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Interatomic Potential and Structural Stability Proceedings of the 15th Taniguchi Symposium, Kashikojima, Japan, October 19-23, 1992 Springer Series in Solid-State Sciences

By -

Springer. Paperback. Book Condition: New. Paperback. 223 pages. Dimensions: 9.0in. x 6.0in. x 0.5in. Structural stability is of fundamental importance in materials science. Up-to-date information on the theoretical aspects of phase stability of materials is contained in this volume. Most of the first-principles calculations are based on the local-density approximation (LDA). In contrast, this volume contains very recent results of going beyond LDA, such as the density gradient expansion and the quantum Monte-Carlo method. Following the recently introduced theoretical methods for the calculation of interatomic potentials, forces acting on atoms and total energies such as the Car-Parrinello, the effective-medium and the bond-order method, attempts have been made to develop even more sophisticated methods such as the order-N method in electronic-structure calculations. The present status of these methods and their application to real systems are described. In addition, in order to study the phase stability at finite temperatures, the microscopic calculations have to be combined with statistical treatment of the systems to describe, e. g. order-disorder transitions on the Si(001) surface or alloy phase diagrams. This book contains examples for this type of calculations. This item ships from multiple locations. Your book may arrive from Roseburg, OR, La Vergne, TN. Paperback.



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