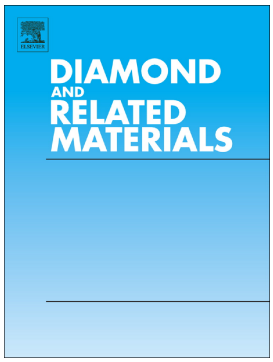

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Molecular dynamics simulations of the thermal conductivity of cross-linked functionalized single- and double-walled carbon nanotubes with polyethylene chains

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Abstract

In this article, for functionalized single- and double-walled carbon nanotubes (SWCNTs and DWCNTs) with cross-linked polyethylene (PE) chains, the thermal conductivity is computed through the molecular dynamics (MD) simulations. Moreover, the effects of different weight percentages of PE chains and distribution patterns on the thermal conductivity are investigated. To calculate the thermal conductivity, an approach for determining the cross-section area is proposed. According to the results, the thermal conductivity decreases by attaching the functional groups to the wall of nanotubes. Additionally, as the weight percentage of functional group increases, the thermal conductivity decreases. It is also observed that increasing the number of nanotube walls results in less sensitivity of thermal conductivity to increasing the weight percentage of functional groups.

Keywords: Thermal conductivity; Functionalization; Carbon nanotube; Molecular dynamics simulations

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