Carbon Family at the Nanoscale

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The science of carbon materials is at an important juncture. The historically independent scientific communities studying graphite-based materials, diamond and fullerene nanotubes merge as their interest converge at the nanoscale. Understanding properties of carbon entities at the nanoscale within a unified framework, including the conditions under which one form transforms into another become a general tendency. According to this tendency, a brif overview of the relative stability of various carbon structures with characteristic sizes in the nanoscale region with major emphasis on nanodiamond structures will be presented.

Due to the rich surface chemistry of nanodiamond particles of detonation origin and their tendency to form agglomerates, it is rather challenging experimentally to study properties of individual nanodiamond particles. Atomistic modeling is a powerful tool to address these challenges as well as outline the routes for development of new carbon-based materials and technologies. Several case studies of diamond nanostructures using analytical and semiempirical approaches for description of interatomic interactions, in some cases performed in conjunction with experimental efforts, will be presented. Relative stability of nanodiamond particles of different shapes, mechanical properties of nanodiamond-polymer composites, feasibility of designing structures composed of nanodiamond clusters and carbon nanotubes as well as determining their electronic properties will be discussed. Finally, based on literature \i ab initio\i0 data, it will be illustrated that diamond nanorods would have a brittle fracture force and stiffness that exceeds carbon nanotubes for radii greater than about 1-3nm depending on the orientation of the diamond nanorod. The energetic stability of diamond nanorods is predicted by molecular modeling to be comparable to single-walled carbon nanotubes. Analysis of thermal conductivity of diamond nanorods depending on their morphology will be reported and compared to heat conduction properties of pristine and functionalized carbon nanotubes. It is concluded that diamond nanorods represent an important and viable target structure for synthesis.