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Softening of nanocrystalline materials at small grain size GEORGIOS KOPIDAKIS, NIKOS GALANIS, IOANNIS REMEDIAKIS, Dept. of Materials Science and Technology, University of Crete — We examine the dependence of the mechanical properties of nanocrystalline materials on grain size. Our extensive atomistic simulations for several nanocrystalline solids show a universal softening at grain sizes of less than a few nanometers. The elastic constants decrease as the average grain size becomes smaller, in analogy with the reverse Hall-Petch effect for nanocrystalline metals. This behavior is explained by the increase of the fraction of grain boundary atoms as grain size decreases. We derive simple scaling laws for various mechanical properties as a function of the grain size by decomposing the energy into contributions from atoms in the bulk of grains and from atoms at the interfaces. Our theoretical predictions fit very well our results from atomistic simulations of different nanocrystalline materials, from nanocrystalline metals to ultrananocrystalline diamond. It is therefore argued, and quantitatively explained, that softening at small grain size is a general nanoscale effect.

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