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Softening of ultra-nanocrystalline diamond at small grain sizes GEORGIOS KOPIDAKIS, Department of Materials Science and Technology, University of Crete, IOANNIS REMEDIAKIS, Department of Materials Science and Technology and Department of Physics, University of Crete, PANTELIS KELIRES, Department of Physics, University of Crete and Dept. of Mechanical Engineering and Materials Science and Engineering, Cyprus University of Technology — Ultrananocrystalline diamond is a polycrystalline material, having crystalline diamond grains of sizes in the nanometer regime. We study the structure and mechanical properties of this material as a function of the average grain size, employing atomistic simulations. Using the bulk and Young's moduli as probes of stiffness, we observe softening of the material as the size of its grains decreases, similar to the reverse Hall-Petch effect observed for nanocrystalline metals. This softening is attributed to the enhanced fraction of interfacial atoms. The calculated scaling of the cohesive energy and bulk modulus with respect to average grain size agrees very well with this picture. Our results suggest that softening at very small grain sizes might be a generic property of nanocrystalline materials.

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