

Proceedings of
THE
ROBERT A. WELCH
FOUNDATION

Conferences on Chemical Research
XXIII. MODERN STRUCTURAL METHODS

NOVEMBER 12-14, 1979

HOUSTON, TEXAS

**PROCEEDINGS
OF
THE ROBERT A. WELCH FOUNDATION
CONFERENCES ON
CHEMICAL RESEARCH
XXIII. MODERN STRUCTURAL METHODS**

W. O. Milligan, Editor

Houston, Texas

1980

THE ROBERT A. WELCH FOUNDATION

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PROGRAM

W. O. BAKER, Presiding

Monday, November 12, 1979

- 9:30 a.m. 1. OPENING REMARKS.
- 9:45 a.m. 2. W. O. BAKER, Introductory Remarks.
- 10:00 a.m. 3. HOMER D. HAGSTRUM, "Basic Studies of Solid Surfaces."
- 2:00 a.m. 4. MICHAEL E. FISHER, "The States of Matter -- A Theoretical Perspective."

Tuesday, November 13, 1979

- 10:00 a.m. 5. HENRI A. LEVY, "Interatomic Distances and Bond Angles -- How Much Do They Mean?"
- 2:00 a.m. 6. L. C. KIMERLING, "Imperfections in Condensed Matter."
- 6:30 p.m. RECEPTION. Grand Ballroom Foyer, Shamrock Hilton Hotel.
- 7:30 p.m. DINNER. Grand Ballroom, Shamrock Hilton Hotel.
- 8:30 p.m. 7. ALAN L. BEAN, "Mankind's Future in Space."

Wednesday, November 14, 1979

- 10:00 a.m. 8. ELMAR ZEITLER, "Looking at Structure with the Electron Microscope."
- 1:30 p.m. 9. GEORGE K. RADDA, "From Molecular Structure to Bio-Dynamics."

ROUND TABLE DISCUSSION LEADERS

1. DEAN E. EASTMAN -- International Business Machines Corporation
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3. PAUL A. FLEURY -- Bell Laboratories
4. H. S. GUTOWSKY -- University of Illinois at Urbana-Champaign
5. MICHAEL HART -- University of London King's College
6. PETER HIRSCH -- University of Oxford
7. WILLIAM N. LIPSCOMB, JR. -- Harvard University
8. ROBERT J. MADIX -- Stanford University
9. S. J. SINGER -- University of California, San Diego
10. BENJAMIN WIDOM -- Cornell University

THE DISCUSSION LEADERS



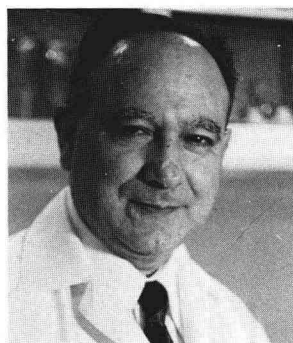
DR. DEAN E. EASTMAN



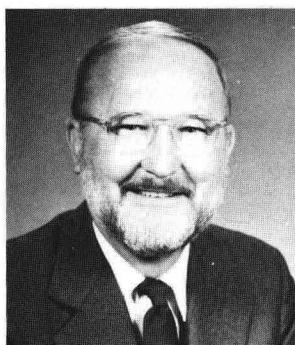
DR. PAUL A. FLEURY



DR. MICHAEL HART



DR. HUMBERTO FERNANDEZ-MORAN



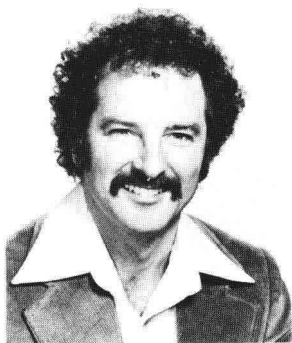
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DR. BENJAMIN WIDOM

P R E F A C E

The Robert A. Welch Foundation is a Trust established by the will of the late Robert Alonzo Welch. The Founder's aims in furthering research in chemistry are best expressed in his own words, as recorded in his will:

"I have been spared to live beyond the allotted span of three score years and ten, and, in that lifetime, by hard work and sacrifice assisted to some extent by good fortune, have accumulated property of substantial value. My desire, now, is to make that disposition of it by will which will result in its being used in the way most beneficial to Mankind. I have long been impressed with the great possibilities for the betterment of Mankind that lay in the field of research in the domain of Chemistry. This is a feeling that I think is widely held by others. It is a popular expression to say that we are living in a 'Chemical World.' Day by day we see marvels wrought in that field."

In 1978-1979 fundamental research in chemistry was being conducted under The Robert A. Welch Foundation grants by a total of 1,585 persons, including 374 principal investigators, 273 post-doctoral and 587 pre-doctoral fellows, and 351 undergraduate scholars. The aggregate yearly cost encompasses approximately forty percent of all private foundation funds devoted to the direct pursuit of non-mission oriented basic chemical research in colleges and universities.

In addition to a program of direct grant-in-aid, a limited number of professorships and scholarships, and special lectureships, the Trustees of The Robert A. Welch Foundation have inaugurated a series of conferences on chemical research with the object of stimulating and encouraging chemical research within the State of Texas.

The general plan of the several conferences in this series, was designed to broaden the scope and interest in chemical research, rather than to more sharply delineate boundaries between chemistry and allied fields of research such as physics and mathematics. We believe that these considerations are entirely in harmony with the current trend of research.

This volume comprises the proceedings of the twenty-third conference held in Houston, November 12-14, 1979. The Trustees of the Foundation have asked me to extend their deep appreciation and thanks to the principal speakers who gave so freely of their time, thereby making possible a successful conference.

This series of conferences has attracted an attendance varying from 500 at the first meeting in 1957 to almost 1600 at later meetings. Participants have come from each of the fifty States and from as many as nineteen Countries.

We appreciate very much the cooperation of all those who were involved in this effort. The Trustees of The Robert A. Welch Foundation are convinced of the value of the scientific research material presented at these Conferences and consider that prompt dissemination is essential. We trust that the completeness of the papers of this volume will compensate the reader for the time required for publication.

W. O. Milligan

December, 1980

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CHAPTER I

OPENING REMARKS

Dr. W. O. Milligan (Director of Research): Ladies and gentlemen, it is my pleasure to open Conference XXIII of The Robert A. Welch Foundation. We welcome all of you here. It is my pleasure at this time to introduce the Chairman of the Board of The Robert A. Welch Foundation, Mr. Roger J. Wolfe, who will welcome you on behalf of the Trustees of the Foundation.

Mr. Roger J. Wolfe (Chairman, The Robert A. Welch Foundation Board of Trustees): Thank you, Mr. Chairman, ladies and gentlemen, on behalf of the Trustees of The Robert A. Welch Foundation, I welcome all of you to Conference Twenty-Three on the subject of "Modern Structural Methods."

We are pleased to announce that there are over thirteen hundred registrants at this meeting. This is most gratifying to us since these conferences were established for the purpose of providing a means for an open and free discussion of research results in a designated area of chemistry, as well as to provide a stimulus to the chemists conducting research in the State of Texas under the general program of the Foundation.

The Robert A. Welch Foundation is an operating foundation, tax-exempt under Section 501 (c) (3) of the Internal Revenue Code. The status of "Operating Foundation carries with it certain responsibilities concerning assurances that the funds granted by the Foundation are used strictly for the specific purpose for which granted to further the specific objectives of the Foundation.

We are pleased that this latter responsibility required no change whatsoever in our operating procedure of over a quarter of a century, as the Trustees and Officers had always felt such moral responsibility in carrying out the dreams and desires of the Founder.

You may be interested to know that our Grant-in-Aid Program is currently supporting nearly 1,600 people, including principal investigators, post-doctoral fellows, pre-doctoral fellow, and undergraduate scholars at over 40 educational institutions within the State of Texas.

We are proud to be your host on this occasion, and I welcome you to Houston and Conference Twenty-three and hope your attendance will be a pleasant and profitable one.

Thank you very much.

Dr. Milligan: I would like to make a few remarks about the particular manner in which our conferences are conducted, and the procedures that make things run as smoothly as possible. Whenever anyone wants to say something in the discussion, we would like to ask him to give his name and location to Mr. Perkins, the stenotype operator, because we are going to print all of the discussion and the proceedings. And

you will, of course, get a copy before it goes to the press so that you will have the opportunity to change what you said to what you intended to say.

Another reason that we would like to get your name and your location in the record is that the famous man who appears so often in scientific conferences and discussions — I'm speaking of the famous Dr. Anon. We love him, but we don't want him to monopolize the discussion completely.

Right now I'm asking Dr. Baker, the Chairman of the whole meeting and other people who do discussing and so on, if they fail to do this, just interrupt him and get it in the record. We will get this material which is taken down to you a lot faster than you think. And if you get it back to us promptly, we could even get the proceedings in print, say, within 90 days. But of course, you understand no matter how fast some people do it, there is always the last one to get the last material in. So that's the rate controlling step.

At this time it is my pleasure to introduce Dr. W. O. Baker, Chairman of the Board of Bell Telephone Laboratories, a member of our Scientific Advisory Board who is essentially responsible for all of the good things that happen. I'm responsible for any bad things that happen.

Dr. Baker.

Dr. W. O. Baker (Speaker) Bell Laboratories: I have to demur at that specification, but otherwise I agree with everything Dr. Milligan has said. And on behalf of my fellow members of the Scientific Advisory Board: who could be present, Dr. Eyring, Dr. Seaborg, and Dr. Marvel it is a privilege to join Chairman Wolfe in welcoming you all to this conference.

I am happy to be able to greet this fine aggregate. Since we are going to talk about structure, it is appropriate to call our conference an aggregate — of those who work nowadays with a large body of knowledge about science and technology. It is widely believed that the knowledge base doubles about every 7 years. The momentum of publishing and the large population of research and technology workers in chemistry and the rest of natural science may obscure simple matters at the roots of science on which this huge superstructure is being busily built. So this year in particular, we welcome a theme that we believe is congenial to the spirit of these occasions and, indeed, to the purposes of the devoted trustees who carry on with high purpose the legacy of Mr. Robert A. Welch. This theme is to criticize and evaluate the very basic concepts of matter, of substance and its transformation by chemical reaction. Do they seem suitable and perhaps even valid? To determine this for our present science, the choice of directions to be taken is manifold, although perhaps not quite so extensive as in the following story. It is said that during a Caribbean cruise that included Mr. Jimmy Durante among the passengers, a violent storm assailed the ship. There was danger of its foundering in the choppy seas near the Gulf Stream. It was decided to consult some notable persons, most particularly Mr. Durante, about what they would do if they had to

take to the lifeboats. In particular, the passengers were asked, "Suppose we have to take to the boats? Where will you go? How will you determine direction?" Jimmy Durante hesitated for only a moment before responding, "I'll row for the horizon; it's better than nothing."

We shall not be quite so global, but I do recommend that we can extend our discussion quite widely within the theme that we have mentioned. We especially appreciate the presence of distinguished delegates from overseas among our speakers and discussion leaders. This matter has great roots and origins all about the globe. And we are looking forward to the introduction of all pertinent points of view.

You may wonder why, then, we are taking these minutes at the beginning to postpone the appearance of the speakers. It is mostly on the good advice of Dr. Milligan to give our conferees time to come in and get settled. We shall be through with these preliminary remarks rather shortly. But an introduction is appropriate.

This XXIII Conference on Chemical Research, sponsored by The Robert A. Welch Foundation, intends to be a modern assessment of our knowledge of chemical and bio fine structures. It is thus a descendant of the earliest conferences, the first of which in 1957 dealt with the structure of the nucleus; the second in 1958 with that of the atom, especially its magnetic and other electronic peculiarities; the third in 1959 treated the structure of the molecule where microwave and electronic spectroscopy highlighted the focus on features of single molecules. In succeeding years, beginning with the IV Conference on "Molecular Structure and Organic Reactions," a wide range of studies was covered, in which the basic structural concepts of the Twentieth Century were applied to the whole arena of chemistry.

So these conferences and their countless coordinates throughout the world remind us, as we come into the next to the last decade of this century, about the fabric of scientific thought and its application in modern technology. For main fibers in this fabric are ideas of the structure of matter. These earlier Welch Conferences have well prepared us to examine incisively what we know, or ought to know, about the way atoms are formed and then put together into molecules. We believe that the succeeding assemblies of such units account for the properties of matter. So we have rather boldly chosen, in this conference, to test our knowledge beyond the traditional probing of expected structure and actions of individual molecules. Rather, we have taken the chemist's view that assemblies and their interactions are the conditions chiefly encountered in chemical transformation and characterization.

Accordingly, in this conference we have sought to join the basic concepts of atomic and molecular units with the principles of how these units must combine to yield chemical and bio substance. As we shall see, our speakers have reacted admirably to this venture — indeed an adventure which will lead us in the next three days to frontiers of understanding how our world of inorganic and organic matter is put together, in its marvelous and manifold modes. And our discussion leaders who follow each presentation will provide coherence and critiques.

So, let us see briefly why we expect to find new pathways, and indeed new beauties, enroute. These new pathways lead to learning how one thing can transform into another -- gas into liquid, acid into salt, oil into vapor of the atmosphere, or the virus crystal into living organism. And it is well to recall also the elaboration of properties which come from structures and their changes. Much of our modern life depends on these, in beneficial forms envisioned by Robert A. Welch, even when the prominent resources of nowadays were mostly unknown. Thus, a world of electromagnetics-based industry and security would be unimaginable without the crystalline (Figure 1) role of copper wires. But a host of other crystals synthesized chemically extend such service into an electronics era. The garnets, such as yttrium-aluminum garnet, provide important media for laser actions beyond their age-old attractions, in other natural forms, as jewel-like minerals (Figure 2). The knowledge of structure of these garnets, with their elaborate and extensive unit cells enabled identification of magnetic and optical properties of highest import to present-day devices, for information processing and communications. By delicately attuned stoichiometry of derivatives of garnets, L. G. Van Uitert and his co-workers have synthesized new classes of insulating ferromagnets. In these, domains similar to those of the ferrites (another useful class of chemical substance) can be converted, astonishingly, by the use of small, external fields into tiny cylinders of magnetism (Figure 3). These are the so-called "bubbles" comprising compact and versatile memory systems for digital computers and other machines.

These memories, fitting into thin film integrated circuitry, are already used in the storage and production of the human voice, for efficient communications service (Figure 4). But they offer, also, through the inventions of A. Bobeck and his colleagues, a valuable supplement to human mentality. This is by storing knowledge, which can be easily, although compared to the human function crudely (but rapidly) retrieved. Here again we see detailed knowledge of structure -- structure once more reflected in cooperative and extended phenomena such as magnetic domains -- serving to enhance, in strictly inorganic substance, the miraculous capabilities of organisms themselves.

No wonder we are excited about ways to peer evermore deeply into the patterns and interactions of chemical units. Happily, the very elegance we see in the qualities of chemical bonding and geometry is itself giving us sharper and sharper methods of accounting for structure. But overall, the total validation will be aided by discussions here. Some recent findings give us added confidence in the reality of these ideas, on which so much of chemical science and its derivatives depend. Thus, on the one hand, the studies of Jackson and his co-workers, reported in earlier Welch Conferences, have been carried forward by Gilmer and associates (J.D. Weeks and George H. Gilmer, *Advances in Chemical Physics*, Vol. 40 page 157) in the modeling of crystal growth. This provides a special example of whether discrete atoms and molecules behave as supposed, in coming from a gas or liquid into a compact condensed array (Figure 5).



FIGURE 1
Copper Crystal

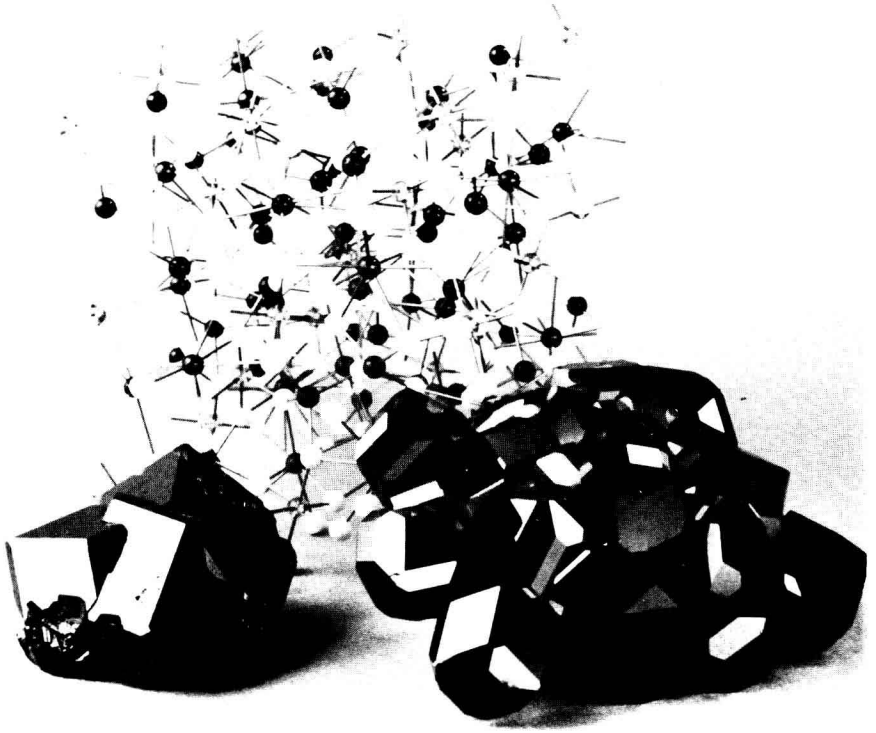


FIGURE 2

Garnet crystals with a model of their crystalline structure. These oxides of the rare earth elements and iron or other metals are a source of magnetic bubbles that may be used in future information-processing devices.

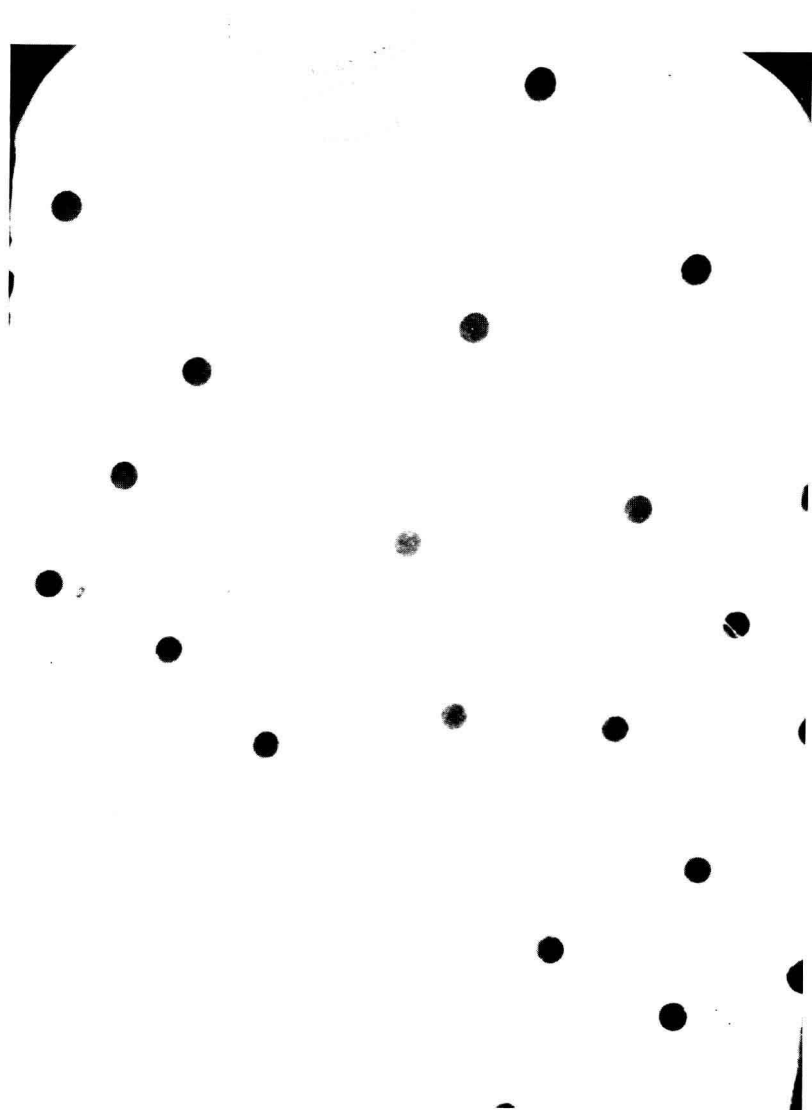


FIGURE 3

Magnetic bubbles. Application of a no. 2 Oe bias field produces tiny cylindrical domains (1.8 mils in diameter) of magnetism in newly synthesized, insulating, ferrimagnetic crystals.

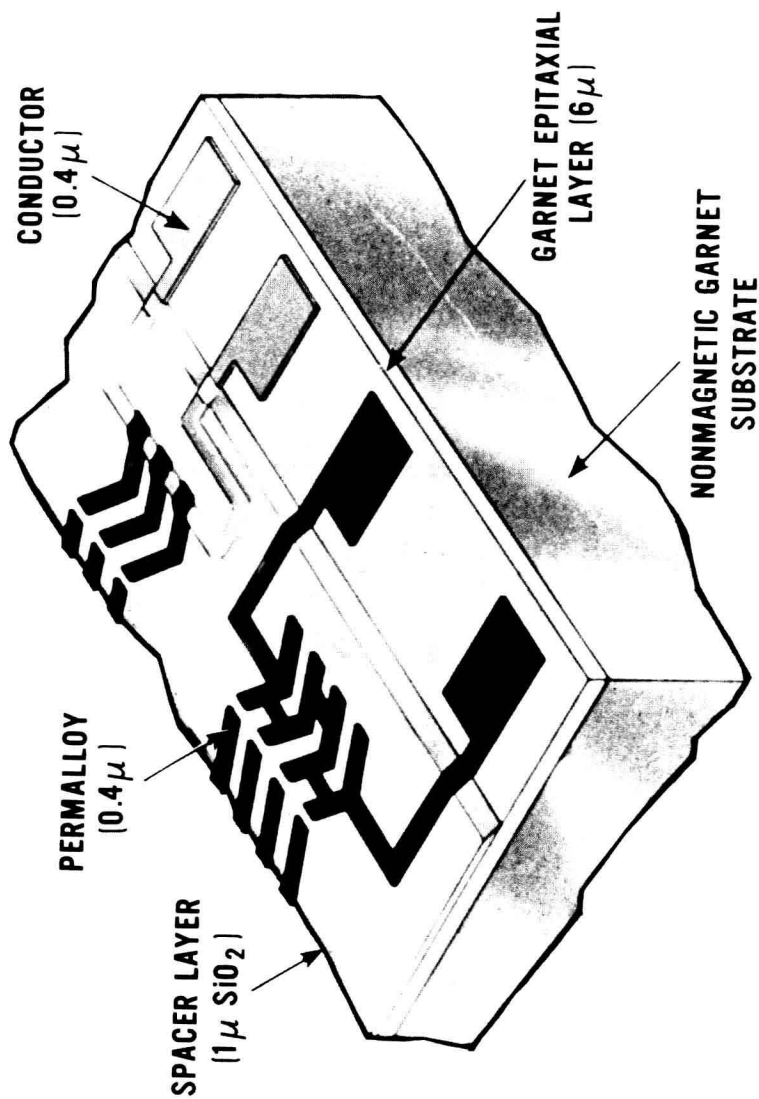


FIGURE 4

Integrated circuit: 2-mask-level bubble chip. Mass memories now being manufactured