经典电介质科学丛书
Classic Dielectric Science Book Series
丛书主编 姚熹 (Yao Xi, Series Editor)

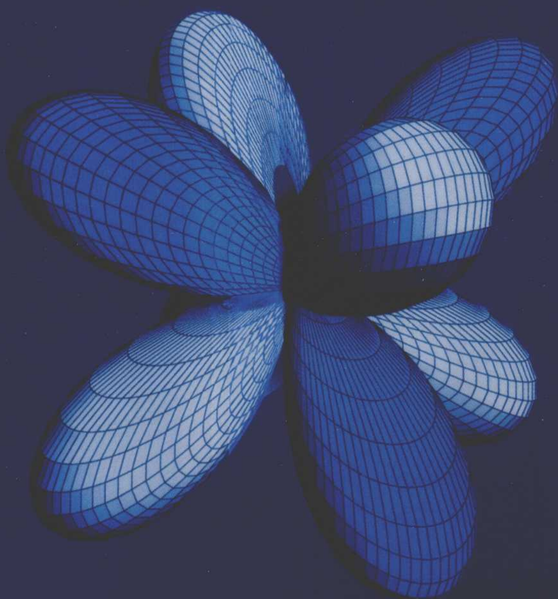
材料性能

各向异性、对称性与结构

Properties of Materials: Anisotropy, Symmetry, Structure

（影印版）

〔美〕 罗伯特·E·纽纳姆 (Robert E. Newnham) 著



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Late professor of Pennsylvania State University
Member of the US National Academy of Engineering
Member of the International Academy of Ceramics
Honorary Lifetime Member of the American Ceramic Society

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内容提要

本书是世界著名材料科学家罗伯特·E·纽纳姆教授为具有中等物理和化学背景的大学理工科学生所写的一本材料科学经典教材。它以张量、矩阵为基本数学工具，以晶体物理和化学为基础理论，以对称性、各向异性和结构与性能的关系为线索，配以丰富的插图和表格，以及大量的实验数据，系统阐述了晶体物理和化学的基本原理以及晶体和其他构型材料的热力学、力学、电学、磁学、声学和光学性能特点，仔细分析了材料的热电、压电、电磁、热磁、声电、光电等各种物理化学效应，讨论了铁性体、声学、非线性光学等其他同类教材很少涉及的主题，介绍了材料的镜像异构、旋光性和化学各向异性等知识。

本书的特色在于以张量和矩阵为数学工具来处理和分析晶体的物理和化学问题，揭示物理现象背后的化学和结构根源，阐明其中的结构与性能的关系，并以大量实验数据验证所做的分析，比较各种不同的结构与性能关系，表述清晰、深入浅出、简明易懂，是一本极为难得的经典教材。

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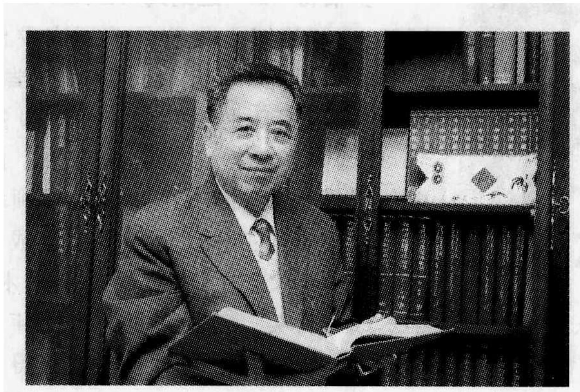
作者简介
ABOUT THE AUTHOR

罗伯特·E·纽纳姆(Robert E. Newnham, 1929-2009)博士生前是美国宾夕法尼亚州立大学材料研究所的Alcoa固态科学荣誉退休教授，美国国家工程院院士，国际陶瓷科学院院士，美国陶瓷学会荣誉终身会士。他是复合压电传感器的发明人，在铁电材料领域做出了享誉世界的研究工作。他一生独立或合作发表了500多篇学术论文，出版了5部学术著作，持有20项专利，获得了数十项学术或教育奖。他在上世纪五十年代早期从哈特威克学院获得了数学学士学位，从科罗拉多州立大学获得了物理学硕士学位，并于1956年获得宾夕法尼亚州立大学物理学博士学位，1960年获得英国剑桥大学晶体学博士学位。他曾在剑桥大学卡文迪许实验室和麻省理工学院电气工程系工作了10年，自1966年起在宾夕法尼亚州立大学任教。

Robert E. Newnham (1929 - 2009) was a late Alcoa Professor of Solid State Science Emeritus in the Materials Research Laboratory at The Pennsylvania State University. He pioneered the development of composite piezoelectric transducers, and his work in ferroelectric materials is known worldwide. A member of the US National Academy of Engineering and the International Academy of Ceramics and an honorary lifetime member of the American Ceramic Society, he has written or co-written more than 500 research papers, 5 books, and 20 patents, several tens awards for his academic or educational contributions. In the early Fifties, Newnham was granted a B. S. of Mathematics from the Hartwick College at Oneonta, N. Y., and a M.S. in physics from Colorado A&M College (now known as Colorado State University) at Ft Collins. He received a Ph. D. in physics from the Pennsylvania State University in 1956 and a Ph. D. in crystallography from Cambridge University in 1960. Prior to joining the Penn State faculty in 1966, he worked at the Cavendish Laboratory of Cambridge University and taught in the Electrical Engineering Department of MIT for 10 years.

丛书主编简介

ABOUT THE SERIES EDITOR



姚熹，1935 年生于中国江苏苏州。1957 年毕业于交通大学电机系，1982 年获美国宾夕法尼亚州立大学固态科学博士学位。1957 年至今在西安交通大学任教，1984 年起任西安交通大学教授。1989 年当选国际陶瓷科学院首批院士。1991 年当选中国科学院院士。2002 年当选美国陶瓷学会会士。2007 年因“在电子陶瓷科学和工程创新方面做出了杰出贡献”当选美国国家工程院外籍院士。

Yao Xi was born in Suzhou, Jiangsu, China, in 1935. He graduated from the department of electrical engineering, Jiaotong University in 1957, and received his Ph.D. of solid state science from the Pennsylvania State University in 1982. He has been a professor of Xi'an Jiaotong University since 1984. Dr. Yao was elected as an Academician in the first election of the World Academy of Ceramics in 1989. He was also elected as a Member of the Chinese Academy of Sciences in 1991 and a Fellow of the American Ceramic Society in 2002. In 2007, Prof. Yao was elected to be Foreign Associate of the US National Academy of Engineering for his "contributions to the science and engineering innovations for electroceramics".

丛书序

五十年前，我坐在交通大学（上海）的一间教室里上一门叫"电介质物理"的课程，讲授者是已故的陈季丹教授，当时参加这门课程学习的同学有 30 位。这是电介质这门学科第一次被介绍到中国的大学里。此后，电介质研究成为中国科技界在发展电气和电子工程的过程中一个重点关注的领域。五十年过去了，中国数以千计的大学生、研究生、教授，科学家和工程师在从事电介质的研究和应用工作。在过去的五十多年里，西安交通大学、上海交通大学、电子科技大学、山东大学、中山大学、四川大学、南京大学、同济大学和中国科学院上海硅酸盐研究所、中国科学院物理研究所等许多单位在电介质研究方面投入了相当大的科研力量，为中国的电介质研究做出了各自不同的贡献。现在中国或许是在电介质研究中包括前苏联和英国在内的最重要的国家之一。已故的陈季丹教授是中国电介质研究的先驱者和奠基人。他的认真、踏实、严谨的学术态度，是中国电介质界最宝贵的财富。我愿借写这篇序言之机，向陈教授表示由衷的敬意。

然而，作为固态科学的一个分支，电介质科学的发展还不尽如人意。我们对实际电介质中电一物理过程的理解还很难超越经典电磁理论。例如，在实际电介质中，电荷的集合以什么方式对外加电场的激励作出反应，这些集合体之间以什么方式通讯和相互作用，都还不清楚；我们对实际电介质中的局域场、缺陷、非均匀性、空间电荷的了解还相当有限；至于电介质材料中的结构一性能关系，我们的认识也很粗浅；我们仍然在为如何计算碱金属卤化物晶体、水以及其他高介电常数材料的介电常数而苦苦努力。和固态科学的其他领域相比，如金属材料、半导体材料和磁性材料，电介质或许是固态材料中理解得最不够深入的一个领域。电介质科学的现状很不能令人满意。电介质科学工作者应该付出更多的努力以赶上 21 世纪现代科学技术的发展。

中国可能是世界上电介质研究群体最大的国家。在过去的几十年里，许多老一代科学家矢志不移地投身电介质研究，贡献了他们毕生的心血。新一代的电介质研究队伍已经越来越成熟和壮大。相比于老一代，他们受到了更好的学术训练，拥有更好的工作条件。中国的电介质学界应该为电介质科学的前进作出更大的贡献。然而，电介质科学直到现在还不是固态科学的主流学科。许多重要的英语著作发表在20—60年以前。其中最早的一本书是德拜的《极性分子》，出版于1928年。现在中国的年轻学者要读到这些重要的经典著作非常困难。为了提升中国的电介质研究，西安交通大学电子材料研究所提出一个推介国外电介质科学重要著作的出版项目，在获得国外原出版社版权许可之后，在中国影印出版这些图书。我很高兴西安交通大学出版社欣然同意支持“经典电介质科学丛书”这一出版项目。我们将尽我们知识和判断力之所能仔细挑选，以保证“经典电介质科学丛书”能够囊括所有重要而有用且不失简明的著作。当然，囿于我们所掌握的知识和信息，或许有些重要著作被遗漏了。因此，我们对读者所提出的任何建议和提议，都深表谢意。

我想借此机会感谢本丛书的国内出版者——西安交通大学出版社，感谢他们对本项目的大力支持，也赞赏他们致力于提升学术水平的远见。同时，我也想感谢牛津大学出版社等原著的出版者，感谢他们慷慨授权这些著作在中国出版。我也要对这些著作的作者们表达崇高的敬意。我们不能一一向他们表达谢意，在此一并致谢并祝他们健康快乐！最后，我要感谢魏晓勇博士和徐卓博士，以及本丛书的责任编辑赵丽萍女士和贺峰涛先生，因着他们的热情和付出的辛勤工作，才使得“经典电介质科学丛书”这一项目得以实现。

姚熹

西安交通大学电子材料研究所

2006年4月20日

Preface to the Classic Dielectric Science Book Series

Fifty years ago, I was sitting in a class at Jiaotong University in Shanghai, China taking a course called "DIELECTRIC PHYSICS" lectured by the late Professor Chen Jidan. I was one of the thirty students sitting in his class taking the course. This was the first time DIELECTRIC study was introduced to Chinese Universities. Since then, dielectric study became one of the major concerns of the science and technology community of China in developing its electrical and electronic engineering. Fifty years past, thousands of students, graduate students, professors, scientists and engineers have been engaged in the studies and applications of dielectrics in this country. In the past fifty years, the Xi'an Jiaotong University, Shanghai Jiaotong University, Electronic Science and Technological University, Shandong University, Zhongshan University, Sichuan University, Nanjing University, Tongji University and the Shanghai Institute of Ceramics, the Beijing Institute of Physics of the Chinese Academy of Sciences were heavily involved in dielectric studies and gave their various contributions to the development of dielectric study in China. Now, China is probably one of the most important countries in dielectric studies among the list of the ex Soviet Union and the United Kingdom. Late Professor Chen was the pioneer and founder of DIELECTRIC studies in China. The staidness, sureness and solemnness of his academic attitude are the invaluable treasure of the Chinese dielectric community. I would like to take the chance of writing this preface to pay my sincere respect to the late Professor Chen.

However, as a branch of solid state science, the advancement of dielectric science is not well satisfied as widely expected. Our basic understanding on the electro-physical process within real dielectrics beyond the classical electro-magnetic theory is still rather poor. For example, the way how the charge assemblies respond to the external stimuli of electric field and the way of the communication and interaction among charge assemblies in real dielectrics are yet to be explored. Our understanding on local field, defects, inhomogeneous, space charges in real dielectric materials is to be profounded. As to the structure-property relationship of dielectric materials is still rather superficial. We are still struggling on how to calculate the dielectric constants of alkali-halogen crystals, water and other high dielectric constant materials. In contrast with other fields of solid state science such as metal, semiconductor and magnetics, dielectrics are probably the worst understood arena of solid state materials. The current status of dielectric science is not satisfied at all. Big efforts should be taken to catch up with the development of modern science and technology in this 21st century.

China is probably the country having the largest community of dielectric study in the world. Many of the old generation have devoted their career life focused on dielectrics in the past several decades. Next generation of dielectric study is now getting more mature and stronger. They have got better training and better working condition than their old generation. The Chinese dielectric community should be able to render more contribution to the advancement of dielectric science. However, dielectric science is now not yet in the main stream of solid state science. Many of the important publications were published twenty to sixty years ago in English. The first published book by P. Debye, Polar Molecules, was published in 1928. These important classics are not easily available to young scholars nowadays. To promote the dielectric studies in China, Electronic Materials Research Laboratory at Xi' an Jiaotong University proposed a publication project to introduce the most important classical publications on dielectrics from abroad and publish them in China, subjected to the consent of their original publishers. I am very pleased that the Xi' an Jiaotong University Press (XJTU Press) kindly agrees to support the publication project of Classical Dielectric Science Book Series (CDSBS). We will carefully select the subjects and topics based on our best knowledge and judgment to keep the CDSBS including all the important and useful publications, while still keeping it concise. Needless to say, due to the restriction of our knowledge and information, there might be pretermissions in searching and collection. Any suggestion and recommendation from the reader of the series would be highly appreciated.

I would like to take the chance to thank the Chinese publisher, the Xi'an Jiaotong University Press, for their kind support of the project and their far sighted vision in promoting academic excellence, as well as the original publishers, such as the Oxford University Press and etc. for their generous consideration to permit the publication of their books in China. Highest esteem will be dedicated to the authors of the books. We may not be able to give our thanks to them individually. We gratitude them and hope them happy and healthy. I would also acknowledge Dr. Wei Xiaoyong and Dr. Xu Zhuo as well as the editors of the book series Ms Zhao Liping and Mr. He Fengtao for their enthusiastic and hard works to promote the CDSBS project being realized.

Yao Xi

Electronic Materials Research Laboratory,
Xi'an Jiaotong University
April 20, 2006

前　言

本书的主题是晶体的各向异性以及性能与结构的关系。基于张量和矩阵提供的数学框架，对称性可以帮助确定哪些（物理性能）系数是否为零，哪些系数必须相等。然而面对其性能参数的大小却无能为力，这更多的取决于原子层面的讨论。我曾经试图指出某些晶体化学要素（例如键长、配位数和电子结构）与性能参数之间的关系。这些关系提供了分子层面的定性理解，对各种工程应用中选择材料有所帮助。

本书共 32 章，约 370 页，涵盖了材料物理性能方面丰富的主题介绍，贯穿其中的是张量和矩阵的使用。我曾经给高年级的本科生和低年级的研究生讲授这些内容。教师可以选择部分内容讲授一个学期，或者选择全书内容讲授两个学期。

本书的先修要求是大学程度的物理和化学，在美国的大学里这些课程通常在第一年或第二年开设。对张量和矩阵代数没有特殊的要求，但最好有基本的晶体学知识。

在讲授这门课程和撰写这本书的时候，我的头脑里产生了如下一些问题：

物理性能如何依赖于晶体的方向？

在数学上，如何描述这些性能，它们的几何表象是什么样的？

矩阵表示和张量描述有什么样的不同？

极张量和轴张量描述的性能有什么不同？什么因素决定了张量的阶数？

如何测量物性参数？这些参数如何被温度、频率、压力和外场等测量条件影响？

对称性如何影响物理性能？

对称性如何影响物性参数使其为零或两两相等，需要多少次测量才能完全确定材料的性能？

各向异性如何与晶体结构及织构关联？

材料物性的取向特征，是否表示结构中存在对应的系列层结构？

张量元的强度如何与键长、键强和化学成分有关?

什么是最重要的工业应用?

什么样的性能组合与“优值”有关?

未来我们如何进一步改善材料的性能?

“分子工程”的目标是依据对材料结构-性能关系的理解,进行材料和器件性能的优化。

许多同事和朋友对我写成此书提供了帮助,尤其要感谢宾州州立大学和香港理工大学的师生,也向美国海军研究办公室持续的支持表示感谢。

我把此书献给我的妻子帕翠西娅,她是两个可爱孩子的母亲和我一生的伴侣,她给了我一个充满温馨的家庭。

Preface

This book is about anisotropy and structure–property relationships. Tensors and matrices provide the mathematical framework, and symmetry is helpful in determining which coefficients are absent, and which must be equal, but they say nothing about the sizes of the property coefficients. Magnitudes depend more on atomistic arguments. I have tried to point out some of the crystallochemical parameters (such as bond lengths, coordination numbers, and electronic structure) that correlate with property coefficients. These relationships provide a qualitative understanding of the molecular mechanisms which underlie the choice of materials for various engineering applications.

The book contains 32 chapters and about 370 pages. It covers a wide range of topics and is suitable as an introduction to the physical properties of materials. The use of tensors and matrices provides a common theme which ties the topics together. I have taught the course at the advanced undergraduate level and to beginning graduate students. Instructors can select topics for a one semester course or use the entire book for a two-semester course.

The only prerequisites for the course are college-level physics and chemistry. Such courses are commonly offered during the first year or two at American universities. No special training in tensor or matrix algebra is required, but knowledge of basic crystallography is helpful.

In teaching the course and in writing the book, I had the following questions in mind.

How do physical properties depend on direction?

How are these properties described mathematically, and what do the geometric representations look like?

How do matrix representations differ from the tensor descriptions?

How do polar tensor properties differ from axial tensor properties? And what determines the tensor rank?

How are the property coefficients measured and how are they influenced by measurement conditions such as temperature, frequency, pressure, and external fields?

How does symmetry influence the physical properties?

Which coefficients are zero by symmetry, which are equal, and how many measurements are required to specify the property?

How is anisotropy related to crystal structure and texture?

Are there chains or layers in the structure that correlate with the directional properties?

How do the magnitudes of the tensor components depend on bond lengths, bond strengths, and chemical composition?

What are the most important engineering applications?

What combination of properties are involved in the "figure of merit"?

How might future improvements be made in the properties?

The goal of this process—a process some call "Molecular Engineering"—is the optimization of materials and devices through an understanding of structure–property relationships.

Many, many colleagues and friends helped me prepare this book: The faculty, staff, and students at the Pennsylvania State University and the Hong Kong Polytechnic University were especially helpful. The sustained support of the Office of Naval Research is also gratefully acknowledged.

I dedicate this book to my wife Patricia, the mother of our two wonderful children, and my lifelong companion in the House of Love and Good Suppers.

目　录