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**Structure of nanocrystals embedded in amorphous carbon** IOANNIS REMEDIAKIS, MARIA FYTA, PANTELIS KELIRES, Physics Department, University of Crete, Heraclion, Crete, Greece, GEORGIOS KOPIDAKIS, Department of Materials Science and Technology, University of Crete, Heraclion, Crete, Greece — Amorphous carbon (a-C) has been often found to contain crystalline regions with diameters in the nanometer scale. The so-called nanostructured amorphous carbon has attracted considerable attention, because of possible applications in MEMS/NEMS and optoelectronic devices. In this work, we study embedded nanocrystals in various a-C matrices using tight-binding molecular dynamics and empirical-potential Monte Carlo simulations. We are especially interested in faceted nanocrystallites, that deviate significantly from a spherical shape. We start by calculating the interface energy between various faces of the crystal and a-C. We then use the so obtained interface energies to predict the shape of the nanocrystal by means of a Wulff construction. Finally, we construct the atomistic configuration of the embedded nanocrystallite and examine its stability as a function of temperature and the nanocrystallite size.

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