

عنوان مقاله:

Effect of torsional deformation on the thermal conductivity of 2D nanomaterials: A molecular dynamics study

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خلاصه مقاله:

The thermal conductivity of nanoscale materials is largely dependent on the applied strain and deformations. In this paper, the effect of torsional deformation and consequent wrinkles on the thermal conductivity of graphene, hexagonal boron nitride (h-BN) and molybdenum disulfide (MoS₂) nanostructures have been investigated by performing non-equilibrium molecular dynamics simulation. It is found that the wrinkles caused by applying the torsion result in reducing the thermal conductivity of nanostructures. Although the effect of created distortions is tangible, these wrinkles have the most influence on the thermal conductivity of MoS₂ and the least on the thermal conductivity of h-BN. The results of this study can be beneficial for estimating the values of applied torsion and wrinkle amplitude by measuring the thermal conductivity variations.

کلمات کلیدی:

thermal conductivity, nanostructures, torsional deformation, wrinkle, molecular dynamics

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