The multiscale analysis of polycrystalline metals and its interface with a-Al2O3 under tension

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Summary

Among many multiscale methods ,we choose the quasicontinuum method to understand the mechanical response at the nanocrystalline of grain boundaries(GBs) under tension. The energetic and mechanical strength of 6 i?"<110> symmetric tilt GBs are investigated in nanocrystalline Cu and Ni. We focus on discussing the interaction of the structural units of symmetric tilt GB for the initial deformation mode and the strength of model. At the basis of the previous, We study the nanocrystalline Cu/a-Al2O3 interface and analyze the relationship during the grains orientations, GB energy and interface. Special emphasis is placed on the crystal slip from the interface across the GB and its influence on GB. These findings provide some insights on the role of GB structure in the deformation processes of nanocrystalline metals.

Keywords: Quasicontinuum method; Nanocrystalline meterials; Grain boundary structure