Detonation Nanodiamond: Modeling and Experiment

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A keen, world-wide interest has developed over the last years in the nanostructured diamond materials and, particularly, in nanodiamonds of detonation origin invented in 60-s in the former USSR. Frequently, new researchers entering the field do not realize initially that there is a wide variety of detonation nanodiamond (DND) produced by different vendors using different synthesis and purification techniques. The different techniques determine the surface chemistry, agglomerate sizes, dispersivity and sedimentation stability in different types of solvents. Particularly, type and content of surface groups as well as a structure of the surface of a DND primary particle are topics of active current research, both theoretical and experimental. Using atomistic modeling, the statistical distribution of the different types of surface groups (such as –OH, –COOH, –C=O, and $-NH_2$) on the surface of a DND particle will be provided and a range of the variation in C-H-N-O content of a DND particle will be discussed and compared with the values reported by different vendors. Based on the statistic of possible surface groups on DND surface, it is possible to predict the electrostatic potential of DND in water solvents, and therefore estimate their stability to sedimentation. Atomistic simulations of the stability of nanodiamond particles will be also discussed including related variations in the non-diamond carbon content in the DND.

From the practical point of view in order to readily utilize DND particulate in many nanotechnology applications it is necessary to modify the surface chemistry and to separate the particles into a more narrow range of particles (fractionalization). As was mentioned above, the surface functionalization and fractionalization are highly dependent upon the DND method of synthesis and purification. In this study we will report on 'dry' methods of modifications resulting in increase of the content of polar or non-polar surface groups. Using high temperature treatment of DND followed by dispersion in water using a high power sonicator and multi-step ultracentrifugation, stable hydrosols were formed from the smallest particle-size fraction (down to 20 nm particles). Several examples of applications of the modified/fractionalized DND in polymer composites, galvanic coatings, cooling nanofluids and biological applications will be briefly discussed.