Multiscale modeling of heat transfer in graphene/h-BN polycrystalline heterostructures

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Abstract

Graphene and atomic layers of hexagonal boron-nitride (h-BN) are revolutionary materials with closest possible atomic structures. Recent experimental study [1] confirms the possibility of fabrication of graphene/h-BN heterostructures using the chemical vapor deposition technique. In this investigation, We proposed a combined atomistic-continuum multiscale modeling to assess the effective thermal conductivity of graphene/h-BN polycrystalline heterostructures. In this approach, non-equilibrium molecular dynamics method is utilized to obtain contact conductance of several grain boundaries with various defects concentrations. In these modeling, we evaluated grain boundary conductance along graphene/graphene, h-BN/h-BN and graphene/h-BN interfaces. In addition, we also obtain the thermal conductivity of pristine graphene and h-BN using the molecular dynamics simulations. In order to explore the effective thermal conductivity of samples at macroscopic level, we constructed relatively large continuum models of polycrystalline heterostructures using the finite element approach. In this regard, obtained properties by molecular dynamics method were used to introduce grains thermal conductivity and grain boundaries contact conductance as well. Comparison with fully atomistic models confirms the applicability and accuracy of the proposed modeling methodology, not only for the evaluation of effective conductivity of macroscopic samples but also for studying the systems at atomic level. Nevertheless, accuracy of the developed multiscale modeling can be yet further improved by considering a more comprehensive sets of grain boundaries in the atomistic modeling step. In our finite element modeling we used Voronoi algorithm to construct polycrystalline sample with random grain configurations. Accordingly, more accurate modeling can be achieved by reconstruction of real microstructures of polycrystalline heterostructures. In response to the remarkably fast growth and interests in the field of 2D materials, the proposed simplified multiscale approach can be considered to efficiently explore the effective thermal conductivity of various 2D structures with complex atomic structures and grain boundaries such as MoS_2 and WS_2.

References

[1] L. Liu, J. Park, D. A. Siegel, K. F. McCarty, K. W. Clark, W. Deng, et al., Science 2014, 343: 163–167.