

Advances in thermal phonon engineering and thermal management

Cite as: Appl. Phys. Lett. **127**, 060401 (2025); doi: [10.1063/5.0281609](https://doi.org/10.1063/5.0281609)

Submitted: 20 May 2025 · Accepted: 29 July 2025 ·

Published Online: 12 August 2025



View Online



Export Citation



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Note: This paper is part of the APL Special Collection on Advances in Thermal Phonon Engineering and Thermal Management.

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ABSTRACT

Recent years have seen major developments in thermal management approaches for semiconductors and thermoelectric materials, which serve as critical technologies for achieving carbon neutrality. Modern electronic and optoelectronic devices require effective heat dissipation and thermal energy conversion to achieve better performance and maintain reliability and efficiency. In particular, as device dimensions continue to shrink to the nanoscale, conventional bulk thermal transport theories become inadequate, necessitating a deeper understanding of phonon transport mechanisms at interfaces, in nanostructures, and across heterogeneous systems. The field of phonon engineering has emerged through the convergence of several scientific disciplines: Theoretical modeling of phonon heat transport together with nanoscale thermal measurement methods, advanced materials development, and materials informatics approaches have driven the development of phonon engineering. The combination of multiple scientific disciplines has sped up advancements in our knowledge and ability to control thermal transport at micro- and nanoscale levels.

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This Special Topic collection presents a variety of research in thermal phonon engineering and thermal management, including both fundamental scientific advances and practical applications. The collection spans a broad range of topics, including interfacial thermal transport,¹ phononic crystals,² nanoscale thermal characterization,³ thermal materials,⁴ and device designs for thermal management.⁵ By providing these diverse but interrelated studies, we aim to provide a comprehensive overview of the current state of the field and to highlight directions for future research and development.

The understanding and controlling thermal transport across interfaces remains one of the most critical challenges in thermal management. Multiple articles in this collection focus on this important aspect, exploring different material combinations and interface engineering strategies. Khan *et al.* investigated the thermal conductance across interfaces between titanium nitride and group IV semiconductors at high temperatures,⁶ which is relevant for high-temperature electronic applications. They illustrated how temperature influences phonon transport across heterogeneous material interfaces. Li *et al.*

demonstrated wafer-scale bonding of GaN–AlN with high interface thermal conductance,⁷ a promising method in thermal management of wide-bandgap semiconductor devices. The relationship between interface structure and thermal conductance was further explored by Yang *et al.* in their study of phonon transport across rough AlGaN/GaN interfaces with varying Al–Ga atomic ratios.⁸ Their work highlights how compositional gradients affect interfacial thermal transport. Tian *et al.* proposed an approach to enhance phonon transport across AlN/SiC interfaces by fast annealing of amorphous layers,⁹ demonstrating a potential method to overcome the thermal resistance typically introduced by interfacial disorder. Interfacial thermal transport in two-dimensional (2D) material systems has also received considerable attention. Li *et al.* reported differences in interfacial thermal transport behavior in MoS₂/Si heterostructures over optical phonon modes,¹⁰ while Zheng *et al.* studied the substrate-independent thermal conductance of Al/graphene/dielectric interfaces over a wide temperature range.¹¹ These works expand our knowledge of how heterogeneous systems can be formed through the integration and use of 2D materials

and still allow for effective heat dissipation. Han and Lee provided important insights into thermal resistance across Si–SiGe alloy interfaces from phonon distribution mismatch,¹² which has implications for thermoelectric and microelectronic applications. Albrigi and Rurali used nonequilibrium molecular dynamics to investigate phonon transport across GaAs/Ge heterojunctions.¹³ Utilizing experimental and modeling techniques, Meng and Yuan studied the role of electron–phonon coupling in interfacial thermal transport, presenting the effects of electron–phonon coupling on thermal boundary conductance in metal–dielectric systems.¹⁴ This paper informs the coupling mechanisms of electronic and phononic thermal transport at interfaces.

The thermal transport characteristics at the nanoscale are different from macroscopic behavior, and this presents both significant opportunities, and, of course, challenges, regarding heat transfer and management. This collection comprises a number of contributions that investigate such matters in a number of different nanomaterials and nanostructures. Wang and Sun measured a large size effect on thermal conductivity in diamond microparticles,¹⁵ showing how effectively the size of crystallites can dictate thermal transport in this material with extremely high thermal conductivity. In Si-based systems, Kurbanova *et al.* examined multiscale phonon thermal transport in nano-porous Si,¹⁶ while Nkenfack *et al.* assessed the thermal conductivity of shape-modulated Si nanowires using a Monte Carlo method and the Green–Kubo formalism.¹⁷ These studies provide a more complete picture of how nanostructuring affects phonon transport in semiconductor materials. The thermal behavior of nanowires in conjunction with other nanostructuring methods has been a particular focus. Chen *et al.*, for instance, investigated the strain effects on the thermal conductivity of 3C–SiC nanowires,¹⁸ with the purpose of showing how mechanical deformation can be used to tune thermal properties. Wang and Bao investigated size-dependent thermal transport properties of advanced metallic nanowire interconnects,¹⁹ which have important implications for thermal management in nanoelectronics. Anufriev *et al.* demonstrated quasi-ballistic thermal transport in SiC nanowires,²⁰ providing evidence for phonon mean free paths exceeding nanowire dimensions under certain conditions. In their work with 2D materials, He *et al.* investigated the effect of hydrogen bond configuration on the lattice thermal conductivity of hydrogenated borophene²¹ and demonstrated that functionalizing the surface was a path to tuning thermal transport. Likewise, Wang *et al.* studied anomalous thermal conductivity in 2D silica nanocages with immobilized noble gas atoms,²² demonstrating avenues for manipulating phonon transport in 2D systems. The thermal properties of thin films were also investigated: thermal conductivity reduction due to phonon geometrical scattering in nano-engineered epitaxial Ge.²³ Advances in computational methods for predicting thermal behavior at the nano-scale were proposed by Takahara *et al.*, who devised an extended volume of fluid scheme to simulate phonon transport in nano-structured thin films.²⁴

The development and characterization of materials with tailored thermal properties constitute a significant portion of this collection. These studies span a wide range of material systems, from conventional semiconductors to advanced compound materials. Several studies focused on SiC-based materials, which are particularly promising for high-temperature and high-power applications. Farzadian *et al.* investigated nanoscale spatially resolved thermal transport in nano-crystalline 3C–SiC,²⁵ providing insights into grain boundary effects on thermal conductivity. The interaction between phonons and structural

features was further explored by Isaiev *et al.*, who examined features of phonon scattering by spherical pores using molecular dynamics.²⁶ Additionally, BN materials, which are widely known for their excellent thermal properties, are well represented in this collection. Guo *et al.* provided first-principles predictions of thermal conductivity in bulk hexagonal BN,²⁷ while Zhang *et al.* explored the phonon properties of cubic BN with vacancy defects and isotopic disorders using neural network potentials.²⁸ These studies advance our fundamental understanding of thermal transport in these technologically important materials. Advanced thermoelectric materials received significant attention. Jin *et al.* investigated anomalous thermal transport and high thermoelectric performance in Cu-based vanadate CuVO₃,²⁹ and Hung explored the role of spin–orbit interaction in the low thermal conductivity in Mg₃Bi₂.³⁰ These materials show promise for efficient thermal energy conversion. Additionally, Yamamoto *et al.* observed phonon drag thermopower persisting over 200 K in FeSb₂ thin films on SrTiO₃ single crystals,³¹ demonstrating remarkably strong phonon–electron coupling effects. Li *et al.* investigated oxide materials with interesting thermal properties, demonstrating wide-range thermal conductivity modulation from protonated nickelate perovskite oxides.³² Shiga *et al.* studied thermal transport and topological properties of heat-carrying modes in amorphous alumina of various densities,³³ providing perspectives on thermal transport in disordered systems. Wang *et al.* contributed to the fundamental understanding of the lattice thermal conductivity of solids by studying the thermal conductivity of CsCl and emphasized the importance of quartic anharmonicity.³⁴ Yang *et al.* utilized machine learning potentials to study the importance of four-phonon scattering in asymmetrical monolayer 1T′–ReS₂,³⁵ thus demonstrating the relevance of higher-order phonon interactions in certain material systems. The thermal properties of more complex systems were also investigated. Donovan *et al.* studied propagon boundary scattering in multiphase GeTe,³⁶ while Hu *et al.* examined topological phonons and thermal conductivity of 2D Dirac semimetal PtN₄C₂.³⁷ Hirt *et al.* investigated thermal conductivity and electron–phonon coupling in AlSc intermetallic phases.³⁸ Each of these studies provides insights into the thermal behavior of metal alloys.

Computational methods and theoretical frameworks play a crucial role in advancing our understanding of thermal transport phenomena. This collection contains several contributions introducing computational methods in thermal phonon engineering. The role of machine learning methods is quickly emerging in this space. Lee and Xia constructed a universal harmonic interatomic potential to predict phonons in crystalline solids via machine learning.³⁹ These findings reinforce that data-driven methods can translate phonon property predictions. Zhou *et al.* investigated the extreme sensitivity of higher-order interatomic force constants and thermal conductivity predictions to the energy surface roughness of exchange-correlation functionals.⁴⁰ These findings are valuable for considering first-principles calculations of thermal properties. Advanced theoretical frameworks were also proposed. Cappai *et al.* introduced the concept of generalized thermal diffusivity to understand coupled heat-charge transport in ionic solutions,⁴¹ extending thermal transport concepts to electrochemical systems. Wu *et al.* focused on optimizing the performance of thermal transistors based on negative differential thermal resistance,⁴² exploring analogies between thermal and electronic transport. Boudan *et al.* compared classical and generalized Kirchhoff's laws in anisothermal structures,⁴³ providing important insights for radiative heat transfer

analyses. Rajabpour *et al.* investigated extreme near-field heat transfer between silica surfaces,⁴⁴ advancing our understanding of radiative thermal transport at nanoscales. The computational prediction of thermal properties in complex systems was demonstrated by Gokhale and Jain, who studied cross-plane thermal transport in layered materials.⁴⁵ Similarly, Shen and Cao proposed a two-temperature principle to assess the electrothermal performance of GaN HEMTs,⁴⁶ which provides a practical approach for thermal management at the device-level.

The practical application of thermal phonon engineering principles to device and system-level thermal management is a critical aspect of this field. Several studies in this collection focus on technologies for efficient thermal control and energy conversion. Luo *et al.* demonstrated scalable capillary-pin-fin structures for efficient flow boiling,⁴⁷ showcasing an innovative approach to phase-change heat transfer enhancement. Wang *et al.* investigated methods for suppressing the Leidenfrost effect using air discharge assisted electrowetting-on-dielectrics,⁴⁸ which has implications for high-heat-flux cooling technologies. In the area of thermal energy conversion, Koike *et al.* developed a planar-type SiGe thermoelectric generator with a double cavity structure,⁴⁹ demonstrating efficient thermoelectric energy conversion. Li *et al.* observed a colossal barocaloric effect in a spin-crossover compound near room temperature,⁵⁰ suggesting potential applications in solid-state cooling technologies. Thermal sensing and detection technologies were also represented in this collection. Bourgault *et al.* developed a thermal detector based on a suspended polyimide membrane for infrared radiation applications,⁵¹ advancing our capabilities for sensitive thermal measurements. The integration of thermal management strategies into electronic devices was demonstrated in several studies. Shwe *et al.* investigated local augmentation of phonon transport at GaInN/GaN heterointerfaces by introducing graded variations of InN mole fraction,⁵² offering a strategy for managing heat in optoelectronic devices. Shen and Cao put forward a two-temperature principle for evaluating the electrothermal performance of GaN HEMTs,⁴⁶ providing a framework for thermal analysis in high-power electronic devices. New approaches for controlling thermal transport were also explored. Song *et al.* demonstrated electrically regulated thermal conductivity in aramid polymer systems,⁵³ showing how external stimuli can be used to modulate thermal properties. Li *et al.* studied *in situ* annealing of nanoporous Si thin films with transmission electron microscopy,⁵⁴ providing insights into the evolution of thermal properties during processing.

This collection showcases the progress and diversity of research in this swiftly evolving field of thermal phonon engineering and thermal management. The papers in this collection illustrate the maturity of our understanding of thermal transport at the nanoscale and its implementation toward practical technologies in thermal management and energy conversion. Looking ahead, this collection presents some exciting trajectories of research. The ongoing advancement of data-driven and machine learning approaches to predicting and optimizing thermal properties presents incredible opportunities for accelerated materials discovery. The utilization of quantum and topological phenomena in phonon transport could lead to emerging thermal functionalities that may not be realized using conventional approaches. The integration of multiple thermal management approaches—materials to devices to systems—will be critical to solve the thermal challenges presented by next-generation electronics, energy systems, and quantum technologies. Phonon transport manipulation through strategic

interfacial and nanostructure engineering will continue to generate research prospects. As demonstrated by several papers, interfaces play a crucial role in determining overall thermal behavior, and strategies to control interfacial thermal resistance could lead to transformative technologies. The thermal management of device technologies, including those based on wide-bandgap semiconductors, 2D materials, and quantum systems, will require continued innovation in both fundamental understanding and practical implementation. The integration of artificial intelligence for real-time thermal management and the development of adaptive thermal systems represent exciting frontiers that build upon the foundation established by the work presented in this collection. At the same time, there is an increasing number of intersections between thermal phonon engineering and their adjacent fields, including spintronics, valleytronics, and quantum information science, that may also lead to hybrid technologies using thermal phonons in conjunction with other physical phenomena.

We believe that this collection provides a valuable snapshot of the current state of thermal phonon engineering and thermal management research and hope that it will inspire further advances in this field. Interdisciplinary and international collaboration will be essential to address the grand challenges in thermal management for a sustainable future.

The authors thank Maria Antonietta Loi, Satoshi Iwamoto, Nikaela Bryan, Jessica Trudeau, and Jaimee-Ian Rodriguez for their technical assistance with publishing.

AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Masahiro Nomura: Conceptualization (equal); Project administration (equal); Supervision (equal); Writing – original draft (equal); Writing – review & editing (equal). **Sebastian Volz:** Validation (equal); Writing – original draft (equal); Writing – review & editing (equal). **Bing-Yang Cao:** Validation (equal); Writing – original draft (equal); Writing – review & editing (equal). **Zhitong Tian:** Validation (equal); Writing – original draft (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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