

Abstract Submitted
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Interface Inducing Interesting Effects on Thermal Transport in Graphene Based Systems¹ HAIYUAN CAO, HONGJUN XIANG, XINGAO GONG, Fudan University — Using nonequilibrium molecular dynamics method (NEMD), we have studied how the interface affecting the thermal conductivity in multilayer graphene nanoribbons and the graphene grain boundaries. In multilayer graphene nanoribbons, the monotonous decrease of the thermal conductivity with the increase of the number of layers can be attributed to the phonon resonance effect of out-of-plane phonon modes. The reduction of thermal conductivity is proportional to the layer size, which is caused by the increase of phonon resonance. The results clearly show the dimensional evolution of thermal conductivity from quasi-one dimension to higher dimensions in graphene nanoribbons. The thermal transport across the asymmetric tilt grain boundary between armchair and zigzag graphene has also been investigated by simulations. We have observed significant temperature drop and ultra-low temperature-dependent thermal boundary resistance. More importantly, we find an unexpected thermal rectification phenomenon. The thermal conductivity and Kapitza conductance is direction-dependent. The effect of thermal rectification could be amplified by increasing the difference of temperature imposed on two sides. Our results show the interface phonon coupling could greatly change the thermal conductivity. Besides that, we have proposed a new promising kind of thermal rectifier and phonon diode based on the asymmetric interface in graphene.

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