Molecular dynamics simulations of dislocation motion[1]

Bin Wen

In material science, a dislocation is a crystallographic defect, or irregularity, within a crystal structure. The presence of dislocations strongly influences many properties of crystalline materials, such as the ability to yield and flow under stress, creep and fatigue, ductility and brittleness, indentation hardness and friction. To study the mechanical behaviors of crystalline materials, it is important to understand the mechanism and the evolution of dislocations in the microstructure.

Several computational methods have been developed to simulate the dislocation motion. One favorable way is Molecular Dynamics (MD), which directly simulates the motion of atoms providing unique insights into the mechanistic and quantitative aspects of dislocation mobility.

In this project, we are interested in the dislocation motion in BCC metals using feasible MD simulation. The simulation cell is a rectangular box of atoms applied with periodic boundary condition (PBC). The atomic configuration is obtained by adopting conjugate gradient relaxation (CGR) algorithm, which avoids the coincidence of the atoms. The dislocation velocity will be extracted from MD simulations. The stress-dislocation velocity relationship and the temperature dependence of dislocation mobility will be observed. The kink mobility is also interested.

The project will duplicate some results demonstrated in the reference [1] and [2]. And fine details can also be found in the reference listed below.

Reference:

[1] J. Chang, Wei Cai, V. V. Bulatov and S. Yip, "Dislocation Motion in BCC Metals by Molecular Dynamics", *Materials Science and Engineering A*, 309-310, 160 (2001).

[2] J. Chang, Wei Cai, V. V. Bulatov, and S. Yip, "Molecular Dynamics Simulations of Motion of Edge and Screw Dislocations in a Metal", *Computational Materials Science*, 23, 111, (2002).

[1] MAE 715 final project presentation, May 2009

[3] Vasily V. Bulatov and Wei Cai, Computer Simulations of Dislocations, Oxford University Press, Oct 2006.