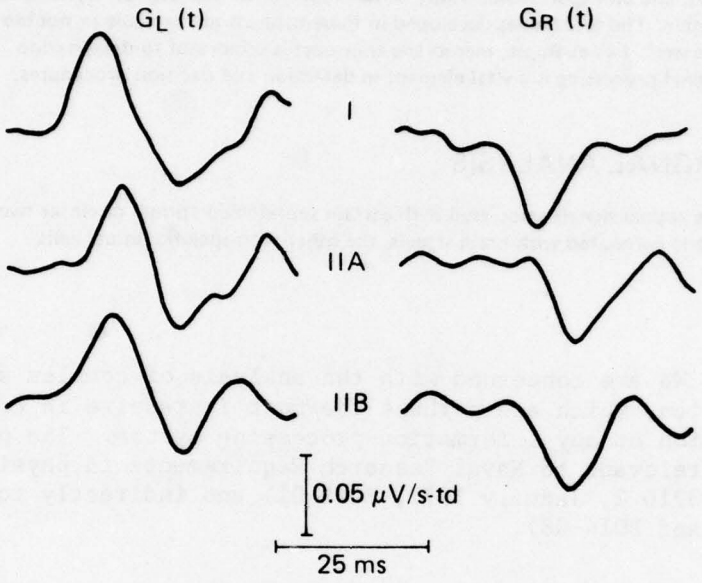


Fig. 1 Green's Functions of Linear (G_L) and Rectifying (G_R) Elements Deduced from ERG Signals in Experiments on Different Monkeys (I, IIA, and IIB)

validity of the analysis is evidenced by the consistency among theoretical determinations from experiments on different monkeys as displayed in Fig. 1. G_L is a strictly linear element, which we can closely correlate with simultaneous brain activity. G_R is a rectifying element, which we can associate with a specific class of retinal cells (amacrines). Thus it emerges that signal analysis techniques seem capable of a noninvasive "dissection" of the retina, which would greatly sharpen the ERG as a physiological/diagnostic tool.

Principal Investigators: J. F. Bird, R. W. Flower, and G. H. Mowbray. Dr. Bird is a senior physicist in the Theoretical Problems Group. Mr. Flower, a senior physicist of the Biomedical Programs Office, and Dr. Mowbray, a senior psychologist no longer associated with the Laboratory, are not supported by the IR&D Program.

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Presentations

1. "Introduction to Spatial-Temporal Aspects of Vision, Part I: Achromatic Brightness," 19 Oct 1977, Vision Psychophysics Seminar, Wilmer Eye Institute, Johns Hopkins Hospital, Baltimore, MD.

2. "Introduction to Spatial-Temporal Aspects of Vision, Part II: The Visual Sensation Field," 30 Nov 1977, Vision Psychophysics Seminar, Wilmer Eye Institute, Johns Hopkins Hospital, Baltimore, MD.

MEMBRANE TRANSPORT

A novel membrane transport cell that we developed is used to examine how membrane structure affects transport. For the particular membrane and solute in our initial study, membrane heterogeneity could be ignored. Also, our theoretical studies indicate that solution nonideality can have significant effects on solute transport.

Problem

Membrane transport is essential to cardiovascular, regulatory, endocrine, and thermoregulatory physiology and thus is relevant to Naval Research Requirements in physiology (ONRINST 3910.2, January 1977, R041-01). Conventional techniques for measuring membrane transport properties are based on the implicit assumption that this barrier is homogeneous, that is, that it is traversed by only one kind of pathway or one size of pore. This is in fact the exception rather than the rule. Our theoretical studies (Ref. 1) have shown that the performance of devices relying on interfacial transport (such as membrane oxygenators or desalination units) can be very different from that predicted by conventional design calculations if the barrier is heterogeneous. There is, therefore, a need to extend our understanding of the influence of structure on membrane transport to permit the more rigorous interpretation of transport experiments and the more confident design of separation devices. In addition, a fundamental understanding of normal membrane processes is important for interpreting the effects of various stimuli (e.g., electromagnetic radiation, hyperbaric pressure, or toxic chemicals) on membrane function.

Objective

The overall objective of our research is to contribute to the understanding of transport processes in complex membrane systems. The goal for the current reporting period was to complete our studies of sucrose transport across a Cuprophan dialysis membrane, thereby assessing the importance of membrane structure to such transport. In addition, theoretical studies were initiated to assess the potential error in flux prediction for nonideal solutions.

Approach

The overall approach couples a theoretical description of transport across membrane structures, based on the principles of irreversible thermodynamics, with experimental transport data obtained in a novel membrane transport chamber (Ref. 2). This chamber uses laser interferometry to measure the solute concentration difference across the membrane in an unsteady experiment. Theoretical studies have shown that the effects of structure are manifested in an unexpectedly high flux of solute when there is a concentration difference across the membrane. The flux is higher than that predicted on the basis of conventionally measured tracer permeabilities and is computed from interferometric measurements of the temporal decay of an initial concentration difference imposed across the membrane in an essentially constant-volume cell. By comparing the true solute flux under a concentration difference with that predicted from conventionally determined transport coefficients, the influence of membrane structure on flux predictability can be determined.

Progress

We have developed a novel membrane transport apparatus that can yield unambiguous transport/design data (cf the 1976 IR&D report, Ref. 3). We have completed our studies of sucrose transport across a Cuprophan dialysis membrane; the results have been reported in Refs. 2 and 4. For this particular membrane and solute, membrane heterogeneity contributes to the effective permeability by no more than 15% when the mean solute concentration is 140 mM.

In membrane performance prediction, solutions are usually assumed to be ideal and dilute. We have recently found that, even for homogeneous membranes, these assumptions can lead to an error in the predicted solute flux if conventionally measured tracer permeabilities are used. We are presently extending these theoretical investigations to study the influence of solution nonideality in heterogeneous membranes. Experimental studies, using our membrane apparatus, are in progress to measure the influence

of membrane structure and solution nonideality on membrane performance for a variety of membrane/solution systems.

Principal Investigators: R. A. Meyer and M. H. Friedman. Mr. Meyer is a special advisor in the Biomedical Program Office, and Dr. Friedman is the Deputy Director of Biomedical Programs.

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PAIN PHYSIOLOGY

A group of peripheral nerve fibers was found that could be responsible for the increased magnitude of pain (i.e., hyperalgesia) evoked by heat stimulation following a first-degree burn.

Problem

The neurophysiological research is aimed at understanding how controlled pain stimuli are encoded into neural signals in the peripheral nerves. Understanding this first level of neural coding is necessary before studying higher order neural centers to which these signals are input. The need for research on this topic is described in the Naval Research Requirements in physiology (ONRINST 3910.2, January 1977, RO41-01), in the Air Force Systems Command Research Planning Guide (Research Objectives) HQAFSC TR 76-01 1.8.3, and in the Army Medical Research Support brochure (U.S. Government Printing Office, 1973, 0-492-688, page 17).

Objective

The long-range objective of the pain research is to develop an understanding of the physiological and psychophysical aspects of pain perception. Our specific objectives are to determine: (a) the peripheral neural coding mechanism for thermal and mechanical pain perception, (b) the peripheral neural mechanism for hyperalgesia induced either from cutaneous injury or peripheral nerve injury, and (c) the effects of therapeutic modalities, such as electrical stimulation of the peripheral nerve, on the activity and responses of primary afferent nociceptive units.

Approach

The pain research employs a laser thermal stimulator, which we had developed previously (Ref. 1), to deliver controlled thermal stimuli to the subject. Standard neurosurgical techniques (Ref. 2) are used to expose the median or lunar nerve of monkeys anesthetized with pentabarbital. The receptive fields of isolated cutaneous units are exposed to a controlled temperature stimulus, and the resultant single-unit neural spike activity is recorded by a computer using standard neurophysiological techniques. The experimental paradigm (e.g., sequence, duration, and repetition rate of thermal stimuli) is modified to fully characterize the neural coding mechanism. Similar paradigms are used with human subjects to determine the significance of particular neural events.

Progress

In our pain research experiments this past year, we identified 189 cutaneous sensory units that responded to heat stimuli. Seventy-seven of the units were "warm" fibers that gave a vigorous neural response to heat stimuli only 2 to 3° above the base temperature. Fifty-eight of the units responded only to high-intensity stimuli and thus are thought to subserve pain sensation (Ref. 2). Fifty-four units did not respond to initial presentations of painful stimuli but developed a response following repeated presentations of painful stimuli, which suggests that these units are responsible for the increased magnitude of pain (i.e., hyperalgesia) evoked by heat stimulation following a first-degree burn (Ref. 3).

Principal Investigators: R. A. Meyer and J. N. Campbell. Mr. Meyer is a special advisor in the Biomedical Program Office. Dr. Campbell is a neurosurgical resident at the Johns Hopkins Medical School.

References

1. R. A. Meyer, R. E. Walker, and V. B. Mountcastle, "A Laser Stimulator," IEEE Trans. Biomed. Eng., Vol. 23, 1976, pp. 54-65.

2. R. H. LaMotte and J. N. Campbell, "Comparison of the Responses of Warm and Nociceptive C-Fiber Afferents in Monkeys with Human Judgments of Thermal Sensation" (accepted for publication, J. Neurophysiol.).

3. R. A. Meyer, J. N. Campbell, and R. H. LaMotte, "Sensitization of A-Delta Nociceptive Afferents to Noxious Radiant Heat Delivered to the Monkey Hand," Abstract, 7th Annual Meeting of the Society for Neurosciences, Anaheim, CA, 1977.

LABORATORY-WIDE RESEARCH AND EXPLORATORY DEVELOPMENT

INTRODUCTION

During the present reporting period, nearly 40% of the Laboratory's IR&D Program was devoted to relatively short-term exploratory investigations carried out in the mission-oriented departments. This component of the IR&D Program fosters initial studies to explore new concepts and techniques. When these investigations are sufficiently promising, direct support is generally solicited for further research and development.

Eighteen projects comprised the exploratory development program during this time period. Many are described in detail in publications that have appeared in print or have been accepted for publication (see Publications Section). Unless otherwise noted, the level of IR&D support for each project was less than about 1/2 professional person for this reporting period.

Of the four projects not discussed below, the largest (level of effort of approximately one person) was devoted to enabling Laboratory personnel to attend meetings and participate in evaluation teams established by the Navy (NAVELEX, PME-106) in connection with classified military programs. The remaining three projects (total level of effort about 1/2 person) were initiated too late in the period to report progress at this time.

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AIR TRAFFIC SAFETY AND CONTROL

An Approach for Multisensor Implementation

Air traffic within the National Aviation System, a mixture of both civil and military aircraft, is increasing at a significant rate. To meet the more stringent safety requirements imposed by this increase in traffic, improved airspace surveillance will be required. Several investigations to date have indicated that multisensor processing of the outputs from existing surveillance sensors offers a cost-effective way to achieve the desired improvement in airspace surveillance. The investigations indicate that the design and implementation of such systems are subject to unexpected effects, especially as a function of sensor site peculiarities. To minimize these unexpected effects, a generic approach for multisensor implementation within the National Aviation System has been derived.

Problem

During the past 7 years, the Laboratory has been applying its expertise to problems of air traffic safety and control. Due to the ever-increasing volume of intermixed air traffic, the problems affect both the military and civilian sectors. One approach to improving air traffic control (ATC) to meet the more stringent safety requirements imposed by the increase in traffic is to improve the airspace surveillance coverage. This can be accomplished by the integrated processing of the outputs from the available electromagnetic sensors. The resultant output may then be presented to the air/traffic controllers on a display that reflects both the best capabilities of each sensor and the overall improved surveillance coverage resulting from the integration of the various sensor outputs. This sensor integration approach has been investigated by the Federal Aviation Administration (FAA) (see Refs. 1 and 2) with the objective of improving airspace safety by providing

1. Improved areal coverage,
2. Improved surveillance system failsoft capability,
3. Improved aircraft tracking across ATC boundaries,
4. Altitude estimates for non-Mode C equipped aircraft, and
5. Improved target resolution.

The integrated approach has been identified as non-colocated multisensor processing chiefly because this approach integrates outputs from several sensor sites in relatively close proximity (15 to 40 nmi separation).*

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* Actually the FAA system is a combination of colocated and non-colocated multisensor processing since at each site the radar and beacon antennas are colocated on the same pedestal.

Such non-colocated multisensor processing is also relevant to the needs of the military, who operate numerous airfields that use the airspace controlled by the National Aviation System.* As is pointed out later, sensors from two such military airfields were included in the multisensor investigations reported in Refs. 1 and 2.

The problem at hand is not one of justifying or quantifying the benefits to be gained from non-colocated multisensor processing. References 1, 2, and 3 adequately address this question. The question at hand is more subtle. During the preparation of Ref. 3, a comparison between similar airspace coverage results from the data bases that were used in the preparation of Refs. 1 and 2 indicated unexpected results. Specifically, the experiment conducted in the Washington, DC, area was designed to collect multisensor surveillance coverage data in an environment in which terrain limitations would not pose problems to electromagnetic energy propagation. The Los Angeles basin experiment (Ref. 2), on the other hand, was specifically designed to include the effects of such an adverse environment. The comparison yielded unexpectedly comparable surveillance results. The questions at hand are, therefore, why the results are comparable and what are the possible implications with respect to air traffic safety and control.

Objective

The objectives of this investigation are to (a) explain the unexpected similarity in the Washington and Los Angeles multisensor coverage results and (b) investigate implications on the future of air traffic safety and control.

Approach

The approach to this problem was straightforward. First, the data bases for Refs. 1 and 2 were examined to construct a picture that would permit valid comparisons. The result was Table 1. Second, Refs. 2 and 3 along with their data and background information were reviewed; the plausible sources for the problem were then articulated. Each was investigated, and the results were evaluated. Last, based on the evaluation, the implications were determined and recommendations formulated.

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* The U.S. Navy has several related developments. One that is currently being implemented and soon will be deployed is a colocated (one ship) multisensor system identified as AN/SYS-1. Work is under way on several other fronts to develop non-colocated (many-ship) multisensor systems to support Force Coordination.

Table 1
Coverage Percentages by Site and Sensor

Washington, DC area, 3 Nov 1972

		Andrews Air Force Base (ADW)				
	Sensor	Radar	Beacon	Radar and Beacon	Not Detected	BAL Totals
Baltimore (BAL)	Radar	8	0	1	12	21
	Beacon	1	1	8	5	15
	Radar and Beacon	1	3	20	3	27
	Not Detected	14	13	10	-	37
	ADW Totals	24	17	39	20	100

Primary source: Ref. 1

Los Angeles basin, 6 Aug 1975

		Los Angeles International (LAX)				
	Sensor	Radar	Beacon	Radar and Beacon	Not Detected	BUR Totals
Burbank (BUR)	Radar	5	1	2	11	19
	Beacon	1	5	5	3	14
	Radar and Beacon	2	8	18	3	31
	Not Detected	14	13	9	-	36
	LAX Totals	22	27	34	17	100

Primary source: Ref. 2

Progress

Background on Experiments. The multisensor experiment in the Washington area was conducted in November 1972 using colocated radar and beacon sensor systems located at Andrews Air Force Base (ADW) and at Baltimore-Washington International Airport (BAL).* The surveillance airspace investigated from a coverage standpoint was the area within 55 nmi of both sensor sites, as indicated on Fig. 1. By design this experiment was to take place in a benign environment as far as terrain effects on electromagnetic propagation were concerned.

The Los Angeles Basin experiment was conducted in August 1975. Data similar to that recorded in the Washington area were recorded at the seven sites noted on Fig. 2; however, for the purpose of this investigation only the Burbank (BUR) and Los Angeles (LAX) Air Surveillance Radar 7 (ASR-7) and beacon sensors were used. By design, this experiment was to take place in a terrain environment with severe effects on electromagnetic propagation.

Data Recording and Reduction. During both experiments, broadband radar video information was recorded, and targets were detected and subsequently tracked. Corresponding recordings of targets detected by the colocated beacon sensors, as extracted by the FAA Automated Radar Terminal System Model III (ARTS III), were also tracked. These radar and beacon track files were used as the primary basis for determining the values of Table 1.

Results. In Table 1, the percentage of tracks detected (coverage percentages) is indicated for each experiment for each sensor and all of the possible combinations of each sensor with the other three sensors. The total base of tracks for each experiment was defined by all tracks detected by at least one of the four sensors. Interpretation of Table 1 can best be explained by examples. The BAL radar detected approximately 21% of the tracks in the area of common coverage that were defined by all four sensors. In addition, this sensor detected 12 of the 20% of the total number of tracks that were not detected by either sensor at ADW. As another example, all four of the sensors at BUR and LAX simultaneously detected 18% of the tracks defined in the common coverage region.

Table 1 is versatile and presents much significant information, the major portion of which has been treated in other forms in Refs. 1 and 2. For the purposes of this investigation, the

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* The Air Traffic Control Radar Beacon System (ATCRBS) is referred to as the beacon.

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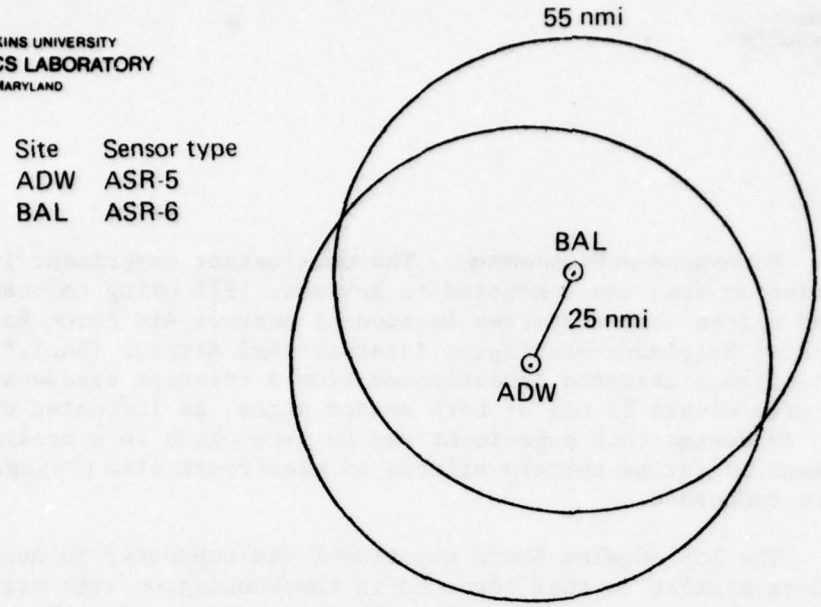


Fig. 1 Baltimore-Washington Area Multisensor Coverage Experiment

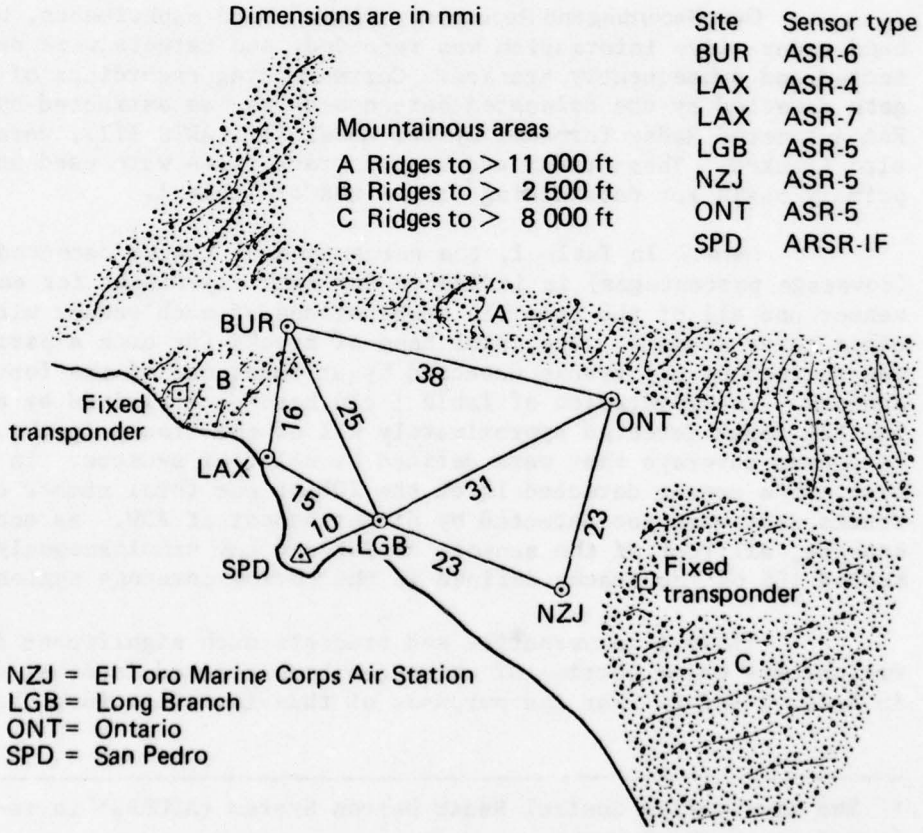


Fig. 2 Los Angeles Basin Multisensor Coverage Experiment

important fact is that the coverage percentages of BAL and BUR and ADW and LAX, taken in pairs, are of similar magnitudes. This was not expected. Prior to the experiments, it was expected that ADW, BAL, and LAX would have comparable coverage performance, with BUR being adversely affected by its terrain limitations.

Analysis. Plausible reasons were explored for the noted results, among them site-to-site geometry, earth curvature, antenna uptilt, sensor performance, data reduction differences, and unsuspected terrain limitations or sensor siting problems.

Evaluation of Results. The site-to-site geometry, earth curvature, sensor performance, and data reduction differences are judged to have had little impact on the problem. Since coverage to the east of BAL does not appear to be adversely affected, it is a good assumption that the antenna tilts at BAL were not set high so as to reduce ground clutter with an attendant loss in coverage. It is judged that the relative placement of the BAL sensors with respect to this ridge significantly affects the BAL coverage as noted in Table 1. In short, the coverage performance of electromagnetic sensors can be materially affected by seemingly small site peculiarities. Such situations are highlighted by and to a certain extent compensated for by multisensor processing.

Implications. *To assure the safe passage* of both military and civil aircraft in an increasingly crowded airspace, especially in hub areas, an increase in the performance of the airspace surveillance system is required. Due to cost benefit considerations, new approaches such as satellite-based sensor systems will most likely have to wait for many years. In the interim, the capabilities of the current surveillance systems will have to be extended. Multisensor processing of existing sensor outputs can provide this requisite capability in most of the areas of concern (see Ref. 1). To do this, however, each configuration of sensor sites will have to be addressed on an individual basis.

Principal Investigator: J. P. Berry. Mr. Berry is an Assistant Supervisor and a senior engineer of the Surveillance Systems Project office of the Fleet Systems Department.

Publications, Presentations, and References

1. "ARTS Enhancement Support Program Multisensor System Study," APL/JHU FS-75-204, Feb 1974.

2. "Los Angeles Coverage Evaluation for Multisensor Design Support," APL/JHU Preliminary Draft FP8-T-039, undated and unpublished.

3. J. T. Miller, Jr., and J. P. Berry, "Multisensor Utilization Investigation," Radar 77 Conference Paper, IEEE Radar-77 Conference, 26 Oct 1977, London, England.

BIOMEDICAL ENGINEERING

A broad spectrum of physiological research is important to both civilian and DoD agencies (e.g., Naval Research Requirements ONRINST 1310.2, January 1977, R041-01, R041-08, and R041-20). For many years the Laboratory has engaged in a wide range of biomedical engineering research and development, funded by the Department of Health, Education, and Welfare (HEW), the National Institutes of Health (NIH), the Veterans Administration (VA), the National Aeronautics and Space Administration (NASA), the Department of Defense (DoD), and private agencies, primarily in collaboration with the Johns Hopkins Medical Institutions.

During the current reporting period, small projects dealing with intracranial pressure measurement and with arterial hemodynamics were carried out under the IR&D Program, at a total level of effort of about 1/2 person/year. In the intracranial pressure project, several prototype sensors have been constructed and their performance has been determined by animal tests. In the arterial hemodynamics project, casts of arteries are being constructed for experiments in investigating correlations between blood flow and arteriosclerotic lesions.

INTRACRANIAL PRESSURE SENSOR

Problem

Elevated intracranial pressure secondary to head injury, surgery, and various pathological conditions can lead to severe brain damage and, in extreme cases, to death. The diagnosis and monitoring of this condition, therefore, have become a problem of national importance and are yet to be fully solved in spite of almost two decades of research and development.

Objective

Our objective is to develop an implantable pressure sensor suitable for both acute and chronic clinical use.

Approach

During the previous reporting period, a concept was devised for a totally implantable, passive pressure sensor that can, following implant, be interrogated at any time to read out or warn of excessive, intracranial pressure. The sensor consists of a passive electrically resonant circuit whose capacitance, and

therefore frequency, varies with intracranial pressure. The technical design of such a device must include a means of establishing a stable reference pressure for comparison with the intracranial pressure.

Progress

At the present time, our concept is based on an absolute pressure reference with the reference pressure gas contained within a very small volume inside the implantable sensor - a volume of approximately 0.016 cm^3. Work continues to determine which combination of reference pressure gas, wall material with which it is in contact, sensor geometry, fabrication techniques, and environmental processing will provide the stability required of this small volume of gas.

Currently, several prototypes have been constructed that confine the reference pressure gas within an all-metal enclosure. Engineering and animal tests indicate that reference pressure drift is less than 3 to 5 mm H_2O/day, which is within limits for acute clinical use. These tests have indicated the major cause of the residual drift, and further redesign is under way. Verification of the redesigned sensors' performance in both acute and chronic clinical use will be undertaken when these prototype sensors are available.

ARTERIAL HEMODYNAMICS AND PULSATILE FLOW

Problem

The distribution of atherosclerotic lesions in the large arteries strongly suggests that blood flow patterns (hemodynamics) adjacent to the vessel wall play a role in the development of the disease. It is not yet clear which aspects of the blood flowfield are most important in this regard, in part because the distribution of these "hemodynamic stress factors" in the vasculature is not known with a resolution comparable to the scale of atherosclerotic foci. Similarly, the mechanisms by which these stresses provoke or contribute to the pathologic response are still speculative, and quantitative response data are extremely limited.

Objective

The first objective of this study is to understand the morphological response of the human vascular wall to hemodynamic stress.

Approach

The objective is to be approached by generating flows, fluid dynamically similar to in vivo arterial flows, through casts of human arteries, measuring the flowfield noninvasively with a laser doppler velocimeter, and comparing the hemodynamic environment at the wall of the cast with histologic observations on the parent vessel from which the cast was made. High-resolution quantitative results correlating hemodynamic stress with arterial morphology can thereby be obtained. Conclusions regarding the mechanisms of hemodynamic insult and arterial response should follow.

Progress

The task was initiated during the last quarter of the reporting period. During that time, a rotating valve was designed to produce a pulsatile flow through the cast, and a cast support was constructed. A casting procedure was evolved to provide a cylindrical section upstream of the cast of the vessel itself; velocity measurements on the center line of the cylindrical section are to be manipulated to give the actual flow wave through the cast. A final casting protocol was developed and used to provide a hard, smooth-surfaced, and clear cast of a human aortic bifurcation provided by Dr. G. M. Hutchins of the Hopkins Department of Pathology. The cast has been mounted in the flow system and is now ready for use.

Principal Investigators: J. T. Massey, M. H. Friedman, J. G. Chubbuck, and L. J. Viernstein. Dr. Massey is the Director and Dr. Friedman is the Deputy Director of the Biomedical Engineering Programs in the Biomedical Programs Office. Dr. Chubbuck is a section supervisor in the Dynamics Analysis Group, and Mr. Viernstein is a senior physicist in the Operational Systems Development Branch, both of the Fleet Systems Department.

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COMMUNITY ANNUAL STORAGE ENERGY SYSTEM

The Community Annual Storage Energy System (CASES) is a scheme to heat and cool communities efficiently. The concept was initially explored with IR&D support; further work has been entirely funded by the Department of Energy. The Norfolk Naval Base is a possible candidate for a prototype system. In brief, CASES employs thermal storage and collects both heat and "cold" when they are available "energy-free" to reduce seasonal energy consumption. Efficiently managed responses to diurnal changes in both the weather and in the hourly heating and cooling requirements of the diverse buildings in the CASES community are also exploited to reduce further the fuel required for heating and cooling. CASES heats small buildings with waste heat from large buildings and cools large buildings with the heat deficit produced when heating small buildngs with heat pumps. Because much of the energy required for heating and cooling is collected energy-free as surplus heat or cold, CASES can reduce energy consumption for heating and cooling by as much as 80%. Most of the fuel saved is natural gas or oil.

Problem

The efficient utilization of power to heat and cool buildings is a problem of national concern and of importance to DoD as well as to civilian agencies (e.g., Naval Research Requirements ONRINST 3910.2, January 1977, RO24, p. 15). The mobility of the U.S. Navy is threatened as the United States becomes even more dependent upon foreign oil. As heating and cooling buildings represents more than 20% of all the energy used in the United States, CASES can save more oil than the U.S. Navy uses.

Objective

The long-range objective of the CASES program is to convert the United States economy from its current practice of supplying heat to buildings with oil and natural gas that are essential petrochemical feedstocks. In the short run, the object of the CASES program is to demonstrate, first by simulation model and then by field test, that the concept is both economical and efficient. These objectives refer to the entire CASES program of which this work is a part.

Approach

CASES is currently being evaluated via hourly simulation of an operating year to define cost and performance characteristics.

The first module of the simulation code calculates hourly heating and cooling requirements of individual building types when subjected to recorded weather data. The second module combines these building types, heating and cooling equipment, and distribution pipelines to convert the entire community into a single equivalent load center. Subsequent modules will model the operation of the central CASES plant and perform detailed cost and performance analyses for the entire system, sponsored by the Department of Energy through the Argonne National Laboratory.

Progress

During the initial exploratory phase, IR&D support was used to address the problem of collecting both heat and cold from the environment with a minimum of electrical energy required. A set of possible concepts for an Environmental Energy Exchanger (EEE) was developed. Also, as part of the EEE, a new concept in ice making called the Flexible Ice Former (FIF) was invented and patented.

The concept's technical methods developed for CASES heating and cooling can be summarized as follows:

Cooling. Water at 40°F is first distributed through pipes that extend throughout the community and then passed through cooling coils in the various buildings. Leaving these cooling coils at a temperature of about 60°F, the water is returned to a central ice deposit where it is again cooled to 40°F prior to being repumpted through the flow loop. The heat imparted to the water when it is used for cooling is saved within the system until needed or until it can be rejected without an energy-consuming heat pump. This is in contrast to conventional air-conditioning systems that remove heat from buildings and eject it by means of a heat pump (air conditioner) into the atmosphere, where it is lost.

Heating. The community is heated by water-source heat pumps. Conventional air-source heat pumps become inefficient when the output air falls below 32°F, but the heat pumps used in CASES remain highly efficient because 60°F water, distributed from the central CASES plant, is always available as a source of heat. The heat pumps extract thermal energy from the water, lowering its temperature to 40°F. The 40°F water is returned to the central facility in the same 40°F mainline used for cooling water, thus avoiding additional piping expense. Likewise, the pipeline used to supply 60°F heat-source water to the heat pumps is the same as the 60°F pipeline used to return water to the central ice store during the cooling cycle. Thus, CASES has only two uninsulated pipelines,

one for 40°F water and one for 60°F water, yet both heating and cooling are always available to all users.

The central CASES facility must be prepared to supply the net heating (60°F) or cooling (40°F) water. One particularly attractive approach is simply to store large quantities of these thermal waters in two separate aquifers. The cold water store can be replenished in winter and the warm water store can be replenished in summer with little consumption of electrical energy. In regions where aquifer storage is impractical, an insulated ice water pond can be used for seasonal storage of heat and cold. As heat is removed by an ice machine heat pump in winter, the water in the pond is converted to ice. In summer when cooling is required, excess heat collected in the buildings is returned to the ice water pond to recharge it with heat (melt ice) as discussed in "Cooling," above.

Principal Investigator: W. R. Powell. Dr. Powell is a senior physicist in the Space Electromechanical Design Group of the Space Department.

Presentations

A presentation of the CASES concept was given to the Naval Facilities Engineering Command Headquarters in Washington (Arlington, Virginia) on 29 December 1977. This presentation resulted in a broader presentation on 24 January 1978, at which personnel from the Norfolk, Virginia, Naval Air Station were in attendance to discuss possible applications of CASES to the Norfolk Naval Base.

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ELECTROMAGNETIC CONDUCTIVITY SURVEY SYSTEM

The Navy's extra low frequency (ELF) transmissions at 45 and 75 Hz provide a unique source of narrowband electromagnetic radiation that is detectable over much of the world. Investigation of the effects of the earth's conductivity anomalies on these (and other) transmissions can provide data valuable for geophysical as well as communication purposes.

Problem

Increased knowledge of the physical nature of the earth's crust and of energy transmitted through the earth's crust are needed to meet civilian as well as DoD requirements, and improved knowledge of electrical conductivity is of particular interest to the Navy (e.g., Naval Research Requirements ONRINST 3910.2, January 1977, RO32-01, p. 19).

Objective

The objective of the investigation was to explore the possibility of utilizing the Navy's ELF transmissions to measure conductivity anomalies of the earth's crust.

Approach

In essence, the proposed technique is to measure and interpret the scattering of electromagnetic waves from subterranean hidden conductivity anomalies. The source of the incident waves is to be the extremely stable ELF radiations from the U.S. Navy's submarine communication transmitter in Wisconsin (originally called SANGUINE, now SEAFARER), which has been operational for many years and is currently broadcasting. The radiation consists of coded pulses at 45 and 75 Hz that propagate with very little loss over most of the earth and penetrate to depths of several kilometers. The advantages of this method are: capitalizing on the enormous investment already made by the United States in this facility; the enhancement of receiver sensitivity available through long-time integration of the extremely narrowband signals (to reject unwanted environmental noise); and the single-point source of the incident signal. These represent significant advantages and flexibility over the conventional magnetotelluric (MT) exploratory technique. The information from these measurements would, however, be combined with any useful data from MT signals (0.01 to 11 Hz) and very low frequency (VLF) (8 to 15 KHz) signals (also from Navy transmitters),

which would add information at both shallower and greater depths. These data would then be combined with data from other anomaly detectors (e.g., gravity and magnetic surveys) for final processing.

The technical feasibility of discovering and measuring certain properties of conductivity anomalies with this technique appears to have only moderate technical risks; however, there is at present less certainty in the interpretation of the resulting data and their correlation with other information to identify prospective geothermal sources or other features of interest. Consequently, in addition to analyzing and experimentally establishing the validity of the wave-scattering measurement techniques, the work plan would include analysis and experiments to learn how to interpret the resulting data.

The electromagnetic prospecting community has exploited MT and audio magnetotelluric (AMT) techniques in the past with varying degrees of success and frankly expressed desire for additional technique. The proposed technique, if successful, should offer a powerful adjunct to current surveying methods for geothermal sources (and possibly other geologic features of interest).

Progress

An exploratory analysis of the effects of anomalies was investigated and reported in Ref. 1. The analysis is a calculation of the scattering of an ELF wave from a subterranean spherical conducting body. This leads to a conceptual ELF receiver system that measures both electrical and magnetic (vector) fields. The study also revealed the basic feasibility of the technique. Further analyses are required to understand the effects of terrain. Analysis could also establish optimum search parameters, such as antenna length and diameter, as well as field procedures, such as swath separation, integration time, search pattern, and the like.

It is conceivable that in a field exercise no conductivity anomalies will be detected. However, it is more likely that too much information will be received from multiple, extended, and other complex anomalies, so that interpretation of data will be very difficult. Several solutions to this difficulty are suggested:

1. The coherence of the incident ELF signals provides the possibility of processing sinusoidal signals from conductivity intrusions to determine the exact location and dimensions of the anomaly, in contrast to the poorly defined estimation of location and size from the "1/R" anomaly signatures in the usual MT and

AMT analysis. The ELF wavelengths in the ground are fairly long (2 to 10 km) and far-field type calculations do not apply in detail, but the first-order calculations are adequate to evaluate the signal-to-noise radio.

2. Each model of an anomaly, from a simple spherical intrusion to segmented dikes, horsts, and grabens, will exhibit a characteristic space modulation pattern. The analysis of such patterns could establish whether sufficient accuracy is available for reliable model building.

3. Data from other survey techniques (e.g., MT or AMT) may be correlated with the ELF (and VLF) antenna data to eliminate returns from uninteresting or nonexistent anomalies. Optimum blending of the data and the inversion of the matrices involved will require careful analysis to determine their scope of application.

4. Should distant sources of background noise (such as thunderstorms) prevent adequate ELF signal reception, it is likely that such interfering signals can be at least partly cancelled by coherently subtracting the received data at one location from the simultaneously received data at another location via clock synchronized recordings, since the scattered field from a single anomaly would be different at the two locations, whereas the interfering signals, being from distant sources, would be the same.

Encouraged by these considerations, an appropriate work plan was submitted to the U.S. Geological Survey (USGS) for support. However, costs were higher than the USGS was prepared to support in view of the considerable technical risk, and it was suggested that a relatively inexpensive feasibility experiment be carried out. Consideration is being given to this suggestion.

Principal Investigators: J. W. Follin, K. Yu, and C. A. Shipley. Dr. Follin is Technical Director, Mr. Yu is a senior physicist, and Mr. Shipley is a senior engineer in the Advanced Research Programs Office.

Reference

1. K. Yu, "An Electromagnetic Conductivity Surveying System," APL/JHU QM-77-007, 17 Jan 1977.

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FEASIBILITY DEMONSTRATION, AUTOMATED MAINTENANCE SUPPORT TOOL

The ability to maintain increasingly sophisticated individual components in a Naval Combat Weapon System frequently limits readiness. Moreover, for smaller ships, equipment maintenance with a small crew results in an effective ceiling on the complexity of the components deployed. Thus, a significant increase in the ability to maintain equipment can result in a direct increase in combat effectiveness. This feasibility demonstration addresses one approach to a general improvement in maintainability by developing an Automated Maintenance Support Tool (AMST) that can interact with and provide broad support to an operator during routine maintenance and diagnostic repair. The project was initiated during the previous reporting period and has now been terminated.

Problem

The problem of shipboard maintenance for Naval Combat Weapon System components is generally treated by training, the preparation of documentation, and the limitation of complexity in the equipment deployed. The concept of the AMST is to organize the information required to maintain the equipment and facilitate the retrieval of appropriate information. Two information storage techniques are used:

1. Digital computer processing to access data by various logical paths and

2. Microform technology to display static information.

By using inexpensive, off-the-shelf equipment, we have demonstrated that the AMST provides a potential avenue for improving the maintenance process.

Objective

The demonstration AMST has shown that a system can be produced that will

1. Provide programmed support for routine maintenance and standard diagnostics for a given equipment set,

2. Provide nonprogrammed access to technical data, including text, drawings, waveforms, and computations, to support troubleshooting in situations for which no diagnosis has been anticipated, and

3. Provide a mechanism by which additional programmed support can be developed for an arbitrary equipment set.

Furthermore, the AMST has been shown to be capable of

1. Displaying diagrams, flow charts, waveforms, text, mathematical equations, and other graphic data,

2. Prompting an operator and processing inputs to select displays, providing further prompting, or performing calculations,

3. Operating with an easily changed data base, thereby allowing the AMST to be essentially independent of the equipment to be maintained, and

4. Being inexpensively mass-produced in a semiportable model that can interface directly with standard test equipment.

Approach

The AMST combines the technology of minicomputers with that of micrographics. The minicomputer is used to

1. Prompt the operator and, based upon the operator response, branch forward and back through a program decision tree,

2. Provide the operator with an unprogrammed information retrieval access to all data in the data base,

3. Address the micrographic device and display the required graphics or text, and

4. Perform computations and analyses using parameters that have been retained, keyed in, or directly interfaced (not demonstrated).

The micrographics device is used to

1. Automatically display graphics and text that cannot be economically retained in a computer readable format,

2. Automatically display manuals and related documents, and

3. Manually peruse micrographic materials.

The AMST uses a data base consisting of a replaceable automated file (floppy disk) and a micrographic file (ultrafiche cassette). A separate data base may be used for every piece or class of equipment to be maintained.

Figure 1 shows the AMST equipment configuration used for the Feasibility Demonstration System (FDS). It consists of three units:

1. An Operator Unit that comprises the microform display, an optional computer display, and a computer input device. All operator inputs and outputs are via this unit. For the FDS, the unit was packaged in three independent elements.

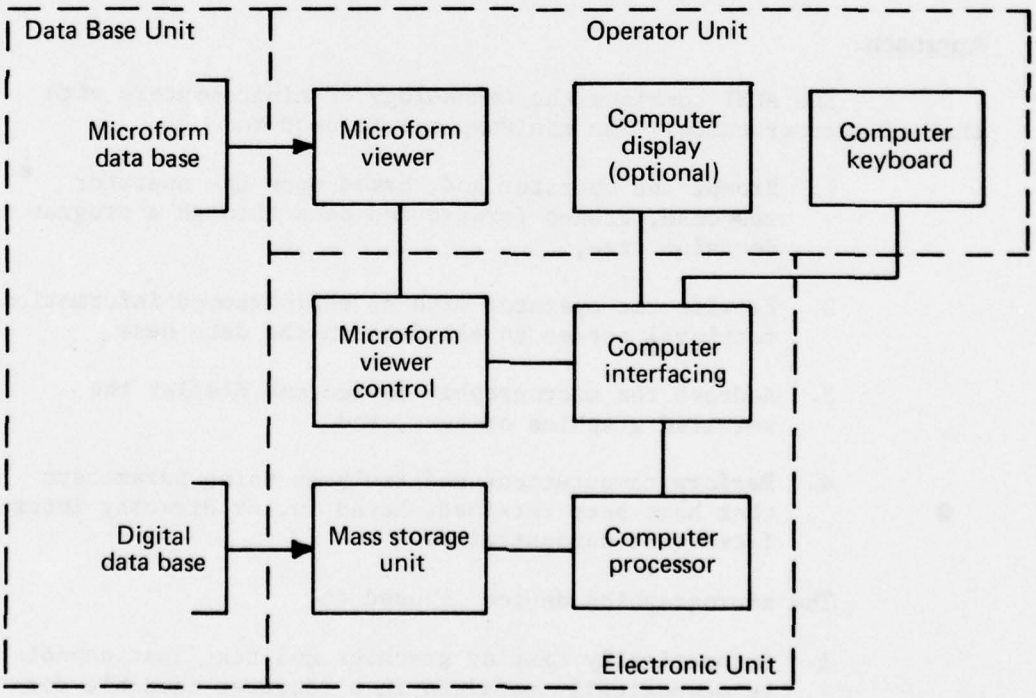


Fig. 1 FDS Automated Maintenance Support Tool Configuration

2. A Data Base Unit that consists of the microform and digital data bases. For the FDS, a single data base with several demonstration capabilities was used. The interchangeability of data bases is, however, a requirement.

3. An Electronic Unit that contains a computer (or microprocessor), a mass storage (floppy disk) device, a microform viewer control element, and appropriate interfacing. The FDS uses a permanently mounted unit; nevertheless, it is shown that the Electronic Unit can be packaged as a portable unit.

Progress

A feasibility demonstration AMST system has been implemented and evaluated. The system uses approximately 2% of its storage capacity for the complete AN/SPS-25 maintenance manual. Using the keyboard entry, the operator can

1. Query the system for instructions in its use,

2. Select a manual or demonstration,

3. Request a specific page, table, or figure in the manual,

4. Request the index to a manual by a key letter or word,

5. Request the table of contents of a manual,

6. Request the next or previous page,

7. Request the last n images displayed, and

8. Provide a mnemonic for selected pages and request them by this mnemonic.

In addition to the basic manual, a fault logic demonstration has been implemented which allows the user to

1. Step through the fault isolation sequence,

2. Review illustrations showing locations of key compoments,

3. Display block diagrams,

4. Access text sections on concept of operations, etc., and

5. View printed circuit board layouts and component lists.

The system is complete and available for demonstration. It has been demonstrated to visiting groups from the Navy and NSA.

Principal Investigator: B. I. Blum. Mr. Blum is a senior mathematician in the Operational Systems Development Branch of the Fleet Systems Department.

Publications and Presentations

1. Users' Manual for the AN/SPS-25 Demonstration, APL/JHU F3C-0-240.

2. B. I. Blum, "Low-Cost Mixed-Media Picture Data Retrieval," Workshop in Picture Data Descriptions and Management, IEEE 77 CH1187-4C, 21-22 Apr 1977.

THE JOHNS HOPKINS UNIVERSITY
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MAGSAT-II

From the study of the Magsat-II mission to date, it appears that satellites at very low altitudes have a distinct advantage in the measurement of the earth's magnetic and gravity fields. To be able to obtain the best data, drag-free satellite operation is highly advantageous. The type of drag-free (DISCOS) system demonstrated in orbit on the Triad satellite appears to be satisfactory for the Magsat-II mission. A pair of satellites (or even more than two) offer additional advantages in obtaining the most accurate data on the earth's magnetic and gravity fields. The data could be used for mapping the earth's gravity and magnetic fields, for geological exploration, and possibly for earthquake prediction.

Problem

APL is studying the requirements and characteristics for a second Magsat (Magnetic Survey Satellite) mission that will provide improved magnetic data and have wider space applications than the Magsat-I mission. The Magsat-I satellite being developed for NASA/Goddard Space Flight Center will provide worldwide data for use in updating and refining magnetic charts, obtaining an accurate quantitative description of the earth's magnetic field, and compiling and interpreting crustal magnetic anomaly maps. The satellite's orbit will have a perigee of 325 km, an apogee of 550 km, and an inclincation of 96.9°. Magsat-II will be designed for a lower, drag-free orbit to meet the objectives listed below.

Objective

Five specific objectives for a Magsat-II mission are

1. An improved model of the earth's magnetic field,
2. Improved magnetic charts for navigation and other purposes,
3. Improved gravity charts,
4. The identification and correlation of magnetic and gravity anomalies, and
5. A more precise measurement of both spatial and temporal variations of the earth's magnetic field.

Each of these objectives is important to the U.S. Geological Survey as well as being recognized Navy and/or Air Force research requirements (Naval Research Requirements ONRINST 3910.2, January 1977, R 032-01, p. 19; Air Force Systems Command Research Planning Guide HQ AFSC TR 76-01, 3.4.1, 3.4.2, 3.4.5, pp. 3-20, 3-21, 3-22).

Other objectives could be

1. Mapping magnetic and gravity anomalies,
2. Exploration for minerals in the earth's crust, and
3. Earthquake prediction.

Approach and Progress

General Design Characteristics for Magsat-II. Table 1 lists some general design characteristics that are appropriate for a Magsat-II mission and that could meet the five specific objectives.

Table I

Magsat-II General Design Characteristics

Orbit inclination:	90°
Orbit altitude:	180 to 400 km
Launch vehicle:	Shuttle
Approximate launch date:	1983-84
Approximate payload weight:	1000 kg
In-orbit station keeping system:	Single-axis DISCOS
Orbit lifetime:	a) 10 years or longer with in-flight refueling b) 1 year if recovered by shuttle
Instrumentation:	a) Magsat-I scalar magnetometer improved to obtain ±0.1 gamma accuracy b) Magsat-I vector magnetometer c) Magsat-I attitude transfer system d) Magsat-I attitude detection system
Tracking system:	GPSPAC
Data acquisition:	TDRSS
Attitude control system:	Aerodynamic stabilization in pitch and yaw; flywheel stabilization in roll.

Discussed in a later section of this report is a configuration consisting of two satellites at lower altitudes, which seems more appropriate for carrying out other applications such as earthquake prediction, magnetic and gravity anomaly mapping, and exploration for minerals in the earth's crust.

Application of Drag-Free Satellite Concepts to a Magsat-II Mission. Figure 1 is an illustration of a disturbance compensation (DISCOS) drag-free system as implemented on the Triad satellite (Ref. 1). A spherical, high-density proof mass is located within a hollow spherical enclosure that shields the proof mass from aerodynamic and solar radiation pressures. The proof mass is then free to follow an orbit determined only by gravitational forces. As drag retards the satellite, a capacitive bridge circuit involving the proof mass is unbalanced, causing the aft thruster on the satellite to accelerate the satellite so as to cause a recentering of the proof mass within the spherical dead zone.

Figure 2 presents actual data from the Triad satellite which shows how the proof mass moved within the spherical dead zone. Approximately 1 min from the start of the data, the proof mass position reached the dead zone surface, actuating the aft valve. The aft thruster then fired, accelerating the satellite to cause a recentering of the proof mass. Approximately 2 min later the total impulse of the drag force on the satellite exceeded the impulse imparted by the firing of the aft thruster, causing the proof mass once again to approach the surface of the dead zone. At times of 5 and 11 min, the aft thruster again fired to maintain the drag-free state. As can be seen, the total translational motion of the satellite from a true drag-free orbit was less than 1 mm. This technique is uniquely suited to obtaining those extremely accurate and predictable orbits that are required for improved knowledge of magnetic and gravity anomalies at very low altitudes. The tracking results show that it was possible to predict the along-track orbit position of the Triad satellite to within 80 m over a period of 60 days and 230 million miles of travel (1 mm per 5000 km along track average).

The problem presented for the Magsat-II is really much simpler since we need only to track the satellite position after the fact rather than the vastly more difficult problem of long-term tracking prediction. For a Magsat-II we would expect to be able to track the satellite to better than 5 m absolute position in spherical coordinates, i.e. in the along-track, cross-track, and vertical directions.

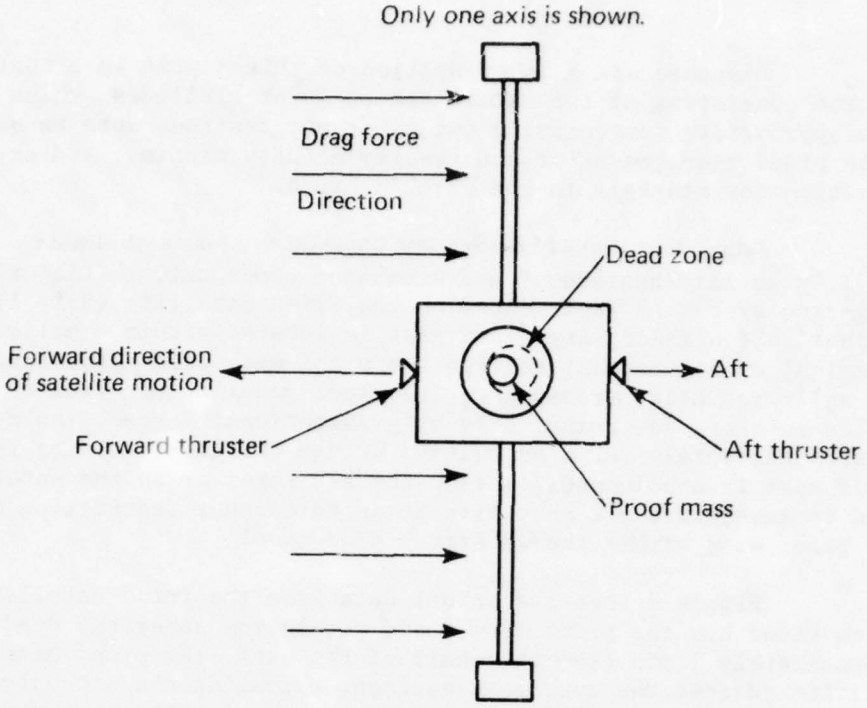


Fig. 1 Illustration of DISCOS as used on the Triad Satellite

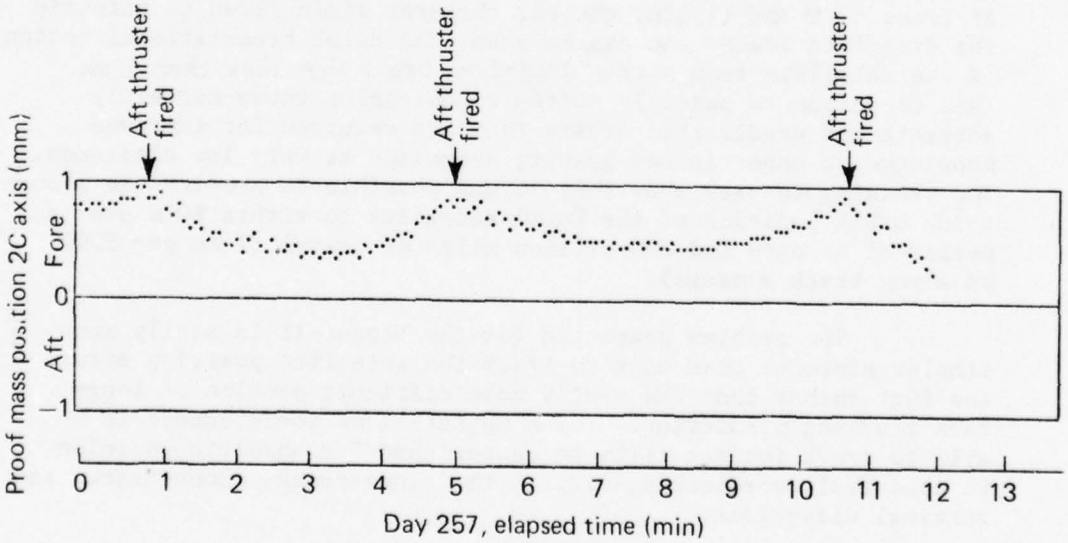


Fig. 2 DISCOS Proof Mass Position

Figure 3 illustrates a single-axis DISCOS system that has been used on the TIP-II and TIP-III satellites. In the single-axis DISCOS, the proof mass is a hollow cylinder levitated by means of eddy currents generated within the proof mass along a single conductor center wire carrying an alternating current. As the proof mass moves forward or aft along the center conductor (whose attitude is controlled along the flight direction), a light detector is covered or uncovered so as to create an unbalanced bridge circuit that results in the firing of a pulse plasma jet as required to recenter the proof mass. Since aerodynamic drag and radiation pressure forces are generally cumulative only along the velocity vector of the satellite, the single-axis DISCOS is a somewhat simpler embodiment of the DISCOS concept. Either the omnidirectional DISCOS or the single-axis DISCOS is applicable for a Magsat-II mission.

Magsat-II Orbit Configuration. Figure 4 illustrates a conceptual orbit configuration for a Magsat-II spacecraft. It is desirable to have as low a projected area to the airstream as possible in order to reduce drag force. A single-axis DISCOS is shown whose purpose is to make the satellite accurately trackable without being affected by the vagaries of drag. Two fuel tanks are shown which could be filled with hydrazine and refueled in orbit by shuttle. Many of the elements of Magsat-I can be used, including the scalar and vector magnetometers and the attitude detection and attitude transfer systems. Only a small fraction of the volume and weight available in the shuttle would be required.

Mission Profiles for Magsat-II. The great weight and volume-carrying capacity of the shuttle allows innumerable mission profiles for Magsat-II. One profile that was presented to the Earth Dynamics Working Group meeting, Boulder, Colorado, in July 1977, is shown in Fig. 5. For this profile, the shuttle would release Magsat-II at a convenient altitude, such as 250 km. When drag forces cause the satellite to reach a preselected altitude, such as 180 km, DISCOS would be turned on, resulting in the maintenance of a constant altitude to obtain data for a nominal period, such as 6 months. Thrust could then be applied using the hydrazine fuel to raise the orbit to a nominal altitude of 400 km. The orbit might then be allowed to decay naturally so that 3½ years later the satellite would again return to a low altitude where DISCOS would again be turned on to maintain a constant altitude and the capability for extremely accurate tracking. Such a mission profile would have the advantage of providing very accurate, worldwide, magnetic measurements for the purpose of obtaining the 5-year updates of magnetic charts as are typically needed by the U.S. Geological Survey. Since on-board propulsion is available, it would not be difficult to include other mission profiles as might be either preselected or conceived after the satellite was placed in orbit.

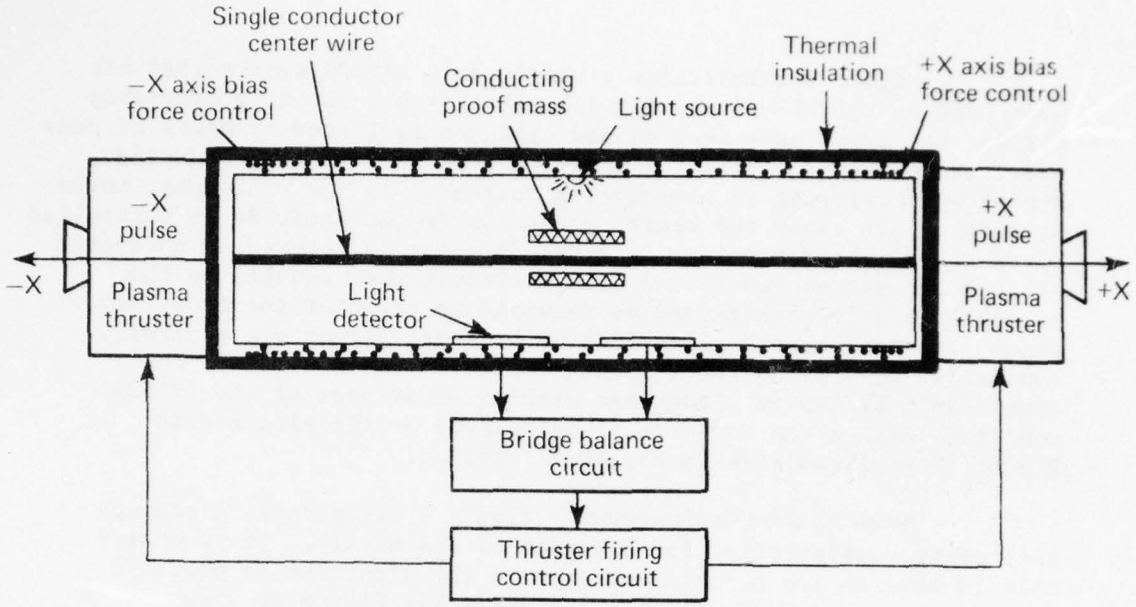


Fig. 3 Diagram of a Single-Axis DISCOS

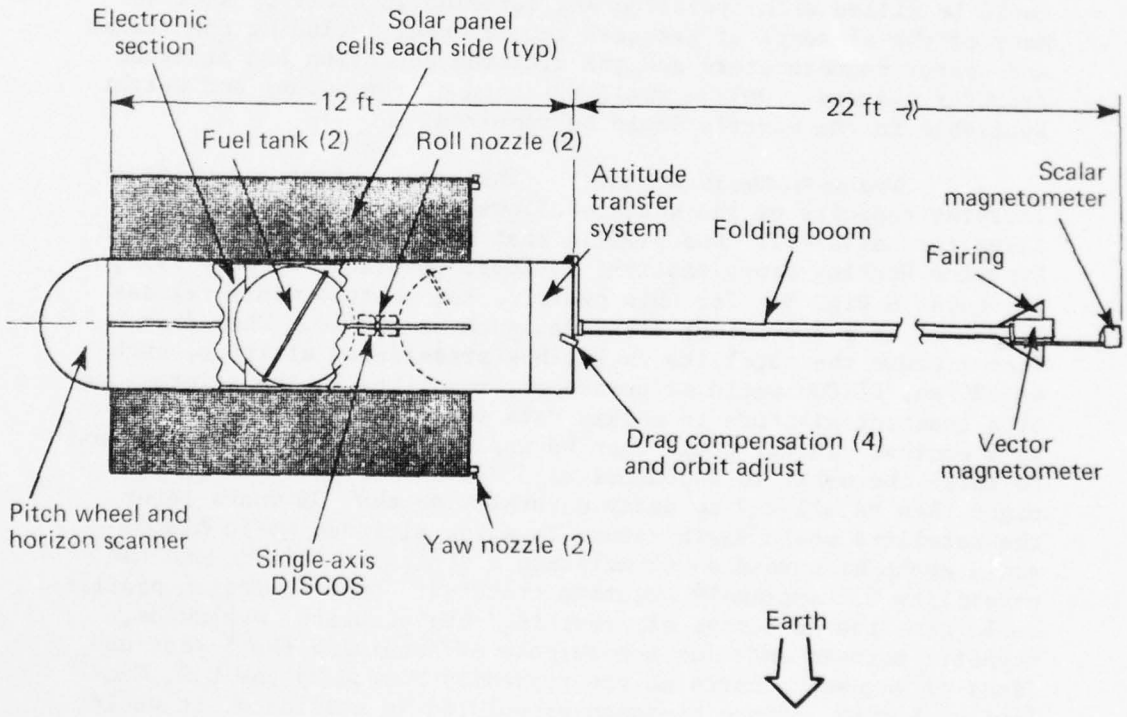


Fig. 4 Magsat-II Orbit Configuration

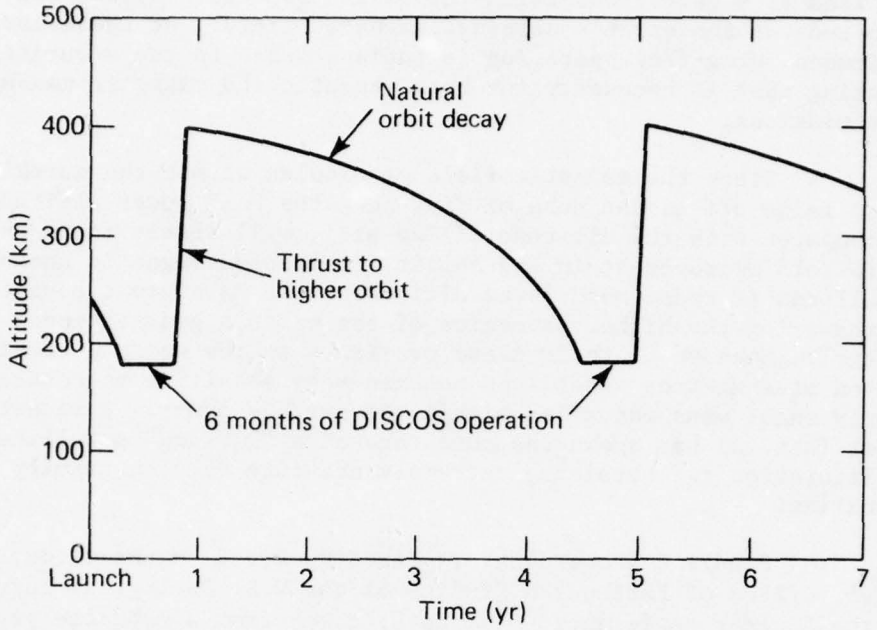


Fig. 5 Possible Mission Profile for Magsat-II

Tracking a Magsat-II. One of the possible means of tracking a Magsat-II would be to use the general-purpose computer (GPS) satellite with on-board satellite equipment known as GPSPAC, which is being developed by The Johns Hopkins University Applied Physics Laboratory for NASA and the Defense Mapping Agency. In its most accurate tracking mode, GPS would allow the orbit computation of satellite position to 5 m when the full GPS satellite constellation is available.

A Two-Satellite Configuration for the Magsat-II Mission. In the three days preceding the presentation of Magsat-II concepts at the Earth Dynamics Working Group meeting in Boulder, a constant interaction with geophysicists working in the areas of geology, earthquake prediction, geodesy, and geomagnetism made it apparent that there are more desirable configurations for a Magsat-II mission than the configuration previously described — in particular, a system of two orbiting spacecraft at an altitude between 120 and 150 km with a 100-km along-track separation. By making a differential magnetic measurement between the two spacecraft, it is possible to eliminate to a large extent the large temporal variations in the earth's magnetic field data. By making measurements from more than one spacecraft simultaneously, one not only gets the

difference field but also the absolute field at each point, which can lead to a better understanding of the sources, extent, and magnitude of the earth's external magnetic field. At these low altitudes, drag-free operation is indispensable to the accurate tracking that is necessary for both geodetic and magnetic measurement missions.

Since the magnetic field of dipoles within the earth's crust falls off as the cube of distance, the much lower altitudes, as compared with the altitude of Magsat-I, will result in an 8- to 10-fold improvement in the ability to resolve magnetic anomalies. Satellites at these much lower altitudes also have great advantages in measuring the higher harmonics of the earth's gravitational potential. Because of their close proximity to the earth's crust, the motion of drag-free satellites becomes very sensitive to comparatively small mass anomalies within the earth's crust. A recent paper (Ref. 2) has shown the advantage of a "low-low" satellite configuration for obtaining extremely accurate data on gravity anomalies.

Figure 6 shows data presented by Dr. R. M. Hamilton, Chief, Office of Earthquake Studies of the U.S. Geological Survey, at the Boulder conference. The data, taken from a magnetic gradiometer against a fault line, indicate the possibility of a magnetic

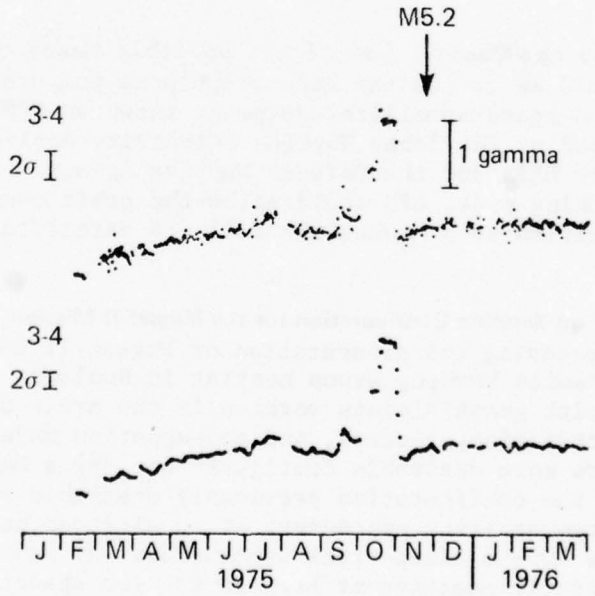


Fig. 6 Differential Magnetic Field Precursor of an M5.2 Earthquake

precursor to earthquakes. This precursor might be caused by a magnetostrictive effect resulting from crustal stress on ferromagnetic materials within the crust. By means of two satellites in differential magnetic measurement mode, it may be easier to detect such stress build-up over large regions as compared with a magnetic differential mode (as was the case in Fig. 6) at a separation distence of only 7 km. It should be remembered, however, that the higher satellite altitude causes the magnetic field from the stressed material to decrease in magnitude. Additional study is required, hypothesizing various magnetization geometries, in order to size the magnitude of the magnetic differential that might be obtained by a pair of satellites at low altitude.

Principal Investigator: R. E. Fischell is Chief Engineer of the Space Development Department.

Presentation

1. R. E. Fischell, "Alternative Post-Magsat Missions," presented at the Earth Dynamics Working Group Meeting, Boulder, CO, 18-23 Jul 1977.

References

1. Staff of Space Department (APL/JHU) and Staff of Guidance and Control Laboratory (Stanford University), "A Satellite Freed of All but Gravitational Forces: TRIAD I," J. Spacecr. Rockets, Vol. 88, No. 9, pp. 637-644, 1974.

2. V. L. Pisacane, "Filtering of Satellite-to-Satellite Observations: Low-Low Configuration," presented at AGU 1977 Spring Annual Meeting, Washington, DC, 30 May-3 Jun 1977.

THE JOHNS HOPKINS UNIVERSITY
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OPTICAL ALTIMETER FOR THE SURFACE EFFECT SHIP WAVE PROFILING SYSTEM

An optical altimeter is being developed for use on board a high-speed surface effect ship (SES). It will be used in conjunction with an inertial ship-motion compensation system to determine accurately the profile of the sea waves directly ahead of the ship. The definition of the encountered sea spectra is important in correlating analytical predictions and measured response of ship performance parameters, fuel consumption, hull structure load distributions, and motions that can affect personnel habitability and effectiveness. The effort was initiated in December 1977. A survey of available equipment has been made, circuit designs have been completed, specific items have been selected and ordered from vendors, and the assembly of components has begun.

Problem

The SES rides on a cushion of air entrained by two hard side walls (keels) and flexible fore and aft seals. The reduced hydrodynamic drag permits speeds that are significantly greater than those of other ships. The SES Project Office (PMS-304) is developing a large, oceangoing SES, with a gross weight on the order of 3000 long tons (3KSES). The design is based on analysis, with correlations from model tests and operating data from two manned test craft, the SES-100A and SES-100B (each weighing approximately 100 long tons). These craft have attained speeds in excess of 80 kt in calm seas.

The SES-100A is being modified to simulate the hydrodynamic and pneumatic lift characteristics of the large 3KSES. It will be operated in the Chesapeake Bay during 1978 to validate its design performance and to provide a crucial data point in the technology extrapolation to the much larger 3KSES. In particular, the operating performance of the modified SES-100A and subsequent correlation with analysis predictions are expected to validate the critical 3KSES development areas of

1. Personnel habitability as affected by ship motions,
2. Ship performance and fuel consumption, and
3. Hull structural integrity and fatigue life.

An onboard wave height sensor will be needed to validate performance and correlate analysis in each of these critical areas. To make any meaningful estimates of ship performance, an accurate description of the test conditions must be available for both the

model (SES-100A) and the ship being modeled (the 3KSES), including time histories and a statistical description of the sea surface encountered during the tests.

The wave profile ahead of the SES can be determined by combining a relative wave surface measurement, referenced to the bow of the SES, with the output of an inertial system mounted at the ship's center of gravity. The development of an inertial system is straightforward; such a unit has been designed and tested and is ready for installation in the SES-100A. The development of a relative wave height sensor is a more difficult task because of stringent requirements on accuracy, beam width, and dynamic response, which are discussed in the following sections.

Objective

The Navy program planned initially to measure the relative wave height with a radar altimeter. However, the altimeter should be capable of measuring the vertical distance from the bow of the ship to a small spot on the water surface as follows:

Altitude operating range	25 ft maximum
Range accuracy	$< \pm 0.5$ in.
Frequency response	> 25 Hz

Radar altimeters presently available cannot meet these requirements. Likewise, it appears that there are no off-the-shelf optical altimeters available that meet these requirements. The objective of this program is to demonstrate a simplified optical ranging system that will satisfy the requirements and to define the necessary components for an onboard system for installation on the SES-100A.

Approach

The optical altimeter to be demonstrated would use a solid state Ga Arsenide laser source ($\sim$15 mW at 0.85 μm) modulated at $\sim$50 MHz. Simple optics would be used to collect, collimate, and expand the transmitted beam to about 2 in. in diameter. The receiver, which is colocated near the source, would be typically a pin-type diode. The demonstration system could use a phase detection processor for range determination with accuracies for ranges up to 25 ft of better than 0.1 in. Application of such a laser system to the SES is quite feasible. The environmental effects of salt spray and the like can be eliminated by enclosing the optics with a tubular arrangement with a positive flow of air down the tubes, and the effects of spurious return signals from the sprays can be minimized by conventional techniques.

Progress

Available lasers, detectors, and other components were surveyed in late 1977. Specific laser devices, optics, and signal processing electronics were selected and ordered from vendors. The equipment has been received and assembled on an optical bench in the electro-optical laboratory, and checkout of the system is under way.

Principal Investigator: T. M. Rankin. Mr. Rankin is a senior engineer in the Control Technology Group of the Fleet Systems Department.

Publications and Presentations

Due to the early stage of the program, there has been no formal reporting of results. Government sponsors and other interested parties will be invited to demonstrations of system operation in the Laboratory. A final report will document the information developed.

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PASSIVE HEIGHT FINDER

For the purposes of air traffic control, it is desired to measure the height of aircraft to an accuracy of ±500 ft at ground ranges out to 20 nmi at all altitudes up to 10 000 ft. For reasons of economy, it is desired to perform this measurement using energy transmitted by existing Airport Surveillance Radar (ASR). Approaches for adding a height-finding capability to the ASR were studied during the previous reporting period, and design studies for a demonstration model have now been completed.

Problem

Both DoD and civilian agencies continue to assign high priority to system developments that promote flight safety (e.g., Air Force Systems Command Research Planning Guide, HQAFSC TR 76-01, p. 4-18). Air traffic is conventionally partitioned into specific dynamic cells within a terminal control volume depending on airplane intention, route, velocity, and altitude. Cell sizes defined by regulations of the Federal Aviation Administration (FAA) are intended to provide an orderly separation of airplanes approaching, departing, or transiting the terminal air space. Air traffic controllers at the terminals maintain and monitor separations by communicating appropriate vectoring instructions to pilots via radio links.

The controllers have two major sources of sensor information to aid in their task, the ASR and the Air Traffic Control Radar Beacon System (ATCRBS). The ASR provides aircraft range and azimuth while ATCRBS provides identification range and azimuth for aircraft equipped with transponders. In addition, ATCRBS can provide altitude for aircraft equipped with Mode C transponders that provide a coded return corresponding to the aircraft's barometrically determined altitude.

Because many aircraft using the air space are not equipped with Mode C beacon transponders, flight safety would be enhanced if aircraft height could be determined by using a ground-based system. Such a system could also be used to compare altitude reports coming via ATCRBS.

An economical method of attaining this increased capability would be to add a height-finding system to the existing ASR. Altitude measurement would be accomplished by establishing the elevation of the radar return scattered from an aircraft target illuminated by the ASR fan beam and then using this information along with the slant range derived from the ASR receiver to calculate altitude. Since the ASR transmitter and antenna provide

target illumination, the height finder would be a passive device requiring a beamsteering array, receiver, and processor to accomplish its task.

Objective

The task was established to determine the best design approach for the ASR add-on capability and to implement a demonstration model of the candidate height-finding system. Evaluation testing of the demonstration hardware to quantify system performance was included in the task.

Approach

Various trade-off studies were performed to aid in establishing the design features for the demonstration model. These studies included calculations of the expected measurement errors in a multipath environment for an amplitude comparison design and for a phase comparison approach. The final design configuration of the demonstration hardware was heavily influenced by the available hardware.

Progress

Design studies for the demonstration model were completed and hardware implementation was started. The elevation error calculations indicate that for the same design constraints there is essentially no difference in the overall accuracy performance of amplitude versus phase comparison designs. For this reason, and since a set of phase (interferometer) receiver hardware was available for modification, it was decided to use phase processing in the demonstration system.

Funding was not provided to build a demonstration model, and work has been suspended pending direct project sponsorship.

Principal Investigator: R. C. LaFever. Mr. LaFever is the Supervisor of the Missile Guidance Fire Control Group of the Fleet Systems Department.

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POWER PLANT WASTE HEAT UTILIZATION

Fifteen percent of the total energy used in the United States is lost as waste heat from thermal-electric power plants. Use of this waste heat for heating homes and offices could significantly reduce the United States' consumption of fossil fuel. Hot water district heating systems have been proposed for the utilization of waste heat from steam electric generating plants (Ref. 1). An ammonia absorption district heating and cooling system has been proposed (Ref. 2) that appears to have some significant advantages over standard hot water district heating systems. Several point designs of such a system have been made and the transmission capital cost of a hot water district heating system has been compared with the transmission capital cost of an ammonia absorption system. The conditions under which the ammonia transmission system has a lower capital cost have been identified.

Problem

Research in energy conversion involving various processes and cycles to provide technical knowledge and data to aid in designing the most effective power systems is important to the DoD as well as to the civilian sector (e.g., Navy Research Requirements 3910.2, R-024, p. 15, January 1977). The 1973 rate of waste heat generation from power plants in Maryland was 495 x 10^8 Btu/hr (14 500 MW) (Ref. 3). It is projected that in the early 1990's the waste heat generation rate will be nearly three times the 1973 rate. It is significant that nuclear power plants may generate up to 150% as much waste heat per unit of busbar electrical energy delivered as a conventional fossil fuel power plant (Ref. 4). Thus as nuclear plants increase, waste heat problems will intensify. Also, as nuclear plants are large for economic reasons, their waste heat output is large. For the proposed Douglas Point nuclear power plant, two generating units will each produce 1180 MW of electricity and 2400 MW of waste heat (32.9% efficiency) (Ref. 5). Theoretically, over 800 000 homes in Baltimore or Washington, DC, could be heated with the waste heat from this one nuclear plant.*

The utilization of waste heat generated by electrical power plants for heating buildings can help solve two major problems: the disposal of waste heat and the conservation of energy resources.

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* The average heating degree day in Baltimore is 32 during January. The average heating load per typical house is approximately 15 000 Btu/degree day. This results in a requirement of 4.8 x 10^5 Btu/day/home (5.9 kW/home).

Although hot water district heating as proposed in Ref. 1 has many advantages, it does have problems, namely:

1. Summer utilization of the heat;

2. Distribution of thermal energy to buildings beyond a radial distance of 25 mi (40 km) from the power plant;

3. Variation of thermal load. Since the thermal loss rate for hot water district heating systems is essentially constant, as the system load decreases the thermal loss rate relative to the load increases, thus decreasing overall system performance; and

4. Mismatch between the electrical load of the power plant and the thermal load of the district heating system. Typically the greatest thermal loads are at night when the electrical load is minimum.

Objective

The objective of the work is to identify a system that will overcome the problems of a hot water district heating system and to determine system parameters that will make it economically viable and environmentally safe.

Approach

The approach was to examine possible "chemical heat pump" systems for district heating and cooling of buildings (Ref. 2). Several chemical systems are possible, and an ammonia-water absorption system is examined in some detail. The ammonia absorption cycle is based upon the molecular affinity between ammonia and water molecules. This affinity is so strong that in one volume of water over 1100 equal volumes of ammonia vapor can be absorbed at standard temperature and pressure. This absorption of ammonia in water is exothermic, yielding over 600 Btu/lb (1.4×10^6 j/kgm) of ammonia vapor.

Figure 1 is a schematic diagram of the basic absorption cycle. The cycle contains five major elements:

1. An ammonia generator,
2. A condensor,
3. An evaporator,
4. An absorber, and
5. A feed pump.

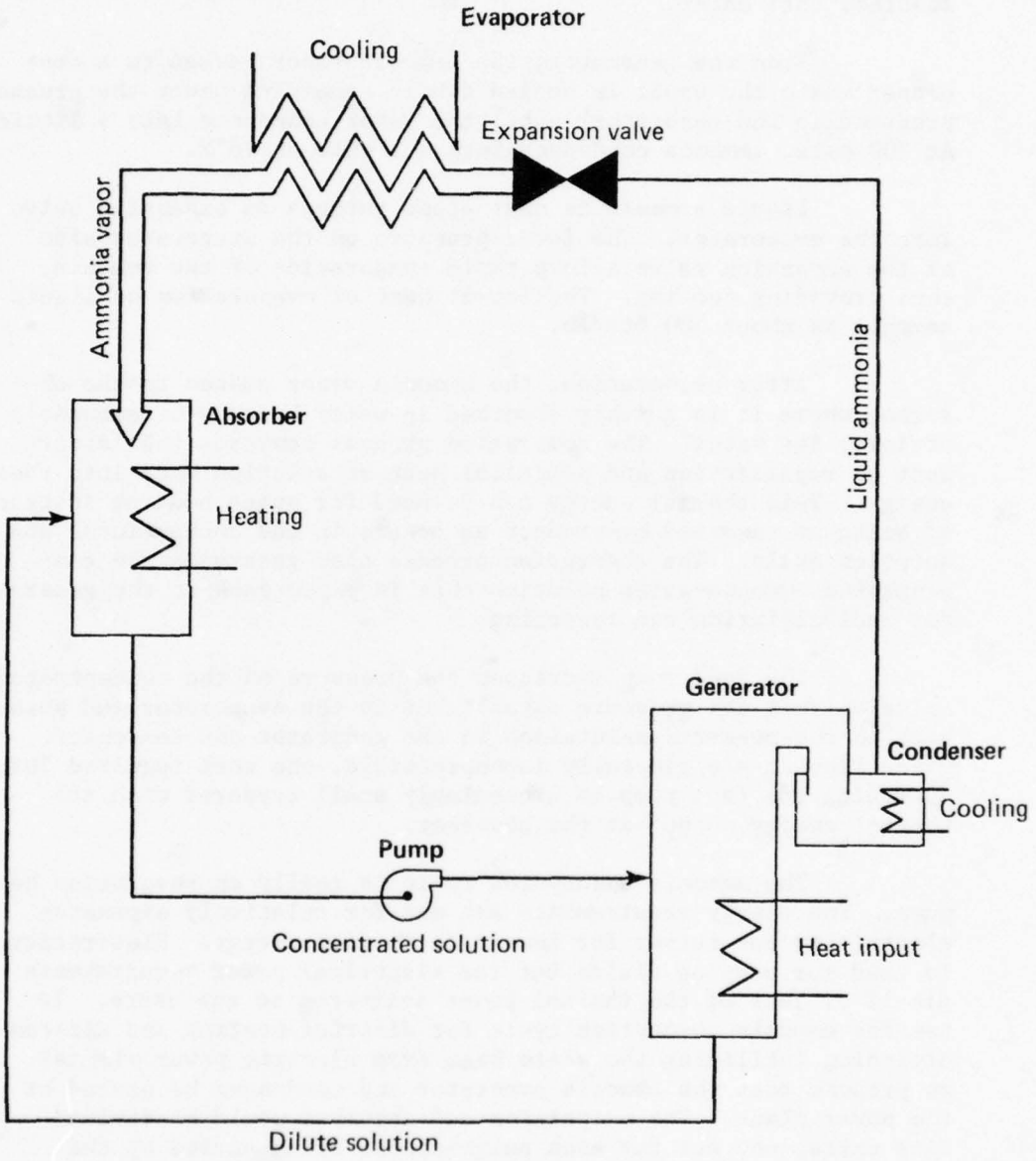


Fig. 1 The Basic Ammonia Absorption Cycle

Low-grade thermal energy from the power plant is used in the generator to distill ammonia from an ammonia-water solution. In this process, thermal energy is converted and stored as latent heat of vaporization in the ammonia vapor and as potential heat of solution, which are both recoverable when the ammonia vapor is re-absorbed into water.

From the generator, the ammonia vapor passes to a condenser where the vapor is cooled (while remaining under the pressure produced in the generator) until the vapor condenses into a liquid. At 200 psia, ammonia condenses into a liquid at 96°F.

Liquid ammonia is next piped through an expansion valve into the evaporator. The lower pressure on the evaporator side of the expansion valve allows rapid evaporation of the ammonia, thus providing cooling. The latent heat of evaporation of liquid ammonia is about 500 Btu/lb.

After evaporation, the ammonia vapor passes to the absorber where it is quickly absorbed in water because of ammonia's affinity for water. The absorption process converts the latent heat of vaporization and potential heat of solution back into thermal energy. This thermal energy can be used for space heating instead of being an unwanted by-product as occurs in the conventional absorption cycle. The absorption process also generates the concentrated ammonia-water solution that is piped back to the generator for redistillation and recycling.

The feed pump increases the pressure on the concentrated solution from the pressure established in the evaporator and absorber back to the pressure maintained in the generator and condenser. Since liquids are generally incompressible, the work required for operating the feed pump is exceedingly small compared with the thermal energy output at the absorber.

The ammonia absorption cycle is really an absorption heat pump. The energy requirements are not for relatively expensive electricity but rather for low-grade thermal energy. Electricity is used for pumping fluids but the electrical power requirements are 1% or less of the thermal power delivered to the users. To use the ammonia absorption cycle for district heating and air-conditioning (utilizing the waste heat from electric power plants), we propose that the ammonia generator and condenser be placed at the power plant. The evaporator and absorber would be divided into units, one set for each neighborhood being served by the system. Two pipes would be used to carry the liquid ammonia and dilute solution (both at ambient temperature) to the neighborhood

heating and cooling center, and a third pipe to return the concentrated ammonia-water solution back to the power plant.

At the neighborhood center, the evaporator cools water for cold water air conditioning or other chilled water needs of the users. The absorber heats water for hot water heating or other hot water needs of the users.

The major advantages of the ammonia absorption system over a typical hot water district heating system are that it

1. Provides cooling as well as heating,
2. Transports "thermal" energy with essentially no thermal losses because the ammonia and ammonia-water solutions are piped at ambient temperatures,
3. Decreases mass flow requirements because the energy density of the ammonia system may be two times the energy density of hot water, and
4. Eliminates system performance degradation with load variation and electrical load/thermal load mismatch.

Progress

The following progress has been made in evaluating the viability of the ammonia system:

1. Several system point designs have been developed and appear technically feasible, and
2. An economic comparison between hot water transmission and ammonia transmission costs has been accomplished.

Figures 2 and 3 show one point design for the ammonia absorption system using an all-liquid system for transport. Figure 2 shows both the ammonia generator and the condenser. The turbine exit steam flow rate shown in Fig. 2 is given as M x 0.252 lb/s, where M is a variable scaling factor. On Fig. 3, k is the fraction of M sent to a neighborhood center. For a crude scaling of a power plant, approximately 2.5 to 3 lb of steam/s are used to generate 1 MW of electricity. Thus, for a power plant that generates N MW of electricity, M is approximately 10 N. This implies 10 N lb/s of 50% ammonia-water solution for the point design shown in Fig. 2. Approximately 2 MW of thermal energy are delivered for every 1 MW of electrical energy generated.

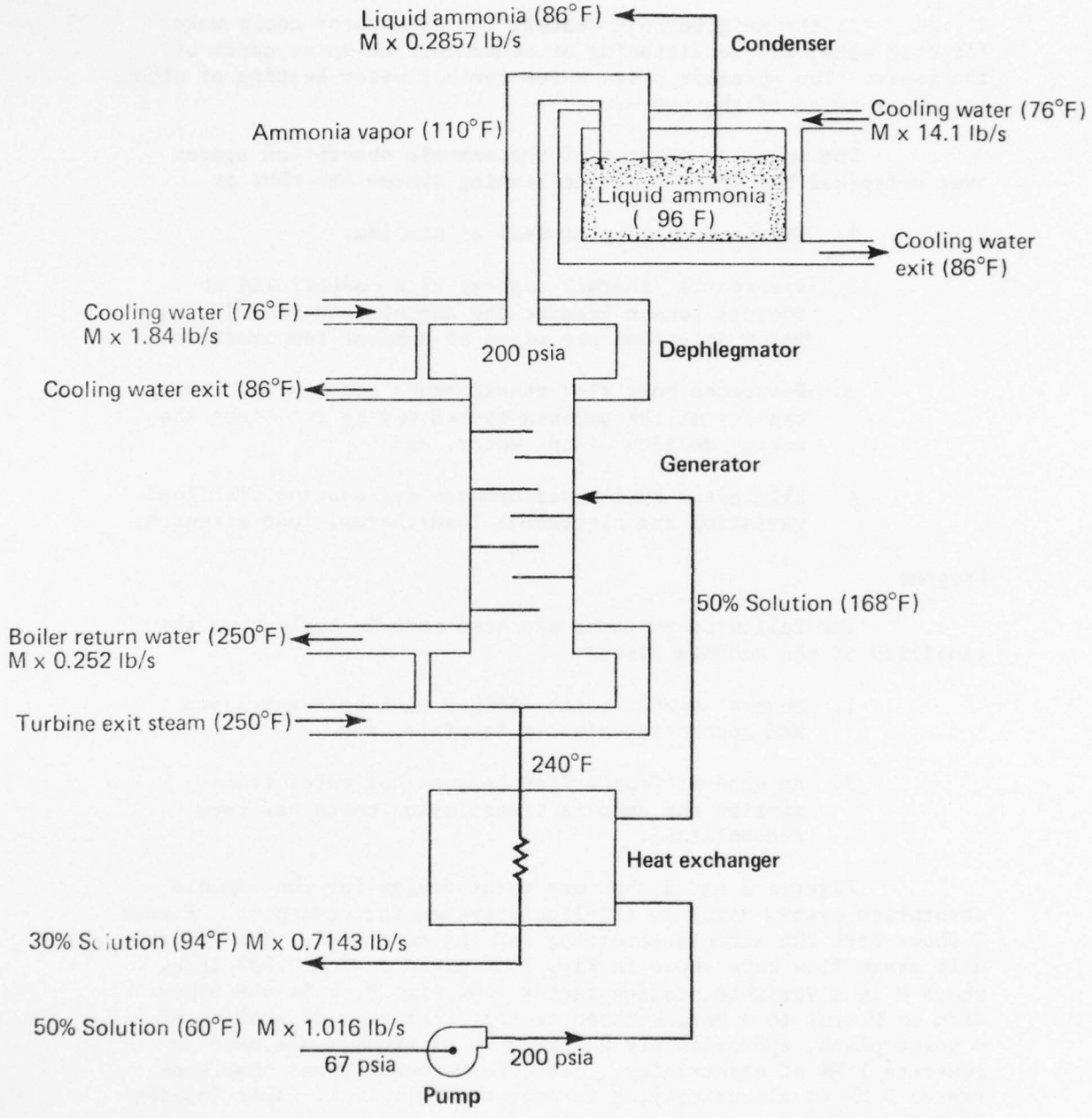


Fig. 2 Generator and Condenser at Power Plant

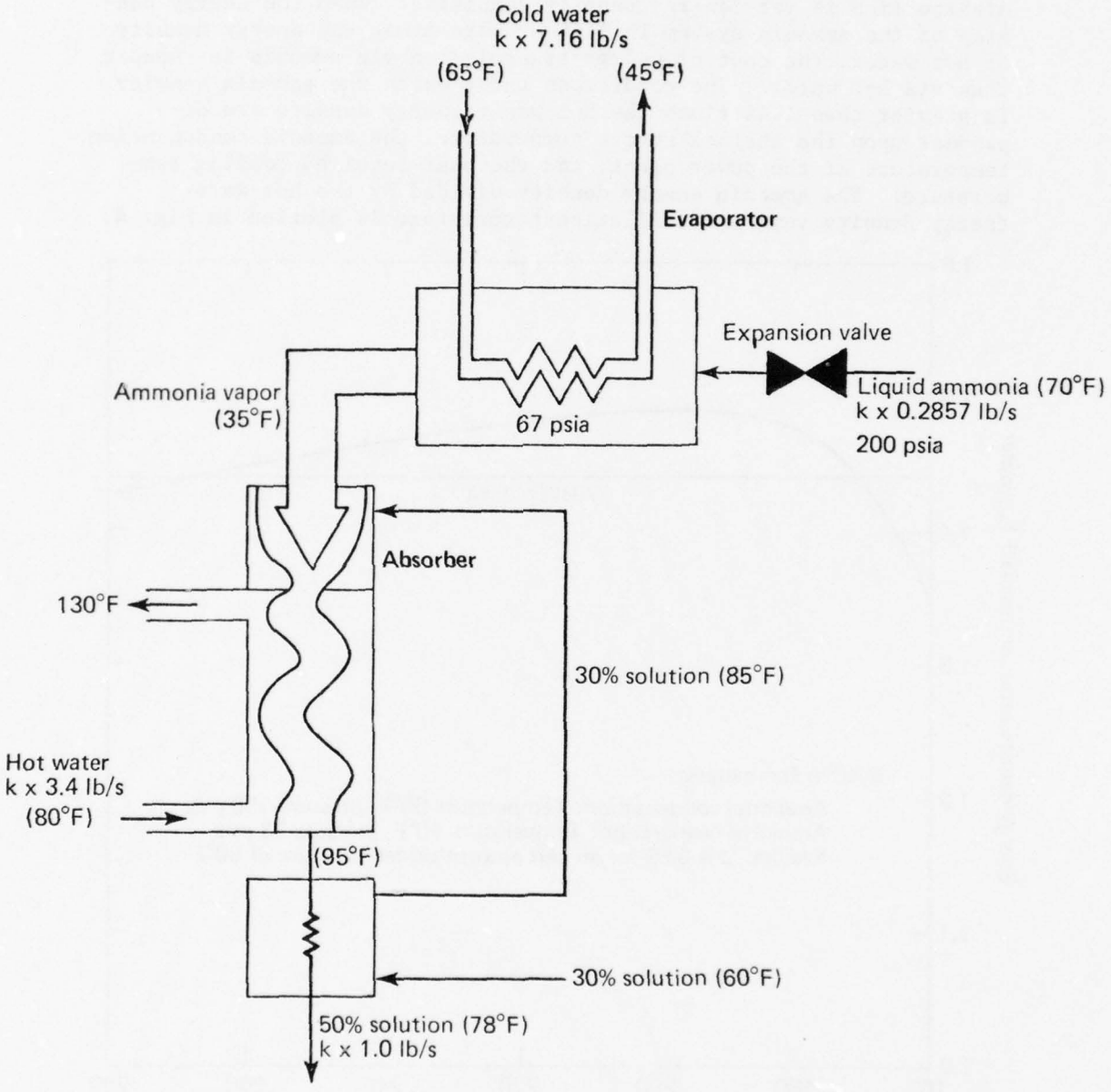


Fig. 3 Evaporator and Absorber at Neighborhood Heating and Cooling Center

An economic comparison between costs for hot water transmission and for an all-liquid transport ammonia absorption system has also been done (Ref. 6). The cost of the ammonia system transmission line is very energy density sensitive: when the energy density of the ammonia system is 1.44 or more times the energy density of hot water, the cost of energy transmission via ammonia is cheaper than via hot water. The conditions under which the ammonia density is greater than 1.44 times the hot water energy density are dependent upon the thermal source temperature, the ammonia condensation temperature at the power plant, and the user-required cooling temperature. The ammonia energy density divided by the hot water energy density versus distillation temperature is plotted in Fig. 4.

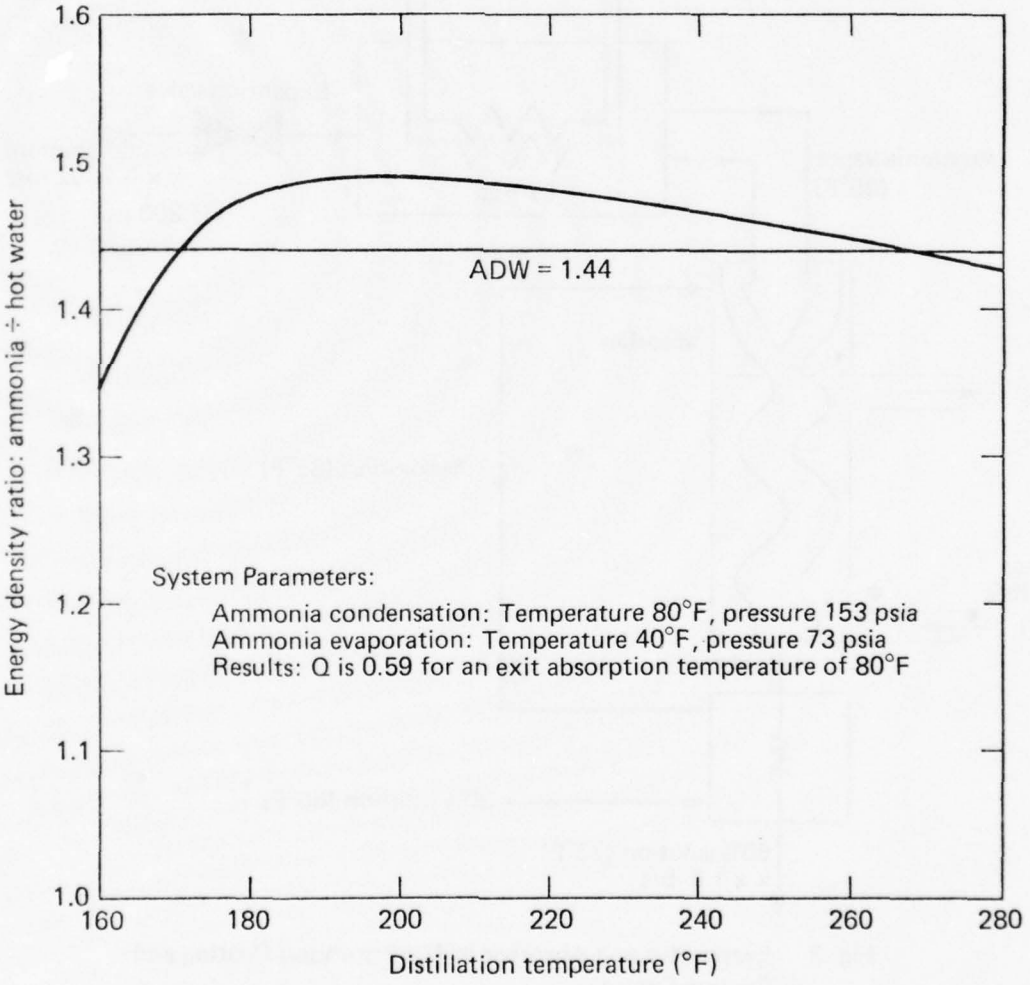


Fig. 4 Energy Density Ratios, Ammonia System Divided by Hot Water System, versus Driving Temperature

The plot is for the case when both systems use steel pipe. Cheaper pipe materials have been proposed. However, for source temperatures above 300°F, steel pipe would probably be required for a hot water system. Since the ammonia system transports the fluids at ground temperature, a cheaper pipe may be used to make the ammonia system much more cost effective than hot water for this case.

The problems and complexity of varying system parameters and evaluating total economic impacts require the next phase of work to utilize a computer simulation, the most practical approach to system design for lowest life-cycle cost.

Principal Investigator: R. J. Taylor. Dr. Taylor is a senior physicist in the Power Plant Site Evaluation Group.

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Presentation

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THE JOHNS HOPKINS UNIVERSITY
APPLIED PHYSICS LABORATORY
LAUREL, MARYLAND

RADIATION HAZARD STUDY

Occupational exposure to significant levels of microwave radiation is common in naval facilities. Personnel assigned to onshore bases and laboratories, as well as to ships at sea, are all subject to this radiation. The Laboratory is attempting to increase its understanding of possible deleterious effects to humans resulting from long-term exposure to relatively low levels* of microwave radiation through a study of the problem, including a radiation survey throughout the Laboratory.

Problem

The effect of occupational exposure of humans to microwave radiation has been considered with increasing concern by a wide range of people and organizations and is of concern specifically to the Navy (Naval Research Requirements ONRINST 3910.2, R041-08) and the Air Force (Air Force Systems Command Research Planning Guide (Research Objectives) HQAFSC TR 76-01, p. 1-43). Standards for allowable exposure limits have been reviewed and discussed with increasing fervor among both lay and trained opinion leaders. Committees have been formed, conferences called, and congressional hearings held to discuss the problem. There seems to be a significant objection to the current standard, but little agreement as to what a reasonable standard might be. The primary problem in setting or revising a "safe" standard is the lack of an adequate scientific basis for any proposed standard. The requisite studies have been sparse and in many instances unscientific in quality, and later attempts to duplicate the same work are often conflicting. Much of the so-called "evidence" cited is at best vague and anecdotal.

A significant portion of the work of the Applied Physics Laboratory involves microwave equipment, in particular naval radar systems. The number of radars installed at the Laboratory has increased over the past 15 years, as has the power associated with the units. Prudent management requires that the spatial patterns and strengths of radiation emanating from local microwave sources be measured and catalogued in a rational manner, using the best currently available technology. Regardless of the value of the finally accepted standard, a radiation survey is necessary to understand the basic microwave environment.

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* "Low levels" in the sense that the power densities are 10 to 1000 times lower than the currently presumed safe standard.

Objective

The objective of this study was two-fold:

1. To review the current literature on the biological effects of microwaves with particular interest in demonstrated effects on humans; and

2. To spot-check radiation levels in occupied areas close to the radiating sources, thereby roughly determining the order of magnitude of existing radiation patterns.

Approach

In the areas of information gathering, numerous sources were contacted in order to receive a wide variety of views. Recognized experts in industrial, governmental, military, and academic institutions were questioned as to their current opinions with respect to the hazard posed by occupational exposure to microwaves. In addition, their views on the safety of the existing standard were solicited, as well as their estimate of whether the standard will be changed. Additionally, academic papers and books were studied with a special emphasis on understanding the basis for the thousand-fold difference between what the East European countries consider safe and the higher United States standard.

The existing radiation levels were measured using standard surveying and monitoring devices. More sophisticated microwave instrumentation was then set up in the areas suggested by the survey devices, and more accurate data were recorded.

Progress

It is believed that an adequate operational understanding of the current state of knowledge of microwave effects has been obtained, recognizing that much of this reflects only opinion, since there is no accepted, unified theory of low-level effects. In numerous instances, qualified investigators have found adverse effects in biological species, but most of these are so specific to the circumstances of the study that they give little if any suggestion of how those observed effects would scale to humans. Effects are observable in humans but the reversibility and indeed the "harmfulness" of the effects themselves have not been adequately measured. An appraisal of the literature leads to the unmistakable conclusion that the scientific community just does not yet know what effect low-level microwave exposure has on humans and that it will probably take quite a long time to find out.

An epidemiological study recently published shows no effect on the mortality rate of occupationally exposed microwave workers when compared to a control group. The scientific community awaits a similar major study being prepared elsewhere for publication in the summer of 1978. The subject population of this investigation is the U.S. Embassy staff stationed in Moscow.

The brief radiation survey at this Laboratory was completed. The levels found in some occupied areas exceeded the Russian "safe" standard but were everywhere less than the level considered safe by most U.S. experts. A plan was devised to acquire additional instrumentation that would facilitate accurately assessing the microwave environment.

Principal Investigators: D. B. Staake and L. G. Knowles. Mr. Staake is Supervisor of and Mr. Knowles is a senior engineer in the Operational Systems Development Branch of the Fleet Systems Department.

THE JOHNS HOPKINS UNIVERSITY
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LAUREL, MARYLAND

SALT DRIFT DEPOSITION STUDIES

Prediction of the transport and fallout of particulate matter through the atmosphere poses several types of problems, including the need for a better data base to provide source term, meteorological, and fallout inputs for parametric computer studies of theoretical models. Our investigation addresses the use of a fluorescent tracer to identify an aerosol source and the use of modeling techniques that this identification facilitates. The experimental method was validated through the use of a natural-draft cooling tower experiment involving salt deposition.

Problem

Improved measurement and modeling of the dispersion of pollutants is of importance to both civilian and DoD agencies. Research is required to provide necessary sensitivity, accuracy, selectivity, and freedom from interferences (Air Force Systems Command Research Planning Guide, HQAFSC TR 76-01, p. 1-44), as well as modeling to correlate source characteristics, transport phenomena, and other phenomena to system effects (p. 1-43). The need for methodologies for quantification of trace quantities is specifically recognized (pp. 1-42 and 1-44).

Objective

The objective is to develop and validate a theoretical model to correlate and predict the dispersion and fallout of aerosol pollutants.

Approach

A multiyear directly funded program is underway at the Chalk Point, Maryland, electric power generating station to determine the environmental effects of salt drift from the natural-drift cooling towers. It is important to determine the probable long-term effects on agricultural crops and the general vegetative covering. The present IR&D work has been undertaken separately to develop and validate drift deposition models for use in predictive studies.

The basic measurements of salt deposition and the study of salt toxicity to vegetation has been undertaken by the University of Maryland in direct response to a certification requirement imposed by the Public Service Commission. The design of a field study to obtain data for model validation was undertaken by APL/JHU.

The unambiguous identification of deposited salt as having originated from the cooling tower necessitated the use of a tracer. Model validation required the preparation of source term, deposition, and meteorological inputs for use in parametric computer studies.

Progress

A dye tracer test was designed and conducted in 1977. It It used a fluorescent dye (Rhodamine WT) to provide positive identification of salt drift from a natural-drift cooling tower as distinguished from salt drift from other on-site sources, including sea salt background. The use of Rhodamine WT required a series of proof of principle tests to determine its suitability under temperature cycling and exposure to light, and during data recovery processes. It was determined that the dye deteriorates in sunlight to a degree requiring that the test be done at night. The dye proved quite stable under temperature cycling, including boiling.

Data were taken to facilitate the validation of salt deposition models. The parameters included source term data; cooling tower basin salinity and dye concentration, exit plume parameters, and salt drift size-number distribution; meteorological data; and the deposited dyed drift. Work has been initiated on the data reduction, analysis, and initial model validation under IR&D funding. The work will continue into 1978; the work done to date is described in detail in Refs. 1 through 4. References 1 and 2 describe the experimental and data reduction work; Refs. 3 and 4 are abstracts accepted by the 1979 Chalk Point Cooling Tower Symposium.

Principal Investigators: M. L. Moon, E. A. Davis, and J. H. Meyer. Dr. Moon is Supervisor, Dr. Davis, senior physicist, and Mr. Meyer, a meteorologist, in the Power Plant Site Evaluation Group.

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THE JOHNS HOPKINS UNIVERSITY
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LAUREL MARYLAND

SPEECH SYNTHESIS

Advances in the state of the art of microelectronics and in physiology have recently raised promising new possibilities in man/machine communications, particularly in the area of machine-generated speech. The speech synthesis project is exploring the applicability of this new technology to Naval tasks that involve a high degree of interactions between sensors, associated computers, and the computer operators. Two areas of immediate promise are (a) augmentation of the usual visual communications channel to commanders in Combat Information Centers (CIC's) and (b) response to operator queries about data in radar track files. The few months of the project have been devoted to performing a technology survey/literature search, to establishing a technology approach, and to acquiring equipment.

Problem

Increasingly complex defense systems of all types require research in pattern recognition, display processing, and data processing (e.g., Naval Research Requirements ONRINST 3910.2, January 1977, RO21-05; Air Force Systems Command Research Planning Guide HQAFSC TR 76-01, pp. 4-18, 4-19, 7-26, 7-32, 7-75, and 7-80).

The CIC of any modern warship contains several consoles that allow the commander and his staff to interact with each other, with the sensors, with the weapons system, and with the supporting computer(s), including those associated with command and control functions. The console provides a mechanism for the equipment to display data and for the operator to control both the data to be presented and the way the data are processed. That is, it is one implementation of a man-machine interface.

Historically, man was more flexible than the machine with the result that men were shaped to fit their machines. But today machines are becoming more flexible and capable. A modern console makes extensive use of the operator's visual and tactile senses so that displays, buttons, and switches cover all usable areas. But no use is made of his hearing.

In the past, the audio channel was not used since there were no adequate techniques to synthesize speech mechanically. Today, however, such units are readily available and are finding increased use in commercial airlines as emergency warning enunciators, by telephone companies to assist in the dissemination of changed and disconnected numbers, and in a few complex machines to aid the operators.

Objective

The long-term objective is to understand, advance, and utilize the technology of mechanical speech, to apply it when it is effective to do so, and perhaps to influence both device technology and future systems so as to benefit both. The short-term goal is to apply mechanical speech to Naval man-machine interfaces to improve today's complex systems. Specifically, the project will investigate the current state of the speech synthesis art, define a particular and limited application area within a CIC, and determine the utility of speech synthesis in that milieu. The next phase will be to investigate the applicability of the current technology to other such complex operational situations within the CIC, within the general framework of Naval command, control, and communications, and in other military and civilian areas.

Approach

The project is oriented toward new-term identification and demonstration of specific applications of importance to the Communications, Command, and Control Project of the Naval Electronics System Command, the Aegis Project, and the Trident Technology Improvement Community. The initial approach involves technology survey and the identification and procurement of the most appropriate speech synthesizer. A detailed plan will then be developed to upgrade the stand-alone capability of the synthesizer to the point of control from a high-level computer program. Practicable performance characteristics will be identified, demonstrated, and evaluated in the context of applications to Naval systems.

Progress

Three accomplishments to date are an overview of the state of the art, selection of a technical approach, and the acquisition of related equipment.

The technology survey separates current mechanical speech generators into two generic classes: recording devices and true synthesizers. The recording devices range from simple analog magnetic tape recorders through devices that digitize the audio signal, remove nonessential components with sophisticated filtering algorithms, and record the result digitally. This permits the automatic generation of messages in the sense that the recorded words can be transmitted in any order. In all of the recording type mechanical speech generators, the words are initially created by a human voice.

The true speech synthesizers, on the other hand, are electronic analogs of the human vocal tract. By controlling parameters analogous to such variables as air flow rates, voicing pitch, and tongue position, "speech" is produced from a sequence of digital signals. This method is characterized by an unlimited vocabulary but a requirement for providing the proper digital inputs.

The second accomplishment was to identify the approach that the project should follow, i.e., the recording technique of the synthesis alternative. True speech synthesis was selected due to its unlimited vocabulary, the more limited requirements for mass storage, less severe computation requirements, and the lower data transmission rates required.

Finally, the most advanced synthesizer currently available has been acquired.

Principal Investigator: M. J. Gralia, Dr. Gralia is a senior engineer in the Computer Systems Group.

SPACE RESEARCH AND TECHNOLOGY

The Applied Physics Laboratory has participated continuously in space science and technology activities since the immediate post-World-War II years when V-2 and Aerobee rockets first carried cosmic ray detectors, magnetometers, and ultraviolet (UV) and optical spectrometers above the earth's atmosphere. The goal has been to understand the fundamental physical and chemical processes related to the earth and interplanetary space, including the sun and the planets.

The space research program of the Laboratory is carried out primarily by the Space Physics and Instrumentation Group of the Space Development Department. The group is comprised of senior research physicists complemented during the present reporting period by three temporary postdoctoral appointees. The total program spans a range of technical fields including atmospheric and magnetospheric sciences, solar-interplanetary physics, radio astronomy, and astrophysics. A portion of this program was supported by the IR&D Program at a level of effort of about four persons during this period.

However, as shown by the manifold authors of the more than 30 publications that appeared during calendar year 1977, the total level of effort devoted to the space research program greatly exceeds that of the group itself through the purely voluntary collaboration of more than 30 scientists at many other institutions in this country and abroad. Collaborative research program teams include scientists from the Universities of Tokyo, Malaya, Calgary, Kiel, New Hampshire, Kansas, and Iowa, the Max-Planck Institutes in Munich and Lindau, the Danish Meteorological Institute, Kiruna Geophysical Institute, the Norwegian Defense Research Establishment, the National Oceanic and Atmospheric Administration, the Air Force Geophysics Laboratory (AFGL), and the Canadian Department of Energy, Mines, and Resources. During the current period, the group hosted more than 30 visitors from 15 countries including the USSR, Malaysia, Argentina, Australia, Japan, and Greece. Representatives from Japan, Denmark, Canada, and West Germany participated in a symposium held at APL in September 1977 in connection with studies of auroral and magnetospheric phenomena using the Triad magnetometer data. Members of the group responded to numerous invitations to present lectures at several international symposia, including the 20th COSPAR meeting in Tel Aviv, Israel, the Gordon Conference on Plasma Reconnection Phenomena in New Hampshire, the NATO Advanced Study Institute on Atmospheric Phenomenon in Spåtind, Norway, the 15th International Cosmic Ray Conference in Plovdiv, Bulgaria, and various American Geophysical Union Meetings.

Research activities have been greatly enhanced by the contributions of postdoctoral fellows/associates: Dr. N. A. Saflekos, R. D. Zwickl, and D. G. Mitchell, and part-time visitors: Prof. C. K. Ng (University of Malaya), Dr. E. Kirsch (Max-Planck Institute/Lindau), Prof. T. P. Armstrong (University of Kansas), Dr. G. Haerendel (Director, Max-Planck Institute/Munich), and Dr. G. Green (University of Kiel), to name only a few. Some of these activities are described in detail in the following reports.

Members of the Space Physics and Instrumentation Group also participated as technical consultants in support of the Space Development Department's primary role in the Navy Navigation Satellite Program. Areas of interest include geomagnetic modeling for satellite attitude determination, energetic particle characteristics for evaluation of radiation damage to satellite components, atmospheric and ionospheric models for evaluation of radio and optical propagation characteristics, and the application of a wide variety of computer numerical and graphic techniques developed for large-data-rate satellite systems to other Laboratory studies.

Support of these activities came primarily from sponsors of academic research, including the National Science Foundation (NSF), National Aeronautics and Space Administration (NASA), Office of Naval Research, Air Force Office of Scientific Research, and the AFGL. Primarily, IR&D funds supported the research projects outlined below and described in detail in the listed publications. However, a small fraction of the IR&D funds also supported participation of the group in prestigious scientific study groups, e.g., Dr. Krimigis in the Space Physics Committee of the National Academy of Sciences; Dr. Potemra in the National Academy of Sciences Committee for the Evaluation of NSF Arctic Research Programs; Dr. Roelof in the Management Operations Science Working Group of NASA Headquarters; and Dr. McEntire in the NASA Science Definition Working Group for the AMPS (Atmospheres, Magnetospheres, and Plasmas in Space) Space Shuttle Program.

REFLECTION OF SOLAR ELECTRONS FROM THE MAGNETOSHPERE

Observations made by near-earth spacecraft have established that solar flare particles exhibit a pronounced variability in their velocity angular distributions. The phenomenon had not been explained. However, detailed analysis now shows that it can be understood in terms of reflections from the earth's magnetosphere.

Problem

Understanding the behavior of solar flare particles poses important problems to Navy communications as well as to astronomy, astrophysics, and atmospheric sciences (Navy Research Requirements ONRINST 3910.2, January 1977, R033, R033-2, R033-03, and R034 through R034-06).

Professor C. K. Ng, on a 6-month sabbatical leave from the University of Malaya, undertook a comprehensive analysis of a phenomenon first identified at this Laboratory in 1973 by Drs. J. C. Armstrong, C. O. Bostrom, and E. C. Roelof. Solar flare particles display a puzzling variability of velocity anisotropic behavior when observed by near-earth spacecraft outside the magnetosphere. Sometimes the particle fluxes are strongly collimated along the interplanetary magnetic field direction, while at other times (often within the same event) the fluxes are nearly isotropic. This behavior is vexatious since the flux anisotropy is an essential clue to interplanetary propagation conditions, which should not be so variable.

Approach

Solar particle flux anisotropy data were available to the Laboratory as measurements of $\sim$ 0.3 MeV protons and electrons from the APL/JHU detectors on the IMP-7 and IMP-8 spacecraft. These data, together with other known data on the earth's magnetosphere, provide the basis for isolating the origin of the variability of velocity anisotropy.

Progress

Through a detailed and comprehensive analysis, Drs. Ng and Roelof demonstrated conclusively that the reduction in flare particle anisotropy occurred whenever the direction of the interplanetary field measured at the spacecraft was such that the linearly extrapolated field line intersected the magnetosphere. Thus the reduction of the anisotropies was not an interplanetary effect, but simply a reflection of the particles from the stronger magnetic field inside the earth's bow shock. Not only does this result clarify the nature of interplanetary propagation, it also provides global information on the 3-dimensional structure of the bow shock, and, by analogy, similar information on particle interactions with propagating shocks in interplanetary space. Publications and presentations resulting from this work are listed in the bibliography.

Principal Investigators: E. C. Roelof and C. K. Ng. Dr. Roelof is a physicist in the Space Physics and Instrumentation Group, and Prof. Ng is with the University of Malaya.

NEW SATELLITE INSTRUMENTATION

Improved instrumentation has been developed and tested in the laboratory for the purpose of measuring the elemental composition and energy spectrum of cosmic radiation. Current activity is directed toward a flightworthy system.

Problem

There is a continuing need to develop improved techniques to detect, analyze, and interpret the energetic particle population in planetary magnetospheres and in interplanetary space. Both the local and interplanetary aspects of the problem fall within the province of NASA, but Naval research requirements also recognize the need for extended and new information about the high atmosphere, specifically including research on solar phenomena and emissions and the naturally occurring radiation background (Naval Research Requirements ONRINST 3910.2, January 1977, R033, R033-02, R033-03, and R034 through R034-06).

Objective

The primary specific objective is to develop spacecraft quality instrumentation that will extend the effective energetic range of particle detection and identification.

Approach

The Space Physics Group has pioneered in the development of an energetic particle time-of-flight telescope using an extremely thin foil as the front element and solid-state detectors as the rear element. The time-of-flight measurement is based on detection of secondary electrons that are emitted when incident particles penetrate the front foil and strike the rear detectors. The general approach to improve the effective energy range is through the use of thinner foils and improved secondary electron optics.

Progress

The experimental program involves measuring the elemental composition and energy spectrum of cosmic radiation using the advanced technique of three-parameter analysis (dE/dx, total energy, and time of flight). Past effort has included the development of the three-parameter solid-state detector telescopes (based on 2 to 5μ thick front elements) chosen for flight on the Galileo (Jupiter Orbiter) and AMPTE (Active Magnetospheric Particle Tracer Explorers) Satellite Missions. Present development efforts are based on using extremely thin foils (5 to 100 $\mu gm/cm^2$) as telescope front elements, with particle detection through the analysis of secondary electrons emitted when incident particles penetrate the foil.

This concept has now been proven in Laboratory trials using a time-of-flight telescope with a microchannel array plate for secondary electron detection and a solid-state detector for the rear element; comprehensive accelerator runs with a number of incident nuclei have shown the suitability of such solid-state total

energy detectors for the range of energy and nuclear charge of interest. Effort is now focused on the rapid development of flight electronics and a flightworthy detector head with improved secondary electron optics, leading to the launch of a prototype instrument deep into the tail of the earth's magnetosphere in late 1979 as a collaborative part of the German "Firewheel" experiment on the second test launch of the European ARIANE space vehicle. The brief orbital data from this flight will not only be of great scientific interest, covering an energy range not heretofore measured with composition instruments in the earth's magnetosphere, they will also serve to validate the detector instrumentation for future long-duration spacecraft missions.

Principal Investigators: R. W. McEntire, J. W. Kohl, S. A. Gary, S. M. Krimigis, and G. Haerendel. Dr. Krimigis is Supervisor, Dr. McEntire and Mr. Kohl are physicists, and Mr. Gary is an engineer in the Space Physics and Instrumentation Group. Dr. Haerendel is Director of the Max-Planck Institute/Garching.

Reference

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SOLAR PARTICLE PROPAGATION, LOW-ENERGY NUCLEON SPECTRA, AND Z-RICH SOLAR PARTICLE EVENTS

The energy spectrum and chemical composition of ions measured in interplanetary space with energies below 10 MeV per nucleon reveal a likely solar origin, but with very high enhancements in abundance relative to solar material. After separating out propagation effects, it was found that energetic ions as heavy as iron must be systematically enriched in solar plasma prior to acceleration to superthermal energies in small solar flares.

Problem

The relative abundances of low-energy solar ions from helium through iron observed in interplanetary space have been extremely puzzling since these ions are often overabundant (relative to hydrogen) by factors of tens, compared to spectroscopic solar abundances. The explanation of this phenomenon must bear directly on plasma and particle acceleration processes basic to solar physics and astrophysics of interest to the U.S. Navy (cf., Navy Research Requirements, ONRINST 3910.2, January 1977, R033, R033-02, R033-03, and R034 through R034-06).

Approach

After concluding that interplanetary propagation does not significantly distort the abundances of energetic ions emitted from the sun, interplanetary measurements from the APL/JHU detectors on the IMP-7 and IMP-8 spacecraft were analyzed, first for the "quietest" nonactive periods and then for a class of small, but Z-rich, events.

Progress

Dr. R. D. Zwickl's first work at APL established the general lack of strong scattering of low-energy solar particles by irregularities in the interplanetary magnetic field over particle rigidities (momentum per charge) varying by a factor of 3000. Next he and Dr. S. M. Krimigis analyzed the "quiet-time" proton and helium spectra measured below 10 MeV/nucleon by the APL/JHU detectors on the IMP-7 and IMP-8 spacecraft in 1975. These spectra, taken on the days of lowest fluxes, remained relatively unchanged from similar measurements taken in 1973 and 1974. Detailed analysis of flux anisotropies and the lack of variation over 3 years ruled out galactic origins, leaving either the sun or planetary magnetospheres as the source. The third problem attacked, again with the IMP-7 and IMP-8 detectors, was the nature of a mysterious class of solar particle events which, although they are low in flux, exhibit remarkable enhancements of heavy ions, $\sim$ 1 MeV/nucleon. These events can be overabundant by a factor of 100 in the iron group ($Z \geq 20$) compared to photospheric abundances. The APL investigators and T. P. Armstrong of the University of Kansas established that these events originated in rather small solar active regions, and that the heavy ion enhancements most likely occurred in the substrate (thermal) plasma prior to acceleration to MeV energies. This result has attracted the attention of Nobel Laureate Hannes Alfvén who considers it a possible verification of a basic cosmogonic mechanism for chemical differentiation in a plasma that he has proposed for the formation of the solar system. The numerous publications and presentations resulting from these studies are listed in the bibliography.

Principal Investigators: R. E. Gold, S. M. Krimigis, E. C. Roelof, R. D. Zwickl, and T. P. Armstrong. Dr. Krimigis is Supervisor and Drs. Roelof, Zwickl, and Gold are physicists in the Space Physics and Instrumentation Group. Dr. Armstrong is at the University of Kansas.

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LAUREL, MARYLAND

RESEARCH CENTER PUBLICATIONS

1 October 1976 - 31 December 1977

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