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

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

CHT-15-150

VIBRATIONAL MODE PROPERTIES IN DISORDERED SOLIDS

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ABSTRACT Due to a lack of short- and long-range order, the vibrational modes in a disordered solid (e.g., alloys, amorphous materials) are not phonons. In this talk, I will discuss how to predict the properties of such vibrational modes, which may be propagating, diffusive, or localized. Both molecular dynamics simulations and lattice dynamics calculations are required. Two case studies will then be presented. First, to assess the virtual crystal approximation, a soft alloy described by a Lennard-Jones potential and a stiff alloy described by the Stillinger-Weber potential are studied. Second, the thermal conductivity accumulation functions for amorphous silica and amorphous silicon are predicted and compared to experimental measurements.