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The effect of extended vacancies on the thermal properties of armchair garaphene nanoribbons

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Abstract

This paper shows a theoretical study of the thermal properties of armchair grapehen nanoribbons in the presence of extended vacancies. Each graphene nanoribbons formed by superlattices with a periodic geometric structure, different size and symmetry of vacancies. The phonon dispersion, specific heat and thermal conductivity properties are described by a force-constant model and also by Landauer theory calculations. Our results show that the geometric structure of the vacancies and their positions have a significant roles in controlling the thermal properties, especially at low temperatures. Moreover, the out-of-plane and in-plane phonon modes exhibit a different role in the heat capacity and thermal phonon transport properties. Moreover, the out-of-plane phonon modes have more contribution in low temperature regime rather than in-plane phonon modes even in the presence of extended vacancies. The result may be useful for the design and improvement of thermal or thermoelectric nanodevices.

Keywords: extended vacancies, armchair graphene nanoribbons, specific heat, thermal conductivity

For full article, refer to the Persian section