

MSE 660 ATOMISTIC MODELING OF MATERIALS

Instructor: Vasek Vitek

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 ATOMISTIC 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

P. R. Adby and M. A. H. Dempster: Introduction to optimization methods, Chapman and Hall, London

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

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

M. P. Allen and D. J. Tildesley: Computer Simulation of Liquids, Clarendon Press, Oxford.

Computer Simulation of Solids, Lecture Notes in Physics, Springer, editors: C. R. A. Catlow and W. C. Mackrodt.

A. P. Sutton: Electronic Structure of Materials, Clarendon Press, Oxford.

D. G. Pettifor: Bonding and Structure of Molecules and Solids, Clarendon Press, Oxford.

J. H. Harding: Computer simulation of defects in ionic solids, Rep. Prog. Phys. 53, 1403, 1990.

Selected recent papers.