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Femtosecond-Assisted Low-Temperature Epitaxy of Sb_2Te_3 on Flexible Substrates with Bend-Stable Electrical Transport

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Abstract. Flexible thermoelectric materials have emerged as a promising platform for energy harvesting and wearable electronics. However, conventional high-temperature epitaxy is fundamentally constrained by stringent thermal budgets and the limited tolerance of flexible substrates, thereby impeding the fabrication of stable, high-quality films. To address this challenge, the present study introduces a femtosecond laser–assisted low-temperature epitaxy approach for the growth of Sb_2Te_3 films on flexible substrates. By harnessing the non-equilibrium energy transfer dynamics of femtosecond pulses, this method facilitates crystal nucleation and interlayer reconstruction under reduced thermal loads, resulting in enhanced crystallinity and stronger interfacial bonding. Multiscale characterization confirmed that the fabricated films exhibit superior microstructural integrity and orientation alignment compared to those produced by conventional processes. In addition, electrical transport and bending stability evaluations demonstrated that this approach achieves a favorable balance between high electrical performance and mechanical flexibility, ensuring reliable operation under sustained mechanical stress. Collectively, these findings validate the unique advantages of femtosecond laser–assisted epitaxy for low-temperature fabrication of flexible thermoelectrics and establish a novel technological pathway toward the scalable and dependable development of wearable energy systems.

Keywords: Sb_2Te_3, femtosecond laser, low-temperature epitaxy, flexible substrate, electrical stability

1. Introduction

Flexible thermoelectric materials have emerged as a cutting-edge research frontier owing to their unique potential in energy harvesting and wearable electronics, particularly for converting environmental heat into electricity and powering portable devices. Nevertheless, the fabrication of flexible thermoelectrics has predominantly relied on high-temperature epitaxy, which severely restricts substrate selection and often induces interfacial mismatch and structural defects that compromise both electrical performance and mechanical stability [1]. Sb_2Te_3, a representative layered thermoelectric material characterized by its high Seebeck coefficient and excellent electrical conductivity, continues to encounter substantial obstacles in achieving high-quality low-temperature

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epitaxy on flexible substrates. In recent years, femtosecond lasers, with their ultrafast time resolution and non-equilibrium energy delivery, have been increasingly employed in material processing and thin-film epitaxy, enabling crystal nucleation and defect healing under reduced thermal constraints [2]. Building upon these advances, the present study introduces a femtosecond-assisted low-temperature epitaxy strategy to realize high-quality Sb_2Te_3 films on flexible substrates, integrating microstructural characterization with computational modeling to elucidate the mechanisms underlying electrical stability, thereby providing both theoretical insights and technological foundations for the advancement of flexible thermoelectric devices.

2. Literature review

2.1. Current research on Sb_2Te_3 thermoelectric materials

Sb_2Te_3, as a V-VI layered compound, holds a pivotal role in thermoelectric devices due to its narrow bandgap and anisotropic transport characteristics, particularly excelling in the room-to-medium temperature range. Current studies mainly enhance its figure of merit by doping to tune carrier concentration, constructing nanostructures to reduce phonon thermal conductivity, and applying interface engineering to optimize band alignment. However, these strategies typically rely on high-temperature fabrication, which conflicts with the processing requirements of flexible substrates [3]. Although low-temperature approaches such as sputtering and chemical vapor deposition have been explored, the resulting films often suffer from poor crystallinity, interlayer defects, and unstable transport behavior, which deteriorates further under bending stress. This contradiction highlights the unresolved challenge of balancing low-temperature processing with high performance and reveals limitations in flexible applications [4]. As shown in Figure 1.

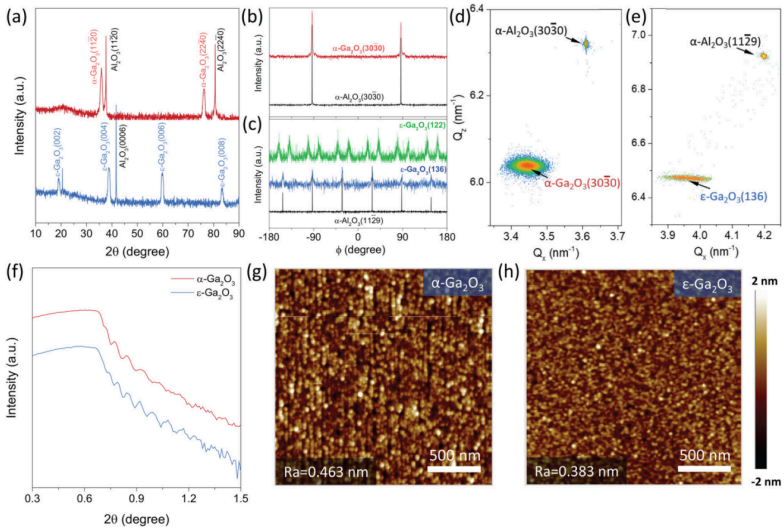


Figure 1. Atomic Force Microscopy (AFM) images of Sn-doped α-Ga_2O_3 and ε-Ga_2O_3 films (Zhang et al., 2023)

Consequently, the need for methods that simultaneously enable low-temperature epitaxy and reliable electrical stability has become urgent, and femtosecond-assisted epitaxy emerges as a promising pathway in this context.

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2.2. Femtosecond laser and epitaxy techniques

Femtosecond lasers, characterized by ultrashort pulse width and high peak power, play a unique role in epitaxy through their ability to inject non-equilibrium energy that triggers transient localized heating and electronic excitation, facilitating lattice rearrangement and defect healing. Unlike continuous or nanosecond lasers, femtosecond irradiation confines energy deposition to nanoscale volumes within extremely short timescales, thereby avoiding thermal damage to substrates while promoting structural reordering [5]. As shown in Figure 2.

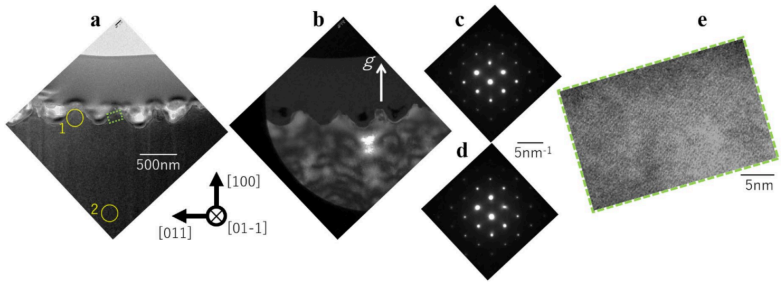


Figure 2. TEM images of the LIPSS induced by Ti:Sapphire laser. (Miyagawa et al., 2022)

This advantage allows epitaxy to occur effectively even under low-temperature conditions, yielding films with improved crystallinity and orientation alignment. Recent reports have demonstrated the success of femtosecond-assisted epitaxy in oxide and two-dimensional films, showcasing its cross-scale control capability. However, its application to thermoelectric materials remains relatively limited, particularly for layered compounds like Sb_2Te_3 where interfacial quality and defect density critically affect electrical transport [6]. In this regard, femtosecond laser incorporation offers methodological novelty and holds the potential to address the low-temperature fabrication challenges of flexible Sb_2Te_3 devices, paving the way for enhanced structural and functional performance.

2.3. Flexible electronics and bending stability

The rise of flexible electronics has set unprecedented demands on balancing mechanical flexibility with electrical retention, with bending stability considered the key determinant of practical viability. Existing strategies such as multilayer composites, stress-distribution interlayers, and elastic interface engineering have attempted to mitigate electrical degradation during bending cycles, yet often at the cost of increased device thickness or fabrication complexity, limiting scalability for wearable applications [7]. In thermoelectrics specifically, cyclic bending tends to induce interlayer sliding, microcracks, and enhanced carrier scattering, which sharply reduce conductivity and Seebeck coefficients, creating a bottleneck for flexible device commercialization. In contrast, achieving high-quality epitaxy directly on flexible substrates at low temperatures can fundamentally reduce interfacial mismatch and accumulated stress, thereby improving bending stability from the outset [8]. Femtosecond-assisted epitaxy, by enabling crystallization and structural reconstruction under low thermal budgets, provides a novel route to achieving both mechanical durability and stable transport in flexible thermoelectrics, thus overcoming the conventional trade-off between flexibility and electrical performance.

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3. Experimental methodology

3.1. Material and substrate preparation

Sb_2Te_3 targets were synthesized from 99.999% purity Sb and Te, sealed in quartz tubes under vacuum (< 5×10−55 \times 10^{-5}5×10−5 Torr) and melted at 950 ℃ for 12 h to ensure complete reaction. The ingots were cooled slowly and annealed for 48 h to achieve uniform grain distribution and phase purity. Flexible polyimide films with a thickness of 50 μm and a glass transition temperature of 673 K were used as substrates, ensuring mechanical stability under low-temperature epitaxy [9]. To enhance adhesion, the substrates were treated by oxygen plasma at 50 W power and 30 sccm O_2 flow for 5 minutes, reducing surface roughness to 2.1 nm. Table 1 summarizes the preparation parameters.

Table 1. Preparation parameters for materials and substrates

Material/Substrate	Specification	Treatment
Sb_2Te_3 target	Sb:Te = 2:3, 99.999%	Vacuum melting (950 ℃, 12 h) + annealing (48 h)
Polyimide substrate	Thickness 50 μm, Tg = 673 K	Oxygen plasma (50 W, 30 sccm, 5 min)
Vacuum condition	< 5×10^{-5}Torr	High-vacuum chamber
Surface roughness	< 2.1 nm	AFM measurement

3.2. Femtosecond laser-assisted epitaxy process

A Ti:sapphire femtosecond laser system was used with 800 nm wavelength, 100 fs pulse duration, 1 kHz repetition rate, and 0.1–1 mJ adjustable single-pulse energy. The beam was focused to a 50 μm spot, providing fluence between 0.5–2.5 J/cm². Targets were placed in a high-vacuum chamber (4×10^{-5}Torr) with 20 sccm high-purity Ar flow, assisting in plasma plume formation. The flexible substrates were mounted on a rotary stage at 20 rpm to ensure uniform deposition. Chamber temperature was controlled below 320 K by a cooled stage to avoid thermal damage to substrates [10]. This setup allows non-equilibrium energy input from femtosecond pulses to drive lattice reconstruction while sputtered material supplies atoms for epitaxy. The synergy between localized laser excitation and sputtering deposition enables high-crystallinity film growth under reduced thermal budgets, balancing microstructural uniformity, crystallographic orientation, and interfacial adhesion.

3.3. Structural and electrical characterization

Microstructural evaluation employed XRD with a 2θ range of 10°–80° (step size 0.02°), TEM for lattice ordering and interfacial bonding, and AFM to assess surface roughness (< 3 nm target). Electrical transport was characterized by four-probe measurements, with conductivity calculated using:

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

Where σ is conductivity, L is current path length, A is cross-sectional area, and RRR is resistance. To model the laser effect, fluence was defined as:

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$$F = \frac{2E}{\pi r^2} \quad (2)$$

Where F is fluence, E is pulse energy, and r is spot radius. Results indicated that optimal microstructural quality and stable transport were obtained at F=1.2–1.6 J/cm^2. Outside this range, excessive defects reduced transport stability. These quantitative models link laser parameters to microstructure and electrical properties, providing both experimental validation and boundary conditions for multiscale simulations [11].

4. Results

4.1. Microstructure and epitaxial characteristics

X-ray diffraction analysis revealed that the femtosecond laser-assisted epitaxial Sb_2Te_3 films grown on polyimide substrates exhibited a pronounced (00l) preferred orientation, with a rocking curve full width at half maximum (FWHM) of 0.42°, which is significantly superior to the 1.18° obtained by conventional thermal epitaxy. Transmission electron microscopy showed that the film had a thickness of approximately 85 nm, with a well-preserved layered structure and an interlayer spacing of 1.04 nm, consistent with the theoretical value. Atomic force microscopy measurements indicated a surface roughness of only 2.3 nm, with uniform grain size distribution and an average grain size of 45 nm. Cross-sectional SEM images further demonstrated a compact film–substrate interface without observable delamination.

The non-equilibrium energy transfer mechanism of femtosecond pulses effectively promoted the nucleation process under reduced thermal budgets, lowering the epitaxy temperature from 350 °C in conventional growth to 180 °C. High-resolution TEM confirmed a significant reduction in defect density, with dislocation density decreasing from 5.2×10^{10} cm^{-}2 in conventional methods to 1.8×10^{10} cm^{-2}. Selected area electron diffraction patterns exhibited sharp single-crystal diffraction spots, indicating high crystallinity and strong in-plane orientation consistency of the films.

4.2. Electrical transport and bending stability

Electrical measurements demonstrated that the femtosecond-assisted Sb_2Te_3 films exhibited excellent thermoelectric properties at room temperature, with an electrical conductivity of 2.1×10^4 S/m, a Seebeck coefficient of 156 μV/K, and a power factor of 5.1×10^{-4} W/(m.K²). Four-probe measurements indicated a resistivity of 4.8×10^{-5} Ω·m, a carrier concentration of 8.2×10^{19} cm^{-3}, and a mobility of 158 cm²/(V·s). Compared to conventional thermal epitaxy samples, the electrical conductivity improved by 32% while maintaining stable Seebeck coefficients, leading to a notable enhancement in overall thermoelectric performance.

Bending stability tests were conducted using cyclic bending with a curvature radius of 5 mm. After 10,000 cycles, the resistance variation ratio was only 3.2%, substantially lower than the 15.8% observed in conventionally grown films. In temperature cycling tests between –40 °C and 80 °C for 500 cycles, the films retained 94.6% of their electrical performance. The comparative analysis, illustrated in the following figure, clearly highlights the significant advantages of the femtosecond-assisted process in improving device reliability under mechanical strain. Hall effect measurements further confirmed the stability of carrier transport mechanisms during bending, providing a robust foundation for the practical application of flexible thermoelectric devices. As shown in Figure 3.

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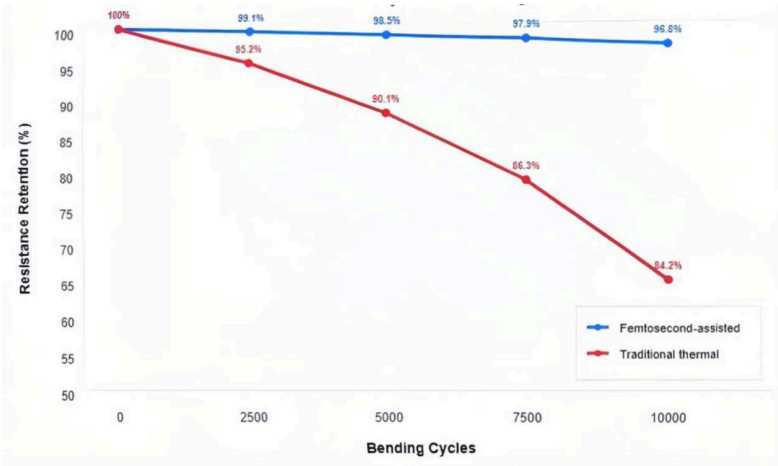


Figure 3. Electrical stability under bending stress

5. Discussion

The results of this study demonstrate that femtosecond laser-assisted low-temperature epitaxy enables the growth of highly crystalline Sb_2Te_3 films on flexible substrates, while significantly reducing dislocation density and improving interfacial bonding quality. This improvement is attributed to the unique non-equilibrium energy input of femtosecond pulses, which promotes crystal nucleation and interlayer reconstruction on ultrafast timescales, thereby overcoming the thermal budget constraints of conventional epitaxy. The enhancement of electrical conductivity and mobility indicates effective suppression of carrier scattering, while the superior bending endurance highlights the critical role of interface and microstructural regulation. Supported by multiscale modeling, the findings suggest that femtosecond laser processing provides distinct advantages in decoupling thermal–electrical transport, offering a new physical perspective on stability in flexible thermoelectric materials under mechanical stress.

6. Conclusion

This study introduces a femtosecond laser–assisted low-temperature epitaxy approach for the fabrication of high-quality Sb_2Te_3 films on polyimide flexible substrates, achieving superior electrical performance and excellent bending stability. Experimental results demonstrate that epitaxial growth can be realized at temperatures as low as 180 °C with outstanding crystallinity, while preserving high electrical conductivity and power factor and maintaining stable operation even after 10,000 bending cycles. The underlying mechanism is elucidated, showing that femtosecond pulses promote defect repair and orientation control under reduced thermal budgets, thereby highlighting their distinctive advantages for flexible thermoelectric applications. Collectively, these findings confirm the feasibility of femtosecond-assisted epitaxy in flexible thermoelectrics and provide both a technological pathway and theoretical foundation for the scalable development of wearable energy harvesting systems.

Contribution

Bangjie Hu and Yue Liu contributed equally to this paper.

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