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Thermal Transport in Kinked Nanowires

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Thermal transport in low-dimensional systems such as nanowires is interesting for applications involving system design at the nanoscale, but the effects of changes like the shape of a nanowire are not completely understood. In this work the behaviour of the thermal conductance of nanowires is investigated by introducing a single kink into an otherwise straight nanowire. The angle of this kink is varied to examine its effects on thermal transport. Kinked systems are constructed and simulated using Molecular Dynamics simulations, phonon Monte Carlo simulations and classical solutions of the heat equation. The effects of lattice orientation within the kink are found to be significant, but an examination of the heat flux field reveals additional complexities. Details of transport modeling, ratio of mean free path to characteristic system size, phonon reflections and system specularity yield differences in thermal behaviour throughout the systems. Comparing the heat flux between phonon Monte Carlo and classical solutions of the heat equation finds that the heat flux in systems where the mean free path of phonons is large compared to the system dimensions (such as those in the Monte Carlo simulation) may have heat flow concentrated in a channel smaller than the dimensions of the system.

Keyword-1

nanowires

Keyword-2

thermal transport

Keyword-3

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