



Interatomic Bonding in Solids: Fundamentals, Simulation, Applications

Valim Levitin

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The connection between a quantum behavior of the structure elements of a substance and the parameters that determine the macroscopic behavior of materials has a major influence on the properties exhibited by different solids. Although quantum theory and engineering should complement each other, this is not always the case. This book aims to demonstrate how the properties of materials can be derived and predicted proceeding from the features of their structural elements, generally electrons. In a sense, electronic structure forms the glue holding solids as whole, and it is central in determining structural, mechanical, chemical, electrical, magnetic and vibrational properties. The main part of the book is devoted an overview of the fundamentals of the density functional theory and its applications to computational solid state physics and chemistry. The author shows in detail the technique of construction of models and the methods of their computer simulation. He considers physical and chemical fundamentals of interatomic bonding in solids and analyzes the predicted theoretical outcome in comparison with experimental data. This is applying the first-principle simulation methods so as to predict the properties of transition metals, semiconductors, oxides, solid solutions, molecular and ionic crystals. Unique in presenting are novel theories of creep and fatigue that help to anticipate - and prevent - possible fatal material failures. As a result, users gain the knowledge and tools to simulate material properties and to design materials with desired characteristics. Due to the interdisciplinary nature of the book, it is suitable for a variety of markets from students and lectures to engineers and researchers.

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