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Collana	Diffusion and defect data. Pt. B. Solid state phenomena, , 1012-0394 ; ; volume 129
Altri autori (Persone)	KozubskiRafa <1955-> MurchG. E ZiebaPawe
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Soggetti	Kinetic theory of matter Materials - Analysis Mathematical models
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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
