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Altri autori (Persone)	TikareVeena
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Nota di contenuto	Theory, Modeling and Numerical Simulation; Preface ; Table of Contents; Atomistic Simulations of the Aluminum-Silicon Interfaces under Shear Loading; Shock Loading of Bone-Inspired Metallic Nanocomposites; Hydrogen Storage in MgH2 Matrices: An Ab-Initio Study of Mg-MgH2 Interface ; First-Principles Calculations of the Atomic and Electronic Structures in Au-Pd Slab Interfaces; In-Diffusion and Out-Diffusion of Oxygen from a Composite Containing Random Traps; Effects of Supports on Hydrogen Adsorption on Pt Clusters; First-Principles Calculations of Pd/Au(100) Interfaces with Adsorbates In-Plane Rotated Crystal Structure in Continuous Growth of Bismuth Cuprate Superconducting FilmDynamical Interaction between Thermally Activated Glide of Screw Dislocation and Self-Interstitial Clusters in Bcc Fe; The Effects of Solute Segregation on the Evolution and Strength of Dislocation Junctions; Physics Mechanisms Involved in the Formation and Recrystallization of Amorphous Regions in Si through Ion Irradiation; Hotspot Formation in Shock-Induced Void Collapse; Molecular Dynamics Simulation of Nanocrystalline Tantalum under Uniaxial Tension

Diffusion Mechanisms near Tilt Grain Boundaries in Ni3Al IntermetallidePhase-Transformation Wave Dynamics in LiFePO4 ; Molecular-Dynamics Analysis of the Structural Properties of Silica during Cooling; Atomistic Simulations of Copper Precipitation and Radiation Induced Segregation in -Iron; Ab-Initio Calculation for the Study of Nano Scale Silicon Based Device Structure; Modelling of Elastic Modulus and Molecular Structure Interrelationship of an Oriented Crystalline Polymer; Reaction Rate as an Effective Tool for Analysis of Chemical Diffusion in Solids
Simulation of the Columnar-to-Equiaxed Transition in Alloy Solidification - The Effect of Nucleation Undercooling, Density of Nuclei in Bulk Liquid and Alloy Solidification Range on the TransitionSimulation of Surface-Enhanced Ordering in Smectic Films; Atomic Scale Modelling of Materials: A Prerequisite for any Multi-Scale Approach to Structural and Dynamical Properties; Morphological Evolution of Intragranular Void under the Thermal-Stress Gradient Generated by the Steady State Heat Flow in Encapsulated Metallic Films: Special Reference to Flip Chip Solder Joints
Effect of C on Vacancy Migration in -IronKeywords Index; Authors Index

Sommario/riassunto

No present-day research and development program is complete without the inclusion of a robust modeling and numerical simulation component. Models and model-based numerical simulations are extensively used to probe complex materials behavior and structure in order to obtain a deeper insight into the fundamentals of materials. Multi-physics models are becoming increasingly common, with advances in computational science, and are rapidly advancing the basic understanding of materials. The aim of this special collection: ""Theory, modeling and numerical simulation of multi-physics behavior"", with