Size dependent phase diagrams of Nickel-Carbon nanoparticles

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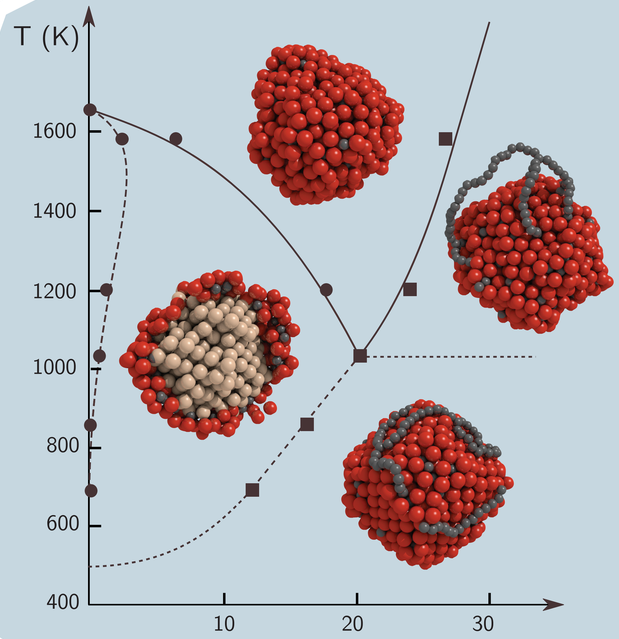
1 Introduction

Under SWNT growth conditions, nanoparticles (NP) are exposed to reactive carbon.
Depending on temperature, carbon chemical potential and nanoparticle size, carbon can either stay adsorbed or diffuse to subsurface or in the core of the nanoparticle, inducing a partial or complete melting.

What is the state of Ni-C NP under SWNT growth conditions ? **Calculation of Phase Diagrams**

Main Results



Deep eutectic

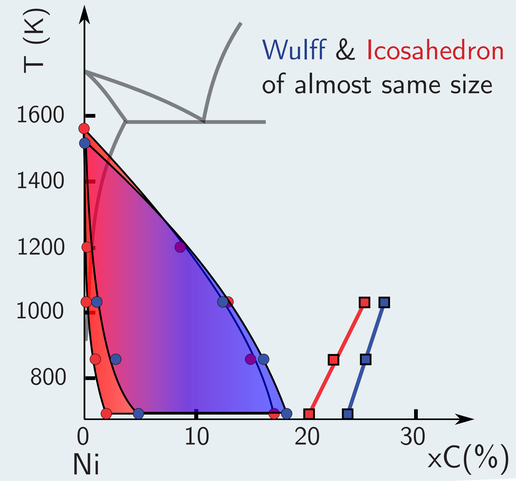
Large Solid core-Liquid shell domain

Segregation from solid NP only below ~900K

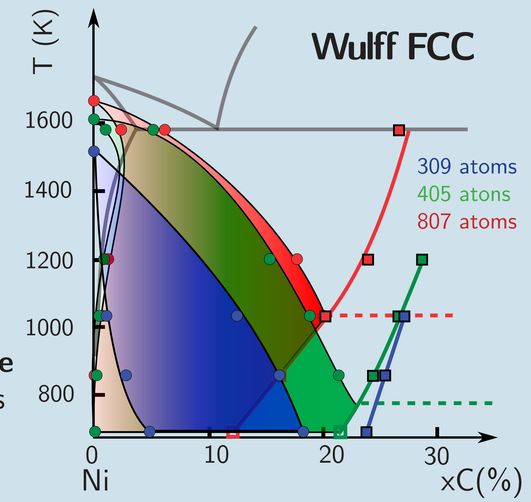
Wulff larger solid phase than icosahedron NP

Icosahedron more compact than Wulff

4



4



Size dependence of phase diagrams

Solid-Liquid order parameter

2

Steinhardt order parameter used to determine Solid or liquid atomic environment

$$q_{6m}(i) = \frac{1}{N(i)} \sum_{j=1}^{N(i)} Y_{6m}\left(\theta(\mathbf{r}_{ij}), \Phi(\mathbf{r}_{ij})\right)$$

Local and directional bond order parameter based on spherical harmonics

$$S_i = \frac{1}{N_b} \sum_{j=1}^{N_b} \frac{\sum_{m=-6}^{6} q_{6m}(i) q_{6m}^{*}(j)}{\left(\sum_{m=-6}^{6} |q_{6m}(i)|^2\right)^{1/2} \left(\sum_{m=-6}^{6} |q_{6m}(j)|^2\right)^{1/2}}$$

$\bar{S}$>0.85 NP Solid

$\bar{S}$<0.25 NP Liquid

Correlation between structures surrounding two particles give the local state of the NP

3

Methodology

Continuous evolution from solid to liquid states
Solid-Liquid phase boundaries determined from order parameter