

Contents

Part I Introduction

Materials Modelling and Design: An Introduction
Vijay Kumar, Surajit Sengupta, and Baldev Raj 3

Part II Methodologies

Computational Modelling of Atomic-Scale Defect Phenomena
in Compound Semiconductors
R.M. Nieminen, T. Mattila, and S. Pöykkö 11

The Generalized-Gradient Approximation to Density Functional
Theory and Bonding
D.C. Patton, M. Pederson, and D.V. Porezag 37

Electronic Structure Calculations and Molecular Dynamics
Using the Real-Space Method
and Optimized Ultra-soft Pseudopotential
T. Hoshi and T. Fujiwara 51

Quantum Simulations Using Linear Scaling Methods:
Clusters on Surfaces
G. Galli, A. Canning, and F. Mauri 59

Electronic Structure of Disordered Alloys
R. Prasad 65

Computer Simulation of Structure and Dynamics
in Complex Materials
S.L. Chaplot 89

Part III Alloys

First-Principles Thermodynamics of Alloys J.M. Sanchez	101
Electronic Structure of Binary Systems G.P. Das	108
First-Principles Phase Stability Study of Metallic Alloys P.P. Singh	121
First-Principles Approach to Ordering and Clustering Behavior in Metallic Alloys: Application to Al-Li and Ni-Mo Systems A. Arya, S. Banerjee, and G.P. Das	127
Thermochemical Modeling of Ternary Alloys from Binary Systems R. Ganesan and S. Vana Varamban	137
Superconductivity in Zr_2Rh and its Hydrides: Theory and Experiment H.G. Salunke, G.P. Das, V.C. Sahni, and P. Raj	142

Part IV Correlated Electron Systems

Ab-initio Approach to Electronic Excitation Spectra in Perovskite $LaMO_3$ Oxides D.D. Sarma and P. Mahadevan	149
Theory for the Interdependence of High- T_c Superconductivity and Dynamic Spin Fluctuations S. Grabowski, J. Schmalian, M. Langer, and K.H. Bennemann	162
Electrical Resistivity and Positron Lifetime Studies in the Kondo Insulating System, $FeSi_{1-x}Ge_x$ A. Bharathi, Y. Hariharan, A. Mani, and C.S. Sundar	170

Part V Clusters and Nanomaterials

Electronic Structure of Magic Metal Clusters and Cluster Assemblies

P. Jena, S.N. Khanna, and B.K. Rao 179

Stability of Molecules and Clusters Studied Through First-Principles Total Energy Calculations

S. Mukherjee, A.P. Seitsonen, and R.M. Nieminen 187

Adsorption on Clusters

Vijay Kumar 193

Ab-initio Molecular Dynamics Study of Impurity in Metal Clusters: Na_nAl ($n = 1-10$)

D.G. Kanhere, A. Dhavale, and V. Shah 202

Lyapunov Exponent at the Melting Transition in Small Ni Clusters

V. Mehra and R. Ramaswamy 209

Monte Carlo Studies of Argon Clusters Confined in Zeolites

R. Chitra and S. Yashonath 214

Structure-Property Relation in Oxide Nanoparticles

P. Ayyub 228

Nanoparticles of II-VI Semiconductors

S.K. Kulkarni, M. Kundu, and P. Borse 236

Cu Doped ZnO Quantum Dots: Intrinsic and Extrinsic Luminescence

S. Mahamuni, K. Borgohain, B.S. Bendre, and S.S. Joshi 244

Carrier Dynamics in Porous and Nanocrystalline Silicon

V.A. Singh and G.C. John 250

Anodisation Time Dependence of Photoluminescence Properties of Porous Silicon

R. Rajaraman, P. Gopalan, B.S. Panigrahi, and M. Premila..... 257

Formation of Nanocrystalline Fe-Cu-Nb-Si-B Alloys N. Bhagat, Ajay Gupta, and P. Duhaj	261
--	-----

Magnetic Properties of Ultra-fine γ' -Fe ₄ N R.N. Panda and N.S. Gajbhiye	265
--	-----

Part VI Surfaces and Interfaces

First-Principles Calculation of Surface Step Energies and Interactions J. F. Annett	271
---	-----

Deposition of Ga and As Adatoms on the Ge(111) and Si(111) Surfaces: A First-Principles Study C. Cheng and K. Kunc	279
--	-----

Steering and Isotope Effects in the Dissociative Adsorption of H ₂ /Pd(100) A. Gross and M. Scheffler	285
--	-----

Growth and Magnetism of Rough Transition Metal Overlayers A. Mookerjee	293
---	-----

Quantum Adsorbates: Helium in Zeolites C. Chakravarty and K.V. Thiruvengadaravi	305
--	-----

Effect of High-Energy Heavy-Ion Irradiation on Fe/Tb Multilayers A. Paul, A. Gupta, R. Gupta, D.K. Avasthi, and G. Principi	309
--	-----

Part VII Phase Transitions

Isostructural Solid-Solid Transition in Crystalline Systems with Short Ranged Interaction P. Bolhuis and D. Frenkel	315
---	-----

Quantum Effects and Phase Transitions in Adsorbed Molecular Layers P. Nielaba	325
---	-----

Anchoring Transitions of Nematic Liquid Crystals Induced by Solid Substrate J. Chakrabarti and B. Mulder	334
Monte Carlo Simulation of the Kinetics of Martensitic-type Restacking Transitions: Dynamic Scaling and Universal Growth Exponents S.P. Shrestha and D. Pandey	339
Structural Transitions of a Soft Solid: The Skyrmion Lattice M. Rao, S. Sengupta, and R. Shankar	348
Electronic Topological Transitions in Elemental Metals and Compounds B.K. Godwal, R.S. Rao, and S.K. Sikka	356
Role of High Pressure in Designing Novel Phases P.Ch. Sahu, K. Govinda Rajan, N.V. Chandra Shekar, and M. Yousuf	365
Pressure-Induced Polymerisation of Fullerenes C.S. Sundar, M. Premila, P.Ch. Sahu, A. Bharathi, Y. Hariharan, D.V.S. Muthu, and A.K. Sood	376

Part VIII Microstructure and Deformation

Microstructural Evolution During Precipitation in Stressed Solids T.A. Abinandanan and R. Sankarasubramanian	387
Modelling of Process for Controlled Microstructure of Material P.V. Sivaprasad	395
Multiscaling in Normal Grain Growth: A Monte Carlo Study S. Koka, P.V. Sivaprasad, V. Sridhar, S. Venkadesan, and K.P.N. Murthy	404
Non-destructive Evaluation of Defects: A Model-Based Approach B. Raj, P. Kalyanasundaram, R. Sivaramanivas, and C. Babu Rao	410

Deformation of Nanostructured Materials	
K.A. Padmanabhan	418
Mechanics of Powder Compaction	
Ch. PavanaChand and R. KrishnaKumar	426
Finite Element Modelling of the Creep Behaviour of Weldments	
A.K. Bhaduri	434
List of Authors	445