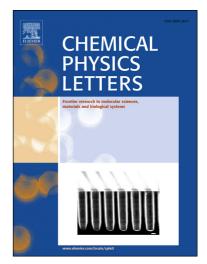
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ACCEPTED MANUSCRIPT

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

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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)

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