

Nanoscale Heat Generation in Silicon via the Monte Carlo Method

Eric Pop, Sanjiv Sinha, Robert Dutton, Kenneth Goodson
Contact: epop@stanford.edu, Stanford University, CA 94305

Modeling heat generation at nanoscales in silicon is of great interest and particularly relevant to the heating and reliability of nanoscale transistors [1]. While the phonon Boltzmann Transport Equation has been used at such scales, its electronic Joule heating term, typically modeled as the dot product of the macroscopic electric field and current density [2], cannot account for the microscopic non-locality of heat generation near a strongly peaked electric field region. It also does not account for branch- and polarization-specific phonon heating.

This work develops a Monte Carlo (MC) simulation method for calculating the Joule heating term in silicon nanostructures. Electrons accelerated by the electric field scatter primarily with optical phonons, yet heat transport out of the region of most intense scattering occurs via acoustic phonons. The MC model makes use of electron energy bands in the non-parabolic approximation and incorporates the appropriate scattering rates of electrons with each phonon branch [3]. Care is taken to implement inelastic (i.e. energy-dissipating) scattering models both with the acoustic and optical phonons. This accounts for the correct non-equilibrium energy exchange between electrons and both phonon branches. Use of the MC method with an electron energy-dependent scattering rate intrinsically accounts for the non-locality of the heat transfer near a strongly peaked electric field. No assumptions have to be made about the shape of the electron distribution, hence semiconductor regions where “hot” and “cool” carriers mix are properly modeled.

The simulator builds histograms of the phonons emitted and absorbed. The majority of the heat resulting from electric current flow in silicon generates optical phonons. Fig. 1 demonstrates this for the simple case of a one-dimensional resistor under constant electric field. Optical phonons dominate electron energy relaxation by about an order of magnitude compared to acoustic phonons for most practical electric fields. However, heat transport in silicon occurs primarily through the faster acoustic modes. Optical phonons decay into acoustic modes on time scales on the order of picoseconds. Under high current levels and strongly peaked fields the optical phonon density can significantly build up and localize, and would consequently affect electron transport.

A histogram of heat generated along the channel of a proposed future generation dual-gate transistor [4] is shown in Fig. 2. The macroscopic $\mathbf{J} \cdot \mathbf{E}$ heat generation model is compared to the heat generation profile extracted by collecting all phonon emission and absorption events from the MC run. Electrons gain most of their energy while traveling through the narrow field region near the drain. On average, they travel another electron-phonon scattering length (several nanometers) before they begin releasing their energy to the lattice. This results in the MC heat generation profile peaking deeper inside the drain. Negative heat generation regions correspond to net energy absorption from the lattice: electrons in the source absorb more phonons than they emit to surmount the barrier of injection at the beginning of the channel.

The MC approach to computing heat generation rates gives direct information on the magnitude and types of phonons that are generated through electronic Joule heating in silicon. The MC method also provides more accurate spatial information about the localization of the heat source,

particularly at length scales on the order of the electron and phonon mean free path. This method has applications in any region of high spatial or temporal non-equilibrium between electrons and phonons and particularly facilitates careful microscopic analysis of heating in the drain of a silicon transistor. The generated phonon distributions may be used as an input to a phonon MC simulator.

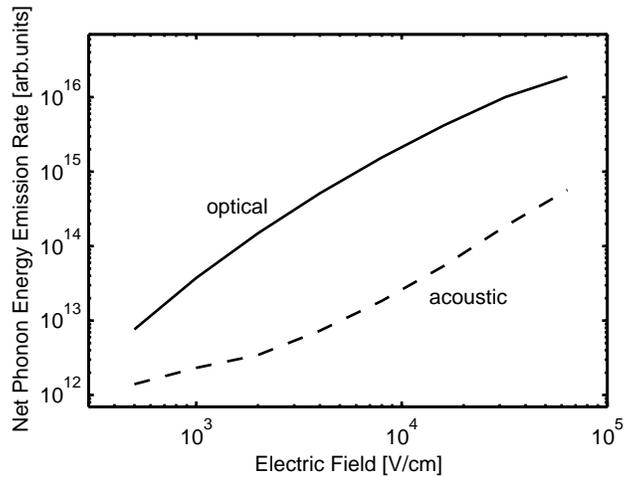


Figure 1: Computed net (emission minus absorption) phonon energy emission rates for optical and acoustic phonons at most practical steady-state electric fields in silicon.

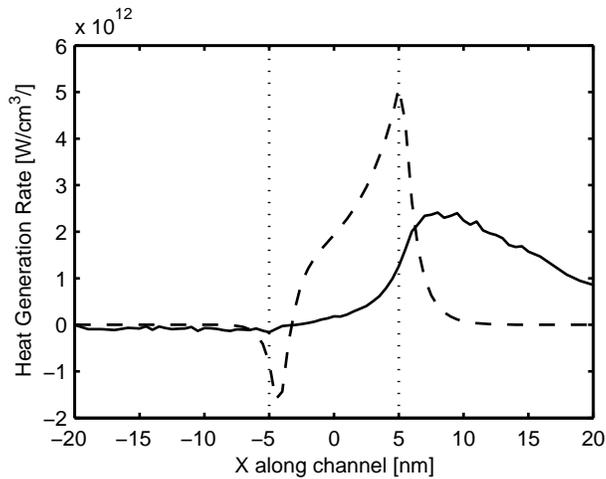


Figure 2: Heat generation profile along the channel of a future 10 nm transistor. The dashed line is the heating rate obtained from the conventional $\mathbf{J} \cdot \mathbf{E}$ model, the solid line is the heating rate profile obtained with the MC method (optical plus acoustic phonons). The source and drain are to the left and right, respectively, of the vertical dotted lines.

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- [4] M. Lundstrom et al, *IEEE Transactions on Electron Devices*, v. 49, p. 133, Jan. 2002