

Non-uniform Thermal Conductivity in Nanoscale Multiple Hotspot Systems

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Abstract

Nanoscale hotspot thermal transport is critical for thermal management of electronic devices. Here, the thermal transport in nanoscale multiple hotspots is investigated by solving the phonon Boltzmann transport equation. To address the limitations of the conventional black-box treatment, a formal local thermal conductivity is proposed, which extends the classical framework to nanoscale non-diffusive regimes. The results reveal a highly non-uniform local thermal transport capability with up to a 13-fold variation across the system. A substantial heat flux deflection is also observed, which significantly deviates from the direction predicted by Fourier's law. Furthermore, closely spaced nanoscale hotspots are found to enhance heat flux by up to 40%. This enhancement arises from a mechanism in which diffuse boundary scattering at hotspot spacing regions can enhance rather than impede thermal transport. This work challenges the long-standing uniform black-box treatment of nanoscale thermal transport and offers fundamental insights for the thermal management of high-power-density integrated circuits.

Keywords: Nanoscale thermal transport, Nanoscale hotspots, Phonon transport, Phonon Boltzmann transport equation

1. Introduction

The rising power density of electronic devices intensifies thermal management challenges [1-3], which are further compounded by heat transport at micro-nanoscale hotspots. When the hotspot size falls below the phonon mean free path (MFP), heat transport deviates from classical Fourier's law [4-6], suppressing the effective thermal conductivity to values drastically below the bulk value [7-10]. Existing studies predominantly focus on isolated single hotspots [11-14], implicitly assuming no interactions between them [15]. However, integrated circuits ubiquitously contain high-density periodic nanoscale hotspots with spacing often smaller than the phonon MFP, and the impact of their interactions on thermal transport remains poorly understood [16].

Recent studies have revealed an anomalous heat transport phenomenon in systems with nanoscale multiple hotspots [17-19]. Although nanoscale hotspots are conventionally viewed as impeding heat dissipation [15], extreme ultraviolet (EUV) scatterometry experiments show that nanoscale closely spaced multiple hotspots can instead enhance heat dissipation [20-23]. Based on molecular dynamics (MD) simulations, Honarvar et al. [16] attribute this enhancement to phonon-phonon scattering between the nanoscale hotspots, which preferentially redirects phonons in the cross-plane direction. However, such MD simulations are limited to length scales far below experimental regimes, leaving the enhancement mechanism at broader scales poorly understood. More importantly, existing experimental observations rely on complex pulsed laser heating, transient thermal relaxation, and Fourier-law-based data fitting [21-24], and whether this enhancement represents a universal behavior under steady-state conditions remains unverified.

These open questions highlight a fundamental bottleneck in the characterization of nanoscale thermal transport. At micro- and nanoscales, classical Fourier's law breaks down for non-diffusive

transport [25-27]. The prevailing global effective thermal conductivity is essentially a black-box treatment that averages the thermal transport capability across the entire system [4,28]. Recent experimental advances have further exposed this critical limitation: local thermal transport at interfaces [29], boundaries [30-32], strained regions [33], and hotspot regions [34-37] deviates markedly from the global average. By collapsing all spatial variations into a single average value, the global effective thermal conductivity obscures such spatially non-uniform behaviors, whose quantitative characterization remains an outstanding challenge.

In this study, the thermal transport in systems with nanoscale multiple hotspots is investigated by solving the phonon Boltzmann transport equation (BTE). First, the formal local thermal conductivity is proposed to characterize the spatial distribution of thermal transport capability. Second, the formal local thermal conductivity is calculated and compared across configurations with a nanoscale single hotspot, nanoscale multiple hotspots, and uniform heating conditions. Finally, systems with varying hotspot spacing and substrate thickness are studied, and the mechanism for the enhanced thermal transport capability with reduced hotspot spacing is analyzed.

2. Methods

In this work, the first-principles-based Monte Carlo (MC) method is employed to solve the phonon BTE [38,39]. Silicon is selected as the substrate material due to its prevalence in chips. First, the harmonic and anharmonic interatomic force constants (IFCs) for silicon are derived from first-principles calculations, implemented using VASP [40]. Second, these IFCs are used as input for the ShengBTE package [41] to obtain the spectral phonon properties. Finally, these spectral properties serve as input for solving the phonon BTE using the linearized deviational MC method [42-46].

Nanoscale periodic hotspots are ubiquitous in integrated circuits, and a typical example is the fin

field-effect transistor (FinFET) array, where heat is generated near the drain of each fin and dissipates into the underlying silicon substrate [11,47]. A schematic illustration of a FinFET array and different heating configurations is presented in Fig. 1. In the simulations, the regions on the top surface corresponding to hotspot locations are set as isothermal boundaries at 310 K to represent the steady-state thermal boundary condition at the substrate entrance, where heat generated near the drain enters the underlying substrate. This approximation is widely adopted in nanoscale thermal transport studies [16,17]. The regions between hotspots are set as adiabatic boundaries with fully diffuse reflection; the heat sink regions are set as isothermal boundaries at 300 K, and all other boundaries are treated as periodic boundaries. In all nanoscale periodic hotspot simulations, the hotspot size S and the spacing L between hotspots are kept equal, so that the hotspot regions and the spacing regions each occupy 50% of the top region. Additional simulation details and validation are provided in the Supplemental Material II and III [48-60].

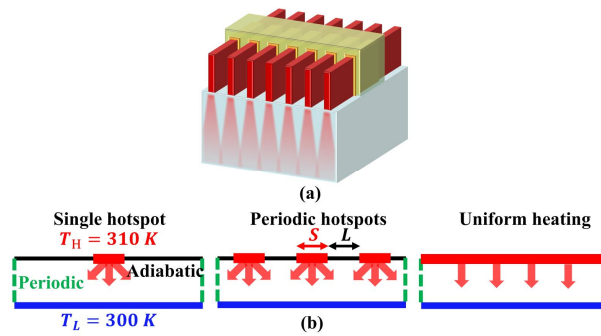


Fig. 1. (a) Schematic illustration of a FinFET array. (b) Schematic diagrams of the single-hotspot, periodic-hotspot, and uniform heating systems. The red regions represent the hotspots of size S , maintained at 310 K as isothermal boundaries. The black regions represent the adiabatic boundaries between hotspots with spacing L . The blue regions represent the heat sinks, set at 300 K as isothermal boundaries. The green dashed lines represent the periodic boundaries.

Given the periodic boundary condition along the z -direction, the system is simplified to a two-

dimensional model. To characterize the spatial distribution of thermal transport capability at the nanoscale, the formal local thermal conductivity is defined by decomposing heat flux along and perpendicular to the temperature gradient. At any position $\mathbf{r} = (x, y)$, the unit vector along the temperature gradient is defined as $\mathbf{e}_T(\mathbf{r}) = \nabla T(\mathbf{r})/|\nabla T(\mathbf{r})|$, and the unit vector along the heat flux direction as $\mathbf{e}_q(\mathbf{r}) = \mathbf{q}(\mathbf{r})/|\mathbf{q}(\mathbf{r})|$. In two dimensions, a local orthogonal coordinate system can be constructed. The direction opposite to the temperature gradient is taken as the first axis, i.e., the Fourier-law expected heat flux direction $\mathbf{e}_\parallel(\mathbf{r}) = -\mathbf{e}_T(\mathbf{r})$. Then, the perpendicular direction is taken as the second axis, obtained via the cross product with the out-of-plane unit normal vector $\mathbf{z}$: $\mathbf{e}_\perp(\mathbf{r}) = \mathbf{z} \times \mathbf{e}_\parallel(\mathbf{r})$.

The heat flux is projected onto these directions, yielding the Fourier-direction component $q_F(\mathbf{r}) = \mathbf{q}(\mathbf{r}) \cdot \mathbf{e}_\parallel(\mathbf{r})$ and the Hall-direction component $q_H(\mathbf{r}) = \mathbf{q}(\mathbf{r}) \cdot \mathbf{e}_\perp(\mathbf{r})$. Corresponding to these two heat flux components, two formal local thermal conductivities are defined:

$$k_F(\mathbf{r}) = q_F(\mathbf{r})/|\nabla T(\mathbf{r})| \quad (1)$$

$$k_H(\mathbf{r}) = q_H(\mathbf{r})/|\nabla T(\mathbf{r})| \quad (2)$$

Here, $k_F(\mathbf{r})$ denotes the formal local thermal conductivity associated with the heat flux component collinear with the temperature gradient, referred to as the Fourier-direction formal local thermal conductivity. Meanwhile, $k_H(\mathbf{r})$ represents the formal local thermal conductivity associated with the heat flux component perpendicular to the temperature gradient, referred to as the Hall-direction formal local thermal conductivity.

The formal local thermal conductivity extends the classical thermal conductivity framework from macroscopic diffusive transport to nanoscale non-diffusive regimes, providing a spatially resolved characterization of local heat transport capability. It is an apparent, formally defined physical quantity

extracted via post-processing, rather than a conventional intrinsic material property under the framework of Fourier’s law. The term “formal” is deliberately adopted to emphasize this distinction: it retains the canonical mathematical form of heat flux divided by temperature gradient, while physically extending the classical thermal conductivity concept to nanoscale non-diffusive regimes. Its value is jointly determined by the intrinsic bulk thermal conductivity of the material and the degree to which each local region deviates from diffusive transport, enabling quantitative, spatially resolved characterization of local thermal transport capability. A comparison of the formal local thermal conductivity with other descriptions is provided in the Supplemental Material I.

3. Results and discussion

The Fourier-direction formal local thermal conductivity k_F distribution for a nanoscale single hotspot is presented in Fig. 2(a). In this case, the region of maximum k_F is located away from the hotspot, with a value reaching 62.2 W/(m·K), which equals k_u , the effective thermal conductivity under uniform heating conditions (a schematic of uniform heating is shown in Fig. 1(b)). Except at the periodic boundaries, the values of k_F near other boundaries are reduced due to boundary thermal resistance, which is consistent with findings reported in previous studies [30,32].

The Hall-direction formal local thermal conductivity k_H distribution for a nanoscale single hotspot is presented in Fig. 2(b). The maximum value of the k_H is only 12.7 W/(m·K), indicating that under the single-hotspot condition, the heat flux and temperature gradient are nearly collinear (as can also be observed from the arrows in Fig. 2(a)), and non-Fourier effects are not prominent.

The k_F distribution for nanoscale periodic hotspots is presented in Fig. 2(c). In this case, the maximum k_F is found in the interstitial regions between hotspots, enhanced to a value of 77.0 W/(m·K). This value is greater than those under both single-hotspot and uniform heating conditions (24% higher).

Furthermore, k_F exhibits a strong spatial non-uniformity, with a more than 13-fold difference between its maximum and minimum values across different regions within the system.

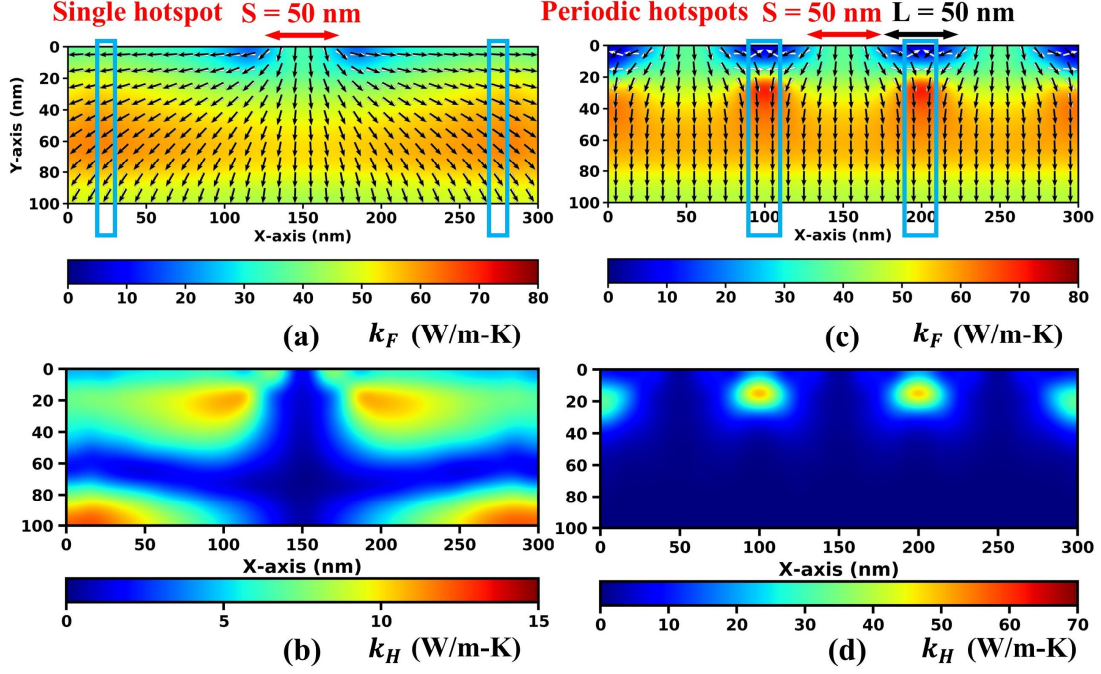


Fig. 2. Distribution of formal local thermal conductivity for a substrate thickness of $D = 100$ nm. (a) k_F and (b) k_H distributions for a nanoscale single hotspot. (c) k_F and (d) k_H distributions for nanoscale periodic hotspots. Black arrows in (a) and (c) indicate the direction of heat flux, while white arrows show the direction opposite to the temperature gradient. The blue box in (a) and (c) marks the region of maximum k_F , which will be analyzed in Fig. 3. For the nanoscale single hotspot system, a total x-direction length of 1200 nm is used to ensure adequate separation from the boundaries; the central 300 nm region is selected for comparison, and the hotspot size is $S = 50$ nm. For the nanoscale periodic hotspot system, both the hotspot size S and the spacing L are 50 nm.

The k_H distribution for nanoscale periodic hotspots is shown in Fig. 2(d). The region of maximum k_H lies directly above the region of maximum k_F . The peak value of k_H reaches 67.0 W/(m·K) which is significantly higher than that observed in single-hotspot. This indicates that the heat flux is strongly

deflected away from the direction predicted by classical Fourier's law. This deflection bears only a phenomenal resemblance to the phonon Hall effect [61-63], with fundamentally distinct physical origins. Unlike the conventional magnetic-field-driven phonon Hall effect, it arises purely from quasi-ballistic transport and is independent of external fields. The underlying mechanism is that phonons near the hotspot regions are dominated by the size and spacing of hotspots rather than by local temperature gradients. Quantitative analysis of the deflection angle and a ballistic phonon model are provided in the Supplemental Material IV.

A key finding of this study is the highly spatially non-uniform thermal transport capability in nanoscale multiple hotspot systems. The widely adopted global effective thermal conductivity, as a black-box averaged metric, inherently obscures such spatial variations by collapsing them into a single average value. As observed in Figs. 2(a) and 2(c), the formal local thermal conductivity cannot be described by a uniform value across the system: it exhibits up to a 13-fold difference between its maximum and minimum local values. This phenomenon, where local thermal transport capability deviates substantially from the global average, has been corroborated by several recent experiments [29,31-34], yet it is consistently overlooked under the oversimplified single-value representation.

For direct comparison, Fig. 3(a) displays the regions of maximum value of k_F for the nanoscale single hotspot, nanoscale periodic hotspot, and uniform heating configurations. It can be observed that the maximum value of k_F in the single hotspot case cannot exceed k_u , whereas in the periodic hotspot case it exceeds k_u by 24%. This enhancement of k_F reveals the presence of non-diffusive thermal transport in periodic hotspot systems.

To further clarify the enhancement of the maximum value of k_F , the heat flux contribution of first-drift phonons is analyzed. First-drift phonons are defined as phonon bundles emitted from hotspots that

have not yet undergone any intrinsic three-phonon scattering or boundary scattering, i.e., they are in their first drift. This descriptive phrase emphasizes that these phonon bundles are in the initial propagation stage from their emission to the first scattering event they experience. For direct comparison with k_F , the Fourier-direction formal local thermal conductivity corresponding to first-drift phonons is calculated by $k_{FS} = q_{FS}/|\nabla T|$, where q_{FS} is the Fourier-direction heat flux contributed by first-drift phonons.

As shown in Fig. 3(b) and (c), nanoscale single- and periodic-hotspot systems exhibit distinct behaviors. Compared with the single hotspot system, the periodic hotspot system shows strong similarity between the trends of its k_{FS}^* and k_F^* curves. Additionally, the contribution of first-drift phonons to the formal local thermal conductivity in the periodic hotspot system is much higher than its counterpart in the single hotspot system. These observations indicate that the enhancement of k_F in periodic hotspot systems is attributed to the increased fraction of first-drift phonons. This occurs because when the hotspot spacing is smaller than the phonon MFP, first-drift phonons emitted from adjacent hotspots can propagate into the central region between hotspots, thereby significantly increasing their fraction in these regions. Conversely, as the hotspot spacing increases (eventually approaching the single-hotspot case when sufficiently large), the fraction of first-drift phonons in the central region between hotspots decreases, since these phonons undergo scattering during propagation. In regions where the fraction of first-drift phonons is higher, the transport behavior is closer to that dominated by ballistic transport. Therefore, this spatial variation of the fraction of first-drift phonons leads to the spatial non-uniformity in thermal transport capability. The increase in the fraction of first-drift phonons can also be intuitively interpreted via the ballistic phonon model detailed in the Supplemental Material IV.

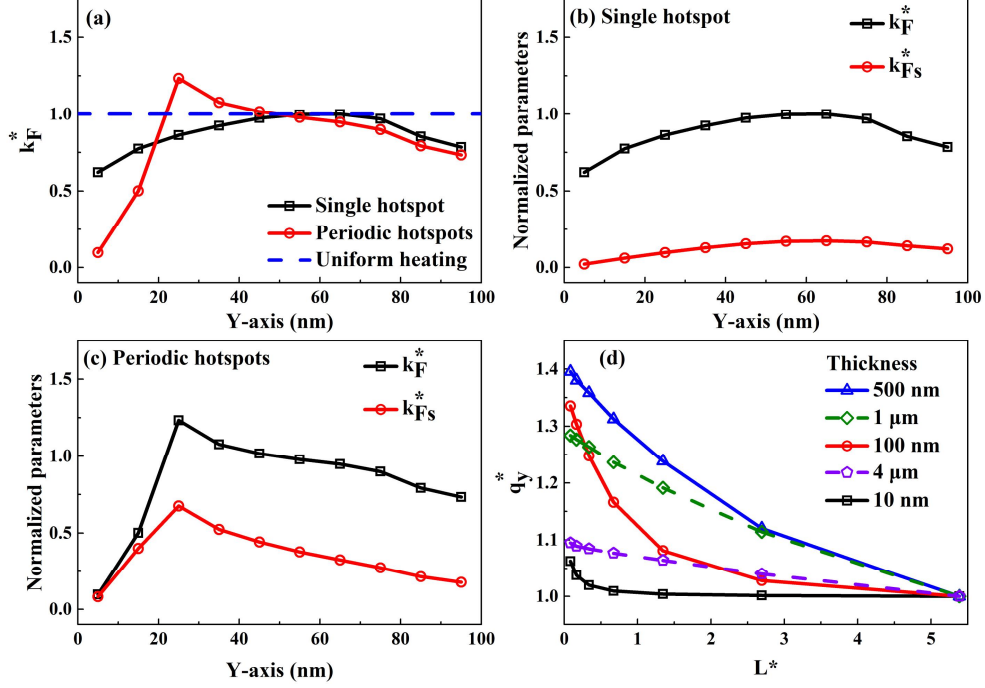


Fig. 3. (a) Normalized k_F^* comparison in the blue-box regions for single-hotspot, periodic-hotspot, and uniform-heating configurations. (b) k_F^* and first-drift phonons contribution k_{FS}^* in the maximum k_F region, corresponding to the blue box in Fig. 2(a) (single hotspot). (c) The k_F^* and k_{FS}^* in the maximum k_F region, corresponding to the blue box in Fig. 2(c) (periodic hotspots). (d) Dimensionless heat flux in the y-direction q_y^* as a function of normalized hotspot spacing L^* for substrate thicknesses D of 10 nm, 100 nm, 500 nm, 1 μ m, and 4 μ m. The k_F^* is normalized as $k_F^* = k_F/k_u$. The k_{FS}^* is calculated by $k_{FS}^* = (q_{FS}/|\nabla T|)/k_u$. The heat flux is normalized as $q_y^* = q_y/q_{min}$, with the normalization performed independently for each thickness, where q_{min} is the minimum value for each thickness. The L^* is normalized as $L^* = L/MFP$, where MFP is the median phonon mean free path, defined as the MFP at which phonons with longer MFPs collectively contribute 50% of the bulk thermal conductivity [8].

To investigate the effect of hotspot spacing on thermal transport in nanoscale periodic hotspot systems, Fig. 3(d) presents the heat flux as a function of hotspot spacing for different substrate thicknesses. As the hotspot spacing L decreases (with both L and S decreasing simultaneously while

being kept equal), the heat flux along the y-direction increases—however, this enhancement shows a clear thickness dependence. At a thickness $D = 10$ nm, the enhancement is only 10%, but it grows with increasing thickness, reaching 40% at a thickness $D = 500$ nm. Further increasing the thickness beyond this value reduces the enhancement. This thickness-dependent enhancement arises from the variation in the fraction of phonons absorbed by hotspots at different thicknesses. In summary, the heat flux is enhanced with reduced hotspot spacing, and the extent of this enhancement first increases and then decreases with increasing substrate thickness.

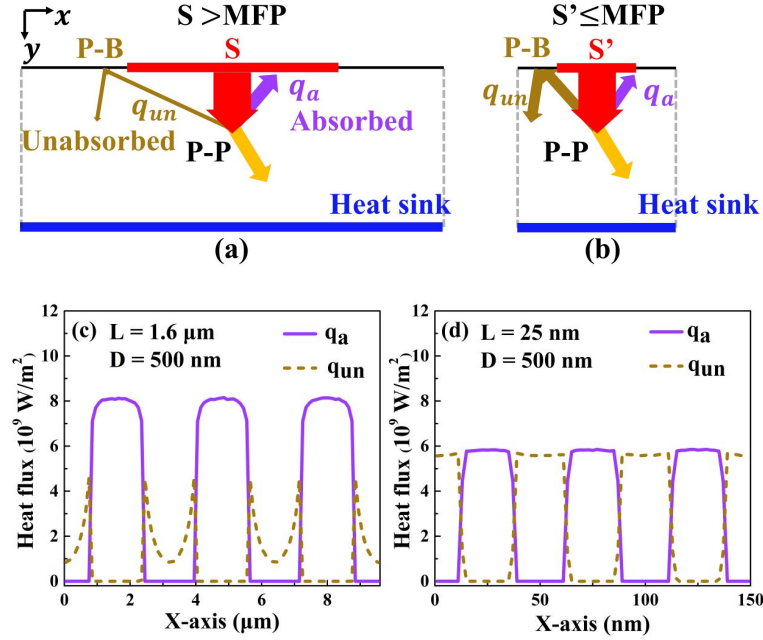


Fig. 4. (a) Schematic of phonon transport in nanoscale periodic hotspot systems with spacing L (equal to hotspot size S) much larger than the phonon MFP. (b) Schematic of phonon transport with spacing L (equal to hotspot size S) comparable to or smaller than the phonon MFP. Phonon-phonon and phonon-boundary scattering are denoted by P-P and P-B, respectively. The absorbed and unabsorbed heat fluxes by hotspots are denoted by q_a and q_{un} , respectively. (c) Distribution of heat flux absorbed by hotspots and heat flux not absorbed by hotspots along the x-axis for hotspot spacing $L = 1.6 \mu\text{m}$ and (d) $L = 25$ nm at a substrate thickness $D = 500$ nm.

To analyze the mechanism of enhanced heat flux with reduced hotspot spacing, phonon transport processes are tracked. As shown in the schematic representation in Fig. 4(a), the case where hotspot spacing L (equal to hotspot size S) is much larger than the phonon MFP is considered. After phonons are emitted from a hotspot, they propagate toward the heat sink. During this propagation, phonon-phonon scattering may occur, randomly altering phonon directions. Some phonons continue moving toward the heat sink (positive y -direction), while others are redirected back toward the hotspot (negative y -direction). These phonons returning toward the hotspot are critical for thermal transport. Given the limited phonon MFP, phonons are nearly unable to reach the boundaries adjacent to the hotspots, as the distance is too far compared with the phonon MFP. Consequently, almost all phonons returning toward the hotspots are absorbed by the hotspots. Mean-free-path-resolved spectral analysis of the enhancement is presented in the Supplemental Material IV.

The typical case with hotspot spacing $L = 1.6 \mu\text{m}$ is analyzed in Fig. 4(c), where L is much larger than the phonon MFP. The heat flux from phonons absorbed by the hotspot is denoted by q_a , while that from phonons scattered by nearby boundaries without being absorbed is denoted by q_{un} . The results show that most phonons moving toward the hotspot (negative y -direction) are absorbed, with only a low fraction remaining unabsorbed.

As shown in the schematic representation in Fig. 4(b), the case where hotspot spacing L (equal to hotspot size S) is comparable to or smaller than the phonon MFP is considered. Here, phonons can reach boundaries near hotspots. This leads to an increased probability of phonon-boundary scattering and a reduced probability of phonon absorption by hotspots. Those phonons scattered by the boundary may continue to propagate toward the heat sink, thereby enhancing the heat flux along the y -direction.

The typical case with hotspot spacing $L = 25 \text{ nm}$ is analyzed in Fig. 4(d), where L is smaller than

the phonon MFP. It can be observed that among phonons moving toward the hotspot (negative y -direction), approximately half are absorbed by the hotspot while the other half undergo phonon-boundary scattering. This reduction in absorbed heat flux increases the heat flux reaching the heat sink, thereby enhancing the thermal transport capability. Trend comparison with experiments and the correspondence between the formal local thermal conductivity and experimentally measurable quantities are discussed in the Supplemental Material V.

4. Conclusions

Here, the thermal transport in nanoscale multiple hotspot systems is systematically investigated by solving the phonon BTE. The formal local thermal conductivity is proposed to characterize the spatially non-uniform heat transport capability in these systems, which extends classical thermal conductivity descriptions to nanoscale non-diffusive regimes. The results reveal a highly non-uniform local thermal transport capability with up to a 13-fold variation across the system. In comparison, the maximum value of formal local thermal conductivity in multi-hotspots exceeds that under uniform heating by up to 24%, due to an increased fraction of first-drift phonons emitted from hotspots. Furthermore, a reduction in hotspot spacing is shown to enhance heat flux by up to 40%, resulting from the changing ratio between phonon-boundary scattering and phonon absorption by hotspots. This study would reveal the long-overlooked spatial distribution of thermal transport capability at the nanoscale and provide broad implications for thermal management in high-power-density integrated circuits.

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Supplemental Material for: Non-uniform Thermal Conductivity in Nanoscale Multiple Hotspot Systems

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I. Definition and Physical Nature of Formal Local Thermal Conductivity

A. Definition and Physical Nature

The discussion begins with the macroscopic Fourier's law and then extends it to the micro/nanoscale, where the formal local thermal conductivity is defined accordingly. Given the periodic boundary condition applied along the z-direction, the system can be simplified and analyzed as a two-dimensional model. In this case, Fourier's law can be expressed as:

$$\begin{bmatrix} q_x \\ q_y \end{bmatrix} = - \begin{bmatrix} k_{xx} & k_{xy} \\ k_{yx} & k_{yy} \end{bmatrix} \cdot \begin{bmatrix} \nabla_x T \\ \nabla_y T \end{bmatrix} \quad (S1)$$

In general, crystalline silicon can be approximated as having isotropic thermal conductivity. Under conditions dominated by macroscopic diffusive transport and in the absence of an applied external magnetic field, the thermal conductivity tensor reduces to a scalar form, where its off-diagonal components (k_{xy} and k_{yx}) vanish and its diagonal components (k_{xx} and k_{yy}) become equal. Under these conditions, the heat flux vector aligns collinearly with the temperature gradient vector, consistent with the description of classical Fourier's law.

In micro-/nano-scale, when the characteristic system dimension approaches or falls below the phonon mean free path (MFP), the dominant phonon transport mechanism shifts from diffusive to quasi-ballistic and ballistic regimes. Non-diffusive transport can cause the heat flux direction to deviate from collinearity with the temperature gradient, and the off-diagonal components of the thermal conductivity tensor may become non-zero.

In micro-/nano- scale heat transport, the tensor form of thermal conductivity does not provide an intuitive representation of the spatial distribution and local directional behavior of heat transport capability. To address this, the thermal conductivity can be locally decomposed into components defined along the temperature gradient direction and its perpendicular direction.

In the following, it is provided a detailed definition of the formal local thermal conductivity. At any position $\mathbf{r} = (x, y)$, the unit vector along the temperature gradient is defined as $\mathbf{e}_T(\mathbf{r}) = \nabla T(\mathbf{r})/|\nabla T(\mathbf{r})|$, and the unit vector along the heat flux direction as $\mathbf{e}_q(\mathbf{r}) = \mathbf{q}(\mathbf{r})/|\mathbf{q}(\mathbf{r})|$. In two dimensions, a local orthogonal coordinate system can be constructed. The direction opposite to the temperature gradient is taken as the first axis, i.e., the Fourier-law expected heat flux direction $\mathbf{e}_\parallel(\mathbf{r}) = -\mathbf{e}_T(\mathbf{r})$. Then, the perpendicular direction is taken as the second axis, obtained via the cross product with the out-of-plane unit normal vector $\mathbf{z}$: $\mathbf{e}_\perp(\mathbf{r}) = \mathbf{z} \times \mathbf{e}_\parallel(\mathbf{r})$.

In this local coordinate system, the heat flux vector $\mathbf{q}(\mathbf{r})$ is projected onto these two orthogonal directions:

$$q_F(\mathbf{r}) = \mathbf{q}(\mathbf{r}) \cdot \mathbf{e}_\parallel(\mathbf{r}) \quad (S2)$$

$$q_H(\mathbf{r}) = \mathbf{q}(\mathbf{r}) \cdot \mathbf{e}_\perp(\mathbf{r}) \quad (S3)$$

Corresponding to these two heat flux components, two formal local thermal conductivities are defined:

$$k_F(\mathbf{r}) = q_F(\mathbf{r})/|\nabla T(\mathbf{r})| \quad (S4)$$

$$k_H(\mathbf{r}) = q_H(\mathbf{r})/|\nabla T(\mathbf{r})| \quad (S5)$$

In the local orthogonal coordinate system, the above relationship can be expressed as:

$$\begin{bmatrix} q_F(\mathbf{r}) \\ q_H(\mathbf{r}) \end{bmatrix} = \begin{bmatrix} k_F(\mathbf{r}) & 0 \\ k_H(\mathbf{r}) & 0 \end{bmatrix} \cdot \begin{bmatrix} |\nabla T(\mathbf{r})| \\ 0 \end{bmatrix} \quad (S6)$$

Here, $k_F(\mathbf{r})$ denotes the formal local thermal conductivity associated with the heat flux component

collinear with the temperature gradient, referred to as the Fourier-direction formal local thermal conductivity. Meanwhile, $k_H(\mathbf{r})$ represents the formal local thermal conductivity associated with the heat flux component perpendicular to the temperature gradient, referred to as the Hall-direction formal local thermal conductivity.

Formal local thermal conductivity extends the concept of thermal conductivity from macroscopic diffusive transport to non-diffusive transport at micro- and nanoscales. In the diffusive regime, thermal conductivity can be regarded as a linear response coefficient that relates heat flux to the temperature gradient, manifesting as a uniform material constant. At the micro-/nanoscale, although the conventional definition breaks down, it can still be regarded as a response function characterizing local heat transport capability. Formal local thermal conductivity is determined jointly by the intrinsic bulk thermal conductivity and the degree to which local regions deviate from diffusive transport, thereby quantifying local thermal resistance in non-diffusive regimes and capturing the transition from diffusive toward ballistic transport.

Formal local thermal conductivity enables direct characterization and analysis of local thermal resistance in integrated circuits and micro-/nanoscale experiments [1-5]. Furthermore, it is also applicable to quantum devices, where understanding and controlling quantum-effect-driven deviations from Fourier's law is essential for their design [6].

B. Distinction from Existing Descriptions

The core distinction between the formal local thermal conductivity and the widely used global effective thermal conductivity lies in whether they provide spatially resolved characterization. In nanoscale thermal transport studies, the prevailing global effective thermal conductivity is essentially a black-box treatment that averages the thermal transport capability across the entire system. This black-box treatment obscures the fact that local transport capability can be significantly higher or lower than the average, as recently evidenced by experiments [1-5].

By contrast, the formal local thermal conductivity is a spatially resolved field quantity that can reveal dramatic variations in thermal transport capability across the system. In this work, it is observed that the maximum and minimum values of k_F within the system can differ by up to 13 times. This core finding is entirely undetectable by any global effective thermal conductivity.

Quantitative local thermal transport characterizations remain rarely reported. One existing approach is the graded thermal conductivity we previously proposed [7,8]. This approach is strictly limited to centrally symmetric single-heat-source geometries. It can only describe one-dimensional radial variation of thermal transport capability. Consequently, it cannot be extended to complex configurations such as periodic multiple hotspots in integrated circuits.

A few studies adopt a definition of a scalar local quantity, which is the total heat flux magnitude divided by the temperature gradient magnitude [9]. They do not decompose the heat flux directionally; instead, they directly disregard the directions of heat flux and temperature gradient and use a scalar form. Such a scalar formulation suffers from inherent physical ambiguity: when heat flux deviates from the direction collinear with the temperature gradient, the scalar value mixes two distinct physical effects—the thermal transport capability along the temperature gradient direction and the heat flux deflection caused by quasi-ballistic phonon transport. Consequently, it is impossible to distinguish whether the variation originates from a change in thermal transport capability or from directional deviation.

By contrast, the formal local thermal conductivity proposed in this work overcomes both the one-dimensional constraint and the directional ambiguity of scalar definitions. It is completely free from the

dimensional constraint and is applicable to arbitrary non-uniform thermal transport scenarios with significantly broader universality.

Furthermore, by decomposing the local heat flux into the Fourier-direction component k_F and the Hall-direction component k_H , it separately quantifies the spatial distribution of local thermal transport capability and the degree of heat flux deflection in two- or three-dimensional space, thereby providing a more comprehensive and physically unambiguous local diagnostic framework for nanoscale thermal transport analysis.

To facilitate intuitive distinction, the three related concepts are briefly summarized as follows.

Effective thermal conductivity is a global lumped parameter that describes the overall average heat transport capability of the whole system, calculated from total heat flux and global temperature difference. It is built on the assumption of spatially uniform transport, and thus cannot capture spatial variations of local thermal performance.

Local thermal conductivity refers generally to all spatially resolved thermal conductivity descriptions that vary with position. Quantitative local thermal transport characterizations of this type remain rarely reported in the literature. Existing scalar formulations define the quantity as the magnitude of the total local heat flux divided by the magnitude of the local temperature gradient, with no directional decomposition of the heat flux vector; other implementations are restricted to one-dimensional symmetric geometries. Both approaches suffer from either ambiguous physical interpretation or limited applicability to complex structures.

The formal local thermal conductivity proposed in this work is a spatially resolved directional quantity. It preserves the canonical mathematical form of Fourier’s law, and decomposes local heat flux into components aligned with and perpendicular to the temperature gradient, enabling independent quantification of local transport capability and non-Fourier heat flux deflection. It applies to arbitrary multi-dimensional non-uniform transport scenarios with no requirement for structural symmetry.

II. Computational Methodology and Simulation Configurations

Over the past few decades, the phonon Boltzmann transport equation (BTE) has been demonstrated to be a reliable method for describing heat transport at the micro-nanoscale [10]. The numerical approaches for solving the phonon BTE fall into two broad categories: deterministic methods and stochastic methods. Deterministic methods, such as the discrete ordinates method (DOM) and the lattice Boltzmann method (LBM), directly discretize the governing equation. Although they yield solutions free of statistical noise, their computational expense grows dramatically with dimensionality, making them prohibitively costly for solving the high-dimensional (time, space, direction, and frequency) BTE [10]. In contrast, stochastic methods, most notably the Monte Carlo (MC) method, solve the phonon BTE by transforming it into a Lagrangian framework and tracking the trajectories and scattering events of phonon ensembles. The computational complexity of the MC method scales approximately linearly, rather than exponentially, with the number of dimensions, rendering it particularly suitable for high-dimensional problems [11].

In conventional MC methods, statistical uncertainties are significant and strict energy conservation is challenging to maintain. The deviational MC method substantially reduces statistical variance by simulating only the deviations from an equilibrium distribution, while rigorously preserving energy conservation, thereby enhancing computational efficiency [12]. The linearized deviational MC method enables independent simulation of each computational particle, improving parallel computing efficiency [13]. Furthermore, this method eliminates the need for time steps and spatial grids, avoiding numerical

errors introduced by discretization and obviating the sampling of local temperatures, thus further boosting computational efficiency [14].

The phonon BTE is expressed as:

$$\frac{\partial f}{\partial t} + \mathbf{V}_g \cdot \nabla f = \frac{f^{loc} - f}{\tau} \quad (S7)$$

where f denotes the phonon distribution function, and f^{loc} represents the equilibrium Bose-Einstein distribution at the local temperature. Additionally, $\mathbf{V}_g$ and τ correspond to the phonon group velocity and relaxation time, respectively.

To enhance computational efficiency and reduce statistical variance, particularly under small deviations from equilibrium, the deviational MC method is introduced. The governing equation is recast in terms of deviational energy [12]:

$$\frac{\partial e^d}{\partial t} + \mathbf{V}_g \cdot \nabla e^d = \frac{(e^{loc} - e_{T_{eq}}^{eq}) - e^d}{\tau} \quad (S8)$$

The deviational energy distribution is defined as $e^d = e - e_{T_{eq}}^{eq}$. Here, $e = \hbar\omega f$, $e^{loc} = \hbar\omega f^{loc}$ and $e_{T_{eq}}^{eq} = \hbar\omega f_{T_{eq}}^{eq}$, with $f_{T_{eq}}^{eq} = [\exp(\hbar\omega/k_b T_{eq}) - 1]^{-1}$ being the Bose-Einstein distribution at the equilibrium temperature T_{eq} , and k_b is Boltzmann's constant.

Further simplification is achieved by using linearized deviational MC method, which is valid when $|T - T_{eq}| \ll T_{eq}$. The linearized form of the deviational BTE is given by [13]:

$$\frac{\partial e^d}{\partial t} + \mathbf{V}_g \cdot \nabla e^d = \frac{\mathcal{L}(e^d) - e^d}{\tau} \quad (S9)$$

where

$$\mathcal{L}(e^d) = (T_{loc} - T_{eq}) \frac{de_{T_{eq}}^{eq}}{dT} \quad (S10)$$

The linearized deviational MC method involves generating phonon bundles sampled from the initial deviational energy distribution. These phonon bundles are propagated through drift and scattering processes. For steady-state simulations, thermodynamic observables such as temperature deviation and heat flux are computed by time-averaging phonon bundle trajectories. In a region of volume V , the temperature deviation from equilibrium T_{dev} and the heat flux component q_y are evaluated using [15]:

$$T_{dev} = \frac{\dot{\epsilon}_{eff}^d}{CV} \sum_i s_i \frac{l_i}{V_{g,i}} \quad (S11)$$

$$q_y = \frac{\dot{\epsilon}_{eff}^d}{V} \sum_i s_i l_{y,i} \quad (S12)$$

where s_i signifies the sign of the deviational energy (positive or negative), l_i is the total path length traveled by the i -th phonon bundle, $l_{y,i}$ is its displacement along the y -direction, C is the volumetric specific heat. Here, $\dot{\epsilon}_{eff}^d = \dot{E}_{tot}^d/N$ is the effective deviational energy rate, and $\dot{E}_{tot}^d$ is the total deviational energy rate, N is the number of phonon bundles in the simulation. Further details regarding the MC method can be found in previous literature [11-15].

In this work, the first-principles-based MC method is employed to solve the phonon BTE, and the process comprises three sequential stages. First, the harmonic and anharmonic interatomic force constants (IFCs) for silicon are derived from first-principles calculations, implemented using VASP [16].

Second, these IFCs are used as input for the ShengBTE software package [17] to obtain the spectral phonon properties, including group velocity, relaxation time, and heat capacity. Finally, these spectral phonon properties serve as input for solving the phonon BTE using the linearized deviational MC method [15].

The IFCs are obtained from first-principles calculations performed using VASP. Projector-augmented-wave pseudopotentials and the Perdew-Burke-Ernzerhof exchange-correlation functional are employed. A $10 \times 10 \times 10$ k-point mesh is used for Brillouin-zone sampling. A plane-wave kinetic energy cutoff of 350 eV is uniformly adopted for all calculations. While a cutoff energy of 319 eV has been adopted for silicon in previous studies [17], a higher value is selected here to ensure robust convergence. Systematic convergence tests confirm that the total energy deviation at 350 eV is approximately 1 meV per atom relative to the fully converged 450 eV reference. The corresponding convergence curve is provided in Fig. S1 (a).

The harmonic (second-order) IFCs are extracted using density functional perturbation theory (DFPT) on a $5 \times 5 \times 5$ supercell. The anharmonic (third-order) IFCs are generated via the finite-displacement method. This involves creating a series of systematically displaced atomic configurations within a $4 \times 4 \times 4$ supercell and calculating the resulting forces using density functional theory (DFT). A displacement amplitude of 0.01 Å is used for the finite-displacement calculations, which is the default recommended value in the ShengBTE software package. The maximum interaction cutoff for anharmonic force constants reaches 9.5 Å, which exceeds the cutoff values reported in prior literature [17] and ensures full convergence of the anharmonic interactions.

These second- and third-order IFCs are then used as input for the ShengBTE package. Two solution schemes for the linearized phonon BTE are implemented in the code: the relaxation-time approximation (RTA) and the full self-consistent iterative method. The iterative scheme, which accounts for the full coupling of phonon scattering channels and delivers higher accuracy than the RTA, is adopted in this work. The phonon properties, including group velocities and relaxation times, are computed by ShengBTE on a $30 \times 30 \times 30$ q-point mesh. Systematic convergence tests over q-point meshes ranging from $10 \times 10 \times 10$ to $32 \times 32 \times 32$ show that the relative change in thermal conductivity is only 1.6% between the $25 \times 25 \times 25$ and $30 \times 30 \times 30$ meshes, confirming sufficient numerical convergence. The convergence curve of thermal conductivity with respect to the q-point mesh is presented in Fig. S1 (b). Isotope scattering is disabled in the primary calculations to isolate intrinsic three-phonon scattering, which dominates thermal resistance in bulk silicon at room temperature. The calculated bulk thermal conductivity of silicon from this framework is 142.3 W/(m·K), in agreement with established values [18,19], thereby validating the phonon properties used in the subsequent MC simulation. Notably, all phonon branches, including both acoustic and optical branches, are taken into account.

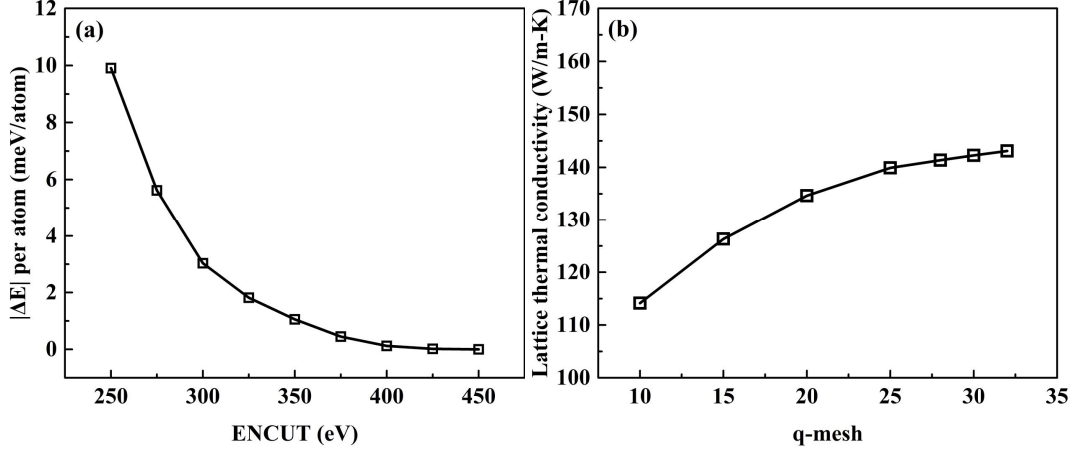


Fig. S1. Convergence validation of first-principles lattice thermal conductivity calculations. (a) Convergence of total energy per atom with respect to the plane-wave kinetic energy cutoff. (b) Convergence of bulk silicon thermal conductivity with respect to the q-point mesh size.

For the single nanoscale hotspot case, the computational model is shown in Fig. S2(a). The system parameters are set with hotspot size $S = 50$ nm, substrate thickness $D = 100$ nm, and system length $LA = 1200$ nm. This length ensures that heat transport near the hotspot is unaffected by x-direction boundaries. In regions far from the hotspot where the temperature exactly equals the ambient temperature and the temperature gradient is 0, the formal local thermal conductivity cannot be calculated. Therefore, a 300 nm region centered on the hotspot is selected for calculating distributions. For calculating the temperature distribution and formal local thermal conductivity distribution, the numbers of meshes in the x-, y-, and z-directions are set to 30, 10, and 1, respectively. In the other regions, no mesh is generated, which improves the computational speed. In these unmeshed regions, phonon bundles can move, but the temperature and heat flux are not calculated. All boundaries in the z-direction are set to periodic for all simulation cases.

For the periodic nanoscale hotspot case, the computational model is shown in Fig. S2(b). Two different computational setups are employed in the various periodic nanoscale hotspot simulations. When the focus is on the internal thermal transport mechanisms, the formal local thermal conductivity distribution needs to be calculated. In such cases, the parameters used are hotspot size $S = 50$ nm, spacing $L = 50$ nm, substrate thickness $D = 100$ nm, system length $LB = 300$ nm, with the numbers of meshes in the x-, y-, and z-directions set to 30, 10, and 1, respectively.

When focusing on the overall heat dissipation of the system rather than local regions, calculating the heat flux is more direct than obtaining the formal local thermal conductivity distribution. This heat flux indicates how much heat is transferred from the hotspots to the heat sink. To investigate the overall heat dissipation at different hotspot spacings, the heat flux values under various spacing conditions are calculated. In periodic nanoscale hotspot systems, the total heat flow in the y-direction is conserved. Consequently, the mean heat flux remains the same when calculated at different cross-sections along the y-axis. To quantify the phonon bundles moving in the negative y-direction that are absorbed or unabsorbed by hotspots, the mean heat flux in the top 1 nm thick region of the computational domain is calculated. This value is denoted as q_y .

In all periodic nanoscale hotspot simulations, the hotspot size S and the spacing L between hotspots are maintained equal, occupying 50% of the top region respectively. This configuration ensures that both S and L are varied simultaneously when adjusting the hotspot spacing.

For the uniform heating case, the computational model is shown in Fig. S2(c). The system is

configured with length $LC = 100$ nm and substrate thickness $D = 100$ nm. Given the identical results at different x -positions under uniform heating, the numbers of meshes in the x -, y -, and z -directions are set to 1, 10, and 1, respectively. The effective thermal conductivity in the central linear temperature region k_u is calculated for comparison, as commonly employed in previous studies [20,21].

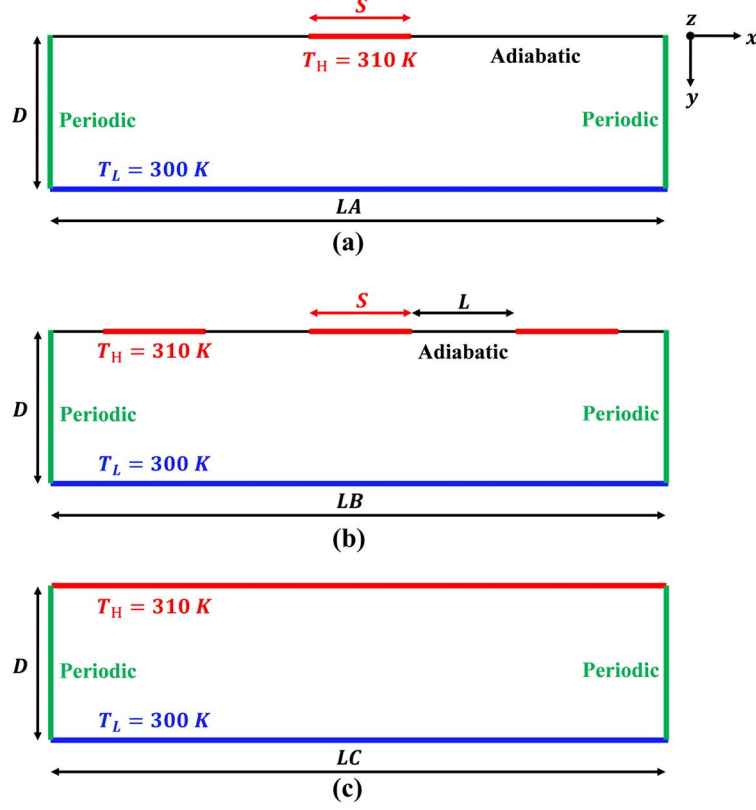


Fig. S2. Computational models for (a) the single nanoscale hotspot system, (b) the multiple nanoscale hotspot system, and (c) the uniform heating system.

III. Numerical Validation and Convergence Tests

The linearized deviational MC method has been extensively validated in prior work, including successful applications to commercial transistor design [22-24] and consistent agreement with time-domain thermoreflectance (TDTR) experiments [14].

In this work, linearized deviational MC simulations were performed using the open-source code MCBTE, whose reliability has been thoroughly validated by its authors and documented in prior literature [15,25]. To further verify the accuracy of the adopted simulation framework, the thermal conductivity of silicon thin films across a range of thicknesses was calculated, and the obtained results show good agreement with previous simulation and experimental data (as presented in Fig. S3). Furthermore, additional validation details can be found in previous work [26].

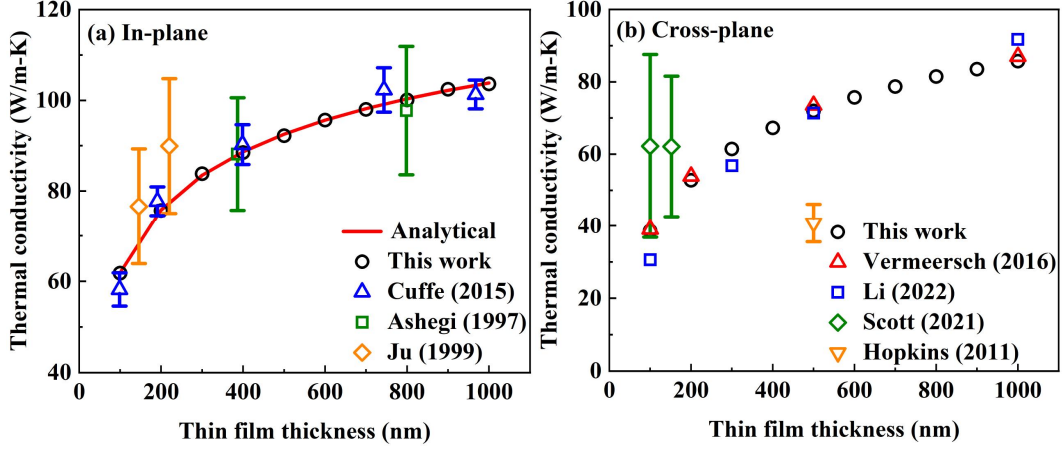


Fig. S3. (a) In-plane thermal conductivity of silicon thin films with varying thickness. Results from this work are compared with analytical solutions [27] and experimental data [19,28,29]. (b) Cross-plane thermal conductivity of silicon thin films with varying thickness. Results from this work are compared with previous simulations [30,31] and experimental data [32,33].

Large temperature differences may introduce additional errors in the linearized deviational MC method. However, for the present work, the error introduced by linearization remains within acceptable limits. Previous error analyses have shown that for silicon with an ambient temperature of 300 K, the relative error due to linearization is approximately 2% and 6% for temperature differences of 30 K and 50 K, respectively [11].

Prior to simulation, the convergence of key results with respect to the number of phonon bundles and the maximum number of scattering events was verified. Insufficient phonon bundles lead to significant statistical errors, while an inadequate maximum number of scattering events prevents the system from reaching steady state.

As shown in Fig. S4(a), to ensure the system reaches steady state, the convergence of q_y with the maximum number of scattering events was tested for the largest system. The largest system is characterized by a length $LB = 9.6 \mu\text{m}$ and a substrate thickness $D = 4 \mu\text{m}$. Convergence is observed when the maximum number of scattering events reaches 1×10^5 . Accordingly, this value is adopted for all simulations.

Fig. S4(b) shows the convergence of q_y with the number of phonon bundles for the largest system, ensuring sufficiently small statistical errors. Convergence is achieved with 1×10^7 phonon bundles.

For the formal local thermal conductivity distribution calculations, where smaller statistical errors are required, the convergence of the maximum Fourier-direction formal local thermal conductivity k_F and Hall-direction formal local thermal conductivity k_H with the number of phonon bundles was separately tested, as shown in Fig. S4(c). Based on these convergence tests, 1×10^8 phonon bundles are used in formal local thermal conductivity distribution calculations.

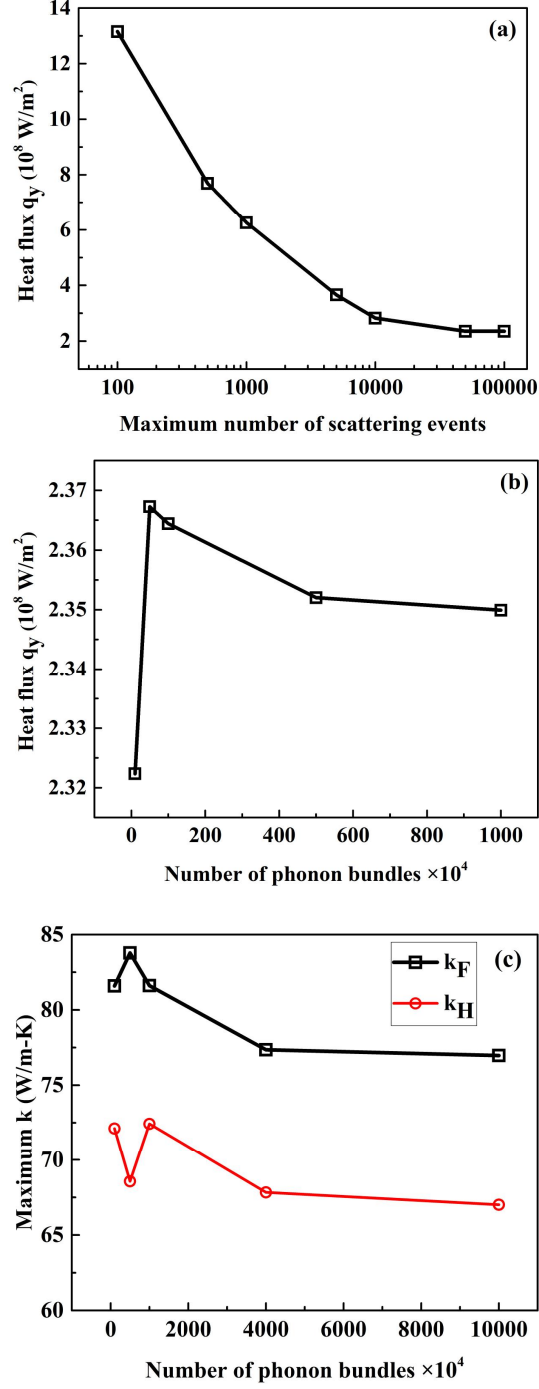


Fig. S4. (a) Convergence of the y-direction heat flux q_y with the maximum number of scattering events. (b) Convergence of the y-direction heat flux q_y with the number of phonon bundles. (c) Convergence of the maximum Fourier-direction formal local thermal conductivity k_F and Hall-direction formal local thermal conductivity k_H with the number of phonon bundles.

The numerical methodology and associated error analysis used to compute the formal local thermal conductivity are described in the following. The steady-state temperature field is obtained by solving the phonon Boltzmann transport equation via the linearized deviational Monte Carlo method [11]. Unlike grid-based deterministic methods such as the finite difference method or the finite volume method, the linearized deviational Monte Carlo method eliminates the need for discrete time steps and spatial grids when solving the governing transport equation, which fundamentally avoids numerical artifacts such as

spurious oscillations, and numerical stability issues induced by spatial or temporal discretization [10,14]. The numerical error of the obtained temperature field is dominated by statistical error, which can be systematically reduced by increasing the number of simulated phonon bundles. The resulting temperature field is numerically stable, even in regions with relatively small temperature gradients [11].

For the post-processing calculation of the local temperature gradient, a second-order accurate central difference scheme is adopted, implemented via the `np.gradient` function from the NumPy scientific computing library. This scheme applies second-order central differencing to all interior grid points:

$$\left. \frac{\partial T}{\partial x} \right|_{i,j} \approx \frac{T_{i+1,j} - T_{i-1,j}}{2\Delta x}, \quad \left. \frac{\partial T}{\partial y} \right|_{i,j} \approx \frac{T_{i,j+1} - T_{i,j-1}}{2\Delta y} \quad (\text{S13})$$

where $T_{i,j}$ is the temperature at grid point (i,j) , and $\Delta x, \Delta y$ are the grid spacings in the x and y directions, respectively.

The leading truncation error for each gradient component is estimated from the Taylor expansion:

$$\varepsilon_{\partial T/\partial x} \approx \frac{\Delta x^2}{6} \left| \frac{\partial^3 T}{\partial x^3} \right|, \quad \varepsilon_{\partial T/\partial y} \approx \frac{\Delta y^2}{6} \left| \frac{\partial^3 T}{\partial y^3} \right| \quad (\text{S14})$$

where $\varepsilon_{\partial T/\partial x}$ and $\varepsilon_{\partial T/\partial y}$ are the upper-bound truncation errors for the respective gradient components, and $|\partial^3 T/\partial x^3|$, $|\partial^3 T/\partial y^3|$ denote the absolute values of the third-order spatial derivatives of temperature.

The gradient magnitude is $|\nabla T| = \sqrt{(\partial T/\partial x)^2 + (\partial T/\partial y)^2}$. When the errors of the gradient components propagate into $|\nabla T|$, the individual error contributions may have opposite signs and partially cancel out, causing an underestimation. To avoid this and obtain a safe, conservative estimate, the absolute values of the coefficients are taken, which gives a practical upper bound:

$$\varepsilon_{|\nabla T|} \leq \frac{|\partial T/\partial x|}{|\nabla T|} \varepsilon_{\partial T/\partial x} + \frac{|\partial T/\partial y|}{|\nabla T|} \varepsilon_{\partial T/\partial y} \quad (\text{S15})$$

where $\varepsilon_{|\nabla T|}$ is the error bound for the gradient magnitude $|\nabla T|$.

Since the formal local thermal conductivity is defined as $k_F = q_F/|\nabla T|$ and the heat flux q_F is obtained directly from the Monte Carlo simulation, its error (dominated by the gradient error in this analysis) satisfies:

$$\frac{\varepsilon_k}{k_F} = \frac{\varepsilon_{|\nabla T|}}{|\nabla T|} \quad (\text{S16})$$

where ε_k is the error in k_F ; this equation states that the relative error of k_F equals the relative error of the gradient magnitude.

Applying this error analysis to our single-hotspot and periodic-hotspot cases (i.e., the examples used for calculating the formal local thermal conductivity in Fig. 2 of the main text) gives global mean relative errors of 1.39% and 0.98%, with maxima of 5.76% and 8.70%, respectively, and no grid point exceeds 10% error. It is noteworthy that these values therefore represent conservative upper bounds for the actual numerical error, rather than the error itself. These quantitative results confirm that the truncation error introduced by the second-order central difference is negligible and does not affect the reliability of the formal local thermal conductivity.

The following analysis evaluates the numerical stability of the formal local thermal conductivity calculation under reduced temperature gradients by comparing results obtained at hotspot temperatures of 301 K and 310 K. In this test, the temperature of the isothermal hotspot boundaries was reduced from 310 K to 301 K while keeping all other simulation settings unchanged. This adjustment markedly lowers the overall temperature gradient across the entire system, creating a more stringent condition for

numerical stability. Using the same post-processing procedure, the formal local thermal conductivity distributions were then recomputed for the same configurations as in Fig. 2 of the main text, and these new results obtained at 301 K were compared with the original distributions computed at 310 K.

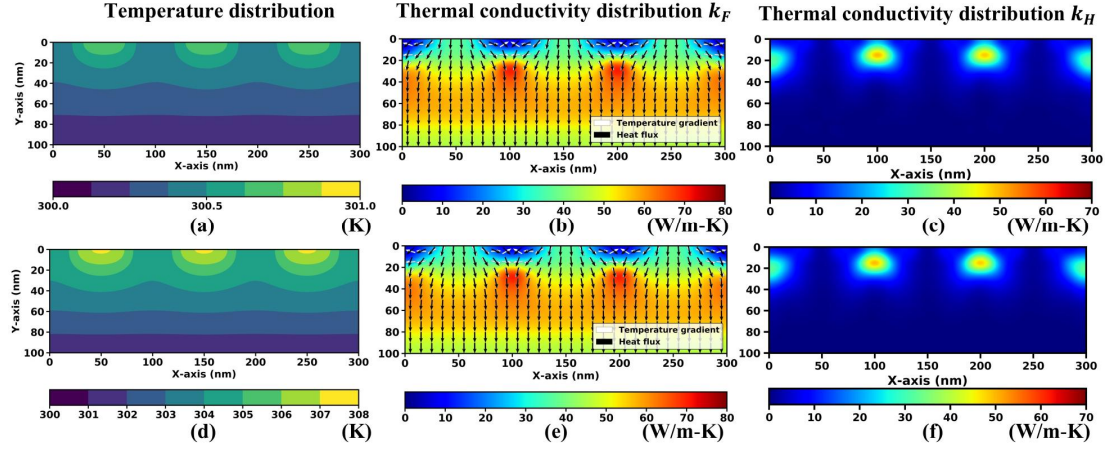


Fig. S5. Comparison of temperature and formal local thermal conductivity distributions for nanoscale periodic hotspots at hotspot temperatures of 301 K and 310 K. (a) Temperature, (b) k_F and (c) k_H distributions at a hotspot temperature of 301 K. (d) Temperature, (e) k_F and (f) k_H distributions at a hotspot temperature of 310 K. Black arrows in (b) and (e) indicate the direction of heat flux, while white arrows show the direction opposite to the temperature gradient.

As shown in Fig. S5, a comparison is made between the cases with hotspot temperatures of 301 K and 310 K. It can be observed that the formal local thermal conductivity differs very little between these two temperatures. For the Fourier-direction formal local thermal conductivity k_F , the average relative difference across all grid points between the two cases is 0.52%, and the maximum relative difference is 9.8%. Notably, the maximum difference appears in regions with very low k_F values, where local thermal transport capability is weak and the results have little impact on the overall heat dissipation performance.

For the Hall-direction formal local thermal conductivity k_H , grid points where k_H is below 3 W/(m·K) in both cases are excluded. These points correspond to regions with negligible non-Fourier effects, where k_H carries little physical significance for our core analysis. For the remaining valid grid points, the average relative difference is 2.4%, and the maximum relative difference is 15.7%. Consistent with the k_F results, the maximum difference also occurs in regions with small k_H values.

These quantitative results fully demonstrate that the calculation of formal local thermal conductivity has excellent numerical stability even under small temperature gradient conditions. The deviations are limited and mainly concentrated in regions with low thermal transport capability, which do not affect the core conclusions of this work regarding the spatial distribution of thermal transport capability and the enhancement mechanism of heat dissipation.

IV. Mechanism Analysis of Thermal Transport in Multi-Hotspot Systems

A. Heat Flux Deflection and Non-Fourier Transport Characterization

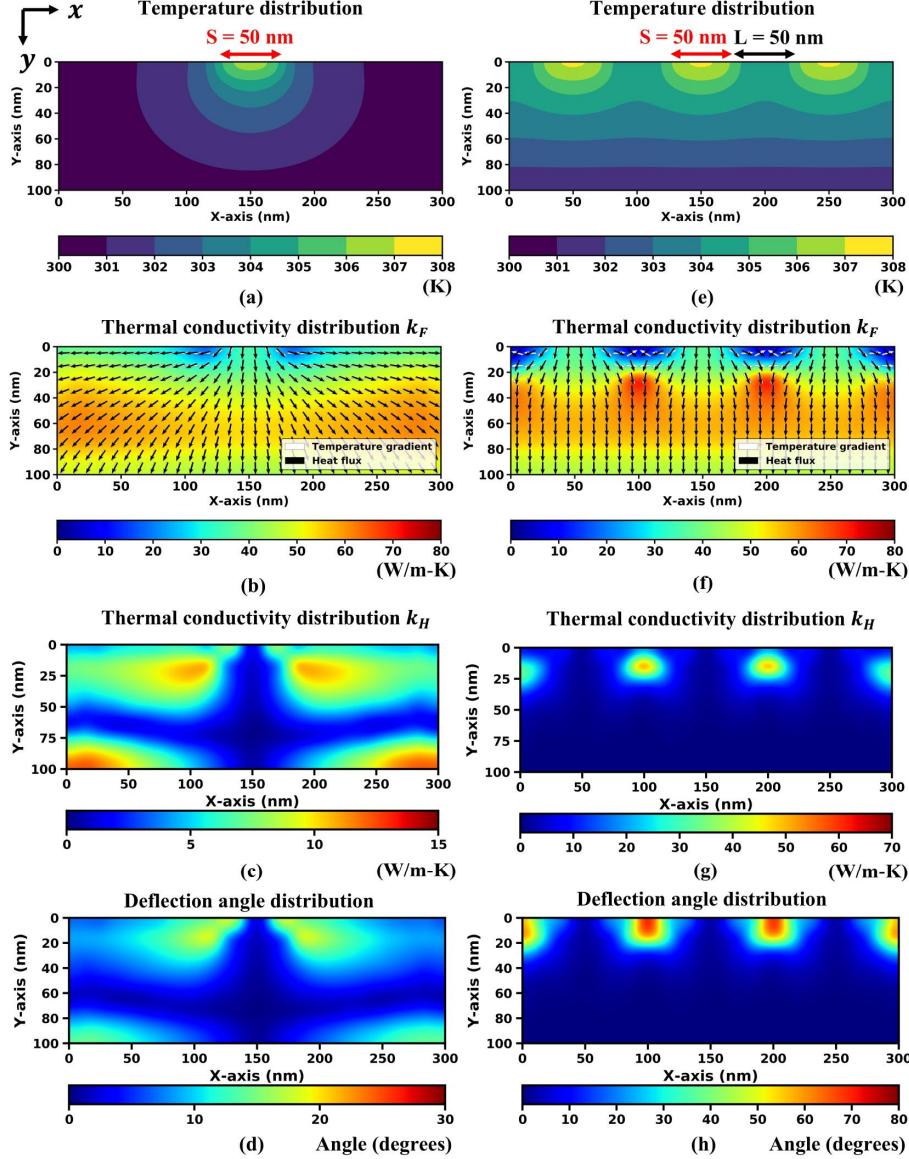


Fig. S6. Distribution of temperature, formal local thermal conductivity and deflection angle for a substrate thickness of $D = 100$ nm. The deflection angle is defined as the angle between the heat flux vector and the direction opposite to the temperature gradient. (a) Temperature, (b) k_F , (c) k_H and (d) deflection angle distributions for a nanoscale single hotspot. (e) Temperature, (f) k_F , (g) k_H and (h) deflection angle distributions for nanoscale periodic hotspots. Black arrows in (b) and (f) indicate the direction of heat flux, while white arrows show the direction opposite to the temperature gradient. For the nanoscale single hotspot system, a total x-direction length of 1200 nm is used to ensure adequate separation from the boundaries; the central 300 nm region is selected for comparison, and the hotspot size is $S = 50$ nm. For the nanoscale periodic hotspot system, both the hotspot size S and the spacing L are 50 nm.

The temperature distribution for a nanoscale single hotspot is presented in Fig. S6(a). A distinct

temperature jump is observed at the hotspot boundaries (boundary temperature significantly lower than hotspot temperature), consistent with previous studies [34].

The temperature distribution for nanoscale periodic hotspots is presented in Fig. S6(e). Compared with the single hotspot case, the temperature jump is reduced by 0.7 K under periodic hotspot conditions, indicating that the boundary temperatures are closer to the hotspot temperature.

Figs. S6(b), (c), (f), and (g) have already been introduced in the main text.

Fig. S6(d) and (h) show the deflection angle distributions between the heat flux vector and the direction opposite to the local temperature gradient for the representative configurations illustrated in Fig. 2 of the main text, further characterizing the non-Fourier transport behavior. In the macroscopic diffusive regime, Fourier's law dictates that the heat flux is precisely collinear with the direction opposite to the temperature gradient, i.e., the deflection angle is 0° . For the single nanoscale hotspot, the maximum deflection angle across the computational domain reaches only 22° . Although moderate in magnitude, this non-zero angle provides direct quantitative evidence of non-Fourier transport, which cannot be captured by the classical Fourier framework. For the periodic hotspot configuration, the maximum deflection angle increases dramatically to 72° . This pronounced deflection originates from the intense quasi-ballistic phonon transport in the spacing regions between adjacent hotspots, where phonon trajectories are dominated by the size and spacing arrangement of the hotspots rather than by the local temperature gradient.

B. Ballistic Phonon Model and Negative Temperature Gradient

A negative temperature gradient phenomenon is observed in our simulations. As shown in Fig. 2(c) of the main text, black arrows denote the direction of heat flux, while white arrows represent the direction opposite to the temperature gradient, which is the heat flux direction predicted by Fourier's law. In the spacing region between periodic nanoscale hotspots, particularly near the top surface, the white arrows point toward the top surface instead of toward the heat sink, whereas the black arrows marking the heat flux still point toward the heat sink.

To elucidate the physical mechanism underlying the negative temperature gradient in the spacing region between adjacent hotspots and its intrinsic link to heat flux deflection, an intuitive ballistic phonon model is constructed under the simplifying assumption of purely ballistic phonon transport, providing a clear physical picture of this non-Fourier phenomenon.

As schematically shown in Fig. S7(a), we consider two adjacent hotspots under the simplifying assumption that all emitted phonons travel ballistically without scattering. For any point along the green dashed line in the spacing region, the local ballistic phonon density is determined by the sum of the view angles from the point to the two hotspots, which is 2α (both angles equal α), as ballistic phonons propagate along straight-line trajectories. Calculating and normalizing this summed angle, 2α , along the green dashed line yields the blue curve in Fig. S7(b). This blue curve thus represents the normalized 2α . The total angle sum 2α reaches its maximum at approximately 40 nm below the surface, corresponding to the highest ballistic phonon density and thus the highest local temperature. This directly accounts for the negative temperature gradient: for periodically arranged hotspots, quasi-ballistic phonons emitted from each hotspot propagate obliquely downward into the spacing region and accumulate at a finite depth, elevating the local temperature there, while the near-surface spacing region remains cooler owing to the absence of direct phonon incidence at its upper adiabatic boundary. Consequently, under quasi-ballistic transport, the temperature peak does not appear at the top surface of the spacing, but at a certain depth beneath it. Notably, both the enhanced formal local thermal conductivity in the spacing region and the

negative temperature gradient share the same physical origin: quasi-ballistic phonon-dominated transport.

Physically, the ballistic phonon density in the spacing region from this view-angle model corresponds directly to the spatial density of first-drift phonons. As first-drift phonons from adjacent hotspots superimpose in the spacing region, the local transport is closer to ballistic transport, leading to a higher formal local thermal conductivity. This also explains the spatial coincidence between the peak of the normalized summed view angle and the peak of k_F^* in Fig. S7(b).

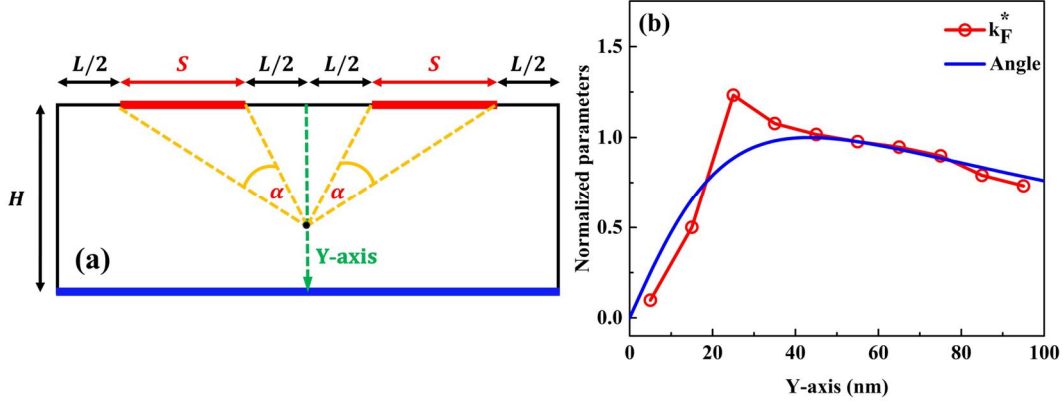


Fig. S7. (a) Schematic of two adjacent hotspots under the assumption of purely ballistic phonon emission, illustrating the view angle α (identical for both hotspots) from an arbitrary point on the green dashed line in the spacing region. (b) Normalized summed view angle 2α (blue curve) and normalized Fourier-direction formal local thermal conductivity k_F^* .

The negative temperature gradient and heat flux deflection are inherently correlated, representing two manifestations of the same underlying physical process. From a mechanistic perspective, both phenomena stem from the same root cause: the propagation direction of quasi-ballistic phonons is determined by their initial direction upon emission from the hotspots, and is not governed by the local temperature gradient.

This correlation is quantitatively captured by the Hall-direction formal local thermal conductivity. As shown in Fig. 2 of the main text, the deviation between the directions of the white and black arrows leads to a significant increase in the Hall-direction formal local thermal conductivity, as this quantity quantitatively characterizes the degree to which the heat flux (black arrows) deviates from the direction opposite to the temperature gradient (white arrows). This indicates that the Hall-direction formal local thermal conductivity can serve as a quantitative metric for the negative temperature gradient phenomenon. Our simulation results also directly verify this spatial correspondence: the region with the most prominent negative temperature gradient coincides with a region of high Hall-direction local thermal conductivity k_H . In other words, the presence of the negative temperature gradient inherently signals the local breakdown of Fourier's law, and heat flux deflection provides a quantitative description of such non-Fourier transport behavior.

C. Saturation Behavior of Heat Dissipation Enhancement

The overall heat flux enhancement with reduced hotspot spacing will not increase without bound. Instead, it will converge to a finite saturation limit governed by the area ratio of the hotspot regions to the spacing regions.

As shown in Fig. S8, taking a substrate thickness $D = 500$ nm as an example, as the hotspot spacing decreases, the absorbed and unabsorbed heat fluxes decrease and increase, respectively, and eventually converge to the same value. It is observed that the increase in the total heat flux is nearly equal in

magnitude to the decrease in the absorbed heat flux. Consequently, as the decrease in the absorbed heat flux converges, the total heat flux cannot increase without bound.

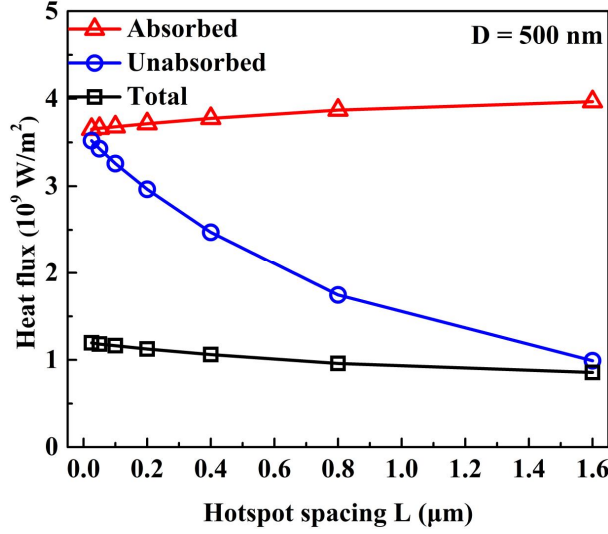


Fig. S8. Absorbed and unabsorbed heat fluxes as a function of hotspot spacing for a substrate thickness $D = 500 \text{ nm}$.

To further demonstrate that the peak formal local thermal conductivity does not diverge as the hotspot spacing approaches zero, its upper physical constraints are analyzed from two core contributing dimensions: the global total heat flux and the local first-drift phonon fraction.

The first contributing factor is the global heat flux enhancement of the system. Heat flux enhancement is a global property that describes the overall heat dissipation capability of the entire system, while the formal local thermal conductivity is a spatially resolved local quantity defined as the ratio of the Fourier-direction heat flux component to the magnitude of the local temperature gradient. The global increase in total heat flux is directly reflected in the magnitude of the local Fourier-direction heat flux component, and thus drives a corresponding rise in the formal local thermal conductivity. As demonstrated in the preceding analysis, the global heat flux enhancement will saturate at a geometrically constrained upper limit, so its contribution to local thermal conductivity will not increase without bound.

The second contributing factor is the local increase in the fraction of first-drift phonons, which further amplifies the formal local thermal conductivity. First-drift phonons are defined as phonons emitted from hotspots that have not yet undergone any intrinsic three-phonon scattering or boundary scattering. When first-drift phonons emitted from adjacent hotspots propagate into the spacing region and accumulate through superposition, they render the transport closer to ballistic transport and thereby increase the formal local thermal conductivity. However, this effect also has a clear physical ceiling: the fraction of first-drift phonons cannot exceed 100%, and their quasi-ballistic transport capacity is fundamentally limited by the phonon mean free path of the material. Once the hotspot spacing shrinks to a sufficiently small scale, the superposition effect of first-drift phonons from neighboring hotspots reaches saturation, and the formal local thermal conductivity cannot increase indefinitely.

With both contributing factors bounded by their respective physical constraints, the peak formal local thermal conductivity will inevitably converge to a finite saturated value, and no divergent behavior will occur as the hotspot spacing approaches zero.

D. Mean-Free-Path-Resolved Spectral Analysis of the Enhancement

To identify the dominant phonon governing overall heat transport, Fig. S9 (a) shows the MFP-

resolved cumulative effective thermal conductivity. To obtain these results, the contribution of each phonon bundle to the heat flux can be determined using Eq. S12, and the total heat flux is the sum of these individual contributions. Because each phonon bundle is associated with a distinct phonon MFP, the heat flux contributed by each phonon bundle can be converted into the heat flux contributed by phonons with different MFPs. In practice, the y -direction heat flux is extracted within a 50-nm-thick region adjacent to the heat sink. Dividing this heat flux by the temperature gradient between the hotspot (310 K) and the heat sink (300 K) then yields the contribution of phonons with each MFP to the effective thermal conductivity. This calculation is performed for hotspot spacings $L = 25, 400$, and 1600 nm at a substrate thickness $D = 500$ nm. The results reveal that thermal transport across the substrate is dominated by phonons with MFPs below 150 nm, which contribute more than 70% to the thermal conductivity. The cumulative effective thermal conductivity rises rapidly as phonons with progressively longer MFPs are included within the 0 – 150 nm range, while a marked slowdown in growth is observed for phonons with MFPs exceeding 150 nm. This behavior is caused by the suppression of long-MFP phonons through boundary scattering imposed by the finite substrate thickness, fully consistent with established nanoscale thermal transport phenomena [35].

To pinpoint the phonon responsible for the heat flux enhancement, Fig. S9 (b) presents the MFP-decomposed heat flux for reduced hotspot spacings. The heat flux is computed within a 50 nm-thick near-hotspot region adjacent to the top hotspots. The heat flux contributed by phonons of different MFPs is quantitatively evaluated for $L = 25, 400$, and 1600 nm. The results demonstrate that reducing the spacing enhances the contributions from phonons with MFPs below 150 nm, but the most dramatic increase occurs for those around 50 nm. Consequently, the heat flux enhancement induced by reduced spacing is predominantly carried by these sub- 150 nm MFP phonons.

This quantitative spectral evidence directly supports the proposed competition mechanism. In the large-spacing case, short-MFP phonons are absorbed by hotspots before reaching the spacing regions and thus make no contribution to the net heat flux toward the heat sink. When the hotspot spacing is reduced to a scale comparable to their MFPs, these phonons can instead reach the adiabatic boundaries of the spacing regions, be reflected, and redirect toward the heat sink. Consequently, short-MFP phonons are the primary contributors to the heat flux enhancement: they are largely absorbed by hotspots in the large-spacing configuration, whereas in the small-spacing case they can be scattered by boundaries and continue to participate in thermal transport.

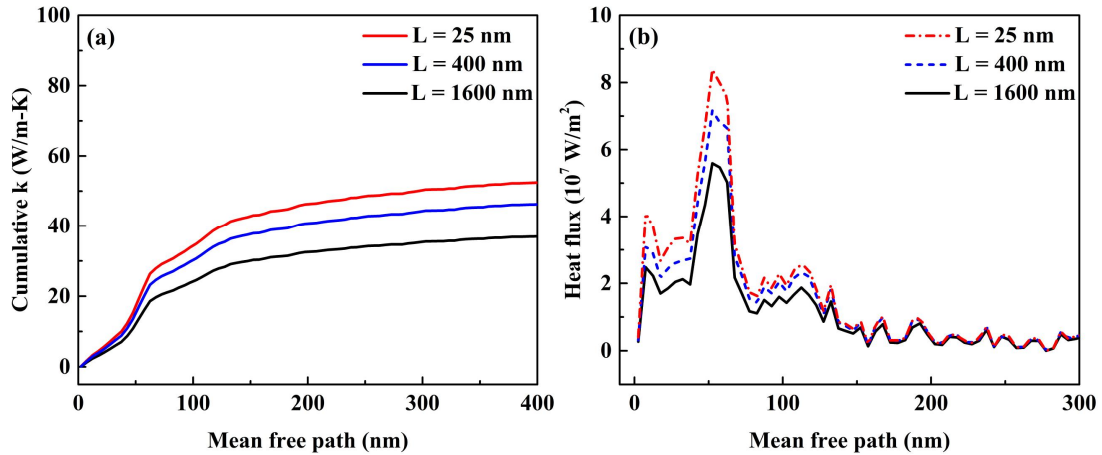


Fig. S9. MFP-resolved phonon transport analysis of heat flux. (a) Cumulative effective thermal conductivity as a function of phonon MFP for hotspot spacings $L = 25, 400$, and 1600 nm. (b) MFP-decomposed heat flux for $L = 25, 400$, and 1600 nm.

E. Thickness Dependence of the Enhancement Effect

This section supplements the Results and Discussion section of the main text, focusing on the heat flux enhancement mechanism and further elaborating on the underlying causes of its thickness-dependent behavior.

As previously discussed, heat flux enhancement from reduced hotspot spacing arises from a competition between phonon-boundary scattering and phonon absorption by hotspots. The main process of this competition is demonstrated in Fig. 4 of the main text, which shows that phonons returning toward hotspots are either absorbed by hotspots or scattered by boundaries, and the relative proportion of these two processes is jointly determined by hotspot spacing and phonon MFP.

This competition reduces the fraction of phonons absorbed by hotspots, and the extent of this reduction also depends on substrate thickness. When thickness is much smaller than the phonon MFP, transport is nearly ballistic and few phonons return to hotspots; when it is much larger than the phonon MFP, extensive phonon-phonon scattering allows phonons to reach distant boundaries. In both limits, the absorbed and unabsorbed fractions approach near-equality, leaving little room for further reduction in absorption. Consequently, the enhancement first increases and then decreases with substrate thickness.

V. Experimental Comparison and Discussion

A. Trend Comparison with Experimental Measurements

The following simulation settings are adopted to closely approximate the experimental conditions. A substrate thickness of $1\ \mu\text{m}$ is selected. In the top region, the isothermal boundary covers 25% of the total period, i.e., a constant 25% duty cycle is maintained. The thermal resistance is calculated by dividing the temperature difference by the heat flux. The temperature difference is taken as the 10 K gap between the isothermal boundary (310 K) and the heat sink boundary (300 K). A lateral region matching the width of the isothermal boundary region is chosen, and the heat flux is extracted from a 50-nm-thick layer adjacent to the heat sink. In experimental measurements, when the hotspot size grows much larger than the dominant phonon mean free path, the extracted thermal resistance converges to that under uniform heating [36,37]. To better replicate the physical scenario probed in experiments, the heat flux is taken from a region that matches the width of the isothermal boundary region. After the thermal resistance is obtained, all values are normalized by the maximum thermal resistance in the series.

The normalized thermal resistance is presented in Fig. S10. The comparison confirms good agreement between the simulation predictions and the experimental trends. For a fixed period with decreasing hotspot size, the normalized thermal resistance increases monotonically as the hotspot size shrinks, consistent with the trend of the experimental results. For the case where both the hotspot size and the spacing decrease simultaneously while a constant 25% duty cycle is maintained, the normalized thermal resistance exhibits clear non-monotonic behavior: it first rises to a peak when the characteristic length matches the dominant phonon mean free path of silicon, then decreases notably as the spacing shrinks further. This directly reproduces the experimentally observed enhanced heat dissipation in closely spaced nanoscale heat sources.

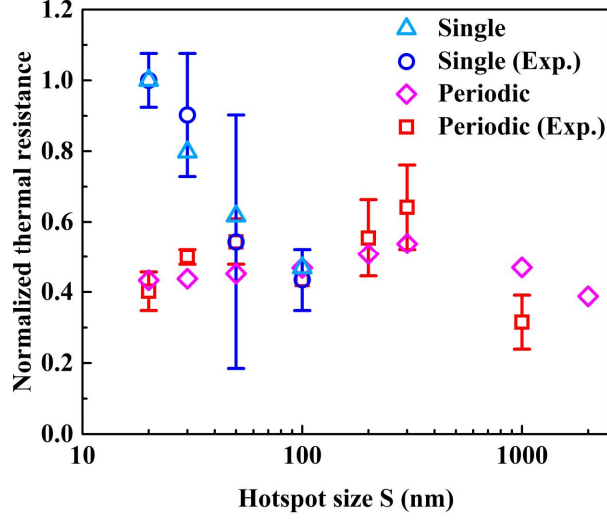


Fig. S10. Comparison of normalized thermal resistance between simulation and experimental results [37].

B. Correspondence between Formal Local Thermal Conductivity and Measurable Quantities

In well-established extreme ultraviolet (EUV) scatterometry studies of nanoscale heat sources, the effective Fourier model (EFM) serves as the standard analytical framework, whose core relation is as shown below, from previous work [37]:

$$r_{eff} = d \ln \left(\frac{P}{L} \right) \left(\frac{1}{K_{nano}} - \frac{1}{K_{bulk}} \right) + r_{tbr} \quad (S17)$$

where r_{eff} is the effective thermal boundary resistivity fitted from experimental relaxation curves; r_{tbr} is the intrinsic interface thermal boundary resistance; K_{nano} is the lumped effective nanoscale thermal conductivity encapsulating all non-diffusive effects; K_{bulk} is the bulk thermal conductivity of the substrate; d is the characteristic depth over which the nanoscale geometry modulates thermal transport; and L and P are the linewidth and period of the heat sources. The geometry-dependent non-diffusive correction term can be explicitly separated:

$$r_{corr} = r_{eff} - r_{tbr} = d \ln \left(\frac{P}{L} \right) \left(\frac{1}{K_{nano}} - \frac{1}{K_{bulk}} \right) \quad (S18)$$

The conventional EFM relies on the simplifying assumption of uniform thermal conductivity beneath the heat sources, yielding only a phenomenological global average. Our proposed formal local thermal conductivity $k_F(x, y)$ generalizes this lumped parameter into a spatially resolved form: physically, the correction term r_{corr} corresponds to the weighted integral of the local thermal resistance deviation along the heat flux path:

$$r_{corr} = \frac{1}{L} \int_0^P \int_0^D \left(\frac{1}{k_F(x, y)} - \frac{1}{K_{bulk}} \right) dy dx \quad (S19)$$

where D corresponds to the empirical parameter d in the EFM formula. This integral relation is a mechanistic correspondence framework rather than a direct quantitative conversion formula. In this substitution, the conventional uniform assumption adopted in EFM can be viewed as a special case of this integral relation under the approximation of spatially invariant thermal conductivity, where the spatially non-uniform $k_F(x, y)$ is simplified to a single lumped effective value K_{bulk} . By resolving the spatial distribution of thermal transport capability, the formal local thermal conductivity breaks through the limitation of this uniform approximation and uncovers the spatially non-uniform physical mechanism behind the phenomenological effective thermal resistance. Notably, direct experimental measurement of

the full spatial distribution of formal local thermal conductivity remains technically challenging at present.

Within this framework, the discrepancies between measurement results from different thermal characterization techniques can be naturally reconciled. Different measurement techniques have inherently different spatial sensitivities: EUV scatterometry is highly sensitive to thermal transport in the topmost region adjacent to the heat source [37,38], while time-domain thermoreflectance probes a deeper range determined by the thermal penetration depth [39,40]. In effect, each technique performs a weighted average of the same non-uniform $k_F(x, y)$ field over its respective sensitive spatial range, leading to different lumped effective values.

We note that this unified perspective offers a plausible physical origin for cross-technique differences, but it does not exclude contributions from other experimental factors such as sample quality, interface roughness, and measurement uncertainties. A complete quantitative reconciliation requires more systematic cross-technique experiments under well-controlled conditions.

C. Material Generality of the Core Conclusions

The core physical mechanism revealed in this work suggests a physically plausible qualitative trend for phonon-dominated semiconductor materials: reducing the spacing between nanoscale hotspots generally enhances overall heat dissipation. While the underlying physical principle is qualitatively generalizable, the specific magnitude of enhancement, the critical length scale at which the effect becomes prominent, and the detailed spatial distribution of formal local thermal conductivity are expected to be modulated by the specific phonon mean free path spectrum and dispersion relation of each material. The enhanced heat dissipation in closely spaced nanoscale hotspots arises from a change in the ratio of phonon absorption by the hotspots to phonon reflection at the adiabatic spacing boundaries. The spatial non-uniformity of formal local thermal conductivity originates from quasi-ballistic transport near nanoscale heat sources. These are intrinsic size effects of phonon transport that consistently emerge when characteristic dimensions (hotspot size and spacing) are comparable to the phonon mean free path, though their quantitative manifestations vary across materials.

Furthermore, this qualitative trend is corroborated by prior experimental observations across different material systems. Hoozeboom-Pot et al. discovered the collectively diffusive regime, in which closely packed nanoscale heat sources exhibit faster cooling, on both silicon and sapphire substrates [36].

D. Outlook on Experimental Validation

This section supplements the Results and Discussion section of the main text, focusing on the challenges and future outlook for experimental validation of the proposed formal local thermal conductivity characterization framework.

The direct experimental mapping of formal local thermal conductivity remains challenging, primarily due to the difficulty in resolving the heat flux field at the nanoscale. Although recent advances in scanning transmission electron microscopy electron energy-loss spectroscopy (STEM-EELS) have enabled sub-nanometer temperature resolution [3,41], measuring local heat flux in periodic hotspots is still formidable [6]. Alternatively, indirect validation can be pursued by comparing the measured temperature gradient fields, obtained via techniques such as STEM-EELS or tip-enhanced Raman thermal measurement [1,42], with those predicted by phonon BTE simulations.

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