Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Movement of solid iron nanocrystal through a constriction in the multiwall carbon nanotube[1] SINISA COH, WILL GANNETT, ALEX ZETTL, MARVIN L. COHEN, STEVEN G. LOUIE, UC Berkeley, Lawrence Berkeley National Laboratory — It has been known for some time that iron (and some other metals) can move inside multiwall carbon nanotube under the application of an external electrical current to the nanotube (B.C. Regan et al, Nature 428, 924 (2004)). Here we report on finding that a solid piece of iron nanocrystal can move through a constriction in the multiwall carbon nanotube that has a smaller cross-sectional area than the nanocrystal itself. Furthermore, we find that during this entire process the core of the nanocrystal remains solid and that the carbon in the nanotube does not chemically interact with iron. We performed kinetic Monte Carlo simulation based on a first principles density functional theory calculation which can reproduce this experimental finding. Additionally, we discuss the nature of the movement of the iron nanocrystal in our simulation and show why the nanocrystal is able to go through a constriction. Also, we compare the dependence of the nanocrystal speed on applied current with available experimental data. From this comparison we are able to estimate the experimental temperature and infer the magnitude of the electromigration force experienced by individual iron atoms for given applied external current.

[1]This work was supported by NSF grant No. DMR10-1006184 and U.S. DOE under Contract No. DE-AC02-05CH11231.

Sinisa Coh
UC Berkeley, Lawrence Berkeley National Laboratory

Date submitted: 07 Nov 2012 Electronic form version 1.4