Strain engineering of thermal transport in two-dimensional grain boundaries

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Abstract

Grain boundaries (GBs) in two-dimensional materials have attracted great attention in recent years due to its unique physical properties [1]. However, many questions are still unanswered about the influence of external factors on their thermal properties. In a previous work, we have shown that functionalization plays an important role in the thermoelectric properties of graphene grain boundaries [2]. Now, we want to provide some insights in understanding the influence of strain on the thermal transport properties of novel two-dimensional materials with grain boundaries. To do this, we employ equilibrium Green's Functions technique combined with density functional tight-binding (DFTB) theory [2]. Our main focuses are grain boundaries in hBN, Phosphorene, and MoS_2 monolayers; which are potential candidates for developing novel approaches to nanoscale electronics and phononics. Among the GBs studied in the present work (5|7 and 4|8), 4|8 GB has the stronger influence on the thermal transport. We have also found an anomalous behavior of the thermal conductance after increasing the uniaxial strain, which can be tuned by considering temperature effects in the grain boundary. This trend is associated to the strain and temperature dependences of the bond length and the force constants of the material. Thus, our result opens up the possibility of controlling the thermal conductance by setting a specific configuration for the experiments. Hence, it is an open question of how strain affects the properties of heterostructures built of graphene and other 2D materials, which will allow novel properties and applications to be explored. It is expected that strain engineering may also shed light to design new type of electronic and phononic devices [3].

References

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Figures

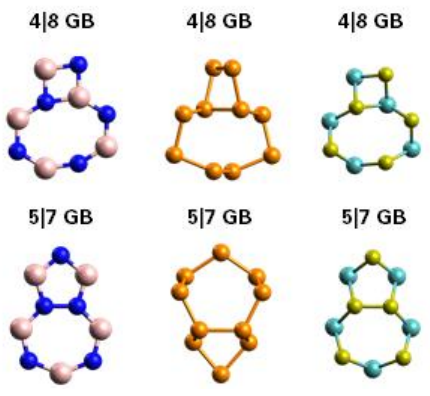

Fig1.- Schematic representations of the grain boundaries (GBs) studied in the present work.

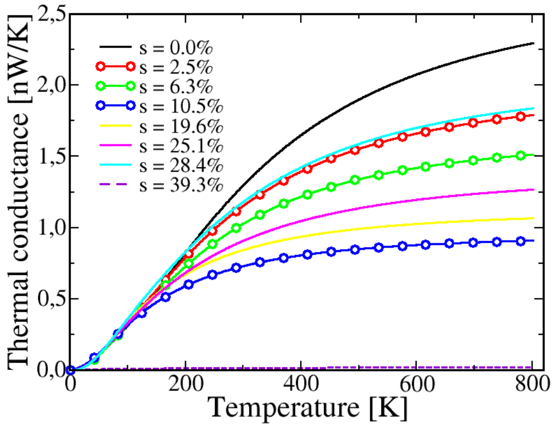

Fig2.- Strain dependence of the thermal conductance for hexagonal boron-nitride 4|8 GB.