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Elasticity and mechanical properties of nanostructured carbon¹ MARIA FYTA, Department of Physics, Harvard University, IOANNIS REMEDI-AKIS, Department of Materials Science and Technology University of Crete, Heraklion, Crete, Greece, PANTELIS KELIRES, Department of Mechanical Engineering and Materials Science and Technology, Cyprus University of Technology, Limassol, Cyprus — We present a theoretical study of nanostructured carbon, emphasizing on diamond nanocomposites. These are materials that consist of diamond nanocrystallites surrounded by a dense amorphous carbon matrix, in a highly stable configuration. We study the properties of such materials by employing a combination of tight-binding molecular-dynamics and empirical-potential Monte-Carlo simulations. We aim to investigate the role of the sp^2 component and the grain size on the mechanical properties of these structures. We calculate the rigidity of these materials and their elastic recovery under hydrostatic pressure, and find them to be considerably high compared to those of dense single-phase amorphous carbon. We find that the inter-grain fracture of these materials under shear and tensile load on these materials occurs at the weakly bonded sp^3 sites in the amorphous matrix.

¹Work done at Physics Department, University of Crete, Heraklion, Crete, Greece.

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