Proceedings of CHT-15
ICHMT International Symposium on Advances in Computational Heat Transfer

May 25-29, 2015, Rutgers University, Piscataway, USA

CHT-15-210

PHONON EIGENSPECTRUM-BASED FORMULATION OF THE ATOMISTIC GREEN'S FUNCTION METHOD

Sridhar Sadasivam[*, §], Umesh V. Waghmare[**] and Timothy S. Fisher[*]
*Department of Mechanical Engineering and Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47906
**Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore 560064
[§]Corresponding author. Email: ssadasi@purdue.edu

ABSTRACT The atomistic Green's function (AGF) method has been widely used to study phonon transport across a wide variety of materials such as Si-Ge interfaces, graphene-graphene nanoribbon interfaces and carbon nanotubes with substitutional impurities. However, most prior studies have focused on obtaining the total phonon transmission function, and predictions of polarization-resolved phonon transmission are scarce. Such polarization-specific phonon transmission functions are expected to aid the interpretation of advanced experiments that can probe phonons of a specific polarization. In this work, we report an eigenspectrum formulation to determine the surface Green's functions in the AGF method. The eigenspectrum formulation leads naturally to the definition of polarization-specific surface Green's functions that are used to obtain polarization-specific phonon transmission functions. We discuss some aspects of numerical implementation of the technique and also demonstrate it by studying phonon transport across a Ge thin film sandwiched between bulk Si contacts and on a C^{12} graphene sheet doped with C^{14} atoms. We also compare the eigenspectrum method with a prior technique to compute polarization-specific transmission functions developed by Huang et al. [2011] and highlight the advantages of the proposed technique.

REFERENCES

Huang, Z., Murthy, J. Y. & Fisher, T. S. [2011], Modeling of polarization-specific phonon transmission through interfaces, Journal of Heat Transfer, Vol. 133, No. 11, p 114502.