A Novel Strategy for Anisotropic Thermoelectric Characterization: Tensor Inversion Method

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Thermoelectric (TE) materials, which enable direct conversion between thermal and electrical energy, have long held promise for applications in waste heat recovery, solid-state refrigeration, and deep-space exploration.[1–3] Their energy conversion efficiency is governed by the dimensionless figure of merit $zT = S^2T/\rho\kappa$, where the Seebeck coefficient (S), electrical resistivity (ρ), and thermal conductivity (κ) are all second-rank tensors with values strongly dependent on crystallographic orientation.[4] In layered materials such as $Bi_2Te_3^5$ and SnSe[6], this anisotropy is particularly pronounced, making accurate characterization of intrinsic properties a persistent challenge. Conventional methodologies rely on single crystals precisely cut along principal crystallographic axes, a process that is not only time-consuming but also prone to orientation errors, mechanical damage, and limitations in reproducing true anisotropic behavior. These constraints have led to significant discrepancies between measured and intrinsic properties, hindering the establishment of reliable structure-property relationships and impeding the development of orientation-optimized materials.

Recently, Qin *et al.* published an Express Letter in *Chinese Physics Letters* that introduces a novel tensor inversion method to overcome these limitations.[7] As shown in Fig. 1, by integrating electron backscatter diffraction (EBSD)-derived Euler angles with transport measurements, this method transforms experimental data between the sample and crystal coordinate systems, allowing direct extraction of intrinsic properties without the need for orientation-controlled cutting. Applied to pure Bi, the reconstructed tensors for ρ, κ, and S exhibit excellent consistency with benchmark data, confirming both the validity and precision of the method.

The core of the tensor inversion framework lies in establishing the rotational relationship between the sample coordinate system (SCS) and the crystal coordinate system (CCS). The research team utilized EBSD to obtain Euler angles of the crystal, constructed a rotation matrix, and ensured physical validity of the transformation through orthogonality verification. Based on the principle of passive rotation, the intrinsic tensor simplifies to a diagonal form in the CCS due to the rhombohedral symmetry of Bi (space group $R\bar{3}m$), requiring only two independent components, T_{aa} (binary axis) and T_{cc} (trigonal axis). The inversion process solves linear equations derived from measurements on arbitrarily oriented samples, yielding intrinsic values with remarkable accuracy.

In experimental validation, the team grew high-quality Bi single crystals via the self-flux method and cut them into in-plane and out-of-plane oriented samples. Transport measurements conducted in the SCS yielded anisotropy ratios (out-of-plane/in-plane) approaching unity, starkly underestimating the true crystallographic anisotropy. After applying tensor inversion, the intrinsic tensor components showed excellent agreement with literature data: ρ and κ perfectly reproduced the anisotropy trends—ρ along the trigonal axis was higher than that along the binary axis, while κ exhibited the opposite behavior. Although the S showed minor deviations from literature values, attributed to the diagonalization assumption omitting transverse TE coupling, the inverted components more faithfully captured the intrinsic anisotropic behavior than direct SCS

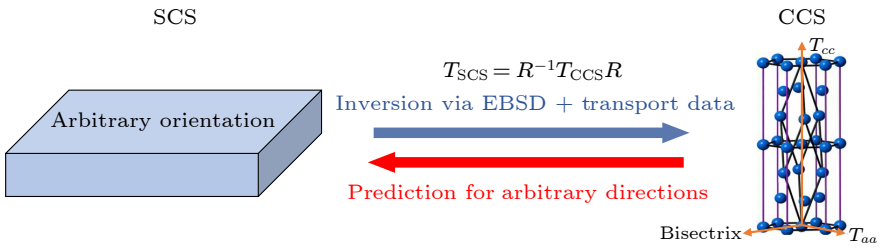

Fig. 1. Tensor inversion framework: bidirectional reconstruction of anisotropic TE properties. Adapted from Ref. [7].

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measurements. Notably, the method possesses bidirectional prediction capability, achieving for the first time the visualization of the complete angular distribution of zT. Results indicated that zT along the trigonal axis direction $\langle 001 \rangle$ reaches 0.6 at 300 K, superior to the traditionally reported value of 0.4, revealing the intrinsic potential of Bi for high-performance applications.

This approach is groundbreaking in its orientation independence, liberating experiments from the constraints of precise crystal cutting. More than just a simplification, it achieves full tensor reconstruction, capturing the complete anisotropic picture. Crucially, the method's bidirectional predictability allows not only the extraction of intrinsic properties from random samples but also the forecasting of performance for any desired orientation. This dual capability culminates in the first panoramic visualization of zT anisotropy, offering an unprecedented tool for optimizing device architecture.

By providing a robust and generalizable pathway to intrinsic property determination, this tensor inversion method transcends the specific case of Bi. It establishes a new paradigm for characterizing a wide range of anisotropic functional materials, promising to accelerate the discovery and optimization of next-generation TE devices.

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