Monte Carlo Simulations of Phonon Transport in Silicon

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Thermal management is one of the main obstacles in the continued reduction of feature sizes in silicon microelectronics. A 'Moore's Law' for heat generation per chip shows that power levels have been rising exponentially to their present ~100 W values, with extrapolation of this trend predicting catastrophically high dissipated powers within the next few years. New technologies, such as silicon germanium and silicon-on-insulator, which are being pursued to obtain improvements in electronic performance, are likely to have a detrimental effect on thermal management, introducing lower thermal conductivities and additional thermal interfaces into the layer structure of individual devices. In this context, detailed modelling of the thermal and electrothermal properties of nanoscale semiconductor structures is required. As the system dimensions are reduced, conventional thermal models, based on diffusive continuum heat flow, become inaccurate, and the microscopic nature of heat generation and heat conduction must be considered. Very little work has been carried out in this area, and many problems remain to be addressed.

In this paper, we describe the development of a computational procedure to simulate thermal transport in small semiconductor structures. On a microscopic scale, heat transport can be described mathematically using a Boltzmann equation for phonons. Direct numerical solution of this equation is difficult, without extensive approximation, because of the quantity and complexity of the anharmonic phonon-phonon interactions. Therefore, we have developed a Monte Carlo simulation approach, analogous to that used for electron transport modelling, which models phonon trajectories and phonon scattering events. The simulation domain is subdivided into cells, and a discretized phonon distribution is monitored in every cell. Anharmonic three-phonon processes (of both 'absorption' and 'emission' type) are simulated for acoustic phonon modes in silicon. For phonon-phonon absorption, a 'partner' phonon must be selected from within the same real space cell to participate in the interaction, in a similar manner to the algorithms used in Monte Carlo simulations of electron-electron scattering. An important difference between electron and phonon transport simulations is the necessity, in the latter case, of simulating Umklapp processes, since these are essential in defining the thermal conductivity. Whereas in previous derivations of analytical approximations for phonon lifetimes and thermal conductivities, it has been very difficult to determine the relative contribution of Normal and Umklapp processes in phonon-phonon interactions, in principle, this information can be extracted directly from a Monte Carlo simulation.

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