

Sarah: Hope this will do. Bob

To: ren1@psu.edu

Subject: AW: Structure-Property Relations Book

Dear Bob,

there is no problem with the book which is out of sale. I am very interested in your new book. Please let me know your ideas.

Best regards,

from Springer

Claus

-----Ursprüngliche Nachricht-----

Von: Robert Newnham [mailto:ren1@psu.edu]

Gesendet am: Freitag, 4. Juni 2004 19:50

An: Ascheron, Claus E., SV

Betreff: Structure-Property Relations Book

Hello Claus: I have several questions about the Structure-Property Relations book I published with Springer in 1975. The book is now long out of print and I am interest in doing two things. 1. I have been asked to put it on the IEEE web and I would like to do so. Is there any copyright problem in doing so? Do I require a letter from the publisher relinquishing the copyright or has the copyright expired by now? Please send me such a letter if one is required. 2. Are you interested in publishing a second edition of the book? If there is interest, I would rewrite it as a textbook with more up-to-date examples together with home problems. Let me know what you think. I'm retired now and have time to do some book-writing. 3. When I looked at the commercial web I saw a few copies of my book offered for sale. These were paperback books which were published in China. Do you know anything about this? I never received any royalty for these paperbacks. Was it an illegal publication? I look forward to hearing from you and perhaps working with you in the future. Sincerely, Bob Newnham

from me

I agree to reproducing the book "Structure-Property Relations on UFFC websites.

Robert Newnham

Crystal Chemistry of Non-Metallic Materials

2

Edited by R. Roy, University Park, PA, USA

Robert E. Newnham

Structure-Property Relations

With 92 Figures



Springer-Verlag Berlin Heidelberg New York 1975

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Preface

As a boy I loved to build model airplanes, not the snap-together plastic models of today, but the old-fashioned Spads and Sopwith Camels made of balsa wood and tissue paper. I dreamed of EDDIE RICKENBACKER and dogfights with the Red Baron as I sat there sniffing airplane glue. Mother thought I would never grow up to make an honest living, and mothers are never wrong. Thirty years later I sit in a research laboratory surrounded by crystal models and dream of what it would be like to be 1 Å tall, to rearrange atoms with pick and shovel, and make funny things happen inside. Professor VON HIPPEL calls it "Molecular Engineering," the building of materials and devices to order:

We begin to design materials with prescribed properties, to understand the molecular causes of their failings, to build into them safeguards against such failure, and to arrive at true yardsticks of ultimate performance. No longer shackled to presently available materials, we are free to dream and find answers to unprecedented challenges. It is this revolutionary situation which makes scientists and engineers true allies in a great adventure of the human mind [1].

This book is about structure-property relationships, more especially applications of crystal chemistry to engineering problems. Faced with the task of finding new materials, the crystallographer uses ionic radii, crystal fields, anisotropic atomic groupings, and symmetry arguments as criteria in the materials selection process. Symmetry is reviewed in the first chapter, emphasizing its influence on physical properties. In general, symmetry is helpful in determining which effects are absent, but not in estimating the relative sizes of property coefficients. Magnitudes depend more on the atomistic arguments presented in later chapters. Using illustrations from present day technology, I have tried to point out the crystallochemical parameters most important to the understanding of molecular mechanisms, and to the choice of new materials.

WILLIAM SHOCKLEY, co-inventor of the transistor, has said it much better [2]. The *modus operandi* of research programs is to seek fundamental understanding while at the same time remaining alert for possible applications. For many solid state problems, it is helpful to ask,

What are the atoms involved and how are they arranged?
How did this arrangement come into being?

How does this arrangement lead to certain mechanisms of electronic and atomic motion?

How do these mechanisms give rise to the observed properties?

Those are the questions I had in mind when I wrote this book, but in looking over the result, I have a sad feeling that it falls far short of the mark. As the Pennsylvania Dutch say, "Ve grow too soon oldt, undt too late schmart."

The preparation of a book requires support in many ways. Looking back, I would like to thank ETHEL CALLAHAN, LOUIS WEBER, RAY PEPINSKY, GEORGE BRINDLEY, HELEN MEGAW, and ARTHUR VON HIPPEL for helping me on my way. There are too many wonderful colleagues here at Penn State to acknowledge each individually, but I want to give special thanks to ERIC CROSS, the originator of most of "my" best ideas. The book would still be submerged among the lunch bags on my desk were it not for the efforts of DOYLE SKINNER, DICK HORSEY, DARIA SESSAMEN, and RUSTUM ROY, the editor of this series. No man is an island—to coin a phrase—and no man has a finer family than mine: Pat, Randy, Rosie, Mom and Dad are wonderful to live with, and except for Zoomer, none are the least big grouchy. Every day is a happy one.

University Park, February 1975

ROBERT NEWNHAM

References

1. VON HIPPEL, A.: Science **138**, 91 (1962).
2. SHOCKLEY, W.: Electrons and holes in semiconductors. New York: D. Van Nostrand Co. 1950.

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