Non-monotonic heat dissipation phenomenon in close-packed 2D and 3D hotspot system

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Abstract

Transient heat dissipation in close-packed quasi-2D nanoline and 3D nanocuboid hotspot systems is studied based on phonon Boltzmann transport equation. Different from previous intuitive understanding of micro/nano scale heat conduction, it is found that the heat dissipation efficiency is not monotonic when the distance between adjacent nanoscale heat sources decreases. The heat dissipation efficiency reaches the highest value when the distance between adjacent nanoscale heat sources is comparable to the phonon mean free path. It is a competition result of two thermal transport processes: quasiballistic transport when phonons escape from the nanoscale heat source and the scattering among phonons originating from adjacent nanoscale heat source.

Keywords: Micro/nano scale heat conduction, quasiballistic phonon transport, Boltzmann transport equation, hotspot systems

1. Introduction

With the fast development of micro- and nanotechnologies [1, 2, 3] and the drastically reduced size of electronic devices [3, 4], the Moore’s law is reaching its limit. Besides, the increase of power density intensifies hotspot issues and increases the demand for heat dissipations. The heat dissipation problem at micro/nano scale has become one of the key bottlenecks restricting the further development of the microelectronics industry. Hence, it is much important to understand the thermal transport mechanisms in microelectronic devices [5, 3] to realize optimal and effective waste heat removal and improve device performance and reliability.

At micro- and nano- scales, the validity of Fourier law of thermal conduction has been questioned in the past decades and the non-Fourier phonon transport can be mainly summarized as following four categories [1, 2, 6, 7, 4]. The first is the ballistic phonon transport [8], which happens when the systems characteristic length/time is comparable to or much smaller/shorter than the phonon mean free path [9, 10, 11, 12] /relaxation time [13, 14, 15, 16]. The second arises from small-scale heat sources [17, 18, 19, 20, 21, 22, 23]. When a hotspot with small size is added in a bulk material, if the phonon mean free path is comparable to or much larger than the size of hotspot, phonons emitted from the hotspot do not suffer sufficient phonon-phonon scattering near the hotspot region so that quasiballistic phonon transport occurs even if there is no boundary or interface scattering inside the systems [19, 20, 22]. The third is the coherent phonon transport [24, 25, 26], which appears when the systems characteristic length is comparable to the phonon wavelength. The fourth is the hydrodynamic phonon transport, which requires that the momentum-conserved normal scattering is much more sufficient than the boundary scattering and the boundary scattering is much more sufficient than the momentum-destroying resistive scattering [27, 28, 29].

Except above situations, recent studies have revealed the importance of the distance between adjacent nanoscale heat sources on heat dissipations in hotspot systems [30, 31, 32, 33, 34]. In 2014, Zeng et al. [32] studied quasiballistic heat conduction for quasi-2D nanoline heat sources periodically deposited on a substrate.
based on the frequency-independent phonon Boltzmann transport equation (BTE) under the single-mode relaxation time approximation model. Their results suggest that the collective behavior caused by closely packed hotspot could counteract the quasiballistic effects present in an isolated nanoscale hotspot. But the result depends on which temperature signal is used as the fitting data of the diffusion equation. In 2015, Hoogeboom-Pot et al. firstly measured this unexpected phenomenon by advanced dynamic extreme UV (EUV) scatterometry experiments. To reveal a comprehensive microscopic understanding of this unexpected heat dissipations, in 2021, Honarvar et al. performed the steady-state molecular dynamics (MD) simulations on silicon samples featuring close-packed nanoheaters. They made a qualitative comparison between the MD simulations and EUV experiments by controlling for equal ratio between the phonon mean free path and geometry size. By using atomic-level simulations to accurately access the temperature, phonon scattering and transport properties, they explained that the phonons emitted from the nanoscale heat source may scatter with each other in the in-plane direction and promote the cross-plane heat dissipations when the distance between two nanoscale heat source is smaller than the phonon mean free path. This heat dissipation phenomenon was also reported by Minnich’s research groups by phonon BTE and time-domain thermoreflectance experiments. Those results suggest that heat dissipations or cooling in nanoscale hotspot systems including integrated circuits might not be as challenging as previously expected.

However, the fundamental physical mechanisms of this novel phenomenon are still not unified. In addition, it’s worth noting that various macroscopic constitutive relationships between the heat flux and temperature are used to fit the experimental data in different research groups. By artificial fitting, an effective thermal conductivity can be obtained, which varies non-monotonously when the distance between the nanoscale hotspot decreases gradually. Usually, the heat diffusion equation with a constant effective thermal conductivity is widely used during data post-processing, as did by Hoogeboom-Pot et al. and Zeng et al., but this model cannot simultaneously fit both amplitude and phase well. Under the semi-infinite assumption, Hua and Minnich obtained a constitutive relationship between the heat flux and temperature by analytically deriving the phonon BTE under the single-mode relaxation time approximation model, which is valid for all phonon transport regimes. However, this analytical strategy is much challenging for complex geometries and hotspot systems with finite size. Beardo et al. used a macroscopic moment equation with adjustable parameters to fit the experimental data, and both the nonlinear and nonlocal terms of the heat flux are accounted in their model. They uncovered the existence of two time scales: an interface resistance regime that dominates on short time scales and a quasiballistic phonon transport regime that dominates on longer time scales. This moment equation is derived from the phonon BTE under the small-perturbation expansion, so that it might be questionable when the systems size is smaller than the phonon mean free path.

Summing up the above, it seems that how to interpret the raw experimental data in the non-diffusive regime with reasonable constitutive relationships is still an open question. As reported by Zeng et al., using the temperature signals in different positions for data post-processing might get a different result. Hence, it is very necessary to obtain the macroscopic physical fields in the whole domain.

Note that there are only a few detection sites in micro- and nano-scale thermal measurement experiments, which indicates that it is hard to measure the whole temporal and spatial macroscopic physical fields. On the other hand, as we all known, the heat dissipations in practical thermal engineering span multiple scales of time and space, for example from picoseconds to microseconds or from transistors at the nanoscale to the heat dissipation of a supercomputer. Although the MD simulations are accurate, it is still too expensive to simulate the dimensions and scales of actual experimental samples or thermal systems. For example, in Honarvar’s work, the transient EUV experiments is usually at hundreds of nanometers but the steady-state MD simulation is below 100 nanometers.

To the best of our knowledge, the phonon particle transport dominates heat conduction in room temperature silicon over tens of nanometers. Simultaneously considering accuracy and computational efficiency, the phonon BTE simulations are conducted in our work to show the temporal and spatial variations of macroscopic physical fields in the whole three-dimensional finite geometry region. We mainly focus on how long it takes for heat to dissipate completely from the heat source. No artificial fitting or effective thermal conductivity is used to avoid possible controversy caused by data post-processing methods and the raw data calculated by phonon BTE is plotted directly.

The rest of the paper is organized as follows. In Sec. 2 the phonon BTE is introduced. Results and
discussions of quasi-2D nanoline (Fig. 1a) and 3D nanocuboid (Fig. 4a) hotspot systems are shown in Sec. 3 and 4 respectively. Conclusions are made in Sec. 5.

2. Phonon BTE

The phonon BTE under the single-mode relaxation time approximation (SMRTA) \cite{14, 15, 39, 16, 37, 36, 40} is used to describe the transient heat conduction in three-dimensional isotropic materials,

\[
\frac{\partial e}{\partial t} + v_g s \cdot \nabla_x e = \frac{e^{eq} - e}{\tau},
\]

where \(v_g\) is the group velocity and \(e = e(x, \omega, s, t, p)\) is the phonon distribution function of energy density, which depends on spatial position \(x\), unit directional vector \(s\), time \(t\), phonon frequency \(\omega\), and polarization \(p\). \(e^{eq}\) and \(\tau\) are the equilibrium distribution function and the relaxation time, respectively. We assume the temperature \(T\) slightly deviates from the reference temperature \(T_0\), i.e., \(|T - T_0| \ll T_0\), so that the equilibrium distribution function can be linearized as follows:

\[
e^{eq}(T) \approx C \frac{T - T_0}{4\pi},
\]

where \(C = C(\omega, p, T_0)\) is the mode specific heat at \(T_0\). The phonon scattering term satisfies the energy conservation, so that we have the following equations:

\[
0 = \sum_p \int \int \frac{e^{eq}(T_{loc}) - e}{\tau(T_0)} d\Omega d\omega,
\]

where the integral is carried out in the whole solid angle space \(d\Omega\) and frequency space \(d\omega\). \(T_{loc}\) is the local pseudotemperature, which is introduced to ensure the conservation principles of the scattering term and can be calculated by

\[
T_{loc} = T_0 + \left( \sum_p \int \int \frac{e d\Omega}{\tau d\omega} \right) \times \left( \sum_p \int \frac{C}{d\omega} \right)^{-1}.
\]

The local temperature \(T\) and heat flux \(q\) can be calculated as the moments of distribution function:

\[
T = T_0 + \frac{\sum_p \int \int e d\Omega d\omega}{\sum_p \int C d\omega},
\]

\[
qu = \sum_p \int \int v e d\Omega d\omega,
\]

3. Quasi-2D nanoline heat source

3.1. Problem description

The heat dissipations in quasi-2D nanoline hotspot systems are investigated numerically, as shown in Fig. 1a. A heat source is added on the top of a rectangle substrate and its sizes in the \(x\) and \(z\) directions are \(L_h\) and \(h\), respectively. The sizes of the substrate in the \(x\) and \(z\) directions are \(P\) and \(H\), respectively. The bottom of the substrate is the heat sink with environment temperature \(T_0\) and the isothermal boundary condition is used (Eq. (A.2)). The left and right boundaries of the substrate are periodic and the others are diffusely reflecting adiabatic boundaries (Eq. (A.3)). We fix \(h/H = 1/8\), \(L_h/P = 1/4\), and the whole domain is a homogeneous material in order to eliminate the thermal interface resistance between two dissimilar materials \cite{41}.
At initial moment $t = 0$, the temperature of the heat source and the other areas are $T_h$ and $T_0$, respectively, where $T_h > T_0$. When $t > 0$, the heat dissipates from the heat source to the heat sink. The temporal evolutions of the average temperature are studied based on phonon BTE, where

$$T^* = \frac{T - T_0}{T_h - T_0}, \quad (7)$$

and $\overline{T}$ is the average temperature over the whole heat source areas. We mainly focus on how long it takes for heat to dissipate completely from the heat source.

Based on dimensional analysis, the transient heat dissipations in the quasi-2D nanoline hotspot systems are totally determined by these length scales, including the phonon mean free path $\lambda = v_g \tau$, the spatial period $P$, height $H$ and the size of hotspot $L_h$. Equation (1) can be written in the dimensionless form:

$$\frac{\partial e}{\partial t^*} + \mathbf{s} \cdot \nabla_x e = \frac{e^{eq} - e}{\text{Kn}}, \quad (8)$$

where the distribution function is normalized by $e_{\text{ref}} = C \Delta T/(4\pi)$ with $\Delta T = T_h - T_0$ being the temperature difference in the domain, the spatial coordinates normalized by $H$, and time normalized by $t_{\text{ref}} = H/v_g$. The dimensionless Knudsen number is

$$\text{Kn}^{-1} = \frac{H}{\lambda} = \frac{H}{v_g \tau} \quad (9)$$

In order to better pinpoint the relationships among various influencing factors, two dimensionless parameters
are introduced and defined as

\[ P^* = P/H, \quad t^* = v_g t / H. \]  \hspace{1cm} (10)\

3.2. Effects of geometric sizes and phonon scattering

The phonon gray model \cite{37, 32} and the linear phonon dispersion are used. The detailed numerical solutions of BTE are shown in Appendix A. In this simulations, the height \( H \) is fixed.

The thermal effects of the spatial period \( P \) is investigated. As shown in Fig. 1(b) with \( Kn = 0.1 \), it can be observed that the heat dissipation efficiency is not monotonic when \( P^* = P/H \) decreases from 8 to 0.01. When \( P^* = 0.1 \) or 0.4, the heat dissipation speed is the fastest. Note that both \( v_g \) and \( H \) are fixed when the spatial period \( P \) changes, so that the dimensionless time \( t^* \) is equivalent to the actual physical time \( t \).

Next, the thermal effects of \( Kn \) is investigated. A number of simulations are implemented with \( Kn = 0.1, 1.0 \) and 10.0, respectively, as shown in Fig. 1(b,c,d). It can be found that the non-monotonic heat dissipation phenomenon still exists with different Knudsen numbers. The present results clearly contradict previous intuitive understanding of micro/nano scale heat transfer, namely, the more densely packed and smaller the electronics, the more difficult it is to dissipate heat \cite{9, 11}.

3.3. Physical mechanisms

The fundamental physical mechanisms of above unexpected thermal transport phenomena in different regimes are discussed. From Fig. 1a or Fig. 2, it can be found that there are two main thermal transport processes when heat is transferred from the heat source to the heat sink: phonons escape from the heat source to the substrate and phonons transport from the substrate to the heat sink. For the first process, the size of the heat source is the key factor, especially \( L_h/h \). For the second process, namely, phonons with high energy are absorbed by the heat sink, the distance \( P \) between nanoscale heat source and height \( H \) determine the heat dissipation efficiency. In addition, the phonon group velocity and relaxation time influence both two transient processes.

**Figure 2:** Schematic of phonon transport and scattering in close-packed hotspot systems.

**Diffusive.**—When the spatial period is much larger than the phonon mean free path (e.g., \( P^* = 8 \)), \( P \gg \lambda \) and \( L_h \gg \lambda \), the phonon scattering is very sufficient inside both the heat source and substrate areas and phonons undergo a diffusive process. Hence, the Fourier’s law is valid and the temperature decreases exponentially.

**Quasiballistic.**—When the spatial period decreases and becomes comparable to the phonon mean free path, the thermal dissipation mechanisms become much complicated. For the first process, \( L_h/h \) decreases so that it becomes difficult for phonons to escape from the heat source areas. For the second process, if there is only a single nanoscale heat source, when phonons escape from the heat source, there is rare phonon-phonon scattering within the spatial range of a phonon mean free path. The insufficient phonon scattering blocks the efficient energy exchange among phonons and a large thermal resistance appears near the outlet position of the heat source.
When a number of heat sources are periodically deposited on a substrate, it should be noted that the distance between two nanoscale heat source decreases if $P$ decreases. The phonons escaped from one nanoscale heat source may scatter with others escaped from the adjacent heat source, as shown in Fig. 2. In other words, when the distance between two nanoscale heat source decreases, the phonon-phonon scattering is instead facilitated within the spatial range of a phonon mean free path. The heat flux in the $x$ direction is cancelled out by phonons coming from opposite directions. And the heat conduction in the $z$ direction is increased unexpectedly, which is totally different from that of a single nanoscale heat source.

**Ballistic.**—When the spatial period is much smaller than the phonon mean free path (e.g., $P^* = 0.01$), $P \ll \lambda$ and $L_h \ll \lambda$, the ballistic phonon transport dominates heat conduction inside both the heat source and substrate areas. Although the smaller distance between two nanoscale heat source could promote scattering, the ratio $L_h/h$ decreases significantly so that the phonon transport is blocked by the diffusely reflecting boundaries and it is much difficult for most of heat/phonons to escape from the heat source to the substrate areas. In other words, the first process totally dominates phonon transport and limits the heat dissipations.

In a word, the heat dissipation efficiency reaches the highest value when the spatial period is comparable to the phonon mean free path, which is a competition result of above two phonon transport processes: quasiballistic transport when phonons escape from the nanoscale heat source and the scattering among phonons originating from adjacent nanoscale heat source.

### 3.4. Silicon materials

The quasi-2D nanoline hotspot systems (Fig. 1a) with room temperature monocrystalline silicon material is studied, and the input parameters of BTE including phonon dispersion and scattering are the same as those mentioned in Refs. [42]. The average phonon mean free path $\lambda = \left( \sum_p \int C_{v_p}^{2} g d\omega \right) / \left( \sum_p \int C_{v_p} g d\omega \right)$ of room temperature silicon is about 171 nm. The thermal effects of the spatial period $P$ on heat dissipations are investigated, and the height is fixed at $H = 300$ nm. From Fig. 3 it can be found that the heat dissipation efficiency is low when $P = 900$ nm or 10 nm, and the efficiency is almost the same when $200$ nm $\leq P \leq 300$ nm, which is consistent with our above theoretical analysis.

### 4. 3D nanocuboid heat source

Last section has predicted the non-monotonic heat dissipation phenomenon in quasi-2D close-packed nanoline heat source, in order to be closer to the heat dissipations in the practical 3D electronic equipments [3], the 3D close-packed nanocuboid heat source is simulated. As shown in Fig. 4a, a number of nanocuboid heat source are arranged periodically on the top of the substrate. The bottom of the 3D geometry is the
Figure 4: (a) Schematic of the transient heat dissipation in 3D nanocuboid heat source with periodic array arrangement. (b,c,d) Heat dissipation process of the average temperature $T_{\text{av}}$, where $t^* = v_g t / H$, $P^* = P / H$.

heat sink with fixed temperature $T_0$ and the isothermal boundary condition is used (Eq. (A.2)). Its front and left views are both the same as the front view plotted in Fig. 1a. The boundaries of the heat source and the top surface of the substrate are diffusely reflecting adiabatic boundaries (Eq. (A.3)). From the top view, there are two concentric squares with side length $P$ and $L_h$, and the boundaries of the substrate are all periodic. The length of the substrate and nanocuboid in the $z$ direction is $H$ and $h = H / 8$, respectively. The basic settings are similar to those in quasi-2D hotspot systems (Fig. 1a). At initial moment $t = 0$, the temperature of the heat source is $T_h$ and the temperature of the other areas is $T_0$. When $t > 0$, the heat dissipates from the heat source to the heat sink.

The detailed numerical solutions are shown in Appendix A. Due to the large computational amount, less numerical cases are simulated compared to those in quasi-2D hotspot systems, and the frequency-independent BTE is solved. The thermal effects of phonon scattering and spatial period $P$ are investigated. From Fig. 4(b,c,d), it can be found that the heat dissipation phenomena are similar to those in Fig. 1. Namely, there is non-monotonic heat dissipation phenomenon when the distance between two adjacent nanoscale hotspot decreases gradually. The fastest heat dissipation speed appears when the spatial period $P$ is comparable to the phonon mean free path $\lambda$. This results show that the non-monotonic heat dissipation phenomena are general in both close-packed quasi-2D and 3D nanoscale hotspot systems.

5. Conclusion and outlook

In summary, the heat dissipation in close-packed quasi-2D nanoline and 3D nanocuboid hotspot systems is studied based on phonon BTE. Against to previous intuitive understanding of micro/nano scale heat conduction, the present results show that the heat dissipation efficiency is not monotonic when the distance
between adjacent nanoscale heat sources decreases. The heat dissipation efficiency reaches the highest value when the distance is comparable to the phonon mean free path. It is a competition result of two processes: quasiballistic phonon transport when phonons escape from the nanoscale heat source and the scattering among phonons originating from adjacent nanoscale heat source. In the future, the heat dissipation in practical electronic devices or electric vehicles with thermal interface resistance will be studied [11, 5, 3].

Author statement

Chuang Zhang: Conceptualization, Methodology, Writing original draft, Investigation, Funding acquisition. Lei Wu: Conceptualization, Methodology, Supervision, Writing original draft, Investigation, Corresponding author.

Conflict of interest

No conflict of interest declared.

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Appendix A. Numerical method for BTE

The discrete unified gas kinetic scheme invented by Guo [43] is used to solve the phonon BTE numerically. Detailed introductions and numerical validations of this scheme can refer to previous studies [14, 15, 16]. For quasi-2D nanoline hotspot systems, the spatial space is discretized with 90 uniform cells in the z direction and 40–200 uniform cells in the x direction. In silicon materials, the spatial space is discretized with 90 uniform cells in the z direction and 40–120 uniform cells in the x direction. For the 3D nanocuboid hotspot systems, similarly, the spatial space is discretized with 90 uniform cells in the z direction and 80–200 uniform cells in both the x and y directions. The number of discretized cells in the x or y direction depends on the spatial period P. Larger the spatial period P is, more discretized cells are used. In addition, the phonon dispersion and scattering in silicon can refer to previous study [42, 16]. The wave vector is discretized equally and the mid-point rule is used for the numerical integration of the frequency space. Total 40 discretized frequency bands are considered.

For all cases, the solid angle space is always three-dimensional, where \( s = (\cos \theta, \sin \theta \cos \varphi, \sin \theta \sin \varphi) \), \( \theta \in [0, \pi] \) is the polar angle, \( \varphi \in [0, 2\pi] \) is the azimuthal angle. The \( \cos \theta \in [-1, 1] \) is discretized with the \( N_\theta \)-point Gauss-Legendre quadrature, while the azimuthal angular space \( \varphi \in [0, \pi] \) (due to symmetry) is discretized with the \( \frac{N_\varphi}{2} \)-point Gauss-Legendre quadrature. In this study, we set \( N_\theta \times N_\varphi = 40 \times 40 \). The van Leer limiter is used to deal with the spatial gradient of the distribution function and the time step is

\[
\Delta t = CFL \times \frac{\Delta x}{v_{\text{max}}},
\]

where \( \Delta x \) is the minimum discretized cell size, CFL is the Courant–Friedrichs–Lewy number and \( v_{\text{max}} \) is the maximum group velocity. In this simulations, CFL = 0.40. Based on previous experience [14, 15, 16], above discretizations of the five- or six- dimensional phase space are enough to accurately predict the transient heat conduction in all regimes.
The isothermal boundary condition is used for the heat sink, where the incident phonons are all absorbed and the phonons emitted from the boundary are the equilibrium state with the boundary temperature $T_{BC}$.

Its mathematical formula is

$$e(T_{BC}, s, \omega) = C(T_{BC} - T_0), \quad s \cdot n > 0,$$  \hspace{1cm} (A.2)

where $n$ is the normal unit vector of the boundary pointing to the computational domain. The diffusely reflecting adiabatic boundary condition controls the total heat flux across the boundary is zero and phonons with the same frequency reflected from the boundary are equal along each direction. Its mathematical formula is

$$e(s, \omega) = C(T_{DBC} - T_0), \quad s \cdot n > 0,$$  \hspace{1cm} (A.3)

where

$$T_{DBC} = T_0 + \frac{-\sum_p \int \int s' \cdot n < 0 v_g c s' \cdot n d\Omega d\omega}{\sum_p \int \int s \cdot n > 0 v_g C_s \cdot n d\Omega d\omega}.$$  \hspace{1cm} (A.4)

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