Phase diagram of Ni-C nanoparticles from computer simulation

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Introduction

Under SWNT growth conditions, nanoparticles 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**

We attempt the liquid/solid phase diagrams for Ni-C nanoparticles and extend our previous calculations[1–3]

Solid-Liquid order parameter

Steinhardt order parameter[4] used to determine solid-liquid fraction of a nanoparticle (NP)

Local and directional bond order parameter based on spherical harmonics

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

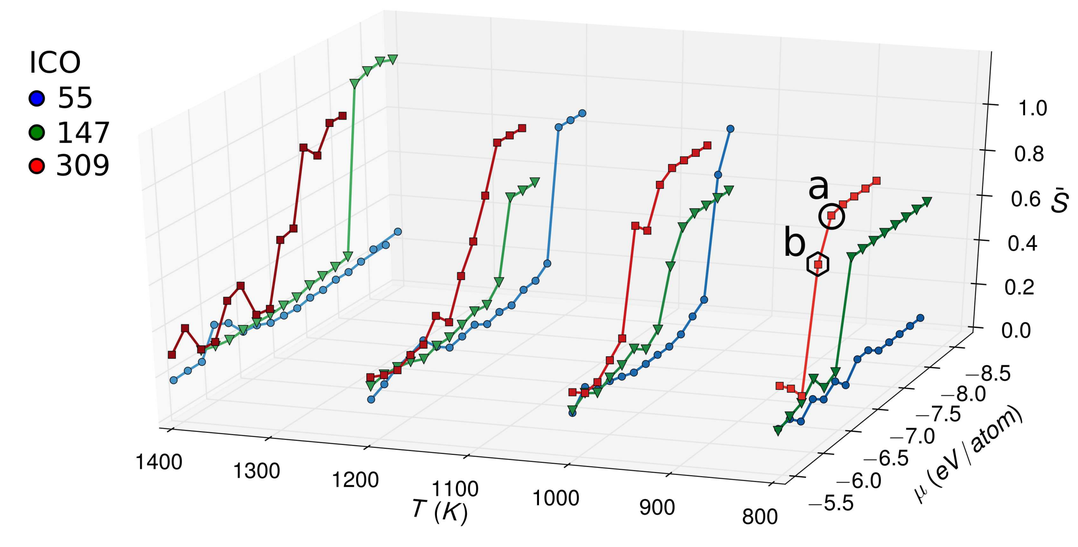
Correlation between structures surrounding two particles give the local state of the NP

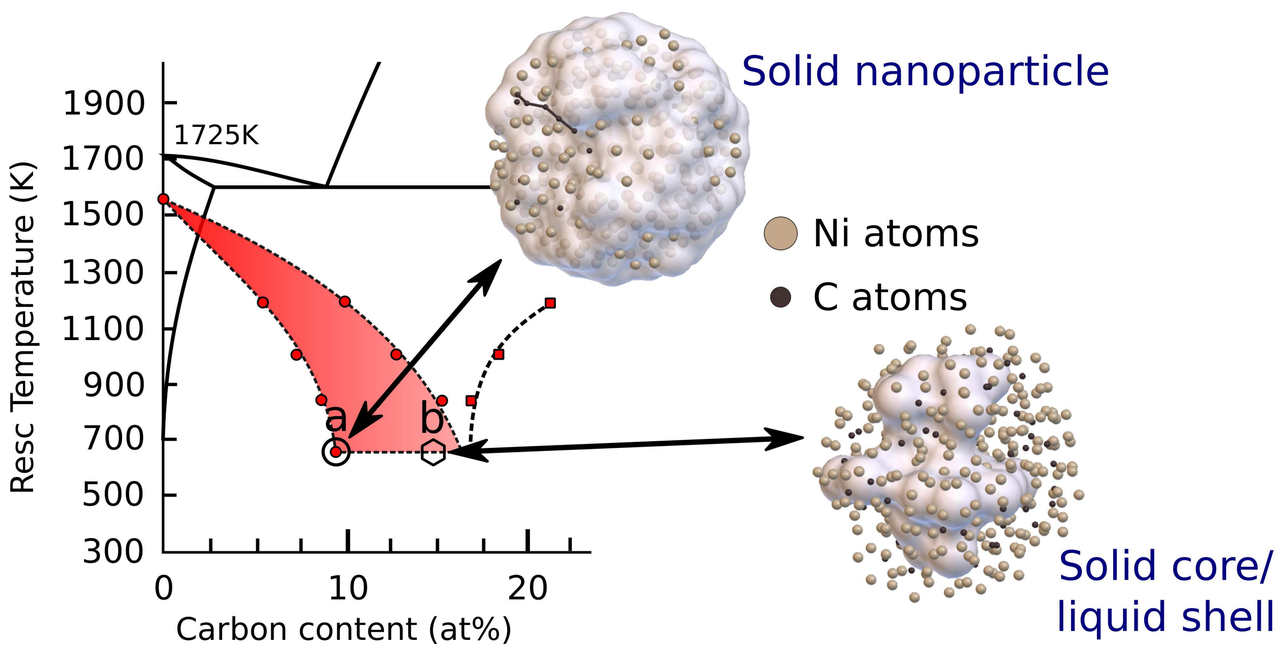
$$S_{ij} = \frac{\sum_{m=-6}^{6} q_{6m}(i) q_{6m}^{*}(j)}{\left(\sum_{m=-6}^{6} |q_{6m}(i)|^2\right)^{1/2} \left(\sum_{m=-6}^{6} |q_{6m}(j)|^2\right)^{1/2}} \longrightarrow$$

$\bar{S} > 0.5$ **NP solid**

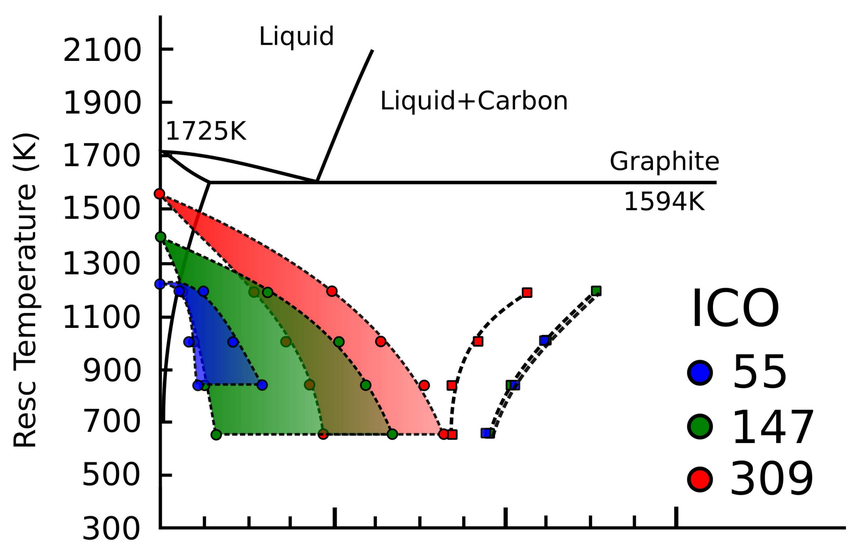
$\bar{S} < 0.5$ **NP liquid**

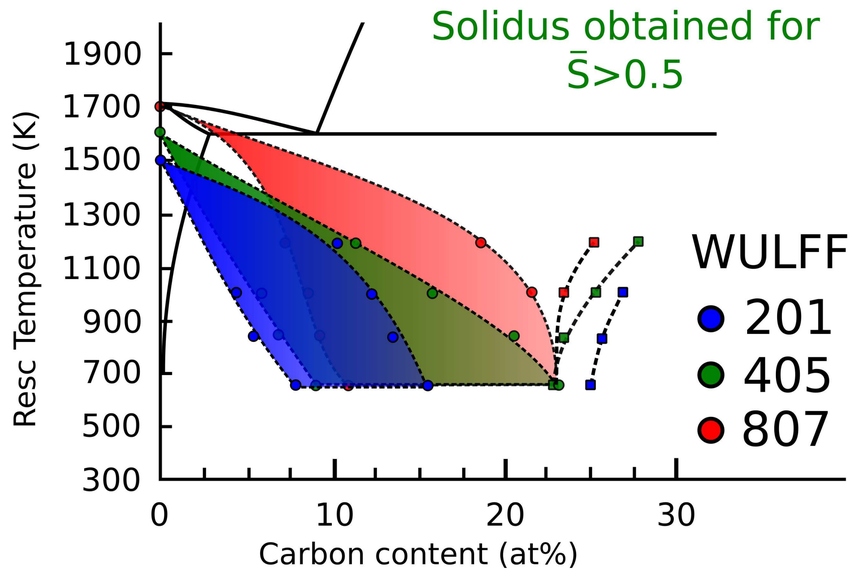
Order parameter function of:
NP sizes and thermodynamic of the system





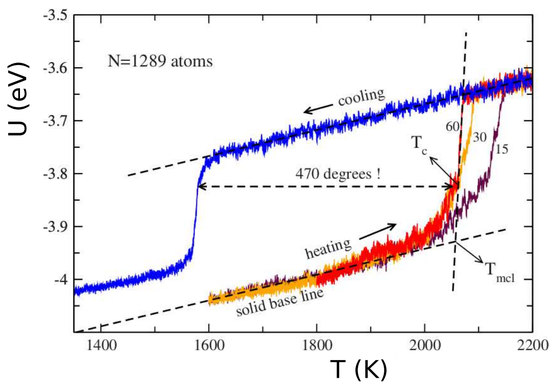
Ni-C NP **phase diagrams** function of**:**
NP structures and sizes

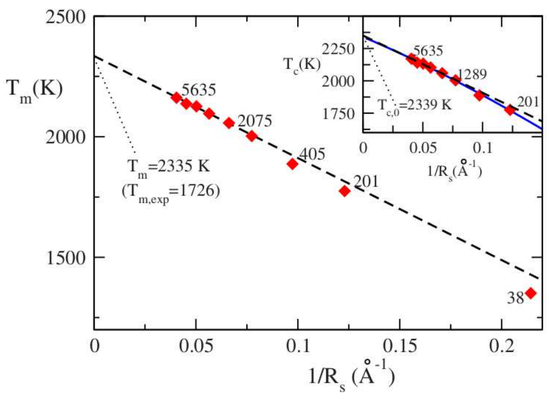




Pure Ni cluster melting temperatures

Melting energies and **temperatures** calculated by Monte Carlo simulations[5] for different **pure Ni cluster** sizes





Conclusion

- **Size dependence** of phase diagrams
- Nanoparticles can be:

  Solid
  Mixed solid core/liquid shell
  Liquid

- **Limit of solulibility** $\sim 25\%$ for NP, $\sim 10\%$ for bulk at the eutectic point
- Solidus difficult to determine

Bibliography

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[5] J. H. Los, R. Pellenq, *Phys. Rev. B* **81**, 064112 (2010)