Many-atom interactions in solids

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Microscopic methods of calculating total energy and interatomic interactions in solids have been widely used recently. These methods are used to study the properties of different types of defects, surfaces, low-symmetry configurations of atoms in crystals, etc. Most of this research is based on the use of computer simulation methods such as molecular dynamics, the Monte Carlo method, and the high temperature annealing method. Until recently, such calculations were mainly done by using phenomenological pair potentials for the interaction between atoms, and most frequently by using the Lennard–Jones potential. This potential describes the properties of inert gases fairly well, but it is poorly suited for describing metallic and semiconductor systems. A number of microscopic approaches for determining pair and many-atom potentials that are suitable for examining both metallic and valence semiconducting systems have appeared recently. First, this is the method for an embedded atom that is based on an examination of the behavior of a single atom and a pair of atoms placed in a uniform electron gas. Further, one may note the effective medium method, which enables one to write the total energy of a system in the form of an adiabatic contribution and contributions from many atoms that are calculated with allowance for the actual electron density distribution for an ideal crystal. Also a number of other approaches for obtaining interatomic interactions exists; these are both purely microscopic and also phenomenological.

Materials from a working symposium in which the researchers that are working most actively in this field took part has been published in the book. About thirty reviews devoted both to general questions of constructing interatomic potentials and their use in investigating the statics and dynamics of crystal lattices, and also to a number of specific problems, such as surface reconstruction and the dynamics of molecular beam epitaxy, have been published. The material of the book is divided into four sections. The first section contains general reviews of the many-atom interaction problem, the material concerning metals has been placed in the second section, reviews of many-atom interactions in semiconductors are in the third section, and the fourth section contains reviews of calculations for surface phenomena.

Translated by Frederick R. West