

Abstract Submitted
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Metal–nanotube interactions – wetting properties¹ RUZENG ZHU, LNM, IMech, CAS., Beijing, China, SHUWEN CUI, ChaoYang school of HSRUC — The wetting properties of metal nanoparticles in large-diameter single Carbon nanotubes (LDSWNT) is studied by considering the size effect on surface tension of the metal cluster. For the case of macro-nonwetting, we get finite critical atom number N such that the metal cluster with any atom number smaller than it has contact angle π , and so it shrinks into a ball. For an experiential formula of the surface tension of cluster expressed by the number of atoms, we determine the parameters in it for Pd and Pt respectively by density functional theory (DFT). Taking a graphene sheet as a representative of LDSWNT and using the known data of the surface tensions of solid and liquid, we obtain solid-liquid interface tension through Berthelot rule. Based on these results, we obtain $N=5$ for Pd and $N=6$ for Pt. For cluster containing 13 Pd atoms and that containing 13 Pt atoms, we use the above mentioned experiential formula to obtain their contact angles in LDSWNT consistent with those shown by the pictures given by DFT (A Maiti and A Ricca, Chem Phys Letters 395 (2004) 7–11), and thus the validity of our method is proved.

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