

Optical Constants of Crystalline and Amorphous Semiconductors

Numerical Data and Graphical Information

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Numerical Data and Graphical Information

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Springer Science+Business Media, LLC

Library of Congress Cataloging-in-Publication Data

Adachi, Sadao, 1950-

Optical constants of crystalline and amorphous semiconductors :
Numeric data and graphical information / by Sadao Adachi

p. cm.

Includes bibliographical references.

ISBN 978-0-7923-8567-7 ISBN 978-1-4615-5247-5 (eBook)

DOI 10.1007/978-1-4615-5247-5

1. Semiconductors--Optical properties. I. Title

QC611.6.06A3 1999

537.6'226--dc21

99-23736

CIP

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Originally published by Kluwer Academic Publishers in 1999

Softcover reprint of the hardcover 1st edition 1999

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Printed on acid-free paper.

To

Yūki, Mai, and Kōya

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PREFACE

Knowledge of the refractive indices and absorption coefficients of semiconductors is especially important in the design and analysis of optical and optoelectronic devices. The determination of the optical constants of semiconductors at energies beyond the fundamental absorption edge is also known to be a powerful way of studying the electronic energy-band structures of the semiconductors.

The purpose of this book is to give tabulated values and graphical information on the optical constants of the most popular semiconductors over the entire spectral range.

This book presents data on the optical constants of crystalline and amorphous semiconductors. A complete set of the optical constants are presented in this book. They are: the complex dielectric constant ($\epsilon = \epsilon_1 + i\epsilon_2$), complex refractive index ($n^* = n + ik$), absorption coefficient (α), and normal-incidence reflectivity (R). The semiconductor materials considered in this book are the group-IV elemental and binary, III-V, II-VI, IV-VI binary semiconductors, and their alloys.

The reader will find the companion book *"Optical Properties of Crystalline and Amorphous Semiconductors: Materials and Fundamental Principles"* useful since it emphasizes the basic material properties and fundamental principles.

The extensive bibliography is included for those who wish to find additional information if required. It is hoped that the book will attract attention of not only device engineers, but also solid-state physicists and material scientists, and particularly students specializing in the fields of semiconductor physics and device engineering.

ACKNOWLEDGMENTS

The author wishes to thank the editors and authors of the following journals and books for permission to reproduce previously published figures: *Physical Review* for Figs. A1-1, A1-5, A3-1, A3-4, A4-1, A4-2, A6-1, A6-2, A8-1, A8-3, B1-1, B2-1, B3-1, B3-2(a), B4-1, B10-1, B11-1, B13-1, B14-1, B15-1, C2-V-2, C2-VI-1, C2-IX-1, C2-X-1, C3-IV-2, C3-IV-3, D1-1, D2-1, D3-1, D4-3, D5-1, D5-2, D6-1, D7-1, D7-2, D9-1, D10-1, D11-1, D15-1, D19-3, D21-1, D22-4, D23-1, D23-2, D23-5, D24-1, D24-4, E1-1, E2-1, E3-1, E4-1, F2-4, F2-5, and F3-4; *Journal of Applied Physics* for Figs. A9-2, C2-I-1, C2-I-2, C2-III-1, C2-VI-2, C2-VII-1, C2-X-2, C2-XIII-1, C3-II-1, C3-II-2, C3-IV-1, C3-IV-4, C3-V-1, C3-V-2, C3-X-1, C3-X-2, C3-X-4, C3-X-6, C3-XI-2, C3-XI-3, C3-XIV-1, C3-XIV-2, D8-1, D14-1, D15-2, D15-3, D17-2, D17-3, D22-1, D23-6, D25-2, E6-4, F3-5, and F4-3; *Solid State Communications* for Figs. B5-1 and D18-1; *Physica Status Solidi* for Figs. B9-1, C2-V-1, D12-1, D19-2, D21-2, and D22-3; *Journal de Physique* for Fig. D20-2; *Applied Physics Letters* for Figs. A2-2, A9-3, B5-2, C2-I-3, C2-X1-1, D14-3, and D24-3; *Japanese Journal of Applied Physics* for Figs. C2-II-1, C2-X-3, C2-X-4, D2-2, D4-2, D16-2, D16-3, D17-1, D18-2, and D18-3; *Soviet Physics Semiconductors* for Fig. D19-1; *Journal of Physics: Condensed Matters* for Figs. C2-IX-2, D23-3, D23-7, and D24-2; *Journal of Crystal Growth* for Fig. D5-3; *Journal of Physics and Chemistry of Solids* for Figs. A4-3, B6-1, B7-1, B8-1, and D4-1; *Chemistry and Physics of Carbon* for Figs. A1-2 and A1-3; *Journal of the Optical Society of America* for Figs. A1-4, A6-3, and A6-4; *Proceedings of the Physical Society* for Figs. A2-1 and A3-2; *University of South Carolina Press* for Fig. A5-1; *Proceedings of the Royal Society* for Figs. A7-1 and A7-2; *Optical Materials* for Fig. A8-4; *Journal of Vacuum Science & Technology* for Fig. A9-1; *Materials Research Society Symposium* for Figs. A9-4 and C2-IX-3; *RCA Review* for Fig. B3-2(b); *Physical Review Letters* for Figs. B3-3 and E6-1; *Materials Science & Engineering* for Fig. B13-2; *Thin Solid Films* for Fig. C2-I-4; *Crystal Research and Technology* for Fig. C2-XIII-2; *Institute of Conference Series* for Fig. C3-XI-1; *Physica Scripta* for Fig. D1-2; *Semiconductor Science and Technology* for Figs. D6-2, D14-2, D23-4, and D25-1; *W. A. Benjamin, Inc.* for Fig. D11-2;

Progress in Quantum Electronics for Fig. D20-1; *Infrared Physics* for Figs. D22-2, E6-2, and E6-3; *International Journal of Infrared and Millimeter Waves* for Figs. E5-1 and E5-2; *Journal of Non-Crystalline Solids* for Fig. F4-1; and *Philosophical Magazine* for Fig. F4-2.

CONTENTS OF THE COMPANION BOOK

OPTICAL PROPERTIES OF CRYSTALLINE AND AMORPHOUS SEMICONDUCTORS:

Materials and Fundamental Principles

Sadao Adachi, Author

Chapter 1 Materials, Properties, and Basic Formulas

Chapter 2 The Reststrahlen Region

Chapter 3 The Interband Transition Region: Crystalline Materials

Chapter 4 The Interband Transition Region: Amorphous and Microcrystalline Materials

Chapter 5 At or Below the Fundamental Absorption Edge

Chapter 6 Concluding Remarks

ABBREVIATIONS AND ACRONYMS

<i>a</i> -	— amorphous-
AFM	— Atomic Force Microscopy
BZ	— Brillouin Zone
<i>c</i> -	— crystalline-
<i>c</i> -	— cubic-
CP	— Critical Point
CPA	— Coherent-Potential Approximation
CVD	— Chemical-Vapor Deposition
DFT	— Density-Functional Theory
DHO	— Damped Harmonic Oscillator
DOS	— Density of States
DP	— Deformation Potential
EMA	— Effective-Mass Approximation
EMA	— Effective-Medium Approximation
ENPM	— Empirical Nonlocal Pseudopotential Method
EPM	— Empirical Pseudopotential Method
ER	— Electroreflectance
ETBT	— Empirical Tight-Binding Theory
fcc	— face-centered cubic
<i>h</i> -	— hexagonal-
HH	— Heavy-Hole
HOA	— Harmonic Oscillator Approximation
HREELS	— High-Resolution Electron-Energy Loss Spectroscopy
IR	— Infrared
KK	— Kramers-Kronig
KSM	— Koster-Slater Method
LA	— Longitudinal Acoustic
LCAO	— Linear Combination of Atomic Orbitals
LDA	— Local-Density Approximation

LEED	— Low-Energy Electron Diffraction
LH	— Light-Hole
LMTO	— Linear Muffin-Tin Orbitals
LO	— Longitudinal Optical
LPE	— Liquid-Phase Epitaxy
LRA	— Linear Regression Analysis
MBE	— Molecular Beam Epitaxy
MDF	— Model Dielectric Function
MOCVD	— Metalorganic Chemical Vapor Deposition
MOVPE	— Metalorganic Vapor Phase Epitaxy
PL	— Photoluminescence
PR	— Photorefectance
RCA	— Radio Corporation of America
rf	— radio frequency
rms	— root mean square
RS	— Raman Scattering
SCP	— Standard Critical Point
SC1(2)	— Standard Cleaning 1(2)
SE	— Spectroscopic Ellipsometry
SO	— Spin-Orbit
STM	— Scanning Tunneling Microscopy
TA	— Transverse Acoustic
TO	— Transverse Optical
UHV	— Ultrahigh Vacuum
UV	— Ultraviolet
VCA	— Virtual-Crystal Approximation
VLSI	— Very-Large-Scale Integration
w-	— wurtzite-
XPS	— X-Ray Photoelectron Spectroscopy
μ c-	— microcrystalline-
1D	— One-Dimensional
2D	— Two-Dimensional
3D	— Three-Dimensional

B6 ALUMINUM PHOSPHIDE (AlP)

B6.1 GENERAL REMARKS

Aluminum phosphide (AlP) remains one of the least studied III-V semiconductors. This is mainly due to the difficulty of growing the crystal in sufficiently pure form and its instability in a humid atmosphere. The few published papers are mainly concerned with crystal growth techniques, but some of them also report measurements on structural, electronic, and optical properties (see Ref. [1]).

B6.2 ELECTRONIC ENERGY-BAND STRUCTURE

AlP is an indirect-band-gap semiconductor with the conduction-band minimum at X and the valence-band maximum at Γ . The electronic energy-band structure of AlP was investigated theoretically by several authors [2-4]. Figure B6-1 shows the band structure of AlP as calculated using the semi-*ab initio* orthogonalized LCAO method by Huang and Ching [3]. This calculated result gives the lowest indirect and direct gaps of $E_g^x=2.51$ eV ($\Gamma_{15}\rightarrow X_1$) and $E_0=3.74$ eV ($\Gamma_{15}\rightarrow\Gamma_1$), respectively. These are in

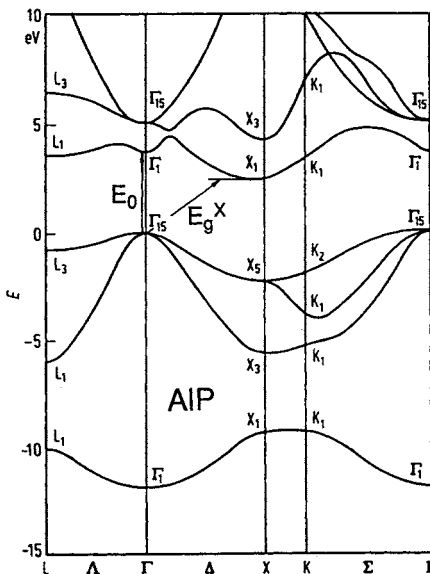


Figure B6-1 Electronic energy-band structure of AlP as calculated using the semi-*ab initio* orthogonalized LCAO method. (From Huang and Ching [3].) The locations of several interband transitions are included by the vertical arrows.

reasonable agreement with Monemar's experimental data of $E_g^x=2.505\pm0.01$ eV and $E_0=3.63\pm0.02$ eV [5].

The theoretical calculation [3] also suggests the higher-lying-gap transitions (CPs), $E_1=4.37$ eV ($L_3\rightarrow L_1$), $E_2=4.78$ eV ($X_5\rightarrow X_1$), and $E_0'=5.09$ eV ($\Gamma_{15}\rightarrow\Gamma_{15}$). Rodríguez and Armelles [6] measured SE spectra of $Al_xGa_{1-x}P$ alloy ($0\leq x\leq 0.53$) to determine the x -composition dependence of the E_0 and E_1 CP energies. Their measured x -dependence data yield, in the limit $x\rightarrow 1.0$ (AlP), $E_0=3.71$ eV (or 3.98 eV) and $E_1=4.17$ eV. However, no further experimental data are available on the CP energies for AlP at present.

B6.3 OPTICAL CONSTANTS

To date, there have been reported no data on the optical properties of AlP in the reststrahlen region. By measuring the long-wavelength n data and using the Lyddane-Sachs-Teller relation, however, Monemar [7] obtained the static and high-frequency dielectric constants of AlP to be $\epsilon_s=9.8$ and $\epsilon_\infty=7.6$.

The $n(E)$ data for AlP from $E=0.5$ to 2.8 eV were measured by Monemar [7]. The AlP crystals were grown by the reaction of PH_3 with liquid Al in an open system at 1500°C. The refractive index was found to vary from 2.75 ± 0.1 at 0.5 eV, to 3.10 ± 0.1 at 2.8 eV. Measurements on the temperature dependence of n for AlP were made by Grimmeiss and Monemar [8]. The resulting coefficient $n^{-1}(dn/dT)$ for $E=0.7$ eV near $T=300$ K was $(3.6\pm 0.3)\times 10^{-5}$ K $^{-1}$.

Measurements on the optical absorption spectra of AlP were carried out by Monemar [7] at 4–300 K and by Lorenz *et al.* [9] at 2–300 K. The AlP crystals used by Lorenz *et al.* [9] were grown by a modified Bridgman technique. The measured absorption spectra showed no clear structures involving phonons near the fundamental absorption edge (i.e., indirect absorption edge) of AlP even at low temperatures [7,9]. On the other hand, Monemar [5] identified some phonon-related fine structures in the PL excitation spectra of AlP at low temperatures [5].

Table B6-1 lists the 300-K values for the optical constants of AlP taken from Monemar [7]. Since the purity of the crystals used by him was not very high, an absorption coefficient of the order 5–20 cm $^{-1}$ in the region 2.0–2.4 eV was believed to have an extrinsic origin [7]. The (ϵ_1 , ϵ_2), (n , k), and α values in Table B6-1 are plotted in Figs. B6-2–B6-4, respectively.

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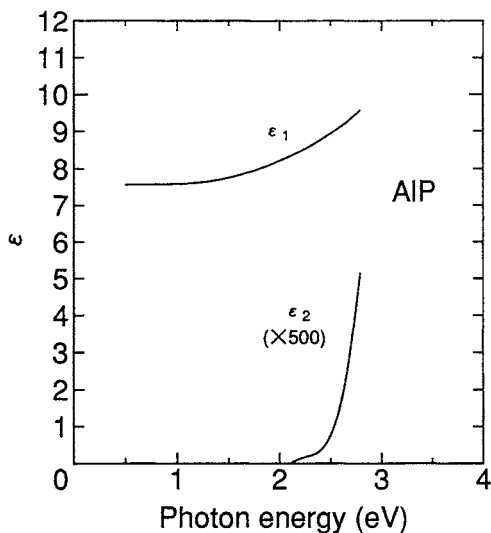


Figure B6-2 $\epsilon_1(E)$ and $\epsilon_2(E)$ spectra for AlP at 300 K.

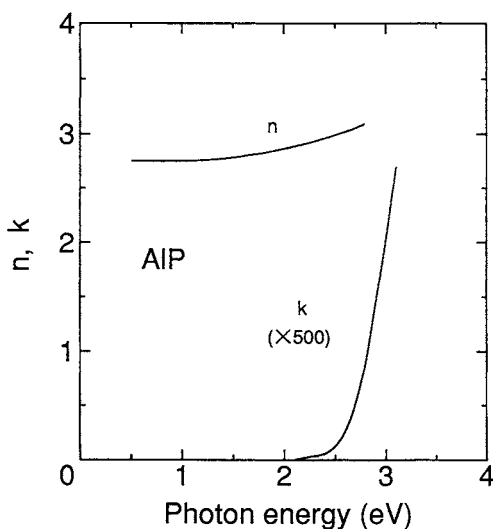


Figure B6-3 $n(E)$ and $k(E)$ spectra for AlP at 300 K.

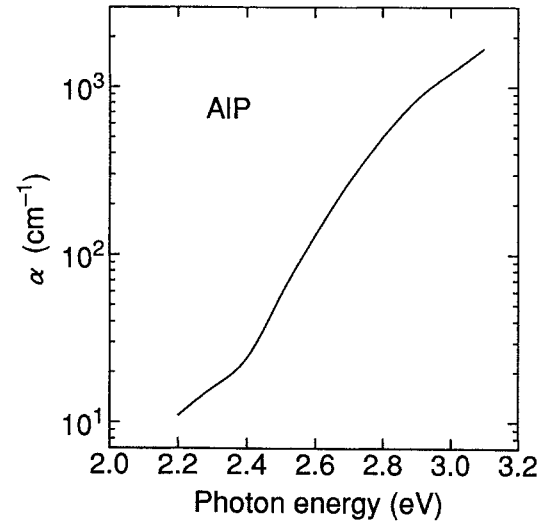


Figure B6-4 $\alpha(E)$ spectrum for AlP at 300 K.

Table B6-1 Optical constants of AlP at 300 K.

eV	ϵ_1	ϵ_2	n	k	α (cm ⁻¹)	R
0.5	7.568		2.751			0.218
1	7.583		2.754			0.218
1.1	7.598		2.756			0.219
1.2	7.620		2.760			0.219
1.3	7.652		2.766			0.220
1.4	7.694		2.774			0.221
1.5	7.754		2.785			0.222
1.6	7.825		2.797			0.224
1.7	7.906		2.812			0.226
1.8	7.993		2.827			0.228
1.9	8.095		2.845			0.230
2	8.210		2.865			0.233
2.1	8.330		2.886			0.236
2.2	8.454	0.00029	2.908	0.000049	1.10E+01	0.238
2.3	8.599	0.00040	2.932	0.000069	1.60E+01	0.241
2.4	8.767	0.00058	2.961	0.00010	2.40E+01	0.245
2.5	8.936	0.0014	2.989	0.00023	5.80E+01	0.249
2.6	9.122	0.0030	3.020	0.00049	1.30E+02	0.253
2.7	9.331	0.0060	3.055	0.0010	2.70E+02	0.257
2.79	9.568	0.0103	3.093	0.0017	4.70E+02	0.262
2.8				0.0018	5.00E+02	
2.9				0.0029	8.40E+02	
3				0.0004	1.20E+02	
3.1				0.0054	1.70E+03	