Thermal Properties of Graphene Nanowiggles

Fereshte Masoodinia, Rouhollah Farghadan*

Department of Physics, University of Kashan, Kashan, Iran

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Abstract

This paper studies the theory of thermal properties of graphene nanowiggles with zigzag- and armchair edges in different size and geometry. In order to calculate the phonon dispersion spectrum, the specific heat, and thermal conductivity properties, we use the four-nearest-neighbor force-constant model and Landauer theory calculations. The results show that the studied thermal properties differ significantly compared to complete nanoribbons, especially at low frequencies. In detail, in acoustic modes, the thermal conductivity and the transmission coefficient of the phonon reduce sensitively due to the special structures of the edge compared to the perfect nanoribbons, which cause the dispersion of the phonon from the edges. There are also significant changes in the thermal capacity, and calculating the out-of-plane and in-plane phonon modes also shows that the in-plane phonon modes play a greater role in the thermal conductivity. These results can be useful in the improvement and design of electronic and thermoelectric nanodevices.

Keywords: graphene nanowiggles, phonon transmission coefficient, phonon thermal capacity, thermal phonon transport coefficient

*Corresponding Author: rfarghadan@kashanu.ac.ir