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Phonon Thermal Conductivity of Si/Ge Nanostructures SHANG-FEN REN, Illinois State University , WEI CHENG, Beijing Normal University — Phonon thermal conductivities of various Si/Ge nanostructures (NSs), including nanocrystals, nanowires, nanovacancies, and Si/Ge nanocomposites, are investigated with three different models: macroscopic approximation, semi-microscopic model that calculates the heat capacity of NCs with a microscopic Valance-Force-Field Model (VFFM), and a full microscopic description of phonon thermal conduction that calculate both heat capacity and phonon group velocity by the VFFM. The results are compared, and the advantages and limitations of each of the models are discussed. It is shown that with full microscopic description, phonon thermal conductivity in Si/Ge nanostructures might be quite different from those obtained with the macroscopic description, mainly depending on the roughness of the interfaces and the size of the nanostructures. This further indicates that it is critically important to investigate phonon thermal conductivities in nanostructures with microscopic models when the roughness is important to consider and the size of the nanostructures is small.

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