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Size effects of mechanical response in thin film samples versus bulk-molecular dynamics simulation study

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ABSTRACT

Understanding the mechanical response of nanocrystalline metals is critical for a wide range of applications and a number of them make a use of nanocrystalline materials in thin film (2D) or wire (1D) form. Despite significant progress in the understanding of the mechanical response of nanocrystals, less is known about how grain-size effects are affected the presence of free surfaces. Here, we characterize the mechanical response of nanocrystalline thin films samples with various grain sizes and at two different strain rates, and then we compare with those in bulk sample. Our simulations show the existence of Hall–Petch maxima for both yield and flow stresses and a quantitative analysis of plastic slip reveal that grain boundary slip decreases while intragranular slip increases with grain size. We also find that Hall–Petch maximum in thin film occur at larger grain size than those in the bulk samples. Our detailed slip analysis shows that the origin of this shift is not the increased grain boundary mobility in the slabs but the weaker size effect of intragranular dislocation-based plasticity.