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WCPM/CSC joint seminar

Interfacial barriers to thermal transport in carbon nanomaterials and polymer-nanotube composites: a molecular modelling study

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Monday, 16th January, 1 p.m.
D202 Seminar room, School of Engineering, 2nd Floor

Abstract: We present numerical simulations of the thermal boundary (or Kapitza) resistance of single wall carbon nanotubes (CNTs) embedded in a polyethylene (PE) matrix, and between graphene sheets in graphite bound by both a standard empirical pair potential (Lennard-Jones) and a registry-dependent many-body potential of the Kolmogorov-Crespi type. The thermal boundary resistance (TBR) in the CNT-PE system is calculated via a lumped heat capacity method using the temperature difference between the CNT and PE matrix obtained from non-equilibrium molecular dynamics simulations. The effects on phonon transport of both the structure of the PE matrix (amorphous or crystalline) and the degree of covalent crosslinking between PE and CNT are investigated. The results show that the boundary conductance is small (~ 12 MW m−2 K−1) for non-crosslinked matrices, and increases linearly for low degrees of crosslinking. For fully amorphous polymer matrices, crosslink densities of between 5-10% are required to achieve optimal interfacial heat transfer. However, the presence of a crystalline layer of polymer at the interface has a significant influence on TBR, and the implications for this these for the production of CNT-polymer composites with more efficient heat transfer at the interfaces are discussed. A similar method is used to study the effects of registry-dependence of inter-layer potential on thermal transport in graphite perpendicular to the basal planes.

A buffet lunch is available from 12:45 pm.

More info: http://warwick.ac.uk/wcpm/seminars

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