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COMPUTATIONAL MATERIALS SCIENCE

SURFACES, INTERFACES, CRYSTALLIZATION

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Rachel Sandford

Computational Materials Science A.M. Ovrutsky, A. S Prokhoda, M.S. Rasshchupkyna, 2013-11-19 Computational Materials Science provides the theoretical basis necessary for understanding atomic surface phenomena and processes of phase transitions especially crystallization is given The most important information concerning computer simulation by different methods and simulation techniques for modeling of physical systems is also presented A number of results are discussed regarding modern studies of surface processes during crystallization. There is sufficiently full information on experiments theory and simulations concerning the surface roughening transition kinetic roughening nucleation kinetics stability of crystal shapes thin film formation imperfect structure of small crystals size dependent growth velocity distribution coefficient at growth from alloy melts superstructure ordering in the intermetallic compound Computational experiments described in the last chapter allow visualization of the course of many processes and better understanding of many key problems in Materials Science There is a set of practical steps concerning computational procedures presented Open access to executable files in the book make it possible for everyone to understand better phenomena and processes described in the book Valuable reference book but also helpful as a supplement to courses Computer programs available to supplement examples Presents several new methods of computational materials science and clearly summarizes previous methods and Computational Materials Science: Surfaces, Interfaces, Crystallization A. M. Ovrutsky, A. S. Prokhoda, M. S. results Rasshchupkyna, 2017-11-13 Computational Materials Science provides the theoretical basis necessary for understanding atomic surface phenomena and processes of phase transitions especially crystallization is given The most important information concerning computer simulation by different methods and simulation techniques for modeling of physical systems is also presented A number of results are discussed regarding modern studies of surface processes during crystallization There is sufficiently full information on experiments theory and simulations concerning the surface roughening transition kinetic roughening nucleation kinetics stability of crystal shapes thin film formation imperfect structure of small crystals size dependent growth velocity distribution coefficient at growth from alloy melts superstructure ordering in the intermetallic compound Computational experiments described in the last chapter allow visualization of the course of many processes and better understanding of many key problems in Materials Science There is a set of practical steps concerning computational procedures presented Open access to executable files in the book make it possible for everyone to understand better phenomena and processes described in the book Valuable reference book but also helpful as a supplement to coursesComputer programs available to supplement examplesPresents several new methods of computational materials science and clearly summarizes previous methods and results Reviews in Computational Chemistry, Volume 17 Kenny B. Lipkowitz, Donald B. Boyd, 2003-04-24 Computational chemistry is increasingly used in most areas of molecular science including organic inorganic medicinal biological physical and analytical chemistry Researchers in these fields who do

molecular modelling need to understand and stay current with recent developments This volume like those prior to it features chapters by experts in various fields of computational chemistry Two chapters focus on molecular docking one of which relates to drug discovery and cheminformatics and the other to proteomics In addition this volume contains tutorials on spin orbit coupling and cellular automata modeling as well as an extensive bibliography of computational chemistry books FROM REVIEWS OF THE SERIES Reviews in Computational Chemistry remains the most valuable reference to methods and techniques in computational chemistry JOURNAL OF MOLECULAR GRAPHICS AND MODELLING One cannot generally do better than to try to find an appropriate article in the highly successful Reviews in Computational Chemistry The basic philosophy of the editors seems to be to help the authors produce chapters that are complete accurate clear and accessible to experimentalists in particular and other nonspecialists in general JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

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Polymeric Nanofibers and their Composites Chandrabhan Verma, Yong X

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