

## **Silicon-Based Materials and Devices**

# Silicon-Based Materials and Devices

Volume 2  
**Properties and Devices**

Edited by

**Hari Singh Nalwa**, M.Sc., Ph.D.  
Stanford Scientific Corporation  
Los Angeles, California, USA

*Formerly at  
Hitachi Research Laboratory  
Hitachi Ltd., Ibaraki, Japan*



**ACADEMIC PRESS**

A Harcourt Science and Technology Company

San Diego San Francisco New York Boston  
London Sydney Tokyo

This book is printed on acid-free paper. ∞

Copyright © 2001 by Academic Press

All rights reserved.

No part of this publication may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopying, recording, or any information storage and retrieval system, without permission in writing from the publisher.

The appearance of the code at the bottom of the first page of a chapter in this book indicates the Publisher's consent that copies of the chapter may be made for personal or internal use of specific clients. This consent is given on the condition, however, that the copier pay the stated per copy fee through the Copyright Clearance Center, Inc. (222 Rosewood Drive, Danvers, Massachusetts 01923), for copying beyond that permitted by Sections 107 or 108 of the U.S. Copyright Law. This consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective works, or for resale. Copy fees for pre-2001 chapters are as shown on the title pages. If no fee code appears on the title page, the copy fee is the same as for current chapters./01 \$35.00

Explicit permission from Academic Press is not required to reproduce a maximum of two figures or tables from an Academic Press chapter in another scientific or research publication provided that the material has not been credited to another source and that full credit to the Academic Press chapter is given.

Requests for permission to make copies of any part of the work should be mailed to the following address: Permissions Department, Harcourt, Inc., 6277 Sea Harbor Drive, Orlando, Florida, 32887-6777.

ACADEMIC PRESS

*A Harcourt Science and Technology Company*

525 B Street, Suite 1900, San Diego, CA 92101-4495, USA

<http://www.academicpress.com>

Academic Press

Harcourt Place, 32 Jamestown Road, London NW1 7BY, UK

<http://www.academicpress.com>

**Library of Congress Catalog Card Number: 00-108486**

International Standard Book Number (Set): 0-12-513909-8

International Standard Book Number (Vol. 1): 0-12-513918-7

International Standard Book Number (Vol. 2): 0-12-513919-5

Printed in the United States of America

01 02 03 04 05 QW 9 8 7 6 5 4 3 2 1

*To my brothers,  
Jagmer Singh  
and  
Ranvir Singh Chaudhary*

---

# CONTENTS

Preface . . . . .	xi
About the Editor . . . . .	xiii
List of Contributors . . . . .	xv
 <b>Chapter 1. OPTICAL ABSORPTION, LUMINESCENCE, AND ESR SPECTRAL PROPERTIES OF POINT DEFECTS IN SILICA</b>	
<i>M. Leone, S. Agnello, R. Boscaino, M. Cannas, and F. M. Gelardi</i>	
1. Introduction . . . . .	2
2. Optical and ESR Activity of Oxygen-Deficient Centers in Silica . . . . .	2
2.1. Introduction . . . . .	2
2.2. Oxygen-Deficient Centers . . . . .	3
2.3. E' Center: ESR and Optical Properties . . . . .	4
2.4. The Absorption Band B <sub>2</sub> and Related Emissions . . . . .	4
2.5. The Absorption Band E . . . . .	6
2.6. Summary . . . . .	7
3. Optical and ESR Spectroscopy of Point Defects . . . . .	7
3.1. Introduction . . . . .	7
3.2. Electronic States of a Point Defect . . . . .	8
3.3. Optical Absorption Spectroscopy . . . . .	9
3.4. Luminescence Spectroscopy . . . . .	12
3.5. ESR Spectroscopy . . . . .	13
4. Experimental Methods . . . . .	15
4.1. Introduction . . . . .	15
4.2. Samples and $\gamma$ -radiation . . . . .	15
4.3. Experimental Techniques . . . . .	16
5. Optical Activity in Natural Silica . . . . .	19
5.1. The 3.1 and 4.2 eV PL Bands Under UV Excitation . . . . .	19
5.2. Excitation of 3.1 eV and 4.2 eV PL Bands in Vacuum-UV Spectral Region . . . . .	24
5.3. Discussion . . . . .	26
6. The Effects of $\gamma$ Irradiation on the Optical and ESR Activity . . . . .	26
6.1. The Intrinsic and $\gamma$ -Induced Optical Activity: A <sub>I</sub> and A <sub>R</sub> . . . . .	26
6.2. Relations between the 4.4 eV Emission and the OA Band E: A <sub>T</sub> Activity . . . . .	31
6.3. Effects of the $\gamma$ Irradiation on the Optical Activity B and Relation with ESR Structures . . . . .	35
6.4. $\gamma$ Induced E' Centers: ESR and Optical Activity . . . . .	38
7. Effects of the Local Environment on the Optical Properties of Luminescent Centers . . . . .	39
7.1. Local Dynamic Properties . . . . .	39
7.2. The Effect of Conformational Disorder on the Photoluminescence Activity of Vitreous Systems . . . . .	43
8. Conclusions . . . . .	46
8.1. Summary . . . . .	46
8.2. Future Aspects . . . . .	48
Acknowledgments . . . . .	48
References . . . . .	48

## Chapter 2. THE REFRACTIVE INDEX OF SILICA GLASS AND ITS DEPENDENCE ON PRESSURE, TEMPERATURE, AND THE WAVELENGTH OF THE INCIDENT LIGHT

*C. Z. Tan and J. Arndt*

1. Introduction . . . . .	51
2. Theories . . . . .	53
2.1. Electric Potential Energy of the Incident Light and the Hamiltonian of the Induced Oscillators in Nonabsorbing Isotropic Dielectrics . . . . .	53
2.2. The Mean Polarizability and Density of Glasses . . . . .	56
2.3. Temperature Dependence of Refractive Index of Glassy SiO <sub>2</sub> in the Ultraviolet and Visible Regions . . . . .	60
3. Experiments . . . . .	63
3.1. Optical Properties of Densified Silica Glasses . . . . .	63
3.2. Determination of Refractive Index of Glassy SiO <sub>2</sub> for Infrared Wavelengths by IR Spectroscopy . . . . .	68
3.3. Optical Phase Change on Reflection at v-SiO <sub>2</sub> -Sn Interface . . . . .	72
3.4. Optical Interference and Refractive Index of Silica in the Infrared Absorption Region . . . . .	74
3.5. Temperature Dependence of Refractive Index of Glassy SiO <sub>2</sub> in the Infrared Wavelength Region . . . . .	77
3.6. Temperature-Dependent Optical Depolarization in Glassy SiO <sub>2</sub> . . . . .	80
4. Implications . . . . .	82
4.1. Faraday Effect in Glassy SiO <sub>2</sub> . . . . .	82
4.2. Measurement of Piezoelectricity in Quartz and Electrostriction in SiO <sub>2</sub> Glass by Interferometric Method . . . . .	85
5. Summary . . . . .	89
References . . . . .	90

## Chapter 3. STRUCTURES AND PROPERTIES OF AMORPHOUS SILICON DIOXIDE — ISSUES ON THE RELIABILITY AND NOVEL APPLICATIONS

*Hiroyuki Nishikawa*

1. Introduction . . . . .	93
1.1 Basic Properties of a-SiO <sub>2</sub> . . . . .	94
1.2 Properties of a-SiO <sub>2</sub> . . . . .	96
2. Characterization Techniques of Defects in SiO <sub>2</sub> . . . . .	97
2.1 Optical Characterization Techniques . . . . .	97
2.2 ESR and Related Techniques . . . . .	100
2.3 Computational Approaches . . . . .	102
3. Reliability Issues . . . . .	103
3.1 Defects and Formation Reactions in a-SiO <sub>2</sub> . . . . .	103
3.2 Optical Applications . . . . .	105
3.3 Electronic Applications . . . . .	110
4. Novel Applications of a-SiO <sub>2</sub> . . . . .	113
4.1 Fiber Gratings . . . . .	114
4.2 Second Harmonic Generation (SHG) . . . . .	116
4.3 Three-Dimensional (3D) Optical Memory . . . . .	116
4.4 Silicon Nanostructures in SiO <sub>2</sub> . . . . .	117
5. Summary . . . . .	117
Acknowledgment . . . . .	118
References . . . . .	118

## Chapter 4. POROUS SILICON MICROCAVITIES

*Claudio Vinegoni, Massimo Cazzanelli, and L. Pavesi*

1. Introduction . . . . .	124
2. Porous Silicon . . . . .	125
2.1. Fabrication of Porous Silicon . . . . .	125
2.2. Structure of Porous Silicon . . . . .	130

2.3. Chemical Properties of Porous Silicon . . . . .	137
2.4. Optical Properties . . . . .	141
2.5. Luminescence in Porous Silicon . . . . .	143
3. Dielectric Multilayers . . . . .	146
3.1. Thin Slab . . . . .	147
3.2. Bragg Reflectors . . . . .	148
3.3. Fabry-Perot Interference Filters . . . . .	149
4. Semiconductor Microcavities . . . . .	151
4.1. Weak Coupling Mode . . . . .	152
4.2. Strong Coupling Mode . . . . .	152
5. Porous Silicon Multilayers . . . . .	153
5.1. Producing Porous Silicon Multilayers . . . . .	155
5.2. Bragg Reflectors . . . . .	158
5.3. Random Bragg Reflectors . . . . .	159
5.4. Fabry-Perot Filters . . . . .	161
5.5. Random Fabry-Perot Filters . . . . .	162
6. Porous Silicon Microcavities . . . . .	164
6.1. Physical Properties . . . . .	164
6.2. Aging Effects in Porous Silicon Microcavities . . . . .	167
6.3. Simulation of the Optical Properties of Porous Silicon Microcavities . . . . .	168
6.4. Time-Resolved Spectroscopy in Porous Silicon Microcavities . . . . .	169
6.5. Temperature Dependence of Porous Silicon Microcavities . . . . .	175
6.6. Coupled Porous Silicon Microcavities . . . . .	178
7. Applications of Porous Silicon Multilayers and Microcavities . . . . .	182
7.1. Waveguides . . . . .	182
7.2. Enhancement of Weak Absorption Signals . . . . .	183
7.3. Optical Nonlinearities . . . . .	183
7.4. Resonant Cavity Light-Emitting Diodes . . . . .	183
7.5. Optical Sensor . . . . .	185
7.6. Color-Sensitive Photodiodes . . . . .	185
7.7. Metal–Porous Silicon Microcavities . . . . .	186
8. Conclusions . . . . .	187
Acknowledgments . . . . .	188
References . . . . .	188

## **Chapter 5. POLYCRYSTALLINE SILICON BASED THIN FILM TRANSISTORS FOR INTEGRATED ACTIVE-MATRIX LIQUID-CRYSTAL DISPLAYS**

*C. A. Dimitriadis*

1. Introduction . . . . .	183
2. Materials for Thin Film Transistors . . . . .	194
2.1. Polycrystalline Silicon . . . . .	194
2.2. Structural Properties . . . . .	196
2.3. Electrical Properties . . . . .	200
3. Polysilicon Thin Film Transistors . . . . .	202
3.1. Grain Boundary Trapping States . . . . .	203
3.2. Threshold Voltage . . . . .	205
3.3. Field-Effect Mobility . . . . .	208
3.4. Subthreshold Swing Voltage . . . . .	209
3.5. Leakage Current . . . . .	211
4. Reliability of Polysilicon TFTs . . . . .	213
4.1. Reliability of Low-Temperature Polysilicon TFTs . . . . .	213
4.2. Reliability of High-Temperature Polysilicon TFTs . . . . .	216
5. Concluding Remarks and Future Trends . . . . .	220
References . . . . .	221

**Chapter 6. LIGHT EMISSION IN SILICON***David J. Lockwood*

1. Introduction . . . . .	225
2. Optoelectronics . . . . .	225
3. Optical Emission in Silicon . . . . .	226
4. Overcoming the Indirect Band Gap Limitations in Silicon . . . . .	227
4.1. Brillouin Zone Folding in Atomic Layer Superlattices . . . . .	228
4.2. Band Structure Engineering via Alloying . . . . .	229
4.3. Luminescence via Impurity Centers . . . . .	230
4.4. Silicon Nanostructures . . . . .	232
4.5. Polymers and Molecules Containing Silicon . . . . .	240
4.6. Hybrid Methods for Integrating Direct Gap Materials with Silicon . . . . .	241
5. Prospects For Silicon-Based Optoelectronic Devices . . . . .	242
References . . . . .	243

**Chapter 7. ERBIUM IN SILICON AND SILICON-GERMANIUM***J. H. Evans-Freeman and A. R. Peaker*

1. Erbium in Silicon and Atomic Luminescence from Erbium . . . . .	247
1.1. Historical Perspective . . . . .	247
1.2. System Requirements . . . . .	248
1.3. Erbium and Luminescence . . . . .	249
2. Incorporation of Erbium into Silicon and Silicon-Germanium . . . . .	250
2.1. Solubility and Diffusivity . . . . .	250
2.2. Incorporation by Diffusion and Epitaxy . . . . .	252
2.3. Ion Implantation and Regrowth . . . . .	254
2.4. Crystal Field Effects, Siting and Complexes . . . . .	257
2.5. Erbium in Amorphous and in Porous Silicon . . . . .	259
3. Electrical Activity of Erbium in Si . . . . .	260
3.1. Erbium as a Donor or Acceptor . . . . .	260
3.2. Excitation of Erbium Atoms in a Silicon Host . . . . .	262
3.3. Temperature Quenching of the Erbium Infra-f-Shell Luminescence . . . . .	265
3.4. Luminescence Decay Mechanisms . . . . .	266
4. Silicon-Based LEDs and Proposed Laser Structures . . . . .	268
4.1. Erbium-Doped Silicon LEDs . . . . .	268
4.2. Erbium-Doped SiGe–Si Structures as LEDs . . . . .	270
4.3. Proposed LASER Cavities . . . . .	271
References . . . . .	272
Index . . . . .	275



---

## PREFACE

*Silicon-Based Materials and Devices* is a follow-up to our recently published 10-volume set, *Handbook of Advanced Electronic and Photonic Materials and Devices*. It presents highly coherent coverage of silicon-based materials, namely, those that have been extensively used for applications in electronic and photonic technologies. This extensive reference provides broad coverage of silicon-based materials including different kinds of silicon-related materials, their processing, spectroscopic characterization, physical properties, and device applications. Fourteen chapters review state-of-the-art research on silicon-based materials and their applications to devices.

The details of amorphous silica are summarized by M. Tomozawa, whereas the structures and properties of amorphous silicon dioxide, which are related to the issues of reliability and novel applications, are discussed by H. Nishikawa. F. Giorgis and C. F. Pirri describe the growth, characterization, and physical properties of noncrystalline and nanostructured silicon-based alloys. Silicon carbide is very useful for tribological and structural applications because of its hardness, wide-temperature-range operation, and corrosion resistance. The structural, optical, and electrical properties of amorphous silicon carbide films are discussed by W. K. Choi, and in “Silicon Carbon Nitrides: A New Wideband Gap Material,” L. C. Chen and coworkers focus on silicon carbide-related materials. M. Masi, C. Cavallotti, and S. Carra discuss the gas phase and surface kinetics of silicon chemical vapor deposition from silane and chlorosilane.

Three chapters focus on processing and physical properties of silicon; they include “Photonic and Magnetic Properties of Spark-Processed Silicon” by R. E. Hummel; “Wet-Chemical Conditioning of Silicon: Electronic Properties Correlated with the Surface Morphology” by H. Angermann, W. Henrion, and A. Röseler; and “Optical Absorption, Luminescence, and ESR Spectral Properties of Point Defects in Silica” by M. Leone, S. Agnello, R. Boscaino, M. Cannas, and F. M. Gelardi. The effect of pressure, temperature, and wavelength of the incident light on the refractive index of silica glasses is extensively discussed by C. Z. Tan and J. Arndt.

Besides many other applications, silicon is a key component of today’s integrated circuit technology. For example, silicon dioxide has been used extensively as an interlayer dielectric material for microelectronic packaging devices, light-emitting diodes, transistors, optical fiber, endoscopy, and so forth. Four chapters focus on the applications of silicon and its related materials in electronic and photonic devices: “Porous Silicon Microcavities” by C. Vinegoni, M. Cazzanelli, and L. Pavesi; “Polycrystalline Silicon-based Thin Film Transistors for Integrated Active-Matrix Liquid-Crystal Displays” by C. A. Dimitriadis; “Light Emission in Silicon” by D. J. Lockwood; and “Erbium in Silicon and Silicon-Germanium” by A. R. Peaker and J. H. Evans-Freeman.

This book covers a broad spectrum of the silicon-based materials and their device applications. Many industries around the world are engaged in silicon-based technology for the new millennium. The applications of silicon and silicon-based materials in present microelectronics and communication technology have been extensively discussed. This reference should be a valuable resource to scientists, graduate and upper level graduate students working in solid state physics, materials science, chemistry, electrical and electronic engineering, optical engineering, microelectronics, data storage, information technology, and semiconductor industries.

Both the editor and the publisher are very grateful to the authors of this project for their outstanding contributions.

Hari Singh Nalwa  
Los Angeles

---

## ABOUT THE EDITOR

Dr. H. S. Nalwa is the Managing Director of the Stanford Scientific Corporation, Los Angeles, California. He was Head of Department and R&D Manager at the Ciba Specialty Chemicals Corporation in Los Angeles (1999–2000) and a staff scientist at the Hitachi Research Laboratory, Hitachi Ltd., Japan (1990–1999). He has authored more than 150 scientific articles and 18 patents on electronic and photonic materials and devices. He has edited the following books: *Ferroelectric Polymers* (Marcel Dekker, 1995), *Nonlinear Optics of Organic Molecules and Polymers* (CRC Press, 1997), *Organic Electroluminescent Materials and Devices* (Gordon & Breach, 1997), *Handbook of Organic Conductive Molecules and Polymers*, Vol. 1–4 (John Wiley & Sons, 1997), *Low and High Dielectric Constant Materials* Vol. 1–2 (Academic Press, 1999), *Handbook of Nanostructured Materials and Nanotechnology*, Vol. 1–5 (Academic Press, 1999), *Handbook of Advanced Electronic and Photonic Materials and Devices*, Vol. 1–10 (Academic Press, 2000), *Advanced Functional Molecules and Polymers*, Vol. 1–4 (Gordon & Breach, 2001), *Photodetectors and Fiber Optics* (Academic Press, 2001), *Supramolecular Photosensitive and Electroactive Materials* (Academic Press, 2001), *Nanostructured Materials and Nanotechnology* (Academic Press, 2001), *Handbook of Thin Film Materials*, Vol. 1–5 (Academic Press, 2001), and *Handbook of Surfaces and Interfaces of Materials*, Vol. 1–5 (Academic Press, 2001). The *Handbook of Nanostructured Materials and Nanotechnology* (Vol. 1–5) edited by him received the 1999 Award of Excellence from the Association of American Publishers.

Dr. Nalwa serves on the editorial board of the *Journal of Macromolecular Science-Physics*, *Applied Organometallic Chemistry* (1993–1999), *International Journal of Photoenergy*, and *Photonics Science News*. He was the founder and Editor-in-Chief of the *Journal of Porphyrins and Phthalocyanines* published by John Wiley & Sons (1997–2000). Dr. Nalwa is a member of the American Chemical Society (ACS), American Physical Society (APS), Materials Research Society (MRS), Electrochemical Society (ECS), and the American Association for the Advancement of Science (AAAS). Dr. Nalwa has been cited in the *Dictionary of International Biography*, *Who's Who in Science and Engineering*, *Who's Who in America*, and *Who's Who in the World*.

---

## LIST OF CONTRIBUTORS

Numbers in parenthesis indicate the pages on which the author's contribution begins.

**S. AGNELLO** (1)

Istituto Nazionale di Fisica della Materia and Department of Physical and Astronomical Sciences, University of Palermo, Palermo, Italy

**J. ARNDT** (51)

Institut für Mineralogie, Freie Universität Berlin, Berlin, Germany

**R. BOSCAINO** (1)

Istituto Nazionale di Fisica della Materia and Department of Physical and Astronomical Sciences, University of Palermo, Palermo, Italy

**M. CANNAS** (1)

Istituto Nazionale di Fisica della Materia and Department of Physical and Astronomical Sciences, University of Palermo, Palermo, Italy

**CLAUDIO VINEGONI** (123)

Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania, USA

**DAVID J. LOCKWOOD** (225)

Institute for Microstructural Sciences, National Research Council of Canada, Ottawa, Canada

**C. A. DIMITRIADIS** (193)

Aristotle University of Thessaloniki, Department of Physics, Thessaloniki, Greece

**J. H. EVANS-FREEMAN** (247)

Centre for Electronic Materials, Department of Electrical Engineering and Electronics, University of Manchester Institute of Science and Technology, Manchester, M60 1QD, UK

**F.M. GELARDI** (1)

Istituto Nazionale di Fisica della Materia and Department of Physical and Astronomical Sciences, University of Palermo, Palermo, Italy

**HIROYUKI NISHIKAWA** (93)

Department of Electrical Engineering, Tokyo Metropolitan Shibaura Institute of Technology, 3-9-1t Shibaura, Minato-Ku, Tokyo 108-8548, Japan

**M. LEONE** (1)

Istituto Nazionale di Fisica della Materia and Department of Physical and Astronomical Sciences, University of Palermo, Palermo, Italy

**MASSIMO CAZZANELLI** (123)

Department of Physics, Trinity College, Dublin, Ireland

**L. PAVESI** (123)

INFN and Dipartimento di Fisica, Università di Trento, Trento, Italy

**A. R. PEAKER** (247)

Center for Electronic Materials and Department of Electrical Engineering and Electronics, UMIST, Manchester, United Kingdom

**C. Z. TAN** (51)

Institut für Mineralogie, Freie Universität Berlin, Berlin, Germany