Simulation and Visualization of Nanodiamond and Nanographite

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Hydrogen plays a significant role in the formation of nanodiamond, terminating diamond surfaces and removing sp^2 bonded atoms from the surface during CVD diamond growth. However, there are only a few calculations that simulate nanodiamond development directly, and even less that do so in a hydrogen-containing environment. Recently, nanoscale graphitic layers emebedded in amorphous carbon were also observed. We carried out a comphrehensive study of nanodiamond and nanographite formation from molten carbon in the presence of hydrogen under varied conditions of external pressure and cooling rate. We found that hydrogen-free nanodiamond crystals are precipitated more readily at increased melt densities and cooling rates, whereas slower cooling rates permit formation of graphitic layers.

Our calculations were made with tight-binding potentials (with the OXON code) and the nanocrystallites were identified with our AViz visualization software. AViz enables colorcoding of different types of carbon hybridization, thereby facilitating the identification.

The most surprising aspect of our study was the initially unexpected formation of the nanographite crystals. In fact we initially suspected an error in our equilibration,(despite all our care) until the experimental nanographite formation was brought to our attention. Movies of the formation of graphitic and nanodiamond structures can be seen at:

`http://phycomp.technion.ac.il/~anastasy/seminar2/graphite.gif`
`http://phycomp.technion.ac.il/~anastasy/seminar2/cluster2.gif`

Additional animations will be placed at:

`http://phycomp.technion.ac.il/~phr76ja/CCP2010`