Mechanical deformation and radiation damage of face-centered-cubic metallic nanowires

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Abstract

Nanowires have received intensive attention in the past decades due to their potential applications in future nanotechnology. The small lateral size and large free surface area of nanowires lead to many unique properties compared to their bulk counterparts. Focusing on face-centered-cubic (FCC) metallic nanowires, this thesis studies mechanical properties of nanowires and the effect of radiation damage in nanowires using molecular dynamics simulations. As a starting point the mechanical properties of twinned copper nanowires are studied, and then the method to generate twin boundaries into nanowires using energetic beams is proposed and demonstrated. The defect evolution in nanocrystalline copper is studied as well to investigate the grain size effect.

Molecular dynamics simulations reveal that twin boundaries do not always strengthen FCC metallic nanowires; whether or not the strengthening takes place depends on the necessary stress required for dislocation nucleation, which in turn depends on the nanowire surface morphology. In nanowires with circular cross-sections, the stress needed for dislocation nucleation is high and dictates the yield strength. The introduction of twin boundaries slightly lowers the dislocation nucleation stress and weakens nanowires. In nanowires with square cross-sections, the presence of sharp edges reduces the stress for dislocation nucleation. The reduced dislocation nucleation stress is not high enough to drive dislocation penetration through twin boundaries, resulting in strengthening effect.

A method to introduce twin boundaries into copper nanowires using energetic beams is proposed. Upon radiation, the local region of a Cu nanowire will melt, and the molten zone recrystallizes after the radiation stops. At the solid-liquid interface, atoms may follow FCC or hexagonal-close-packed (HCP) stacking. Once a twin boundary (i.e., an HCP layer) nucleates, it tends to grow. Within a nanowire, the twin boundary can easily expand across the entire cross-section and becomes stable. The demonstration starts with the ion radiation in copper nanowires. With increasing PKA energy, the defect production under ion radiation corresponds to ballistic collision, surface viscous flow and self-organization. The corresponding defect structures are dispersed point defects, dislocation loops and twin boundaries, respectively. Subsequent electron radiation

simulations show that the formation of twin boundaries is due to the thermal melting and completes in three steps: nucleation of HCP layer, growth of the HCP layer, and interaction of nearby HCP layers. This twinning method offers a new mechanism of improving the mechanical strength of metallic nanowires.

A crossover behavior is predicted in the grain size dependence of defect production in nanocrystalline copper under radiation. With the same number of defects produced, the resulted vacancy concentration first increases and then decreases with increasing grain size. The smaller the grain size, the higher the sink strength of grain boundaries is and the more vacancies are absorbed by grain boundaries. On the other hand, more SIAs survive with larger grain size in the form of clusters, which recombine with vacancies and lead to lower vacancy concentration. The competition between grain boundary absorption and recombination of vacancies with SIA clusters results in the crossover behavior.

To summarize, the molecular dynamics simulation studies in this thesis demonstrated unique properties of copper nanowires, including: **(1) surface morphology dependent twin boundary strengthening effect** (Y. F. Zhang and H. C. Huang, nanoscale research letters 4, 34 (2009))**, (2) yield strength asymmetry** (Y. F. Zhang, H. C. Huang and S. N. Atluri, CMES 35, 215 (2008))**, (3) radiation induced twin formation** (Y. F. Zhang and H. C. Huang, Submitted)**,** and **(4) Crossover behavior in the grain size dependence of defect accumulation in nanocrystalline copper.** The collection of these results enhances the understanding of the properties of FCC metallic nanowires and guides the future applications of nanowires.