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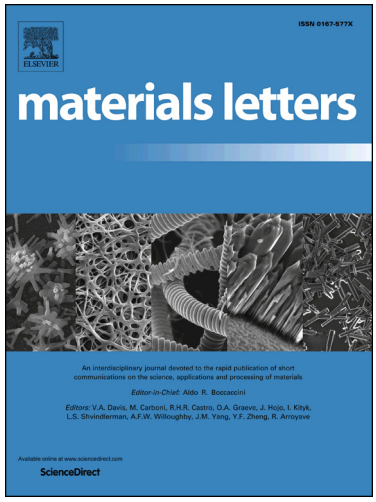

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Molecular Dynamics Simulation of Double-Layered Graphene-Carbon Nanotube Junctions for Thermal Rectification

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Abstract

By using molecular dynamics simulations, we have studied the thermal rectification in double-layered Graphene-Carbon Nanotube (DGN-DWCNT) Junctions. It is found that DGN-DWCNT junctions exhibit significant thermal rectification under both large and small thermal bias. Even under a small thermal bias $|\Delta| = 0.1$, a rectification ratio as high as 300.6 % can be achieved. The influences of the geometric parameters on the thermal rectification of the DGN-DWCNT junctions are discussed, and the underlying mechanism of the significant thermal rectification is explored. These results open a door in the applicability of DGN-DWCNT junctions and their based pillared graphene system in nanoscale engineering of thermal transport devices.

Keywords: Carbon materials; Thermal rectification, Graphene-carbon nanotube junction, Local resonance, Molecular dynamics, Thermal properties

1. Introduction