ABSTRACT

The basic understanding of the underlying techniques of growing Carbon Nanotubes (CNTs) with a specific chirality is still obscure and needs to be understood so as to properly harness its potentials. Using both Classical Molecular Dynamics (MD) simulation with empirical force fields and a geometry optimization based on ab initio forces, we show that the dynamics involved in the growth of CNT on iron nanoparicles is non linear but complex. For a good geometry, the growth depends on the deposition rate of the carbon atoms on the iron nanoparticles. Observations show that defects in the CNT first appear in the cap formed and then propagate through the wall of the growing tube. Partial results from ab initio show the formation of a cap which is a precursor of an armchair type CNT.