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Nota di contenuto	CONTENTS; Foreword; Preface; Dislocation Dynamics in 2 + Dimensions: Slip Planes, Thin Films, and Grain Boundaries Yang Xiang, Siu Sin Quek, Yong-Wei Zhang, Adele T. Lim and David J. Srolovitz; Contents; 1. Introduction; 2. Peierls-Nabarro models for dislocations; 2.1. Classical Peierls-Nabarro model for straight dislocations; 2.2. Generalizations of Peierls-Nabarro model for straight dislocations; 2.3. Generalizations to curved dislocations; 2.4. From the Peierls-Nabarro model to a continuum dislocation dynamics model in a slip plane 2.5. Conclusions of Peierls-Nabarro models of dislocations3. Dislocation dynamics in thin films; 3.1. Dislocation dynamics simulation in thin film: A brief review; 3.1.1. Front-tracking methods; Two dimensions; Three dimensions; 3.1.2. Phase field method; 3.1.3. Level set method; 3.2. Level set simulation of dislocation dynamics in thin films; 3.2.1. Dislocation half-loop in a stationary film; 3.2.2. Pair of coplanar identical half-loops in a stationary film; 3.2.3. Non-

identical coplanar half-loops in a stationary film
3.2.4. Dislocation half-loops on intersecting glide planes in a stationary film3.2.5. Dislocation evolution during single-layer film growth; 3.2.6. Dislocation evolution during bilayer film growth; 3.3. Conclusions of dislocation dynamics in thin films; 4. Dislocation models for low-angle grain boundary migration; 4.1. Introduction to dislocation models for LAGBs; 4.2. Simulation model and method for LAGB migration; 4.2.1. 2-d dislocation dynamics for LAGB migration; 4.2.2. 3-d dislocation dynamics for LAGB migration; 4.3. 2-d dislocation dynamics simulation results
4.3.1. One set of intrinsic dislocations4.3.2. One set of intrinsic dislocations + extrinsic dislocations; 4.3.3. Two sets of intrinsic dislocations; 4.4. 3-d dislocation dynamics simulation results; 4.4.1. Two sets of intersecting intrinsic dislocations; 4.4.2. Mixed LAGB + extrinsic dislocations; 4.5. Conclusions of dislocation models for LAGB migration; 5. Conclusions; Acknowledgments; References; Introduction to Molecular Dynamics Simulations Xiantao Li; Contents; 1. Introduction; 2. Statistical mechanics basis; 2.1. Micro-canonical (NVE) ensemble; 2.2. Canonical (NVT) ensemble
2.3. Modeling canonical ensemble2.4. Linear response and dynamic quantities; 3. Numerical methods for molecular dynamics simulation; 3.1. Non-dimensionalization; 3.2. Time integration for Hamiltonian systems; 3.3. Force calculation; 3.4. Boundary conditions; 4. Non-equilibrium molecular dynamics models; 4.1. Boundary condition for non-equilibrium molecular dynamics; 4.1.1. Exact boundary condition; 4.2. Exact boundary condition; 4.2.1. Approximate boundary condition; 4.2.2. Finite temperature boundary condition; 4.3. Coarse-grained molecular dynamics model; 4.4. A one-dimensional example
5. Summary and discussions

Sommario/riassunto

The Institute for Mathematical Sciences at the National University of Singapore hosted a two-month research program on "Mathematical Theory and Numerical Methods for Computational Materials Simulation and Design" from 1 July to 31 August 2009. As an important part of the program, tutorials and special lectures were given by leading experts in the fields for participating graduate students and junior researchers. This invaluable volume collects four expanded lecture notes with self-contained tutorials. They cover a number of aspects on multiscale modeling, analysis and simulations for problems