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## *Lattice Dynamics Kit*

**This revised and updated edition of the well-received book by C. Klingshirn provides an**

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introduction to and an overview of all aspects of semiconductor optics, from IR to visible and UV. It has been split into two volumes and rearranged to offer a clearer structure

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of the course content.  
Inserts on important  
experimental techniques as  
well as sections on  
topical research have been  
added to support research-  
oriented teaching and

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learning. Volume 1 provides an introduction to the linear optical properties of semiconductors. The mathematical treatment has been kept as elementary as

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possible to allow an intuitive approach to the understanding of results of semiconductor spectroscopy. Building on the phenomenological model of the Lorentz oscillator,

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the book describes the interaction of light with fundamental optical excitations in semiconductors (phonons, free carriers, excitons). It also offers a broad

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review of seminal research  
results augmented by  
concise descriptions of  
the relevant experimental  
techniques, e.g., Fourier  
transform IR spectroscopy,  
ellipsometry, modulation

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spectroscopy and spatially resolved methods, to name a few. Further, it picks up on hot topics in current research, like quantum structures, monolayer semiconductors or



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Perovskites. The experimental aspects of semiconductor optics are complemented by an in-depth discussion of group theory in solid-state optics. Covering subjects

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ranging from physics to materials science and optoelectronics, this book provides a lively and comprehensive introduction to semiconductor optics. With over 120 problems,

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more than 480 figures,  
abstracts to each chapter,  
as well as boxed inserts  
and a detailed index, it  
is intended for use in  
graduate courses in  
physics and neighboring

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sciences like material science and electrical engineering. It is also a valuable reference resource for doctoral and advanced researchers. Zeitschrift für

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Kristallographie.  
Supplement Volume 41  
presents the complete  
Abstracts of all  
contributions to the 29th  
Annual Conference of the  
German Crystallographic

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Society in Hamburg  
(Germany) 2021: - Plenary  
Talks - Microsymposia -  
Poster Session Supplement  
Series of Zeitschrift für  
Kristallographie publishes  
Abstracts of international

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conferences on the  
interdisciplinary field of  
crystallography.

This book presents the  
state-of-the-art in  
supercomputer simulation.  
It includes the latest

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findings from leading researchers using systems from the High Performance Computing Center Stuttgart (HLRS) in 2017. The reports cover all fields of computational science



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and engineering ranging from CFD to computational physics and from chemistry to computer science with a special emphasis on industrially relevant applications. Presenting

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findings of one of Europe's leading systems, this volume covers a wide variety of applications that deliver a high level of sustained performance. The book

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covers the main methods in high-performance computing. Its outstanding results in achieving the best performance for production codes are of particular interest for

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both scientists and engineers. The book comes with a wealth of color illustrations and tables of results.

The Lattice Boltzmann Method

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Combining Computational  
Fluid Dynamics and  
Magnetic Resonance Imaging  
Data Using Lattice  
Boltzmann Based Topology  
Optimisation  
Future Directions of

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**Nonlinear Dynamics in  
Physical and Biological  
Systems  
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## Infra-Red and Raman Optical Processes of Insulating Crystals Scientific and Technical Aerospace Reports

This handbook delivers an up-to-date, comprehensive and

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authoritative coverage of the broad field of surface science, encompassing a range of important materials such metals, semiconductors, insulators, ultrathin films and supported nanoobjects. Over 100 experts from



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all branches of experiment and theory review in 39 chapters all major aspects of solid-state surfaces, from basic principles to applications, including the latest, ground-breaking research results. Beginning with the fundamental

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background of kinetics and thermodynamics at surfaces, the handbook leads the reader through the basics of crystallographic structures and electronic properties, to the advanced topics at the forefront of current research. These

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include but are not limited to novel applications in nanoelectronics, nanomechanical devices, plasmonics, carbon films, catalysis, astrochemistry and biology. The handbook is an ideal reference guide and instructional aid for a

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wide range of physicists, chemists, materials scientists and engineers active throughout academic and industrial research.

Semiannual, with semiannual and annual indexes. References to all scientific and technical literature

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coming from DOE, its laboratories, energy centers, and contractors. Includes all works deriving from DOE, other related government-sponsored information, and foreign nonnuclear information. Arranged under 39 categories, e.g.,

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Biomedical sciences, basic studies;  
Biomedical sciences, applied  
studies; Health and safety; and  
Fusion energy. Entry gives  
bibliographical information and  
abstract. Corporate, author,  
subject, report number indexes.

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New Scientist magazine was launched in 1956 "for all those men and women who are interested in scientific discovery, and in its industrial, commercial and social consequences". The brand's mission is no different today - for its

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consumers, New Scientist reports, explores and interprets the results of human endeavour set in the context of society and culture.

Issues in General Physics

Research: 2012 Edition

Phonon Physics The Cutting Edge



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18th International Conference, Euro-Par 2012, Rhodes Island, Greece, August 27-31, 2012. Proceedings  
Research in Progress  
Lattice Dynamics  
Elastic and Inelastic Scanning  
Tunneling Spectroscopy on Iron-

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## Based Superconductors

*This book constitutes the thoroughly refereed proceedings of the 18th International Conference, Euro-Par 2012, held in Rhodes Islands, Greece, in August 2012. The 75 revised full papers presented were carefully reviewed and selected from 228 submissions. The papers are*

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*organized in topical sections on support tools and environments; performance prediction and evaluation; scheduling and load balancing; high-performance architectures and compilers; parallel and distributed data management; grid, cluster and cloud computing; peer to peer computing; distributed systems and*

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*algorithms; parallel and distributed programming; parallel numerical algorithms; multicore and manycore programming; theory and algorithms for parallel computation; high performance network and communication; mobile and ubiquitous computing; high performance and scientific applications; GPU and*

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*accelerators computing.*

*Reissue of Encyclopedia of*

*Physics/Handbuch der Physik, Vol.*

*XXV/2b I am very pleased that my book is now to be reprinted and rebound in a new format which should make it accessible at a modest price to students and active researchers in condensed matter physics.*

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*In writing this book I had in mind an audience of physicists and chemists with no previous deep exposure to symmetry analysis of crystalline matter, non to the use of symmetry in simplifying and refining predictions of the results of optical experiments. Hence the book was written to explain and illustrate in all*

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*necessary detail how to: 1) describe the space group symmetry in terms of space group symmetry operations; 2) obtain irreducible representations and selection rules for optical infra-red and Raman and other transition processes. On the physical side I redeveloped the traditional theory of classical and quantum lattice dynamics,*

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*illustrating how space-time symmetry designations in the equations of motion can: 1) simplify and rationalize calculations of the classical eigenvectors of the dynamical equation; 2) permit classification of the eigenstates of the quantum lattice-dynamic problem; 3) give specific selection rules for optical infra-*



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*red and Raman lattice processes, and thus make "go, no-go" predictions including polarization of absorbed or scattered radiation; and 4) simplify the modern many-body theories of optical processes. Properties of systems with long range interactions are still poorly understood despite being of importance in most areas*

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*of physics. The present volume introduces and reviews the effort of constructing a coherent thermodynamic treatment of such systems by combining tools from statistical mechanics with concepts and methods from dynamical systems. Analogies and differences between various systems are examined by considering a large range of*

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*applications, with emphasis on Bose--Einstein condensates. Written as a set of tutorial reviews, the book will be useful for both the experienced researcher as well as the nonexpert scientist or postgraduate student. From fundamental research to practical applications*

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*Theory of Crystal Space Groups and  
Lattice Dynamics*

*Lattice Dynamics of Molecular Crystals*

*International Series in Natural Philosophy*

*The Physics of Phonons*

*Dynamics and Thermodynamics of*

*Systems with Long Range Interactions*

Includes Part 1, Number 1: Books

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and Pamphlets, Including Serials  
and Contributions to Periodicals  
(January - June)

Solid State Physics

The vibrations of atoms inside  
crystals - lattice dynamics - is basic  
to many fields of study in the solid-

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state and mineral sciences. This book provides a self-contained text that introduces the subject from a basic level and then takes the reader through applications of the theory.

Principles and Practice

*Page 46/146*

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Proceedings of the International Conference Held at Copenhagen, Denmark, August 5-9, 1963

Study of Lattice, Spin and Charge Dynamics in Cr- and Ni-based Pnictide Superconductors

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Metallic Microlattice Structures  
Growth, Structure and Lattice  
Dynamics of Iron Silicide  
Nanostructures

This volume describes the  
increasing role of in situ  
optical diagnostics in thin film



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processing for applications ranging from fundamental science studies to process development to control during manufacturing. The key advantage of optical diagnostics in these

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applications is that they are usually noninvasive and nonintrusive. Optical probes of the surface, film, wafer, and gas above the wafer are described for many processes, including plasma etching,

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MBE, MOCVD, and rapid thermal processing. For each optical technique, the underlying principles are presented, modes of experimental implementation are described, and

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applications of the diagnostic in thin film processing are analyzed, with examples drawn from microelectronics and optoelectronics. Special attention is paid to real-time probing of the surface, to the

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noninvasive measurement of temperature, and to the use of optical probes for process control. Optical Diagnostics for Thin Film Processing is unique. No other volume explores the real-time

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application of optical techniques in all modes of thin film processing. The text can be used by students and those new to the topic as an introduction and review of the subject. It also serves as a

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comprehensive resource for engineers, technicians, researchers, and scientists already working in the field. The only volume that comprehensively explores in situ, real-time, optical probes

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for all types of thin film processing Useful as an introduction to the subject or as a resource handbook Covers a wide range of thin film processes including plasma etching, MBE, MOCVD,



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and rapid thermal processing  
Examples emphasize  
applications in  
microelectronics and  
optoelectronics Introductory  
chapter serves as a guide to  
all optical diagnostics and

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their applications Each chapter presents the underlying principles, experimental implementation, and applications for a specific optical diagnostic

Lattice Dynamics covers the

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proceedings of the 1963 International Conference on Lattice Dynamics, held at the H.C. Ørsted Institute of the University of Copenhagen on August 5-9. This book is composed of seven parts that

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focus on a better fundamental understanding of the interactions between atoms in solids and their role in lattice dynamics. The major topics covered include phonon dispersion curves,

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anharmonic effects, optical and dielectric effects, influence of defects on lattice vibrations, elasticity, and developments. Papers on the study of vibrational spectra by infrared absorption, X-ray and

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neutron scattering and the electron tunneling effects as well as papers on the influence of defects and on a variety of other problems in lattice dynamics are included. This book will prove useful to

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applied physicists and researchers in the field and related fields of lattice dynamics.

Issues in General Physics Research / 2012 Edition is a ScholarlyEditions™ eBook that

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delivers timely, authoritative, and comprehensive information about Physics Research. The editors have built Issues in General Physics Research: 2012 Edition on the vast information databases of



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informed, and relevant. The content of Issues in General Physics Research: 2012 Edition has been produced by the world's leading scientists, engineers, analysts, research institutions, and companies.

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confidence, and credibility.

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Lectures on Solid State  
Physics

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1965: January-June

Transactions of the High  
Performance Computing  
Center, Stuttgart (HLRS) 2017  
Springer Handbook of Surface  
Science  
Proceedings

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Linear Optical Properties of  
Semiconductors

**Lectures on Solid State  
Physics is a compilation  
of lectures concerned with  
various branches of solid  
state physics. It aims to**

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develop basic physical ideas that lead to a better understanding of phenomena and effects. Comprised of 11 chapters, this book discusses several topics on solid

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state physics: structure of solids; interference effects in crystals; lattice dynamics; perfect and imperfect crystals; electrons and electron theory of metals;



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semiconductors; electrical contact effects; transport phenomena, and magnetism. Students, physics graduates, electrical engineers, chemists, and metallurgists will find

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this book invaluable.  
The lattice dynamics of  
molecular crystals has  
undergone an enormous  
progress in these last  
twenty years or so. The  
experimental and

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theoretical advances have been realized by two different approaches. From one side molecular spectroscopists have been primarily interested in the vibrational properties

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of the molecules themselves subjected to the perturbing influence of the crystal environment. From the other side the lattice dynamical theory familiar

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in solid state physics for atomic lattices has been extended to molecular arrays. Although the overlap between the two approaches has been considerable the reference

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material is rather scattered in specialized papers. The purpose of this book is to partly fill this gap and to discuss the lattice dynamical theory of

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molecular crystals in a compact and specialized form. As such, the book is not intended exclusively for researchers and specialists in the field but also for graduate

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students entering an activity in solid state molecular spectroscopy. Early in 1990 a scientific committee was formed for the purpose of organizing a high-level scientific



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meeting on Future  
Directions of Nonlinear  
Dynamics in Physical and  
Biological Systems, in  
honor of Alwyn Scott's  
60th birthday (December  
25, 1991). As preparations

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for the meeting proceeded, they were met with an unusually broad-scale and high level of enthusiasm on the part of the international nonlinear science community,

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resulting in a participation by 168 scientists from 23 different countries in the conference, which was held July 23 to August 11 1992 at the Laboratory of Applied

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Mathematical Physics and  
the Center for Modelling,  
Nonlinear Dynamics and  
Irreversible  
Thermodynamics (MIDIT) of  
the Technical University  
of Denmark. During the

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meeting about 50 lectures and 100 posters were presented in 9 working days. The contributions to this present volume have been grouped into the following chapters: 1.

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Integrability, Solitons,  
and Coherent Structures 2.  
Nonlinear Evolution  
Equations and Diffusive  
Systems 3. Chaotic and  
Stochastic Dynamics 4.  
Classical and Quantum

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Lattices and Fields 5.  
Superconductivity and  
Superconducting Devices 6.  
Nonlinear Optics 7.  
Davydov Solitons and  
Biomolecular Dynamics 8.  
Biological Systems and

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Neurophysics. AI Scott has made early and fundamental contributions to many of these different areas of nonlinear science. They form an important subset of the total number of the



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papers and posters  
presented at the meeting.  
Other papers from the  
meeting are being  
published in a special  
issue of Physica D  
Nonlinear Phenomena.

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Growth, Structure and  
Lattice Dynamics of  
Epitaxial Rare Earth Films  
and Nanostructures  
Manufacture, Materials and  
Application  
Consolidated Reprint of

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Citations and Abstracts  
from NBS SP305 and Its  
Supplements 1-8  
Solid State Physics  
Energy Research Abstracts  
Contemporary Classics in  
Physical, Chemical, and

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## Earth Sciences

**The first two volumes in this series published twenty years ago contained chapters devoted to anharmonic properties of solids, ab initio calculations of phonons in metals and insulators, and surface phonons. In the intervening years**

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**each of these important areas of lattice dynamics has undergone significant developments. This volume is therefore concerned with reviewing the current status of these areas. Chapter one deals with the path-integral quantum Monte-Carlo method as a numerical**

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**simulation approach and looks at how this has been applied successfully to the determination of low temperature thermodynamic properties of anharmonic crystals and to certain dynamical properties as well. Chapter two is concerned with the calculation of static and**

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**dynamic properties of anharmonic crystals in the quantum regime. Chapter three discusses intrinsic anharmonic localized modes that have been intensively studied recently. Two topics, ab initio calculations of phonons in metals, and surface phonons are dealt with**

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**in the next chapter. The remaining two chapters are devoted to topics that have not been treated in previous volumes. One is phonon transport and the second is phonons in disordered crystals. The work described in the six chapters of this volume testifies to the**



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**continuing vitality of the field of dynamical properties of solids nearly a century after its founding. This review volume consists of scientific articles representing the frontier and most advanced progress in the field of semiconductor physics and lattice**

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**dynamics. Contents:Modern  
Physics and Warm Friendship (C N  
Yang)Semiconductor Surfaces and  
Interfaces Studied with Synchrotron  
Radiation (R Bachrach et al.)A  
Perspective of the Development of  
Semiconductor Superlattices and  
Quantum Wells (L L Chang)Laser**

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**Phononiton: A New**

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Semiconductors under Intense  
Pump Conditions (J L Birman & B S  
Wang)Realistic Calculation on the  
Second Order Nonlinear  
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Wang)Molecular Dynamics and**

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**Point Defects and Recombination in Semiconductors (J M Langer)**  
**Optical Transitions in Very Short Period GaAs-AlAs Superlattices (M D Sturge et al.)**  
**Two-**

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Heterojunction (R Q Han & X Y  
Liu)Hydrogen in Crystalline Silicon  
and Gallium Arsenic (G G  
Qin)Interaction Effects and  
Influence on Magnetoresistances in  
Two-Dimensional Hole Systems (H**

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**Z Zheng)Lattice and Spin  
Relaxation Approach in Low-  
Dimensional Physics (Z B Su & L  
Yu)and other papers Readership:  
Physicists and condensed matter  
physicists. Keywords:Lattice  
Dynamics;Semiconductor  
Physics;Synchrotron Radiation**

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**This work reviews the current state of the art in metallic microlattice structures, manufactured using the additive manufacturing processes of selective laser melting, electron beam melting, binder jetting and photopolymer wave guides. The emphasis is on structural**



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**performance (stiffness, strength and collapse). The field of additively manufactured metallic microlattice structures is fast changing and wide ranging, and is being driven by developments in manufacturing processes. This book takes a number of specific structural**

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**applications, viz. sandwich beams and panels, and energy absorbers, and a number of conventional metallic materials, and discusses the use of additive manufactured metallic microlattice structures to improve and enhance these structural performances. Structural**

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**performances considered includes such non linear effects as plasticity, material rupture, elastic and plastic instabilities, and impact loading. The specific discussions are put into the context of wider issues, such as the effects of realisation processes, the effects of structural**

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**scale, use of sophisticated analysis and synthesis methodologies, and the application of existing (conventional) structural theories. In this way, the specific discussions are put into the context of the emerging general fields of Architected (Architected)**

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**Superconductors**

**Introduction to Lattice Dynamics**

**Optical Diagnostics for Thin Film**

**Processing**

**Festschrift for Professor Kun**

**Huang**

The reason to perform calculations in material science usually falls into one

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of two categories: to predict or explain the origin of material properties. This thesis covers first-principle calculations for solids at extreme conditions, from both of the two mentioned categories. I primarily have studied the effects of high-pressure and high-temperature on lattice

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dynamics, mechanical and electronic properties. To treat the effects of temperature, ab initio molecular dynamics (AIMD) simulations and self-consistent phonon calculations, based on density functional theory, have been utilised. These approaches account for the temperature effects by



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considering thermally excited supercells as samples of a statistical ensemble. To extract properties from this representation, I have used methods which maps the supercell data to a unit cell representation or fits it to a simple model Hamiltonian. The small displacement method was used

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to analyse the dynamical stability for nitrides and polymorphs of silica, synthesised at high-pressure in a diamond anvil cell. The nitride compounds consist of a high amount of nitrogen either as chains, forming a porous framework together with transition metal atoms or as dinitrogen

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molecules, occupying the channels of the framework. The nitrogen chains consist of single- or double-bonded nitrogen atoms, making these compounds highly energetic.

Polymorphs of silica can be used to model deep Earth liquids. These new polymorphs, named coesite-IV and

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coesite-V, consist of four-, five-, and six-oriented silicon. Some of the octahedra of the six-oriented silicon atoms, of these new phases, are sharing faces, which according to Pauling's third rule would make them highly unstable. My phonon calculations indicate these phases to

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be dynamically stable. Furthermore, my calculations predict higher compressibility for these new phases compared to the competing ones. By modelling silicate melts with coesite-IV and coesite-V, a more complex and compressible structure is expected, affecting the predicted seismic

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behaviour. I studied Kohn anomalies for body-centered cubic niobium by simulating this material with self-consistent phonon calculations. The electronic structure was studied by using a band unfolding technique, for which I obtained an effective unit cell representation of the electronic

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structure at elevated temperatures. Temperature primarily smeared the electronic states but did not induce significant shifts of the bands. In parallel, the anharmonicity of this system was studied using the temperature dependent effective potential method. Even close to the

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melting temperature, this element is remarkably harmonic. The experimentally observed disappearance of the Kohn anomalies with increased temperature is predominantly dependent, according to my calculations, on the temperature-induced smearing of the electronic



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states. Using stress-strain relations, accurate high-temperature elastic properties were predicted for  $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ . The simulations were performed with AIMD. The stresses were fitted using the least-squares method to a linear expression from which the elastic constants were

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derived. The results were compared with previously performed calculations that employed additional approximations. The results of the symmetry imposed force constant temperature dependent effective potential (SIFC-TDEP) method agrees well with our results. I also compared

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my results with TiN calculations that employed a similar methodology. My and the SIFC-TDEP results are reporting lower values for the polycrystalline moduli than the calculations for TiN. The data I generated were also used for a machine learned interatomic potential

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method, where moment tensor potentials were trained and evaluated, using this data. Den här avhandlingen handlar om beräkningar för material. När materialberäkningar utförs är det antingen för att förutsäga eller förklara egenskaper. De beräkningar som jag har gjort i denna avhandling är

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baserade på fundamentala fysiska lagar. Detta betyder att de är rent baserade på teori, och inte har anpassats efter resultat av experiment. Jag har i mitt arbete använt mig mycket utav en teori som kallas gitter dynamik. Den är definierad för periodiska material, det vill säga att

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atomerna i dessa material upprepas i periodiska mönster. Vi kan då anta att det finns en jämviktspunkt för alla atomerna, som de vibrerar omkring. Dessa vibrationer kan beskrivas som om atomerna påverkar varandra med fiktiva fjädrar. Genom att beräkna styrkan för dessa fjädrar kan vi

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beskriva vibrationerna av atomerna. Dessa vibrationer i sin tur är avgörande för materialets egenskaper. För att beskriva ett material vid en specifik temperatur har jag använt mig utav olika metoder för att simulera det. En simulering kan ses som ett "dator experiment". Problemet är dock hur vi

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ska mäta egenskaperna i simuleringen. Ju större och mera komplex en simulering är, desto svårare blir det att beräkna egenskaperna av det simulerade materialet. Vi hamnar i en situation likt den vi skulle befinna oss om vi hade gjort ett experiment i verkligheten, och



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tvingas använda förenklade modeller för att kunna tolka resultatet. Jag har därför använt mig utav metoder för att utvinna vibrationer av atomer, elektrontillstånd eller elastiska egenskaper, specifikt utvecklade för att användas på denna typ utav simuleringar. Mitt arbete har kretsat

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kring hur dessa egenskaper påverkas av extrema temperaturer och tryck. De beräkningar jag har utfört vid höga tryck har varit för nyupptäckta nitrider och faser av kiseldioxid. Nitriderna är porösa material som innehåller en stor mängd kväve. Det höga kväveinnehållet gör så att det lagras en stor mängd

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kemisk energi i enkel- och dubbelbindningar mellan kväveatomerna. De nya faserna av kiseldioxid har en betydelse för vår förståelse av jordens inre. Deras existens öppnar upp för att det kan finnas mera komplexa och ihoptryckbara flytande material, under

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jordens nedre mantel, än vad tidigare har varit antaget. Mina beräkningar har bekräftat strukturerna för dessa nyupptäckta material. Vid höga temperaturer har jag studerat för metallen niob hur vibrationerna av atomerna är relaterade till olika elektrontillstånd. För specifika

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vibrationer ökar frekvensen med ökad temperatur. Detta är något ovanligt eftersom vibrationernas frekvenser vanligtvis brukar minska med ökad temperatur. Mina simulering för denna metal överensstämmer med resultat från experiment. Orsaken till varför visa vibrationers frekvenser ökar kan

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jag förklara med att elektrontillståndens enskilda energier varierar över tid på grund av den ökade temperaturen. Jag har även använt mig av simuleringar för att beräkna elastiska egenskaper av legeringen  $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ .  $\text{Ti}_{1-x}\text{Al}_x\text{N}$  legeringar används som beläggningar

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på skärverktyg som används för metall. För att öka effektiviteten av beläggningen, behövs det detaljerad kunskap av dess mekaniska egenskaper för den temperatur som de används vid. Jag beräknade därför så noggrant som möjligt de elastiska egenskaperna för  $\text{Ti}_{0.5}\text{Al}_{0.5}\text{N}$ . Dessa

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beräkningar är avsedda för att användas som en referens för andra beräkningsmässigt billigare metoder. Datan som genererades från mina simuleringar användes även för en sådan metod, baserad på maskininlärning.

Computational Fluid Dynamics: A



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