Hall-Petch Effect and Dislocation Evolution in Gradient-Structured Polycrystalline Copper under Uniaxial Tension

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Abstract

Gradient nanostructures in metals represent an effective strategy to alleviate the trade-off between strength and ductility. Here, we investigate the effects of grain size gradient and twin thickness gradient on uniaxial tensile deformation behaviors of gradient-structured (GS) polycrystalline copper by using molecular dynamics simulation. Simulation results show that the flow stress of gradient nanograined (GNG) or gradient nanotwinned (GNT) model is linearly dependent on $\bar{d}^{-1/2}$ ($\bar{d}$, the mean grain size) or $\bar{\lambda}^{-1/2}$ ($\bar{\lambda}$, the mean twin boundary spacing) with different slopes, i.e., the relationship follows the normal Hall–Petch relation (with $\bar{d} > d_c$ or $\bar{\lambda} > \lambda_c$) or the inverse Hall–Petch relation (with $\bar{d} < d_c$ or $\bar{\lambda} < \lambda_c$). The transformation of boundary-mediated mechanism to dislocation-based counterpart for accommodating deformation with increasing the applied strain is observed in the GNG model. In the grains with small twin boundary spacings, the twin boundary migration and annihilation dominate the plastic deformation; while in the grains with large twin boundary spacings, the deformation is accommodated by the dislocation multiplication in the GNT model. Furthermore, the microstructural evolution demonstrates the gradient distribution of strain and the compatibility of deformation induced by the spatial gradient distribution of grain boundary or twin boundary. Those findings reveal the underlying mechanisms between the gradient nanostructure and mechanical properties in GS metals. The supports from the National Natural Science Foundation of China (Nos. 11772082, 11672062 and 11672063) are gratefully acknowledged.

References

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