Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

New empirical potentials between iron nanoparticles and oxide substrates[1] AIQIN JIANG, NEHA AWASTHI, ALEKSEY KOLMOGOROV, Duke University, KIM BOLTON, Goteborg University, Sweden, ELENA MORA, Ohio State University, TOSHIO TOKUNE, AVETIK HARUTYUNYAN, Honda Research Institute, USA, STEFANO CURTAROLO, Duke University — Interaction of iron catalyst nanoparticles with a substrate may influence nucleation and growth mechanism of carbon nantobutes (CNT) by shifting the melting temperature of the supported iron particles. To account for this effect we have used ab initio calculations to develop empirical potentials between iron nanoparticles and oxide substrates. Simulations have been performed on Fe/Al_2O_3 system with Al_2O_3 substrate fully relaxed. We have demonstrated that the surface rearrangement effects are significant but can be naturally incorporated into a simple Morse potential, which describes the total nanoparticle-substrate binding. The influence of different substrate surface terminations and positions of Fe layers on the strength of binding are discussed. Potentials for Fe and other oxide substrates are also being evaluated.

[1]Research sponsored by Honda Research Institute

Aiqin Jiang
Duke University

Date submitted: 29 Nov 2005 Electronic form version 1.4