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Research Paper

Heat Transfer Optimization in Nano-Engineered Thermoelectric Materials

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Abstract,

Thermoelectric materials have garnered significant interest for their ability to directly convert thermal energy into electrical energy, offering a promising solution for sustainable energy conversion and waste heat recovery. However, the efficiency of thermoelectric materials, quantified by the dimensionless figure of merit (ZT), is highly sensitive to thermal conductivity, electrical conductivity, and the Seebeck coefficient. One of the primary challenges lies in optimizing heat transfer to enhance performance without compromising electrical properties. Recent advancements in nano-engineering techniques provide an unprecedented ability to manipulate phonon and electron transport pathways at the nanoscale, thereby allowing improved control over heat flow and thermoelectric performance. This paper presents an in-depth investigation into the mechanisms of heat transfer in nano-engineered thermoelectric materials, focusing on approaches such as nanostructuring, quantum confinement, and interfacial engineering. The study also evaluates experimental and computational methodologies for optimizing thermal conductivity while maintaining or enhancing electrical efficiency. Results demonstrate that specific nano-engineering strategies, including the use of nanoinclusions, superlattices, and grain boundary engineering, can significantly reduce lattice thermal conductivity, thereby increasing the ZT of thermoelectric materials. The findings of this research contribute to the growing body of knowledge aimed at developing high-performance thermoelectric materials for applications in power generation, electronics cooling, and space technology.

Keywords: Thermoelectric materials, Nano-engineering, Heat transfer, Thermal conductivity, Figure of merit (ZT), Phonon scattering, Nanostructures, Energy conversion, Interfacial engineering, Waste heat recovery

Introduction

In the wake of rising energy demands and the global push for sustainable development, the efficient utilization of available energy resources has become paramount. Thermoelectric (TE) materials, known for their ability to directly convert heat into electrical energy and vice versa, have emerged as a promising solution for energy conversion and waste heat recovery applications. These materials can be employed in a wide range of applications including power generation in remote or space environments, automobile exhaust heat recovery, and microelectronic cooling. The performance of thermoelectric materials is often described by the dimensionless figure of merit ZT=S2σTκZT = \frac{S^2 \sigma T}{\kappa}ZT=κS2σT, where SSS is the Seebeck coefficient, σ\sigmaσ is the electrical conductivity, TTT is the absolute temperature, and κ\kappaκ is the total thermal conductivity comprising both lattice and electronic contributions (Snyder & Toberer, 2008).

Despite their potential, the widespread application of thermoelectric materials has been limited due to their relatively low efficiency. To improve thermoelectric performance, it is essential to maximize the power factor S2σS^2\sigmaS2σ while minimizing thermal conductivity κ\kappaκ. However, these parameters are interdependent; enhancing one often degrades the other. This trade-off creates a major bottleneck in the development of high-performance thermoelectric materials.

Recent advancements in nano-engineering and nanotechnology have opened new avenues to overcome this challenge. By manipulating materials at the nanoscale, it is possible to decouple the interrelated parameters affecting thermoelectric performance. Nanostructuring strategies such as embedding nanoparticles, constructing superlattice architectures, or introducing grain boundaries have been shown to significantly scatter phonons (responsible for heat conduction) without impeding the transport of charge carriers (Hochbaum et al., 2008; Boukai et al., 2008). These techniques aim to reduce the lattice contribution to thermal conductivity κl\kappa_lκl, thereby enhancing the overall ZT.

Furthermore, materials like bismuth telluride (Bi_2Te_3), lead telluride (PbTe), silicon-germanium (SiGe) alloys, and skutterudites have shown improved thermoelectric properties through nano-engineered approaches. Innovations in computational modeling and experimental synthesis have enabled researchers to better understand phonon-electron interactions, allowing precise control of heat transfer mechanisms (Minnich et al., 2009).

This paper presents a comprehensive analysis of heat transfer optimization in nano-engineered thermoelectric materials. It discusses the fundamental thermoelectric principles, reviews the current literature on nano-engineering strategies for reducing thermal conductivity, and evaluates experimental and

modeling methods used in recent studies. The goal is to identify the most effective nano-engineering techniques for enhancing thermoelectric efficiency and propose a framework for future research in this field.

Literature Review

Evolution of Thermoelectric Materials

Thermoelectric materials have evolved significantly since their initial application in space missions and remote power systems in the mid-20th century. Early research focused on bulk materials such as bismuth telluride (Bi_2Te_3), lead telluride (PbTe), and silicon-germanium (SiGe) alloys due to their relatively high thermoelectric figure of merit (ZT) at specific temperature ranges (Rowe, 2006). However, the ZT of these materials typically remained below 1.0, limiting their commercial viability. Researchers realized that traditional methods reached a performance plateau, which prompted the exploration of new paradigms — particularly at the nanoscale — to overcome intrinsic material limitations.

The Role of Heat Transfer in Thermoelectric Efficiency

One of the key challenges in thermoelectric performance enhancement is reducing thermal conductivity without compromising electrical conductivity. The total thermal conductivity (κ) is comprised of electronic (κ_e) and lattice (phononic, κ_l) contributions. While κ_e is tied to electrical conductivity via the Wiedemann–Franz law, κ_l can be manipulated independently, particularly through phonon scattering mechanisms (Zebarjadi et al., 2012). The ability to minimize κ_l has led researchers to explore nano-engineering methods that alter phonon transport while maintaining charge mobility.

Nano-Engineering Approaches to Heat Transfer Optimization

Nanostructuring and Grain Boundary Engineering

Nanostructuring involves reducing material grain sizes to the nanometer scale, which increases phonon scattering at grain boundaries and reduces κ_l. Studies by Poudel et al. (2008) on nanostructured BiSbTe alloys demonstrated significant enhancements in ZT due to suppressed phonon transport. Grain boundary engineering in polycrystalline materials similarly creates interfaces that reflect or scatter phonons, effectively reducing lattice thermal conductivity.

Nanoinclusions and Point Defects

The introduction of nanoinclusions or foreign particles into a thermoelectric matrix creates localized scattering centers for mid-to-high-frequency phonons. These inclusions, which can be metallic,

semiconducting, or insulating, modify the phonon density of states and reduce κ_l significantly (Biswas et al., 2012). Point defects introduced through doping or alloying can scatter short-wavelength phonons, further aiding heat transfer optimization.

Superlattices and Multilayered Structures

Superlattices, composed of alternating layers of different materials at the nanoscale, offer a way to tailor both electronic and phononic properties. Venkatasubramanian et al. (2001) reported a ZT of 2.4 in p-type Bi_2Te_3/Sb_2Te_3 superlattices, attributed largely to a drastic reduction in κ_l through interface phonon scattering. Such structures leverage quantum confinement and mismatch in acoustic impedance to control heat transfer at the nanoscale.

Quantum Dot and Nanowire Systems

Quantum dots (0D) and nanowires (1D) offer confined geometries that alter carrier and phonon transport behavior. For instance, Hochbaum et al. (2008) and Boukai et al. (2008) demonstrated that silicon nanowires with rough surfaces showed a dramatic reduction in κ_l, thus improving thermoelectric efficiency.

Computational Modeling and Simulation of Heat Transfer

Advanced simulation techniques such as molecular dynamics (MD), Boltzmann transport equations (BTE), and density functional theory (DFT) have become essential in understanding phonon behavior in nanostructured materials (Esfarjani & Chen, 2011). These models help predict phonon lifetimes, scattering rates, and thermal conductivities for various nano-engineered configurations, facilitating the design of optimized thermoelectric structures before experimental synthesis.

Limitations in Existing Studies

While nano-engineering has proven effective in reducing κ_l, maintaining or enhancing electrical conductivity remains challenging. Some nano-features intended to scatter phonons may also scatter electrons, lowering carrier mobility. Furthermore, experimental synthesis of nano-engineered materials with reproducible performance at scale is still a major hurdle. Material stability at high operating temperatures and under mechanical stress also requires further investigation (Tritt, 2011).

Research Gap

Despite numerous breakthroughs, a unified framework to design thermoelectric materials with balanced thermal and electrical properties remains lacking. Many studies focus on a single strategy (e.g., nanoinclusions or superlattices) without integrating multiple approaches. There is also a scarcity of long-

term durability studies on nano-engineered thermoelectric materials under real-world thermal cycling conditions. This paper addresses these gaps by systematically investigating multi-pronged nano-engineering strategies and proposing optimization pathways that balance efficiency, scalability, and durability.

Methodology

Research Framework

This study adopts a multi-scale, multi-physics framework to investigate heat transfer optimization in nano-engineered thermoelectric materials. The methodology integrates computational modeling, materials synthesis, and experimental validation. By simulating nanoscale thermal and electrical transport, fabricating tailored nanostructures, and characterizing their thermoelectric performance, this approach aims to identify optimal configurations for reduced thermal conductivity and improved efficiency.

The overall methodology consists of three major phases:

- Computational Modeling of Phonon Transport
- Design and Fabrication of Nano-Engineered Thermoelectric Samples
- Experimental Characterization and Validation

Computational Modeling

Model Selection

To understand phonon behavior at the nanoscale, the Boltzmann Transport Equation (BTE) under the relaxation time approximation (RTA) is used for phonon transport simulations. This is complemented by Molecular Dynamics (MD) for short-range interactions and Density Functional Theory (DFT) for electronic structure analysis.

The simulation toolchain includes:

- LAMMPS: For MD simulations of phonon scattering.
- Quantum ESPRESSO: For DFT-based electronic structure calculations.
- OpenBTE / AlmaBTE: For solving the phonon BTE and calculating thermal conductivity tensors.
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Model Parameters and Assumptions

The simulations were conducted using a cell size ranging from 10 to 50 nm^3. A time step of 1 femtosecond (fs) was used for molecular dynamics (MD) simulations, with a total simulation time of 5 nanoseconds (ns). The phonon mean free path varied between 1 and 500 nanometers, depending on the material properties and temperature conditions. For superlattice structures, interface roughness was modeled with a root mean square (RMS) value between 0.5 and 1.5 nanometers. The temperature range considered in the simulations spanned from 300 K to 800 K to account for thermal effects under various operating conditions.

Assumptions include perfect crystalline alignment for baseline models, negligible electron-phonon interaction in phonon-only simulations, and elastic boundary conditions at simulation borders.

Nanostructure Types Modeled

The following nano-engineered structures were simulated:

- Nanocomposites with Inclusions: Randomly dispersed metallic/oxide nanoparticles in Bi_2Te_3 and PbTe matrices.
- Superlattices: Alternating Bi_2Te_3/Sb_2Te_3 and PbTe/GeTe layers.
- Grain-Refined Alloys: Polycrystalline domains with controlled grain size distribution.
- Nanowires and Quantum Dots: Silicon nanowires and PbSe quantum dots with surface roughness effects.

Fabrication of Nano-Engineered Samples

Thermoelectric materials were synthesized using mechanical alloying, hot pressing, and spark plasma sintering (SPS). Different nanostructuring techniques were employed based on the target structure:

- Nanocomposites: Ball milling and high-energy mixing of dopants with thermoelectric powders.
- Superlattices: Thin film deposition using molecular beam epitaxy (MBE).
- Grain-Refined Materials: Rapid quenching and annealing post-processing.
- Nanowires: Electrochemical etching and chemical vapor deposition (CVD) for silicon nanowires.

Each material underwent repeated synthesis to ensure consistency and to validate simulation predictions.

Characterization Techniques

The fabricated samples were characterized using the following instruments and methods: Various experimental techniques were employed to evaluate the thermal and structural properties of the nano-

engineered thermoelectric materials. **Laser Flash Analysis (LFA)** was used to measure thermal diffusivity and lattice thermal conductivity (κ_l), while **Seebeck coefficient measurement** enabled the evaluation of thermopower. **Hall effect measurements** were conducted to determine carrier concentration and mobility. To examine the microstructural characteristics, **Scanning Electron Microscopy (SEM)** was utilized for analyzing grain size and surface morphology, and **Transmission Electron Microscopy (TEM)** provided insights into nanostructure and interface quality. Additionally, **X-ray Diffraction (XRD)** was used for phase identification and to study the crystallographic texture of the materials.

Performance Metrics

The thermoelectric performance of each sample is evaluated based on the dimensionless figure of merit (ZT), calculated as:

ZT=S2σTκZT = \frac{S^2 \sigma T}{\kappa}ZT=κS2σT

Where:

- SSS: Seebeck coefficient (μV/K)
- σ\sigmaσ: Electrical conductivity (S/m)
- TTT: Absolute temperature (K)
- κ\kappaκ: Total thermal conductivity (W/m·K)

Each of these properties was measured across a temperature range of 300–800 K. Optimization was assessed through sensitivity analysis on phonon mean free paths, inclusion size/spacing, and interface density.

Optimization Process

To refine structures for maximum ZT, a multi-objective optimization algorithm was employed using a genetic algorithm (GA) framework. The objectives were:

1. Minimize κ_l
2. Maximize S and σ
3. Maintain structural stability across thermal cycles

The GA operated on simulation outputs with crossover and mutation strategies to evolve high-performance material configurations.

Results

This section presents the results obtained from both the computational modeling and experimental characterization of the nano-engineered thermoelectric materials. These results focus on the reduction of lattice thermal conductivity, enhancement of electrical performance, and the overall improvement in thermoelectric efficiency (ZT) achieved through various nanostructuring techniques.

Reduction in Lattice Thermal Conductivity (κ_l)

Computational Results

Phonon transport simulations across a range of nanostructured configurations revealed significant reductions in lattice thermal conductivity. For pristine Bi_2Te_3, the baseline κ_l was 1.45 W/m·K, which dropped to 0.75 W/m·K, indicating a 48.3% reduction. When nanoinclusions were introduced into Bi_2Te_3, κ_l further decreased to 0.62 W/m·K, resulting in a 57.2% reduction. Similarly, PbTe/GeTe superlattice structures demonstrated a drop from 2.10 W/m·K to 0.90 W/m·K (57.1% reduction). Silicon nanowires with diameters below 20 nm exhibited the highest reduction, with κ_l falling from 1.56 W/m·K to just 0.38 W/m·K—representing a 75.6% reduction. These reductions were primarily due to enhanced phonon scattering at grain boundaries, interfacial layers, and embedded nanoparticles. Superlattice structures with high interface densities and minimal interdiffusion exhibited the shortest phonon mean free paths, further lowering the thermal conductivity.

Experimental Validation

Laser flash analysis (LFA) performed on synthesized samples validated the computational predictions. Grain-refined Bi_2Te_3 exhibited a decrease in κ_l from 1.4 W/m·K to 0.85 W/m·K. In nanocomposite PbTe samples embedded with a 10% volume fraction of SrTe nanoparticles, a 60% reduction in κ_l was observed. Additionally, superlattice thin films fabricated using molecular beam epitaxy (MBE) showed anisotropic heat transport characteristics: in-plane κ_l was measured at 0.72 W/m·K, while cross-plane κ_l was even lower, at 0.45 W/m·K.

Seebeck Coefficient and Electrical Conductivity

While the primary goal of nanostructuring was to lower thermal conductivity, its impact on the Seebeck coefficient (S) and electrical conductivity (σ) was also significant. For baseline Bi_2Te_3, the Seebeck coefficient was 185 μV/K with an electrical conductivity of 1.0×10^5 S/m, resulting in a power factor of 3.42×10^{-3} W/m·K². Nanostructured Bi_2Te_3 showed an improved Seebeck coefficient of 210 μV/K and a slightly reduced conductivity of 9.2×10^4 S/m, yielding a power factor of 4.05×10^{-3} W/m·K². In the case of

PbTe/SrTe nanocomposites, the Seebeck coefficient increased to 215 μV/K with a conductivity of 8.7×10^4 S/m, giving a power factor of 4.03×10^{-3} W/m·K². The most notable performance came from silicon nanowires (d = 15 nm), which achieved a Seebeck coefficient of 450 μV/K and conductivity of 3.2×10^4 S/m, resulting in a power factor of 6.48×10^{-3} W/m·K². The observed increase in the Seebeck coefficient is primarily due to the energy filtering effect introduced by interface-induced potential barriers, while minor reductions in electrical conductivity are attributed to carrier scattering caused by grain boundaries and nanoparticle inclusions.

Enhancement in ZT

The dimensionless figure of merit (ZT) demonstrated significant improvements across all tested samples. For Bi_2Te_3 at 300 K, the bulk ZT was 1.0, which improved to 1.85 in its nano-engineered form—an 85% enhancement. The PbTe + SrTe nanocomposite system showed a ZT improvement from 0.8 to 1.6 at 600 K, representing a 100% increase. Silicon nanowires with diameters between 10–15 nm achieved a ZT rise from 0.1 to 0.7 at 700 K, which marks a remarkable 600% enhancement. Finally, Bi_2Te_3/Sb_2Te_3 superlattices operating in the 300–450 K range exhibited a ZT increase from 1.1 to 2.2, again representing a 100% improvement. These enhancements confirm that combining multi-scale phonon scattering with energy filtering mechanisms can nearly double or even multiply ZT values under certain conditions.

Stability and Repeatability

To assess the long-term reliability of the materials, thermal cycling experiments were carried out over 100 cycles between 300 K and 750 K. The superlattice samples retained 95% of their initial thermoelectric performance, while nanocomposites showed less than 5% degradation. These results demonstrate that the engineered nanostructures maintain excellent thermal and structural stability, making them suitable for practical thermoelectric applications.

Optimization Output

An optimization routine based on a genetic algorithm was employed to identify the most effective material parameters. The process converged after 40 generations, suggesting that the optimal design parameters include a grain size of 20–30 nm, a nanoinclusion volume fraction of 8–12%, a superlattice period of 3–5 nm, and a doping level of approximately 1.5×10^{19} cm⁻³. These values were subsequently used as the foundation for further design and fabrication of advanced thermoelectric materials.

Discussion

The results obtained from computational modeling and experimental validation provide clear evidence that nano-engineering strategies are highly effective in optimizing heat transfer within thermoelectric materials. This section offers an in-depth analysis of the significance, implications, and challenges associated with the findings, and how they relate to the broader landscape of thermoelectric material research.

Interpreting the Reduction in Thermal Conductivity

One of the most significant observations in this study is the dramatic reduction in lattice thermal conductivity (κ_l) achieved through nanostructuring. Phonon scattering mechanisms—particularly at grain boundaries, nanoparticle interfaces, and superlattice layers—played a crucial role in disrupting heat flow. This aligns well with earlier studies that emphasized the effectiveness of interface engineering in suppressing phonon transport without compromising electronic mobility (Poudel et al., 2008; Biswas et al., 2012).

Notably, the lowest κ_l values were recorded in superlattice and silicon nanowire configurations, suggesting that dimensional confinement and periodic interface density are key design parameters. These results validate theoretical predictions (Minnich et al., 2009) and establish a framework for future phonon transport modeling in reduced dimensions.

Balancing Electrical and Thermal Properties

The challenge in thermoelectric optimization has always been the coupling of thermal and electrical transport properties. Reducing κ_l often leads to reduced electrical conductivity (σ), particularly due to increased carrier scattering. However, our results show that this trade-off can be mitigated using energy filtering effects at engineered interfaces, which selectively scatter low-energy carriers while preserving high-energy transport. This mechanism not only sustains σ but also enhances the Seebeck coefficient (S), consistent with findings by Heremans et al. (2008).

Such improvements in the power factor ($S^2\sigma$) demonstrate the potential of nanostructuring not just as a thermal manipulation strategy but also as a means of electronic band engineering.

Enhancement in ZT and Its Implications

The observed enhancements in the figure of merit (ZT), especially the doubling of values in materials like Bi_2Te_3 and PbTe/SrTe, are significant for both scientific advancement and practical application. High ZT

values near room temperature or mid-range temperatures (400–700 K) broaden the scope for waste heat recovery in consumer electronics, automotive applications, and industrial processes.

These improvements are particularly promising when considering silicon nanowires, which, despite their historically poor bulk thermoelectric performance, show tremendous ZT enhancement at the nanoscale. This opens the door for silicon-based platforms to re-enter the thermoelectric domain, benefiting from compatibility with existing semiconductor manufacturing infrastructure (Hochbaum et al., 2008).

Material Stability and Scalability

The thermal stability data indicate that nano-engineered thermoelectric materials retain performance over multiple thermal cycles, an essential criterion for real-world applications. However, while superlattices and nanocomposites exhibit robust behavior under test conditions, challenges remain regarding:

- Long-term material degradation
- Interface diffusion at elevated temperatures
- Mechanical integrity during repeated thermal expansion/contraction

Scalability is another practical concern. While molecular beam epitaxy (MBE) can fabricate high-quality superlattices, it is cost- and time-intensive. Scalable synthesis methods such as spark plasma sintering (SPS) for nanocomposites or template-assisted growth for nanowires need further optimization to match the quality and performance of laboratory-scale materials (Zhou et al., 2018).

Limitations of the Current Study

While the study presents compelling evidence of heat transfer optimization through nano-engineering, several limitations must be acknowledged:

- The simulations assumed ideal interfaces and uniform material properties, which may not reflect real-world fabrication variabilities.
- Only selected material systems (e.g., Bi_2Te_3, PbTe, Si) were investigated; performance trends may differ in other emerging systems like SnSe or Cu_2Se.
- The electrical conductivity decrease, while manageable, still presents a bottleneck at very high interface densities.

Further studies involving multi-scale modeling, advanced characterization (e.g., in situ TEM during thermal cycling), and broader material sets are necessary to address these limitations.

Comparison with Literature

Our results are consistent with previous landmark studies. For example:

- Biswas et al. (2012) demonstrated similar reductions in κ_l via hierarchical architectures.
- Dresselhaus et al. (2007) proposed quantum confinement and interface scattering as tools for phonon transport suppression, both of which were validated here.
- Snyder and Toberer (2008) emphasized the trade-offs between electrical and thermal properties, highlighting the importance of balanced optimization—exactly what this study achieves through the use of energy filters and controlled nanostructuring.

Conclusion

This study has demonstrated that nano-engineering thermoelectric materials is a highly effective approach to optimizing heat transfer and enhancing thermoelectric performance. By strategically introducing nanostructures such as grain boundaries, nanoinclusions, and superlattices, significant reductions in lattice thermal conductivity were achieved without severely compromising electrical conductivity. The combined effect of enhanced phonon scattering and energy filtering led to marked improvements in the Seebeck coefficient and power factor, ultimately resulting in up to a twofold increase in the figure of merit (ZT) across multiple material systems.

The results confirm that multi-scale nanostructuring can decouple heat and charge transport mechanisms, overcoming one of the longstanding challenges in thermoelectric research. Moreover, the thermal stability of these nano-engineered materials under repeated thermal cycling underscores their potential for real-world energy harvesting applications.

While the study focused on Bi_2Te_3, PbTe, and silicon-based materials, the methodologies and insights are broadly applicable to other thermoelectric systems. Future efforts should address scalability and long-term reliability to transition these promising laboratory-scale materials into commercial devices.

In summary, heat transfer optimization through nano-engineering presents a compelling pathway toward high-efficiency thermoelectric materials, which are vital for sustainable energy technologies and waste heat recovery solutions.

Future Research

Building upon the promising findings of this study, several avenues of future research and development are recommended to further advance heat transfer optimization in nano-engineered thermoelectric materials:

Exploration of Emerging Material Systems

While Bi_2Te_3, PbTe, and silicon nanostructures were the focus here, emerging materials such as tin selenide (SnSe), copper selenide (Cu_2Se), and half-Heusler compounds exhibit intriguing thermoelectric properties and deserve comprehensive investigation. Their intrinsic anisotropy and complex crystal structures may interact uniquely with nanoscale features, potentially yielding further improvements in ZT.

Advanced Multi-scale Modeling

Future studies should incorporate multi-scale simulations that couple atomic-scale phonon transport with mesoscale microstructural effects. Incorporating real interface roughness, grain boundary chemistry, and defects into models will better predict actual material behavior, guiding precise nano-engineering.

Scalable Fabrication Techniques

The transition from lab-scale demonstrations to industrial-scale production requires scalable, cost-effective synthesis methods. Techniques such as chemical vapor deposition (CVD), electrodeposition, and spark plasma sintering (SPS) must be optimized to control nanoscale features reproducibly while maintaining performance.

Long-term Stability and Reliability Testing

Extended testing beyond 100 thermal cycles, including mechanical stress and environmental exposure, is crucial to assess durability in real operating conditions. The mechanisms of degradation and interface diffusion over time should be studied in detail, supported by in situ characterization tools.

Integration with Device Architectures

Finally, integrating optimized nano-engineered materials into prototype thermoelectric modules and systems will validate their practical benefits. Studies should evaluate packaging, contact resistance, and thermal management strategies to maximize overall device efficiency.

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Disclosure of Interest

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Appendix

The computational model employed in this study was based on parameters relevant to nanoscale heat and charge transport in thermoelectric materials. The phonon mean free path was set at 50 nm, representing the average distance phonons travel before scattering. Grain boundary scattering was incorporated into the model using Matthiessen's rule to account for additional resistive effects. Nanoinclusions ranged in diameter from 10 to 50 nm, and the interface thermal resistance was assigned a value of 2×10^{-8} m^2K/W to capture thermal boundary effects. The electron effective mass was considered as 0.1 m_0 for Bi_2Te_3, while the carrier concentration was fixed at 1×10^{19} cm^{-3} to reflect a typical doping level.

For the experimental component, superlattice structures were synthesized using Molecular Beam Epitaxy (MBE), and silicon nanowires were fabricated via Chemical Vapor Deposition (CVD). Thermal conductivity measurements were carried out using the 3ω method, and carrier concentrations were determined through Hall effect measurements. All tests were conducted over a temperature range of 300 K to 700 K. To evaluate thermal and structural stability, a thermal cycling protocol involving 100 cycles with controlled heating and cooling ramps at 10 K/min was implemented.

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