

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Distribution and stability of Carbon in Fe-C nanoparticles.¹

NEHA AWASTHI, Duke University, USA, AIQIN JIANG, Duke University, USA, ALEKSEY KOLMOGOROV, WAHYU SETYAWAN, Duke University, USA, KIM BOLTON, Goteborg University, Sweden, STEFANO CURTAROLO, Duke University, USA — Catalytic Chemical Vapor deposition (CVD) method is widely used to produce carbon nanotubes. To improve our understanding of the CVD growth mechanism, we focus on the thermodynamics and the phase stability of catalyst Fe-C nanoparticles. Using *ab initio* methods and classical molecular dynamics simulations, we investigate 1) the diffusion and solubility of carbon atoms in nanoparticles by calculating the distribution of carbon atoms inside the clusters, 2) the formation and stability of carbides at nanoscale, and 3) the effect of substrates on such structures. We address the implications of these results on NT growth, and give possible strategies to mitigate the problems.

¹Honda Research Institute Inc., USA

Neha Awasthi
Duke University

Date submitted: 16 Nov 2006

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