Transient thermal modeling of a nanoscale hot spot in multilayered film

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A subcontinuum based lattice Boltzmann method is used to accurately model the transient thermal response of a nanoscale hot spot in solids. We developed the numerical scheme for the hot spot in a thin uniform material and extended the approach to study the multilayered materials. We observed that subcontinuum effects of high temperature rise become more prominent as the size of the film reduces to the scale of carrier mean free path. The thermal transport through a double layer is also considered, both for constant temperature difference across the double layer and hot-spot generation in one of the layers, using the diffusive mismatch scattering model at the interface. A finite temperature jump is observed at the interface whose magnitude depends upon the dimensions and properties of the material on the either side of the interface. The insight into the nanoscale thermal modeling, acquired in this work via a relatively simple model, will be critical for the design and operation of complex data storage and electronic systems, dealing with subcontinuum systems.


In state-of-the-art data storage and electronic devices an increased emphasis has been focused on achieving higher operation speed and smaller size, which has forced the characteristic length of the devices to nanometer scale. At these scales the subcontinuum effects of ballistic thermal transport and temperature slip at the boundaries become very prominent and energy management plays a crucial role in the operation and reliability of the system. Continuum based Fourier equation (FE) is inadequate to describe these phenomena and it is desirable to formulate a generic, physics based model to simulate these multilength/time scaled phenomena.

The Boltzmann transport equation (BTE) with the single relaxation time approximation\(^1\) is used to accurately simulate energy transport as long as the particle assumption for the heat carriers is valid; that is, when the time scale is longer than the collision time, characteristic of a scattering event, and the characteristic length is larger than the carrier wavelength. The BTE is, however, difficult to solve and, in general, a large computational effort is involved in the solution of even its most simple geometries. This has led to the development of the lattice Boltzmann method (LBM),\(^2\) which, in essence, discretizes the BTE, maintaining its accuracy while reducing its computational effort. This method has been used in fluid mechanics applications with great success.

In this article, we are utilizing LBM\(^3\) for nanoscale energy transport predictions for hot spots in solids. A uniform thin film is considered to examine the transient thermal profile of a nanoscale hot spot. The size of the hot spot is varied and the deviation of the thermal prediction from the FE is reported. Then the model is extended to a double layer to incorporate and study the effects of an interface. The effect of the film thickness and the material properties on the thermal transport through the interface is observed. This relatively simple system can provide essential physics of the multilayered systems and will provide crucial insight into the design and operation of the complex, state-of-the-art data storage and electronic systems, e.g., heat assisted magnetic recording (HAMR), giant magnetoresistive (GMR) heads, and silicon-on-insulator (SOI) transistors, where thermal effects play a subtle role.

Since LBM is inherently transient, easy to hybridize with other physical models and length scales, and inherently parallel in nature, we have chosen LBM as our simulation tool. LBM is based on BTE with the single relaxation time approximation, which is given by\(^1\)

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = \frac{f^0 - f}{\tau} + g. \tag{1}
\]

Here \(f\), \(\mathbf{v}\), \(\tau\), and \(f^0\) are the carrier distribution function, velocity, relaxation time, and equilibrium distribution function, respectively, and \(g\) is the rate of generation of carriers due to external sources. The \(f^0\) is given by the Bose–Einstein
distribution for phonons and Fermi–Dirac distribution for electrons. This form of the BTE is transformed to an equation on carrier energy density \( e \) as

\[
\frac{\partial e}{\partial t} + v_e \frac{\partial e}{\partial x} = \frac{e^0 - e}{\tau} + Q. \tag{2}
\]

Here \( Q \) is the energy density generation rate due to external sources. The conventional definition of temperature is not valid under nonequilibrium condition; therefore, we must resort to an alternative definition of the equivalent temperature so that the total energy of carriers is equal to the energy of the equilibrium carrier distribution at the equivalent temperature.

LBM is obtained from BTE, the detailed derivation can be found in our previous work. The derived lattice Boltzmann formulation can be written as

\[
e_i(x + \Delta x, t + \Delta t) = (1 - W_i) e_i(x, t) + W_i e_i^0(x, t) + Q\Delta t.
\tag{3}
\]

Here, weighting factor, \( W_i = \Delta t / \tau \), and the term \( e_i(x, t) \) correspond to the discrete carrier energy distribution, which is defined as the population of the carriers associated with a specific direction in the lattice and \( e_i^0(x, t) \) is the equilibrium carrier energy distribution. Notice that the total carrier energy density, \( e(x, t) \), is the sum of discrete carrier energy distributions, \( e_i(x, t) \), over all the lattice directions \( D \)

\[
e(x, t) = \sum_{i=1}^{D} e_i(x, t).
\tag{4}
\]

The equilibrium carrier energy distribution can be derived from Eq. (4) by taking the isotropic distribution assumption

\[
e_i^0(x, t) = \frac{e(x, t)}{D}.
\tag{5}
\]

Equations (3) and (4) are solved at all lattice sites to obtain carrier energy density distribution, which can be converted into the equivalent temperature. These equations are solved for the energy carriers using their respective velocities and \( \tau \) on their respective grids.

Extension of the model to the double layer is essentially a multigrid problem and additional physics is required to treat the interface accurately. Since the velocities of the carriers are different on either side of the interface and we are using the same time step, there is a mismatch of the lattice sites at the interface. Since, generally there is a considerable difference in the thermal properties of the adjacent film and the interface also introduce nonuniformities in the structure, all the carriers become diffusively scattered at the interface. This leads us to use the diffusive mismatch model for the carrier scattering at the interface. The idea of ghost lattice sites at the interface is utilized to incorporate this model. Using the diffusive mismatch model, the transmission probability \( \alpha_i \) \((i = 1, 2)\) of phonons from side \( i \) is calculated as:

\[
\alpha_i = \frac{c_i^{-2}}{\sum_i c_i^{-2}}.
\tag{6}
\]

Here \( c_i \) is the phonon group velocity on the side \( i \) of the interface.

To study the effect of hot-spot size on the thermal transport, phonon LBM is solved for the case of a hot-spot generation in a thin silicon film. The mean free path, relaxation time, and group velocity of the phonons, in silicon, used in our simulation are 41.79 nm, 6.53 ps, and 6,400 m/s, respectively. The results are presented in the Fig. 1, where %deviation from FE is given by

\[
%\text{deviation} = \frac{|\Delta T_{\text{LBM}} - \Delta T_{\text{FE}}|}{\Delta T_{\text{FE}}}
\tag{7}
\]

Here, \( \Delta T_{\text{LBM}} \) and \( \Delta T_{\text{FE}} \) are the peak temperature rise at the center of the hot spot as predicted by the LBM and FE, respectively. We observed that, when the hot-spot diameter is large as compared to the phonon mean free path both LBM and FE give similar predictions but as the hot-spot diameter becomes equal to or smaller than the phonon mean free path, only the LBM is able to capture the subcontinuum effect of higher temperature rise where as the FE fails to do so. Therefore, our current formulation will give useful guidelines for the HAMR design. These results show a close similarity with the results presented by Sverdup et al. where the ratio of subcontinuum to Fourier temperature rise is presented.

Accurate modeling of thermal transport through the interface is very critical to the state-of-the-art data storage devices, such as HAMR and GMR heads, as they are composed of nanometer scale thin multilayered films. Therefore, we extended our model to incorporate an interface in the domain which separates two regions with different thermal properties. A representative oxide layer with a lower mean free path and group velocity (27.86 nm and 4,270 m/s, respectively) with similar relaxation time of 6.53 ps is attached to the silicon layer with the mean free path, relaxation time, and group velocity of 41.79 nm, 6.53 ps, and 6,400 m/s, respectively. We incorporated a diffusive mismatch model for the carrier scattering at the interface and observed the thermal transport through the interface by applying the temperature...
difference between the two ends of the double layered film. The left half of the domain is taken as silicon and the right half is the oxide layer. Figure 2 presents the steady state temperature, $\theta$, for the case where the height of the double layer is kept at 800 nm and its thickness, $L$, is decreased from 1600 to 66.7 nm. It can be observed that for the 1600 nm thickness, the oxide layer exhibits a higher temperature drop due to the lower mean free path, which translates into lower thermal conductivity. Also, the subcontinuum effects of temperature slip at the interface and the boundaries are negligible due to the high thickness of the double layer. But as the thickness is reduced to 400 nm and subsequently to 66.7 nm, we observe the introduction of a high temperature slip at the interface and the boundaries which increases as the thickness decreases. The inset in the figure shows the interface temperature slip for the dual layer thickness of 66.7, 200, 400, 800, and 1600 nm. It can be clearly seen that the temperature slip increases drastically as the thickness is reduced. In our previous work, we have captured the subcontinuum effect of temperature slip at the boundaries for a uniform thin film\textsuperscript{10} and developed an expression for it,\textsuperscript{11} which is extended for the interfaces as

$$T_{\text{slip}} = \frac{1}{2} \left( \frac{1 + P_L \Lambda_L}{1 - P_L \Lambda_L} \frac{\partial T}{\partial x}_L + \frac{1 + P_R \Lambda_R}{1 - P_R \Lambda_R} \frac{\partial T}{\partial x}_R \right),$$

where subscript $L$ and $R$ represents the left and right half of the double layer. $P$ and $\Lambda$ are specularity ($=0$ for both right and left boundaries in our simulation) and mean free path of the carriers and $\partial T/\partial x$ is the temperature gradient at the interface. This expression predicts the temperature slip at the interface to within 10% of the simulation results. Similar results are also applicable to the thermal design of GMR heads.

Figure 3 presents the simulation results for the case where a hot spot is introduced in silicon thin film. Figure 3(a) represents the transient temperature profile in a thin uniform silicon layer, 800 nm high and 800 nm thick, at 2.04 ns and Fig. 3(b) represents the temperature profile in the silicon–oxide double layer of the same dimensions and at the same time. It can be clearly observed that the introduction of the interface not only introduces a temperature slip, shown as the broken isothermal contours at the interface, but also causes confinement of heat in the silicon layer, illustrated by compression of contours in silicon near the interface.

These subcontinuum effects of higher temperature rise in hot spot, temperature slip at the interfaces, and boundaries and confinement of heat by the interfaces reiterates the importance of using an accurate thermal model as the film thicknesses are reduced in the state-of-the-art data storage and electronic devices.

A discrete, transient, and subcontinuum model based on LBM is used to capture the thermal behavior of the nanoscale thin double layered solid films. We observed that the continuum based approaches, such as FE, fail to capture the subcontinuum effects, e.g., temperature jumps at the boundaries and the interfaces and confinement of energy in the hot spots. This leads to the development of subcontinuum models, like LBM, which are derived from the physics of the energy carriers and thus accurately capture the thermal behavior of the state-of-the-art devices where the characteristic lengths are already reaching the subcontinuum domain. We presented a test case of hot spot in a silicon thin film and elucidated the subcontinuum effect of energy confinement when the hot-spot diameter becomes on the order of or less than the phonon mean free path. Also, we studied the thermal transport across an interface between two thin films with different thermal properties, both for a uniform temperature difference across the double layer and for a hot spot in the silicon layer. This relatively simple case provides essential physics for the accurate thermal modeling of the complex data storage and electronic systems with multilayered thin films, e.g., HAMR, GMR, and SOI transistors.

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\textsuperscript{8}E. T. Swartz and R. O. Pohl, Rev. Mod. Phys. 61, 605 (1989).

