

Contents

Part I	Introduction	
Introduction to This Volume		
By F. Yonezawa	3
The Development of Molecular Dynamics Simulations in the 1980s		
By S. Nose	11
Part II	Supercooled Liquid and Glass Transition	
Molecular Dynamics Studies of Diffusion in Liquids		
By J.-L. Barrat (With 3 Figures)	23
Molecular Dynamics Study of Self-Diffusion and the Liquid-Glass Transition		
By Y. Hiwatari (With 8 Figures)	32
Molecular Dynamics Study of Fluctuation and Relaxation in Disordered Systems – Liquid and Glass		
By F. Yonezawa and S. Sakamoto (With 10 Figures)	49
Part III	Oxides and Multi-component Materials	
Molecular Dynamics Simulation of Amorphous Silica		
By R.G. Della Valle and H.C. Andersen (With 2 Figures)	67
Pressure-Induced Structural Transformations and Diffusion Mechanism in Silica		
By S. Tsuneyuki (With 4 Figures)	78
Interatomic Potential Models for Molecular Dynamics Simulations of Multi-component Oxides		
By K. Kawamura (With 3 Figures)	88
Transport and Dynamical Correlations in Glassy States and the Liquid-Glass Transition of Li_2SiO_3		
By J. Habasaki, I. Okada, and Y. Hiwatari (With 5 Figures)	98

Part IV	Fluids and Hydrodynamics	
Simulation of Sub-molecular and Supra-molecular Fluids		
By D. Frenkel (With 4 Figures)	111	
Dynamics of Liquid Water: Fluctuations and Collective Motions		
By I. Ohmine and H. Tanaka (With 7 Figures)	130	
Ab Initio Hydrodynamics via Atomistic Simulation		
By D.C. Rapaport (With 2 Figures)	139	
Part V	Ab Initio Molecular Dynamics Simulations	
Ab Initio Molecular Dynamics		
By M. Parrinello (With 2 Figures)	151	
Density-Functional Molecular Dynamics Calculations for Defects in Si and Al		
By T. Oguchi and T. Sasaki (With 6 Figures)	157	
Optimum Adsorption Sites and Electronic Structure of Alkali-Adsorbed Si(001) Surfaces		
By K. Kobayashi, K. Terakura, and S. Blügel (With 4 Figures)	167	
Full Potential KKR: Applicability to Simulated Annealing Model		
By H. Akai, B. Drittler, and P.H. Dederichs	177	
Application of the Car-Parrinello Molecular Dynamics to Some Microclusters		
By C. Satoko (With 8 Figures)	186	
Part VI	Nonequilibrium Molecular Dynamics	
Response Theory, Lyapunov Instability and Rheology		
By D.J. Evans, E.G.D. Cohen, and G.P. Morriss (With 8 Figures)	199	
Two-Phase Coexistence of String and Liquid Phases in Planar Couette Flow		
By S. Nosé and T. Yamada (With 4 Figures)	210	
Part VII	Interfaces and Ionic Conductors	
Simulation Studies of Interfacial Phenomena – Melting, Stress Relaxation and Fracture		
By S. Yip (With 6 Figures)	221	
Computer Experiments on Systems Containing Surfactants		
By T. Kawakatsu and K. Kawasaki (With 10 Figures)	235	

Collective Motion and Mechanism of Diffusion in Superionic Conductors	
By Y. Kaneko and A. Ueda (With 6 Figures)	249
Index of Contributors	257