Grain Boundaries Applied in Attenuation of Mechanical Transverse Wave Propagations in Graphene

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Abstract

Due to the two-dimensional nature and various extraordinary properties, graphene has potential applications in nanosensors, nanoresonators, and other nanoelectromechanical devices. Generally, these sophisticated devices are extremely susceptible to the effects of acoustic noises in graphene, especially terahertz noises. Therefore, the ability to attenuate the acoustic waves would be necessary and allow the creation of nanoscale devices with improved performances or new functionalities. As we all know, macroscale and microstructured materials are enough to handle sound, ultrasound and hypersound waves, whereas to manipulate mechanical vibrations of much higher frequencies (> 0.1 THz), nanostructured modifications are necessarily required. One approach to modify the graphene nanostructure is to introduce grain boundaries. In this report, using molecular dynamics simulation and frequency spectrum analysis, the effects of grain boundary (GB) on the mechanical transverse wave propagation in graphene sheet are studied. We demonstrate two fundamental mechanisms, scattering and resonance, in the procedure of GB attenuating terahertz waves. The scattering impairs waves slightly and can be well described by Rayleigh scattering in a certain frequency range. Whereas, the resonance, occurring locally near GB, significantly reduces the amplitude responses, displaying a special frequency-selective filter-like behavior. Besides, the amplitude losses were found proportional to the GB buckling heights, which correspond to different graphene chiralities and GB misorientation angles. Our findings should provide a guideline for manipulating terahertz noises via nanostructured modifications in graphene-based nanodevices.

Keywords: Graphene, Grain Boundaries, Molecular Dynamics Simulation, Attenuation, Transverse Wave