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Surface effects in atomistic mechanical simulations of Al nanocrystals

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Abstract— Detailed knowledge of the mechanical properties of nanocrystals is crucial for understanding the behavior of micromachining devices. Determining experimentally the elastic and plastic properties of nanocrystals can be very challenging. In this work, we present molecular-dynamics simulations of mechanical properties of Al nanocrystals, both using Lennard-Jones and embedded-atom method potentials. We show that this kind of tests borrowed from mechanical engineering provide helpful insight on the mechanical behavior of nanocrystals. We also provide evidence suggesting that the small scale effects, mainly due to the small surface-to-volume ratio of nanocrystals, are crucial. The main results of our work are the failure of the thermodynamical relations connecting the applied stress and the material strain (additionally, we introduce a simple mathematical framework to account for this effect), the nonequilibrium behavior at the onset of the plastic deformation related to the appearance of long tails (power law) in the distribution of dissipated heat and, finally, the existence of conditions under which the system can experience reversible load-unload cycles in the plastic state.

Index Terms—

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