First-Principle-Based Phonon Transport Properties of Nanoscale Planar Grain Boundaries

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Abstract
Over the last years, two-dimensional materials have attracted considerable interest due to the fact that they offer a new broad playground to explore and develop nanoscale devices with tailored electrical, optical and thermal properties [1]. Recently, many prototypes have been proposed for thermal devices (diodes, transistors, and logic gates) based on graphene [2]. Advanced computational methodologies such a non-equilibrium Green's functions (NEGF) have successfully helped to gain a deep insight into the mechanisms governing their transport properties.
In the present work, we investigate the integrity of phonon transport properties of large graphene (linear and curved) grain boundaries (GBs) under the influence of structural and dynamical disorder [3]. To do this, we combine density functional tight-binding (DFTB) method with atomistic Green's function technique. The results show that curved GBs have lower thermal conductance than linear GBs. Its magnitude depends on the length of the curvature and out-of-plane structural distortions at the boundary, having stronger influence the latter one. Moreover, we have found that by increasing the defects at the boundary, we can strongly reduce the thermal conductance in comparison to the effect produced by heating up the boundary region. This is due to the large reduction of the phonon transmission for in-plane and out-of-plane vibrational modes after increasing the structural disorder in the grain boundaries. For comparison, results obtained for other 2D materials (e.g., phosphorene and MoS_2 monolayer) will also be discussed.

References

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Figure

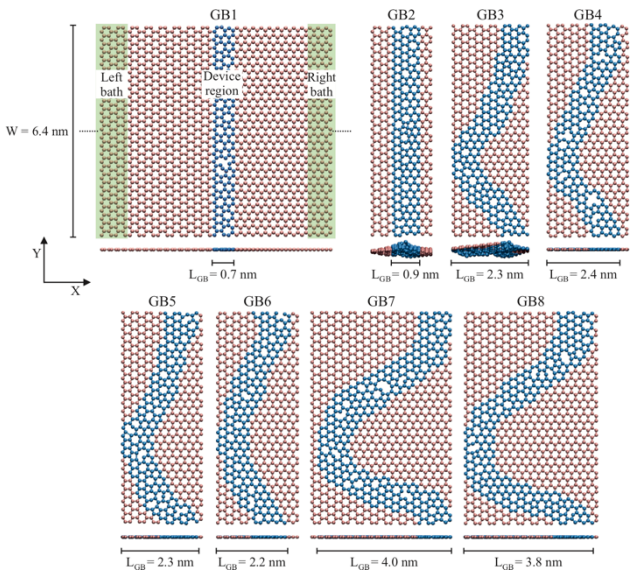

Figure 1: Top and side views of the structures of linear (GB1 and GB2) and curved (GB3-GB8) graphene grain boundaries. L_{GB} is the length of the grain boundary.