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Particle-Based Simulations of Phonon Transport in Silicon

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INTRODUCTION

Thermal management is one of the main issues which must be overcome in order to maintain the continued reduction of feature sizes in silicon microelectronics. Developments in size and structure of silicon devices has led to ever increasing power levels(currently $\approx$100W per chip), the power dissipation is predicted to rise exponentially and will reach catastrophic levels in the near future. New materials and device architectures, such as silicon-on-insulator and strain silicon/silicon-germanium devices being used to archive better performance have had a detrimental effect on thermal management due to higher thermal resistances and additional thermal interfaces. As a result thermal modelling is becoming increasingly important for understanding device properties. Current thermal models, based on diffusive continuum flow, are inaccurate at the nanoscale and a model which considers the microscopic nature of heat generation and heat tansport must be used.

RESEARCH

In this paper we describe the development of thermal transport model for small semiconductor structures. On the microscale, heat transport can be described by the Boltzmann transport equation for phonons. The complexity and quantity of the phonon anharmonic interactions make a direct numerical solution difficult without numerous approximations. We have developed a Monte Carlo simulation approach to this problem, modeling phonon trajectories and three phonon scattering events.

The simulation domain is subdived into cells and a discretized phonon distribution is monitored in every cell. The relaxation time for each phonon is calculated using third order elastic constants [1] [2] and used to simulate the anharmonic three-phonon processes (both 'absorption' and 'emission' type)for acoustic phonon modes in silicon. Phonon-phonon absorption events are performed by selecting a 'partner' phonon from within the same real space cell that satisfies momentum and energy conservation, similarly to the algorithms used for electron-electron scattering. The difference between phonon and electron transport is the necessity, in the latter case, of simulating the 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 difficult to determine the relative contribution of Normal and Umklapp processes in phonon-phonon interactions, in principle, this information can be extracted directly from the Monte Carlo simulation.

REFERENCES

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