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MOLECULAR DYNAMICS SIMULATIONS OF NANOCRYSTALLINE TANTALUM UNDER UNIAXIAL TENSION

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ABSTRACT

Over the past two decades, nanocrystalline (NC) metals (average grain size d <100nm) have been the subject of considerable interests due to their many extraordinary properties in comparison to the coarse-grained (CG) counterparts. The results have shown that there is a shift in deformation mechanisms from dislocation motion to grain boundary activities for nanocrystalline metals especially when the grain size is less than about 10-15nm, leading to a reverse Hall-Petch effect. However, up to date, our knowledge of mechanical properties, especially the deformation mechanisms of NC metals is predominantly based on the studies of FCC metals. Little is known about NC BCC metals. We believe that the technological importance of many BCC metals, and our current limited knowledge about their mechanical properties, particularly plastic deformation behaviors of NC BCC metals, merit further elaborated investigations.

In the present work, molecular dynamics method is used to simulate the uniaxial tensile behavior of NC tantalum (Ta). An embedded-atom method (EAM) potential developed by Guellil and Adams in 1992 was used to describe the inter-atomic interactions of Ta. Seven cubic samples with different grain sizes are generated using the space-filling technique based on Voronoi construction and common neighbor analysis method are used to analyze the local arrangement of the deformed configuration where all atoms can be classified into four groups (FCC, BCC, HCP and Other kinds of atoms).

From the simulation, we found that both the 5% offset stress and the maximum stress in the stress-strain curves decrease with decreased average grain size, revealing an inverse Hall-Petch effect within the grain size regime investigated (6.5 – 13 nm). The mechanical strength of the NC-Ta exhibits strong rate dependence. We can take this observation as an indicator of grain boundaries activities as the predominant plastic deformation mechanisms, though dislocation activities and deformation twinning are also occasionally observed in the deforming samples.

Stress-induced phase transitions from BCC to FCC and HCP atoms are observed during the deformation process of NC-Ta at very low temperatures. Such transitions are reversible with respect to stress, namely, the FCC and HCP structures reverse back to the thermodynamically stable BCC structure upon unloading. Increased strain rate appears to delay the formation of FCC clusters to larger strains, but increase the maximum fraction of the FCC atoms. For FCC atoms in the deforming NC-Ta, a linear relation can be established between their fractions and the maximum stress, revealing a close link between phase transitions and stresses. Such phase transitions are found to occur only at relatively low simulation temperatures, probably because

at high temperatures, Atoms can re-arrange their positions through thermal activations to accommodate the plastic strain, whereas at low temperatures, this process is thermally forbidden. Inter granular fractures are also found during the deformation processing of NC-Ta. Which means the plastic deformation of NC-Ta not only comes from the dislocation motion, grain boundary activities just like the NC-FCC metals, but also from the contribution of inter granular fracture. And the existence of inter granular fracture leads to the decrease of flow stress.