The interplay between strain and size effects on the thermal conductance of grain boundaries in graphene

Tang, Shengjie; Kulkarni, Yashashree, University of Houston, United States

ABSTRACT

Graphene possesses exceptional electronic, optical, thermal, and mechanical properties which make it an outstanding material for next-generation energy, electronics, and thermal management applications. Although there is a strong drive towards fabricating supersized single-crystal domains, recent advances in large-scale production of monolayer graphene sheets via chemical vapor deposition typically result in polycrystalline graphene whose properties can be drastically affected by the presence of grain boundaries. In this discussion, we present a study of the effect of strain on the thermal transport across grain boundaries in graphene using molecular dynamics simulations. The thermal boundary conductance is found to decrease significantly under biaxial tension as expected. In contrast, under biaxial compression, the thermal boundary conductance is strongly affected by the dimensions of the graphene monolayer, increasing with strain for specimen with length-to-width ratio of <20 and being insensitive to strain for length-to-width ratio >20 . This rather unexpected size-dependence under biaxial compression is found to be a result of geometric instabilities.