Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Domain boundary formation in helical multishell gold nanowire
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— Helical multishell gold nanowire (Y. Kondo and K. Takayanagi, Science 289, 606 (2000)) is studied by molecular dynamics simulation with electronic structure ("ELSES" http://www.elses.jp/), so as to explore formation mechanism of helical domain boundary. We have proposed a model for the formation of helical multishell gold nanowires with molecular dynamics simulation with electronic structure (Y. Iguchi, T. Hoshi, T. Fujiwara PRL 99, 125507 (2007)). In this paper, we show simulation results with lager samples, of which the rod length is more than 10 nm and the number of rod atoms is more than one thousand. Unlike the results of shorter rods in the previous paper, a well-defined domain boundary between helical and (non-)helical regions appears, when an atom moves from a inner shell into rod surface. The inserted atoms on the rod surface causes a surface reconstruction on rod surface and introduces a helical region with a domain boundary. Such an inserted atom is a possible candidate of mechanism for forming a helical rod from an ideal (non-helical) one.

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Date submitted: 17 Nov 2008 Electronic form version 1.4