

Abstract Submitted
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Thermal conductivity of Si nanocrystals¹ SHANG-FEN REN, Illinois State University, WEI CHENG, Beijing Normal University — Thermal conductivities of spherical Si nanocrystals (NCs) are investigated with three different models: a macroscopic approximation, a 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 these models are discussed. It is shown that for spherical Si NCs, the macroscopic approximation is quite good for NCs with a diameter larger than 1.33 nm. For smaller NCs, the VFFM predicts that the thermal conductivity increases quickly when the size decreases, opposite to the macroscopic approximation, and VFFM also predicts that the minimum of thermal conductivity for spherical Si NCs occurs at a diameter of 1.33 nm, the limit at which the macroscopic approximation applies.

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