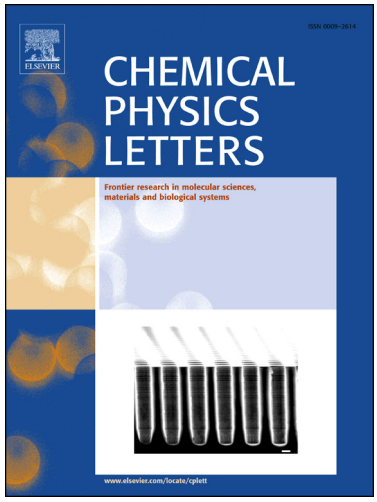

Collision-induced fusion of two single-walled carbon nanotubes: A quantitative study

Chao Zhang, Fei Mao, Xiang-Rui Meng, Dong-Qi Wang, Feng-Shou Zhang

PII: S0009-2614(16)30404-3
DOI: http://dx.doi.org/10.1016/j.cplett.2016.06.009
Reference: CPLETT 33918

To appear in: *Chemical Physics Letters*

Received Date: 21 March 2016
Revised Date: 25 May 2016
Accepted Date: 2 June 2016

Please cite this article as: C. Zhang, F. Mao, X-R. Meng, D-Q. Wang, F-S. Zhang, Collision-induced fusion of two single-walled carbon nanotubes: A quantitative study, *Chemical Physics Letters* (2016), doi: http://dx.doi.org/10.1016/j.cplett.2016.06.009

Collision-induced fusion of two single-walled carbon nanotubes: A quantitative study

Chao Zhang[a,b,*], Fei Mao[c], Xiang-Rui Meng[b], Dong-Qi Wang[d,*], Feng-Shou Zhang[e]

[a] *School of Materials Science and Engineering, Anhui University of Science and Technology, Huainan 232001, China*
[b] *School of Mining and Safety Engineering, Anhui University of Science and Technology, Huainan 232001, China*
[c] *School of Nuclear Science and Technology, University of South China, Hengyang 421001, China*
[d] *Multidisciplinary Initiative Center, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China*
[e] *The Key Laboratory of Beam Technology and Material Modification of Ministry of Education, College of Nuclear Science and Technology, Beijing Normal University, Beijing 100875, China*

Abstract

The coalescence processes of two (6,0) single-walled carbon nanotubes are investigated via coaxial collision based on the self-consistent-charge density-functional tight-binding molecular dynamics method. According to the structure characteristics of the nanotubes, five impact cases are studied to explore the coalescence processes of the nanotubes. The simulation shows that various kinds of carbon nanomaterials, such as graphene sheets, graphene nanoribbons, and single-walled carbon nanotubes with larger diameters, are created after collision. Moreover, some defects formed in the carbon nanomaterials can be eliminated, and even the final configurations which are originally fragmented can almost become intact structures by properly quenching and annealing.

1. Introduction

The coalescence of carbon nanotubes (CNTs) [1] has been extensively studied in recent years. There are several common methods for coalescing CNTs, such as introducing some defects [2], thermal treatment at high temperature [3, 4, 5], applying pressure or external force [6, 7], coaxial collision [8], and so on. Terrones *et al.* [2] have observed the coalescence of single-walled CNTs at high temperature by *in situ* transmission electron microscope (TEM), and studied the fusion process by employing the tight-binding molecular dynamics (MD)

*Corresponding author. Fax: +86 554 666 8649
Email addresses: chaozhang@mail.bnu.edu.cn (Chao Zhang), dwang@ihep.ac.cn (Dong-Qi Wang)