NANOSCALE INTERFACIAL MATERIALS FOR THERMAL TRANSPORT APPLICATIONS

by

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ABSTRACT

Using a variety of modeling techniques, including molecular dynamics (MD) simulations, phonon wave-packet dynamics, and continuum equation based analysis, we explore concepts allowing us to tailor thermal transport properties of interfacial and nanoscale materials.

In the first part of the work we expose phonon interference effects in thermal transports across a self-assembled monolayer (SAM) of alkanethiol molecules covalently bonded to (111) gold substrate and physically bonded to silicon. In particular, we show that the thermal conductance of SAM-Au interface depends on the bonding strength at the SAM-Si interface and that the phonon transmission coefficients show strong and oscillatory dependence on frequency, with oscillatory features diminishing with increasing SAM thickness. The generality of this behavior is analyzed within an analytical solution of a phonon transmission across a simple model of a point junction between one-dimensional chains obtained via the scattering boundary method.

In the second part of the work, using molecular dynamics simulations and model graphene layers in an organic matrix we demonstrate that interfacial thermal resistance determined via "*thermal relaxation method*" is up to an order of magnitude larger than that determined from "*direct simulation method*" of heat transfer across the matrix-graphene-matrix interface. We provide an explanation of this difference based on the spectral analysis of the frequency dependent vibrational temperature. The importance of our finding lies in the fact that the *relaxation method* mimics experimental laser based pump-probe measurements of the interfacial thermal resistance, while the *direct simulation method* provides information relevant to predicting and understanding thermal conductivity of nanocomposites.

Finally, in the third part of the work we demonstrate that despite relatively high interfacial thermal resistance between the filler and the matrix the thermal conductivity enhancement of the nanocomposite can be very significant. Our results suggest that agglomeration and low aspect ratio of the conductive nanofiller additive are primarily responsible for the limited conductivity enhancement reported to date. Mapping of the simulation results on the homogenization model accounting for interfacial resistance

allows us to predict the full potential of the nanocarbon filler addition for thermal conductivity enhancement.