

| | |
|-------------------------|---|
| 1. Record Nr. | UNINA9910808853603321 |
| Titolo | Multiscale kinetic modelling of materials : proceedings of the symposium "Multiscale Kinetic Modelling of Materials", organised within the EMRS Fall Meeting 2006 held in Warsaw, Poland, 4-8 September 2006 / / edited by R. Kozubski, G.E. Murch and P. Zieba |
| Pubbl/distr/stampa | Stafa-Zuerich : , : Trans Tech Publications, , [2007] ©2007 |
| ISBN | 3-03813-142-3 |
| Descrizione fisica | 1 online resource (171 p.) |
| Collana | Diffusion and defect data. Pt. B. Solid state phenomena, , 1012-0394 ; ; volume 129 |
| Altri autori (Persone) | KozubskiRafa <1955-> MurchG. E ZiebaPawe |
| Disciplina | 620.11 |
| Soggetti | Kinetic theory of matter Materials - Analysis Mathematical models |
| Lingua di pubblicazione | Inglese |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
| Note generali | Conference proceedings. |
| Nota di bibliografia | Includes bibliographical references and indexes. |
| Nota di contenuto | MULTISCALE KINETIC MODELLING OF MATERIALS; Participants; Committees; Preface; Table of Contents; Bridging Different Length and Time Scales in Diffusion Problems Using a Lattice Monte Carlo Method ; Electro-Mechano-Chemistry; Transport Problem in Four Time Scales ; Concurrent Multiscale Kinetic Monte Carlo-Continuum Models for the Evolution of Solids via Diffusion ; Comparison of the Strain Distribution Obtained from Multi Scale and Conventional Approaches to Modelling Extrusion ; Energetic Landscapes and Diffusion Properties in FeCu Alloys Multi-Lattice Kinetic Monte Carlo Simulation of Interface Controlled Solid-State Transformations Cluster Dynamics Modeling of Materials: Advantages and Limitations; Interdiffusion of Two L10Phases without Long-Range Order Decrease: Experiments and Molecular Dynamics Simulations; Orientation of Interstitials in Clusters in -Fe: A Comparison between Empirical Potentials ; Anisotropy of the Vacancy |

Migration in Ti, Zr and Hf Hexagonal Close-Packed Metals from First Principles ; Monte Carlo Simulation of Texture and Microstructure Transformation during Annealing of Steel

A Phase Field Model for grain Growth and Thermal Grooving in Thin Films with Orientation Dependent Surface Energy An Extensive Study of Charge Effects in Silicon Doped Heterofullerenes ; Interface Shape Change and Shift Kinetics on the Nanoscale; Analysis of Oxygen Segregation at Metal-Oxide Interfaces Using a New Lattice Monte Carlo Method ; Materials Hardness Estimation by Simulation of the Indentation Process ; Stability of Hollow Nanospheres: A Molecular Dynamics Study ; First Principles Study of Al(100) Twisted Interfaces Interface Dynamics of Melt Instabilities on Semiconductor Surface Grain Boundary Migration in Nanocrystalline Iron ; Multiscale Plastic Deformation near a Fatigue Crack from Diffraction ; Statistical Model of Grain Growth in Polycrystalline Nanomaterials ; Keywords Index; Authors Index

Sommario/riassunto

The inspiration for this book was to gather together the efforts of those physicists, materials scientists/engineers and other scientists who are carrying out interdisciplinary research into multiscale modelling of time-evolving phenomena in materials. The resultant collection focuses on the principal topics of: 1. The current development of theoretical and model approaches to structural kinetics (links between quantum electron theories of solids and non-equilibrium thermodynamics); 2. Computer simulations as an effective tool for studying atomistic mechanisms of structural kinetics (Monte Car
