

Structural and Electronic properties of nanodiamond : first principles simulations

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Nanometer sized diamond has been found in meteorites, proto-planetary nebulae and interstellar dusts , as well as in residues of detonation and in diamond films. Remarkably, the size distribution of diamond nanoparticles appears to be peaked around 2-5 nm, and to be largely independent of preparation conditions. We have carried out ab-initio calculations of the stability of nanodiamond as a function of surface hydrogen coverage and of size [1] and we have found that at about 3 nm, and for a broad range of P and T conditions, particles with bare, reconstructed surfaces become thermodynamically more stable than those with hydrogenated surfaces, thus preventing the formation of larger grains. Our findings provide an explanation of the size distribution of extra-terrestrial and of terrestrial nanodiamond found in ultradispersed and ultra-crystalline diamond films. They also provide an atomistic structural model of these films, based on the topology and structure of 2-3 nm bucky diamonds [2]. In addition work is in progress to study the effect of nitrogen impurities on the structural and electronic properties of nanodiamond.

[1] J.Y Raty and G.Galli, Nature Materials (2003)

[2] J.Y.Raty, G.Galli, C.Boedest, A.Van Buuren and L.Terminello, Phys.Rev.Lett. 2003

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