Size dependent phase diagrams of Ni-C nanoparticles

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Carbon nanotube synthesis critically depends on the chemical and physical states of the catalyst particle from which they grow. In the temperature range (600-1000˚C) of SWNT synthesis, pure isolated Ni nanoparticles are solid. Under CVD synthesis conditions, reactive carbon may stay adsorbed on the surface, or diffuse to subsurface or in the core of the nanoparticle, thereby inducing a partial or complete melting.

On the basis of the tight binding model developed for the Ni-C system coupled with grand canonical Monte Carlo simulations [1, 2, 3], we calculate size dependent phase diagrams for Ni-C alloys. For NP sizes of about 3 nm, we find that i) the eutectic point lies around 1000K, much lower than the bulk one, ii) a large solid core / molten or amorphous shell domain is found instead of the two phase solid liquid region and iii) carbon segregation from a solid NP surface can take place only at temperatures below 850 K. We discuss the consequence of these findings on our understanding of the SWNT growth mechanisms.

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