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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