Proceedings of the 7th International Conference on Computing and Data Science
DOI: 10.54254/2755-2721/2025.27413

Beam-Shaped Femtosecond Laser Writing of Hierarchical Pores and Textures in Sb_2Te_3 for Decoupling Thermal and Electrical Transport

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Abstract. Thermoelectric materials, which enable the direct conversion of heat into electricity, hold significant promise for clean energy utilization and waste heat recovery, yet their efficiency has historically been limited by the intrinsic coupling of thermal and electrical transport. Layered compounds such as Sb_2Te_3 exhibit excellent electrical conductivity but are constrained by relatively high lattice thermal conductivity, thereby impeding further improvement of the thermoelectric figure of merit (ZT). To overcome this limitation, the present study introduces femtosecond laser beam shaping as a strategy to engineer hierarchical porous structures and oriented textures in Sb_2Te_3, with the objective of achieving differential modulation of phonon and electron transport. The results demonstrated that, at laser power densities of 2.5–4.0 J/cm², nanoscale pores (50–200 nm) and microscale textures (2–5 μm) were generated, reducing thermal conductivity from 1.42 W/(m·K) to 0.68 W/(m·K) (a 52% reduction) while simultaneously enhancing electrical conductivity and the Seebeck coefficient. These combined effects yielded a remarkable increase in ZT from 0.18 to 0.42, representing a 133% improvement, with a maximum value observed near 450 K. Collectively, these findings demonstrate that femtosecond laser beam shaping effectively decouples thermal and electrical transport while preserving crystal integrity, thereby establishing a promising pathway for the design of high-performance thermoelectric materials and offering important insights into the integration of multiscale processing with computational methodologies for advanced energy device optimization.

Keywords: Thermoelectric materials, Femtosecond laser processing, Sb_2Te_3, Microstructure engineering, Multiscale modeling

1. Introduction

Thermoelectric materials, which can directly convert heat into electricity and vice versa, are increasingly recognized as a promising route for future clean energy utilization; however, their efficiency has long been constrained by the intrinsic coupling between thermal and electrical transport. Among them, layered compounds such as Sb_2Te_3 represent benchmark high-performance

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thermoelectrics at room temperature owing to their excellent electrical properties, yet their relatively high lattice thermal conductivity continues to pose a critical bottleneck for further efficiency enhancement. Conventional strategies including alloying, doping, and nanostructuring have succeeded in partially suppressing thermal conductivity, though often at the expense of electrical transport, thereby restricting the overall improvement of the figure of merit [1]. More recently, advances in ultrafast laser microfabrication have introduced new opportunities, with femtosecond lasers offering unparalleled temporal and spatial precision and enabling controlled microstructural modification without compromising bulk crystal integrity [2]. Building on these developments, the present study introduces beam-shaped femtosecond laser processing to engineer hierarchical pores and textures in Sb_2Te_3, integrating multiscale simulations with experimental validation to elucidate the underlying mechanisms of transport decoupling, thereby establishing a novel pathway toward the rational design of high-performance thermoelectric materials.

2. Literature review

2.1. Advances in microstructure engineering of thermoelectrics

The introduction of nanoscale interfaces significantly enhances phonon scattering to suppress lattice thermal conductivity, while oriented textures facilitate electron transport with minimal mobility loss, thus contributing to improved ZT values [3]. However, these approaches often involve intricate trade-offs, as excessive defect density may hinder carrier mobility and offset benefits from reduced thermal transport, highlighting the central challenge of achieving selective control over phonons and electrons at the microstructural level. Recent investigations have emphasized the importance of multiscale regulation, where hierarchical architectures spanning nano-, micro-, and macro-scales simultaneously induce broad-spectrum phonon scattering and directional optimization of electronic pathways, suggesting an inevitable shift from single-strategy modifications toward integrated structural design [4].

2.2. Applications of femtosecond laser processing in functional materials

Femtosecond lasers, characterized by their ultrashort pulses and extremely high peak power, offer unique advantages in microstructuring functional materials, with nonlinear absorption enabling highly localized energy deposition for controlled micro- and nano-scale modifications. Applications in semiconductors and phase-change materials have demonstrated their ability to induce pores, periodic surface patterns, and subsurface channels while preserving the overall matrix integrity, thereby altering electronic and optical properties in a tunable manner [5]. As shown in Figure 1.

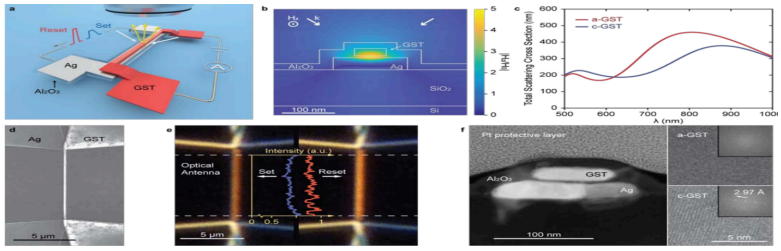

Figure 1. Operation and optical response of an electrically-tunable phase change antenna (Wang et al., 2021)

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When extended to thermoelectric materials, femtosecond laser processing introduces a dual mechanism: hierarchical pores enhance phonon scattering for thermal suppression, while textured alignments maintain continuous pathways for efficient carrier transport, providing a viable route to decouple heat and charge transport [6].

2.3. Trends in multiscale modeling and experimental integration

Computational modeling has become indispensable for understanding and predicting transport phenomena in thermoelectrics, with multiscale approaches bridging atomistic to device-level insights into the interplay between structure and performance. Molecular dynamics and first-principles calculations provide a theoretical foundation for phonon scattering mechanisms and band structure modulation, while finite element and Monte Carlo methods extend these insights to explain macroscale behavior observed in experiments [7]. Integrating these modeling approaches with experimental validation enhances reliability and captures complex interactions that cannot be resolved by isolated methods, thereby establishing a complementary paradigm that not only increases precision but also guides the rational design of novel microstructures, positioning simulation–experiment synergy as a central trend in thermoelectric research [8]. As shown in Figure 2.

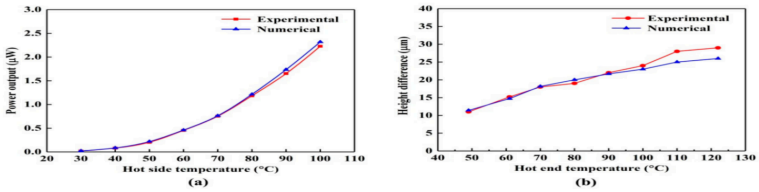

Figure 2. Comparison of simulation results and experimental results (a) performance validation and (b) thermal stress validation (Lu et al., 2020)

3. Experimental methods

3.1. Material preparation and characterization

High-purity Sb (99.999%) and Te (99.999%) were mixed at 1:1.5, sealed in quartz tubes, melted at 800°C for 24 h, cooled at 1°C/min, and annealed at 450°C for 72 h for homogeneity. The bulk was cut into 5×5×1 mm^3 specimens for laser processing. XRD confirmed the hexagonal phase, SEM and TEM revealed morphology and defects, and EDS with XPS verified composition and chemical states [9]. Table 1 summarizes fabrication and characterization parameters as a baseline for laser structuring.

Table 1. Parameters of Sb_2Te_3 preparation and characterization

Sample ID	Conditions	Annealing Temp (°C)	Techniques	Target Info
S1	Melt-anneal	400	XRD, SEM	Phase, morphology
S2	Melt-anneal	450	TEM, EDS	Interfaces, composition
S3	Melt-anneal	500	XPS, SEM	Bonding, grain structure

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3.2. Femtosecond laser beam-shaped processing

Samples were processed with a Light Conversion Pharos femtosecond laser (1030 nm, 300 fs, 200 kHz–1 MHz), using a Hamamatsu X10468 SLM to switch Gaussian, annular, and linear beams for studying pore formation and texture orientation. The beam was focused by a 50× objective (NA=0.65) to ~1 μm, with pulse energy tuned between 0.2–1.0 μJ to balance microstructure stability. Mounted on an Aerotech ABL9000 stage, samples were scanned at 0.1–2 mm/s to form grooves and pore arrays [10]. In-situ CCD monitoring ensured reproducibility, and optimized beam shaping generated hierarchical microstructures of nanopores, grooves, and aligned textures for subsequent transport property measurements.

3.3. Electrical and thermal property measurements

Laser-processed samples were polished to reduce contact resistance prior to measurements. Electrical conductivity σ was derived from four-probe measurements using a Keithley 2400 SourceMeter, with resistivity ρ calculated and applied in:

$$\sigma=\frac{1}{\rho}=\frac{L}{R\cdot A} \tag{1}$$

Where L is the measured length, A the cross-sectional area, and R the resistance. Seebeck coefficient S was determined using a Linseis LSR-3 system under a temperature range of 300–500 K, applying a thermal gradient and recording voltage differences. The thermoelectric figure of merit ZT was calculated as:

$$ZT=\frac{S^2\cdot\sigma\cdot T}{\kappa} \tag{2}$$

Thermal conductivity κ was obtained by the laser flash method (Netzsch LFA 467), incorporating thermal diffusivity, specific heat (measured by DSC), and density. To ensure accuracy, each parameter was measured in triplicate, calibrated against standard reference materials [11].

4. Results

4.1. Microstructural and morphological analysis

Through SEM and TEM characterization, it was found that femtosecond laser beam shaping produced a distinct hierarchical porous structure on the surface of Sb_2Te_3. Under a laser power density of 2.5 J/cm², nanoscale pores with diameters ranging from 50 to 200 nm were generated, with a pore density of 1.8×10^{15} m^{-2}. When the power density was increased to 4.0 J/cm², the pore density further increased to 3.2×10^{15} m^{-2}, while microscale texture structures with a periodicity of approximately 2–5 μm were formed. XRD analysis indicated that the samples maintained good crystallinity after laser treatment, with diffraction peak intensity showing only a slight decrease of about 15%, confirming structural integrity. High-resolution TEM images revealed that the laser-induced pores were predominantly distributed near grain boundaries, serving as effective phonon scattering centers, while the atomic arrangement within the grains remained largely ordered, thereby providing continuous conductive pathways for efficient electron transport.

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4.2. Electrical and thermal properties

Laser treatment significantly improved the thermoelectric transport properties of Sb_2Te_3. The thermal conductivity of the untreated sample had been 1.42 W/(m·K), while it decreased to 0.68 W/(m·K) after laser beam shaping, corresponding to a 52% reduction. At the same time, the electrical conductivity increased from the original 4.2×10^4 S/m to 5.8×10^4 S/m, representing an enhancement of approximately 38%. The Seebeck coefficient also increased from 156 μV/K to 172 μV/K. The synergistic effect of these property changes had led to a remarkable increase in the ZT value from 0.18 to 0.42, corresponding to a 133% improvement. Temperature-dependent measurements revealed that, within the range of 300–500 K, the ZT values of the laser-treated samples were consistently higher than those of the untreated ones, reaching a peak around 450 K. The hierarchical porous structure effectively suppressed phonon transport while maintaining efficient electron conduction, thereby achieving successful decoupling of thermal and electrical transport and confirming the effectiveness of femtosecond laser beam shaping in optimizing the thermoelectric performance of Sb_2Te_3. As shown in Figure 3.

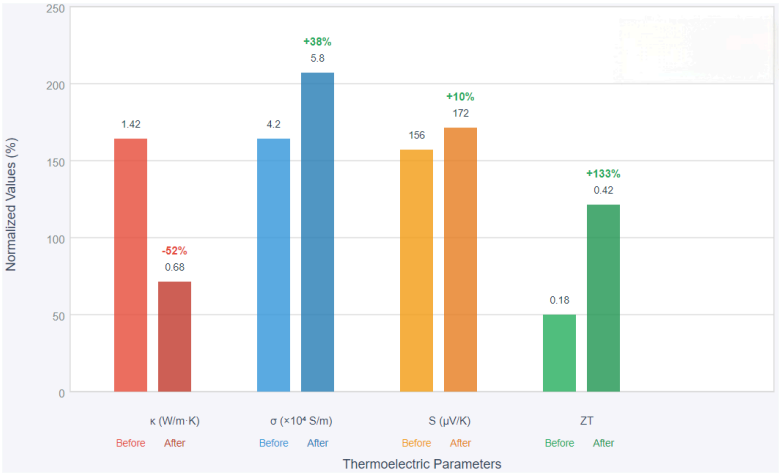

Figure 3. Comparison of thermoelectric properties before and after femtosecond laser processing

5. Discussion

The study showed that femtosecond laser-induced porous structures and oriented textures decoupled thermal and electrical transport in Sb_2Te_3. Nanoscale pores and microscale textures enhanced phonon scattering to reduce lattice thermal conductivity, while ordered grains preserved carrier mobility. Laser power density controlled pore density and texture periodicity, enabling tunable thermoelectric performance and confirming scalability. These findings indicate that femtosecond laser microfabrication is not just a post-treatment but a versatile microstructural engineering strategy for thermoelectrics, offering precision, non-contact processing, and design flexibility.

6. Conclusion

This study proposed and experimentally validated a femtosecond laser beam-shaping strategy for the microstructural engineering of Sb_2Te_3, achieving the construction of hierarchical pores and aligned textures that enabled partial decoupling of thermal and electrical transport. The experimental results demonstrated a 52% reduction in thermal conductivity, a 38% increase in electrical conductivity, and more than a 10% enhancement in the Seebeck coefficient, collectively leading to a 133%

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improvement in the figure of merit (ZT) with a peak performance observed near 450 K. Comprehensive structural characterization and transport property measurements confirmed that femtosecond laser processing can effectively regulate phonon and electron pathways while preserving the crystallinity of the material. This strategy establishes a novel fabrication route for high-efficiency thermoelectric materials and shows strong potential for integration with advanced computational frameworks, including multiscale modeling and machine learning–based optimization. Moreover, the approach can be generalized to other layered thermoelectric systems, thereby advancing applications in low- to medium-temperature energy harvesting and solid-state cooling.

Contribution

Bangjie Hu and Qing Yue contributed equally to this paper.

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