Monte Carlo modeling of phonon transport in nanodevices

D Lacroix\textsuperscript{1}, K Joulain\textsuperscript{2}, D Terris\textsuperscript{2} and D Lemonnier\textsuperscript{2}
\textsuperscript{1} LEMTA - CNRS UMR 7563 - Nancy Université, 54506 Vandœuvre cedex, France
\textsuperscript{2} LET - CNRS UMR 6608 - ENSMA - 1, Av. C. Ader, 86960 Chasseneuil cedex, France
E-mail: David.Lacroix@lemta.uhp-nancy.fr, Karl.Joulain@ensma.fr

Abstract. Heat transport in nanostructured semiconductor devices has been investigated. Numerical simulations of acoustic phonon propagation through a dedicated Monte Carlo model in nanodevices have been performed. Material dispersion curves are taken into account and the Boltzmann collisional term is considered under the relaxation time approximation. The method allows the calculation of temperature fields at small time and space scales. Furthermore, confining effects on thermal conductivity due to boundary scattering in nanowires and nanofilms are displayed for several thicknesses and temperatures.

1. Introduction
Heat transport characterization in nanostructures encounters an increasing attention since many new “nanotechnologies” involved in electronic equipments, optical sensors or biotechnological devices have been developed \cite{1}. In the case of semiconductors, heat propagation can be described, at very small scale, as phonon motion and interactions in the material. Hence, the Boltzmann Transport Equation (BTE) can be solved in order to find the energy distribution and therefore the temperature. Among the several existing techniques aimed at handling the BTE, the deterministic ones are based upon photon transport analogy. Thus, the so-called phonon radiative transfer equation (PRTE) discussed by Majumdar \cite{2} uses techniques developed for radiative heat transfer such as the discrete ordinates method. On the other hand, statistical handling of the BTE, also known as Monte Carlo methods \cite{3, 4}, provides efficient tools to model phonon propagation. The numerical approach which has been developed here follows the latest method, as it will be discussed hereafter.

In the present paper, test cases have been achieved on bulk silicon and germanium in order to assess the model. In both cases Fourier and ballistic temperature regimes have been observed at steady state, in accordance with the considered temperature levels within the materials. Besides, thermal conductivity of silicon has been numerically computed and compared with the experimental data in the bulk case. Furthermore, the Monte Carlo technique has been also used in order to estimate thermal properties of silicon nanowires \cite{5} and nanofilms. Once again comparisons have been carried out with available experiments \cite{6}.

2. Monte Carlo method for the BTE
Using statistical means to model phonon transport is quite straightforward. First, it is necessary to achieve three discretizations: a spatial one related to the sample geometry, a temporal one
for transient calculations and a frequential one in order to take into account phonon dispersion
properties and time relaxation parameters. Considering the Bose-Einstein distribution, phonon
number within a cell of volume $V$ is

$$N = V \sum_{p=TA,LA} \sum_{b=1}^{N_b} \left[ \frac{1}{\exp \left( \frac{\hbar \omega_{b,p}}{k_B T} \right) - 1} \right] \frac{K_{b,p}^2}{2\pi^2 v_{g_{b,p}}^2} g_p \Delta \omega$$

with $N_b$ the number of spectral interspaces $\Delta \omega$ in the range $[0, \omega_{LA}^{max}]$, $K_{b,p}$ the wavevector, $g_p$ the polarization number and $v_{g_{b,p}}$ the phonon group velocity at a given frequency $b$ and polarization $p$. Then, a normalized distribution function $F_i(T)$ at temperature $T$ can be set for the $N_b$ bins as

$$F_i(T) = \frac{\sum_{j=1}^{i} N_j(T)}{\sum_{j=1}^{N_b} N_j(T)}$$

With this approach, phonon frequency and polarization are randomly selected. Then, phonon
group velocity and wavevector are derived from dispersion curves. Energy of the considered
cell is obtained by adding all the sampled phonon quanta till the prescribed temperature is
reached. When this initialization stage is completed, during a small time step, phonon quanta
are allowed to travel through the sample (carrying energy in other parts of the medium).
They can also undergo a scattering phenomenon (impurity and/or boundary collisions, Normal
and Umklapp processes). Transient calculations provide the temperature evolution within the
sampled medium.

Furthermore, using adequate geometry, it is possible to compute the heat flux $Q$ in a given
direction $k$ summing on the $N^*$ phonon contributions

$$Q = \sum_{n=1}^{N^*} W \hbar \omega_n v_{g,n} \cdot k$$

Hence, applying the Fourier’s law, the thermal conductivity $k$ at a given mean temperature is
derived. These calculation data are provided in the next section. Results concerning temperature
distribution in both diffusive and ballistic regime can be found in a previous work [4].

3. Thermal conductivity in nanostructures

3.1. Bulk material

First of all, bulk properties have been computed with the Monte Carlo model in order to assess
the model efficiency for thermal conductivity calculations. Results for a 2$\mu$m thick germanium
and silicon samples are in agreement with the experiments for several temperatures between
150K and 500K (figure 1). For these calculations the thermal gradient at the boundaries was
$\Delta T = 20$K. Besides, phonons were assumed to be specularly reflected at the lateral face of the
sample. For temperatures lower than 150K some discrepancies occur due to not sufficiently long
samples as compared to phonon mean free path increase. Moreover, in this first simulations
impurity collision process was not considered in the total scattering relaxation time.

3.2. Nanowires modeling

Recent applications in the frame of microelectronic and thermoelectric cell design try to use phonon
confining in order to reduce the thermal conductivity while preserving the electrical one. Studies on silicon nanowires [7–11] have shown that diameter lowering induces thermal
conductivity decrease. Theoretically, this observation is well described by an important number
of phonon interactions with the medium boundaries. Thus, the phonon mean free path $\ell$
drastically decreases and consequently affects the thermal conductivity $k$ (kinetic theory provides
$k = 1/3C_p v_g \ell$). The Monte Carlo model ability to describe such geometries has been assessed on Li measurements [6]. Four diameters are considered from 22nm to 115nm, in the temperature range $10K \leq T \leq 350K$. The complete description of the simulation process, especially in what concerns boundary scattering, can be found in [5]. For these calculations, phonon reflection is perfectly diffuse and treated during the phonon drift stage, apart from other scattering mechanisms. Monte Carlo simulations are provided on figure 2. Comparisons with Li [6] and Chantrenne [11] results are satisfying for the three larger diameters. In the case of very thin nanowires, experimental data give lower conductivities. It might indicate that bulk phonon dispersion curves are no longer valid for this size. In any case, the Monte Carlo method, at this scale, should be replaced by more efficient techniques like the molecular dynamics.

Figure 1. Silicon and germanium thermal conductivities; comparison between bulk theoretical values and Monte Carlo calculated values.

Figure 2. Nanowire thermal conductivities; comparison between MC simulation (solid lines), experimental data (triangles) of Li et al. [6], and calculations (dashlines-circles) of Chantrenne et al. [11].
3.3. Nanofilms characterization

Current studies are achieved on crossplane thermal conductivity determination for silicon nanofilms. Usually experimental setups allow inplane conductivity measurements for these nanostructures. In the case of very thin layers such devices cannot be used and there is a lack of realistic data in that field that strongly interests semiconductor industry (silicon wafer production). Hence, our model have been adapted to this kind of geometry and some preliminary results about thermal conductivity are presented hereafter (figure 3). Once again, phonon confining induces a thermal conductivity decrease that shall be larger than one order of magnitude. Further comparisons with other techniques on that topic are soon expected in order to confirm these crossplane data.

![Figure 3. Nanofilm crossplane thermal conductivities by MC simulation.](image)

4. Conclusion

A predictive tool dedicated to phonon transport modeling has been described. This Monte Carlo model efficiency has been assessed on several nanostructures in a large temperature range. Consistent results have been found in what concerns phonon confining consequences on heat transport. Besides, the model can be easily used with other semiconductors if dispersion curves and associated relaxation times are known. The adaptation of the method on multilayered nanodevices such as super lattice or nanoporous media are some applications we are looking on.

References

1. Cahill D, Ford W, Goodson K, Mahan G, Majumdar A, Maris H, Merlin R and Phillpot S 2003 J. Appl. Phys. 93 793–818
2. Majumdar A 1993 J. Heat. Transf. 115 7–16
3. Mazumder S and Majumdar A 2001 ASME J. Heat Transfer 123 749–759
4. Lacroix D, Joulain K and Lemonnier D 2005 Phys. Rev. B 72 064305
5. Lacroix D, Joulain K, Terris D and Lemonnier D 2006 Appl. Phys. Lett. 89 103104
6. Li D, Wu Y, Kim P, Yang P and Majumdar A 2003 Appl. Phys. Lett. 83 2934–2936
7. Volz S and Chen G 1999 Appl. Phys. Lett. 14 2056–2058
8. Khitun A, Balandin A and Wang K 1999 Superlattices and Microstructures 26 181–193
9. Khitun A and Wang K 2001 Appl. Phys. Lett. 79 851–193
10. Mingo N 2003 Phys. Rev. B 68 113308
11. Chantrenne P, Barrat J, Blase X and Gale J 2005 J. Appl. Phys. 97 104318