Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

Defects nucleation and its relation to internal stress in nanocrystalline materials

Li, Mo, mo.li@mse.gatech.edu, Georgia Institute of Technology

ABSTRACT

Although grain boundaries become increasingly important of nanocrystalline materials, dislocations still play a crucial role in their mechanical properties. However, in the nanoscale materials with large interface-to-volume ratio, the knowledge of how the complex microstructure is related to the defect process and eventually the mechanical properties remains largely incomplete. In this discussion, I will elucidate the connection through the internal stress calculated using large-scale atomistic modeling. We show that the internal stress in nanocrystalline materials indeed emerges significantly from the disordered grain boundaries, and moreover, we can further sort out and relate the internal stress to more detailed microstructures in addition to the grain boundaries, i.e., triple junction lines and vertex points. We show that internal stresses associated with these microstructure entities are different in not only magnitude but also their effect on the overall mechanical properties. One striking case discovered from this study is that dislocation nucleation is primarily dominated by the internal stress at the vertex points, followed by that at the triple junction lines in three dimensions. Our observation of dislocation activity, which is often done in two dimensions, can be easily erroneous, such as the so-called “grain boundary dislocation nucleation”. If time permits, I will also discuss how we could utilize the knowledge to design new nanocrystalline materials via microstructure tailoring.