Atomistic Simulation of the Growth of Defect-free Carbon Nanotubes

Ziwei Xu [1], Feng Ding [2], Tian ying Yan [3]

[1] School of Material Science & Engineering, Jiangsu University

[2] nstitute of Textiles and Clothing, Hong Kong Polytechnic University, Hong Kong, The People's Republic of China

[3] Institute of New Energy Material Chemistry , Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Nankai University,Tianjin 300071, The People's Republic of China

Contact e-mail: *ziweixu2014@ujs.edu.cn*

Atomistic simulation of defect-free singlewalled carbon nanotube (SWCNT) growth is essential for the insightful understanding on the SWCNTs growth mechanism. Despite the extensive efforts paid in the past two decades, the goal has not been completely achieved, due to the huge time scale discrepancy between atomistic simulation and the experimental synthesis of SWCNT, as well as the lack of accurate potential energy surface (PES). Here, we report atomistic simulations of defect-free SWCNT growth by using a new generation of carbon-metal potential and a hybrid method, in which a basin-hopping strategy is applied to facilitate the defect healing during the simulation. The simulations reveal a narrow diameter distribution and an even chiral angle distribution of the growth of SWCNTs from liquid catalyst, which is in agreement with most known experimental observations.