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SESSION 1: MODELS AND METHODS, SALON A

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Multiscale modeling of thermal properties for graphene–polymer nanocomposites

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ABSTRACT

In this study, we developed a multiscale method combining molecular dynamics (MD) and finite element (FE) for the investigation of the thermal properties for graphene–polymer nanocomposites. We used NEMD simulation for the investigation of thermal contact resistance (Kapitza resistance). The influences of sample size, layer number, and polymer density on the interfacial thermal transport are studied. The simulation results show that the interfacial thermal resistance is insensitive to the sample size as well as the layer number, while it can be reduced by increasing the polymer density. Using MD, we also performed spectral analysis to explore the mechanism of thermal transport. Using the results obtained by the MD, we developed the three-phase graphene–polymer RVE model including the interface thermal resistance. The effective thermal conductivity in different filler concentrations, orientations was calculated. Compared with experiment results in the literature, the proposed approach is more accurate than the traditional two-phase model.

KEYWORDS: multiscale method, molecular dynamics, finite element, Kapitza resistance, nanocomposite