The Open Access Journal of Science and Technology

Abstract

Graphene Thermal Conductivity Dependence on Using Non-Equilibrium Molecular Dynamics Simulations

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Abstract:

Due to the increasing thermal management has become a serious problems in electric devices, especially in nanodevices. Graphene has been considered as a potential heat transfer material. However, the thermal conductivity in graphene demonstrates the discrepancy between the simulated value and the experimental results. We computed the thermal conductivity of graphene (from length of 21.84 nm to 43.78 nm) on nanoscacle size using NEMD method. The results demonstrate obvious edge type (zigzag edge and armchair edge) and nanostructure size dependence of thermal conductivity. With graphene length << MFP (Phonon mean free path), thermal conductivity increase with the length increasing and is strongly limited by the sample size owing to a dominant boundary scattering. Besides, the thermal conductivity of graphene with zigzag edge is larger than the armchair edge, which is because of the higher phonon group velocities.

Biography:

Xianqi Wei is a lecturer of Jiangsu Ocean University. She has completed his PhD from Xi'an Jiaotong University

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13th International conference on Smart Material and Polymer technology ; February 19-20 2020, Paris, France

Citation: Zhongwei Q ref; Graphene Thermal Conductivity Dependence on Using Non-Equilibrium Molecular Dynamics Simulations Smart Materials 2020; February 19-20 2020, Paris, France