

# A molecular dynamics study of metal coating on SWNT

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Metal coating on an SWNT is an important element technology in CNT-based electric and thermal device integrations. With the strong motivation, vacuum-evaporation experiments of various metals onto SWNT have been reported [1,2], and the observed metal morphologies have been explained based on the static energetics. However, in order to grasp the full picture of the coating mechanism, one would also need to consider the contribution of dynamics, and thus, molecular dynamics approach is useful [3]. In the current simulations, we take a similar MD model to the previous report [3] with Brenner bond order potential [4] for carbon covalent bonds, but use different metal models; the GEAM potential [5] for metal-metal, and Lennard-Jones fitted potential for the carbon-metal interactions. The coating processes were simulated for various metal kinds, temperatures, and deposition conditions such as initial cluster sizes and deposition rates.

The morphology of the deposited metal strongly depends on the metal kind as seen in Figure 1. For these cases, the metal morphologies are confirmed to be insensitive to temperature in a realistic range. While Ti atoms cover the entire SWNT, Au and Fe atoms locally cling onto SWNT and forms clusters, where Au clusters are more spherical than Fe ones. The results of Ti and Au are consistent with the metal coating experiments [1,2], though that of Fe is not. The deposition processes will be presented for various parameters and conditions, and the mechanism will be discussed, also for the cases with bundled SWNTs.

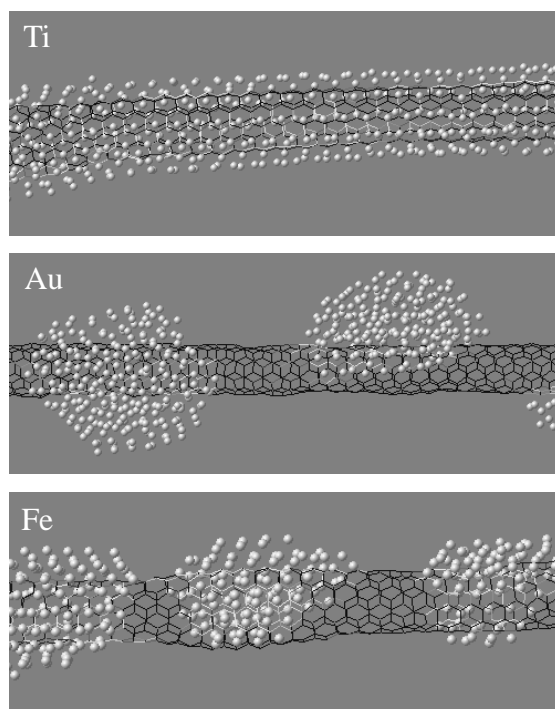


Fig. 1 Various metals deposited on SWNT

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