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Analysis of Diamond Nanocrystal Formation from Multi-walled Carbon Nanotubes ANDRE MUNIZ, TEJINDER SINGH, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — A systematic analysis is presented of the nanocrystalline structures generated due to the inter-shell C-C bonding between adjacent concentric graphene walls of multi-walled carbon nanotubes (MWCNTs). The analysis combines a comprehensive exploration of the parameter space determined by the geometrical characteristics of the individual graphene walls comprising the MWCNTs with density functional theory calculations of inter-shell C-C bonding and molecular-dynamics relaxation of the resulting nanocrystalline structures. We find that these structures can provide seeds for the nucleation of the cubic-diamond and hexagonal-diamond phase in the form of nanocrystals embedded in the MWCNTs. The resulting lattice structure is determined by the relative alignment of adjacent graphene walls in the MWCNT. These crystalline phases are formed over the broadest range of nanotube diameters and for any possible combination of chirality of graphene walls. The generated nanocrystal size is determined by the chiral-angle difference between adjacent graphene walls in the MWCNT.

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