PIMS / AMI Seminar

Friday, April 5, 2013
3:00 p.m.
CAB 657

"A Molecular Dynamics-Continuum Coupled Model for Heat Transfer in Composite Materials"

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Abstract

The heat transfer problem in composite materials has been investigated which contains the nano-scale interface. A molecular dynamics-continuum coupled model is developed to study the heat transport from the macro- to the micro-scales. The model includes four major parts: (1) A reverse non-equilibrium molecular dynamics (RNEMD) is used to calculate the physical parameters such as the thermal conductivities on the interface. (2) The homogenization method is applied to compute the homogenized thermal conductivities of composite materials. (3) The temperature field in the global structure of the composite materials is determined with the multiscale asymptotic method for the macroscopic heat transfer equation. (4) A molecular dynamics-continuum coupled model has been developed to reevaluate the temperature field of composite materials, in particular, the local temperature field near the interface.

Numerical results in one-, two- and three-dimensional structures of the composite materials including the nano-scale interface are presented. The computational results of the proposed coupled algorithm are in good agreement with the full MD simulation, demonstrating the accuracy of the present method and its potential applications in the thermal engineering of composite materials.

Refreshments will be served in CAB 649 at 2:30 p.m.