WHY ATOMIC LEVEL MODELING?

Structural studies. Linking structural studies with experimental observations and providing means for interpretation of the observed structures. Computer experiments

PART 1. METHODS OF COMPUTER MODELING

(1) Molecular statics  
(2) Molecular dynamics  
(3) Monte Carlo  
(4) Lattice Dynamics

INTERPRETATION AND ANALYSIS OF COMPUTER MODELS

(1) Structural analysis  
(2) Evaluation of physical quantities in molecular statics, dynamics and Monte Carlo studies

PART 2. TOTAL ENERGY AND INTERATOMIC FORCES - A PRECURSOR TO ATOMIC LEVEL MODELING

(1) Quantum mechanical foundations  
(2) Pair potentials in molecules and metals  
(3) Pair potentials in ionic crystals (ceramics)  
(4) Many-body central force potentials  
(5) Tight-binding methods and non-central potentials

PART 3 SPECIFIC ATOMIC MODELINGS

Examples of topics of modeling  
Point and extended defects (grain boundaries) in metals, metallic alloys and ionic crystals (ceramics), segregation, link with electron microscopy  
Dislocations in metals and metallic alloys, structure and motion under the applied stress  
Surfaces and interfaces in semiconductors (Si and Ge)  
Friction and adhesion in metallic and ceramic materials  
Structure of zeolites, modeling of catalysis
LITERATURE


D. W. Heerman: Computer Simulation Methods in Theoretical Physics, Springer.

D. C. Rapaport: The Art of Molecular Dynamics Simulation, Cambridge University Press


Selected recent papers.