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Title: Enhancing Thermoelectric Efficiency of Nanostructures through In-Situ and Ex-Situ interfacial alloying

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Enhancing Thermoelectric Efficiency of Nanostructures through *In-Situ* and *Ex-Situ* interfacial alloying

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Overview and Motivation

Enhancing Thermoelectric Efficiency of Nanostructured Bi_2Te_3

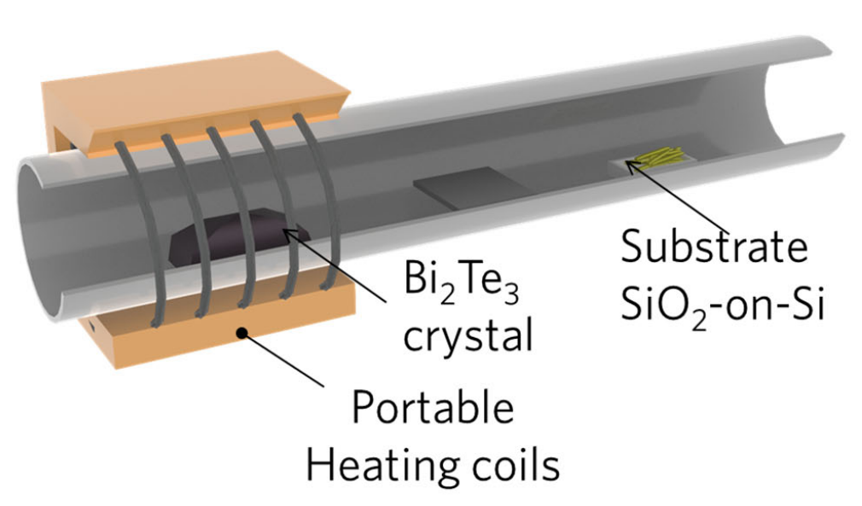
Enhancing the thermoelectric efficiency of materials, nanostructured Bi_2Te_3, aiming to increase the thermoelectric figure of merit (zT) for improved waste heat conversion.
Challenges related to defects, impurities, and surface oxidation in nanostructures need to be addressed to achieve high-performance thermoelectric materials efficiently converting heat into electricity.
The goal is to surpass the performance of bulk material and unlock the full potential of nanostructured Bi_2Te_3.

Controlling Surface Chemistry and Potential

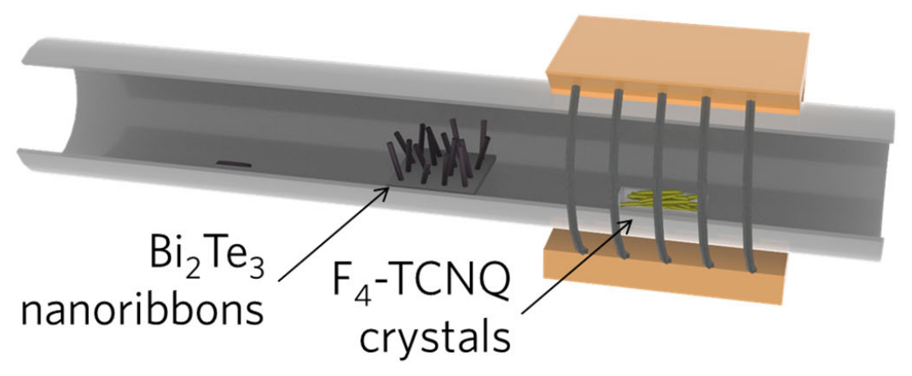
Controlling the chemical potential of nanostructured surfaces, especially in Bi_2Te_3, to create long-lasting and high-performance thermoelectric materials and devices.
Surface state doping technique was performed by both *In-Situ* doping of *p*-type carrier donor (F_4-TCNQ) and *Ex-Situ* interfacial alloying of metal film (Cr).
Achieving control over the surface potential and carrier density of low-dimensional materials is the central challenge in this endeavor.

In-Situ surface doping

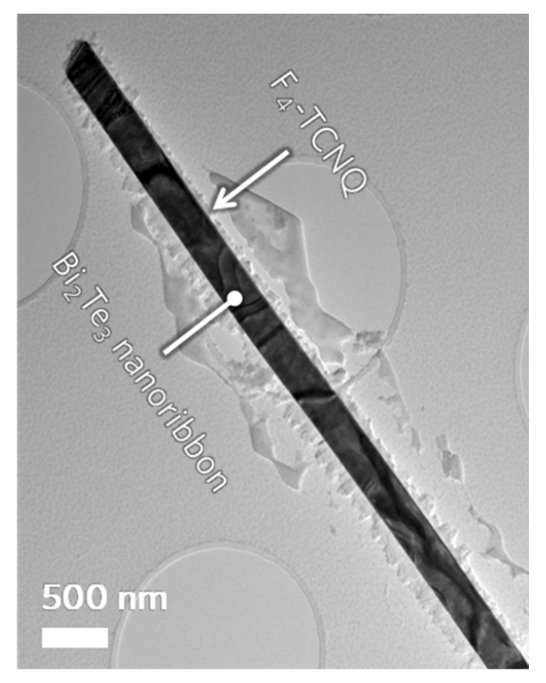
(i) Phase 1
Growth of nanoribbon cores



(ii) Phase 2
Coating dopant layer



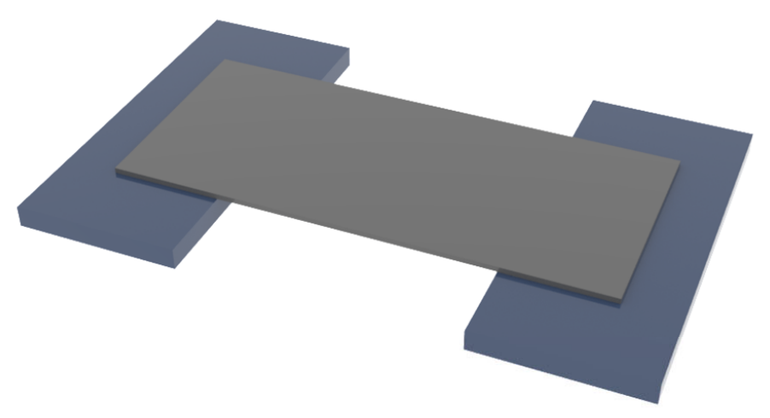
TEM profile



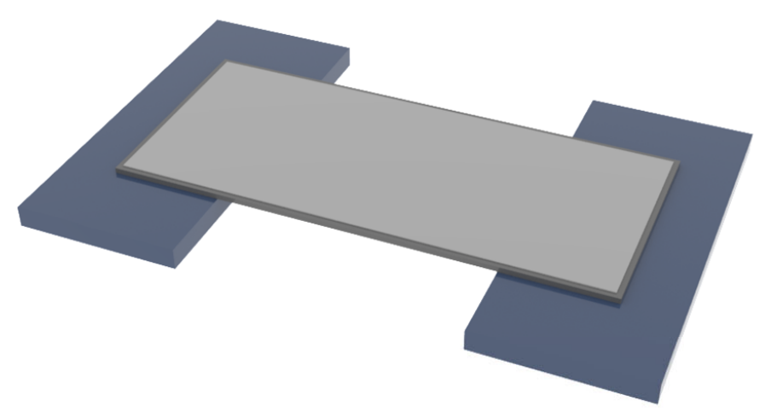
(i) Bi_2Te_3 nanoribbon cores were grown on a SiO_2-coated silicon wafer in high vacuum.
(ii) Electronegative molecule (F_4-TCNQ) layer was *in-situ* coated onto the nanoribbons by re-orienting the quartz tube inside the furnace.

Ex-Situ surface doping

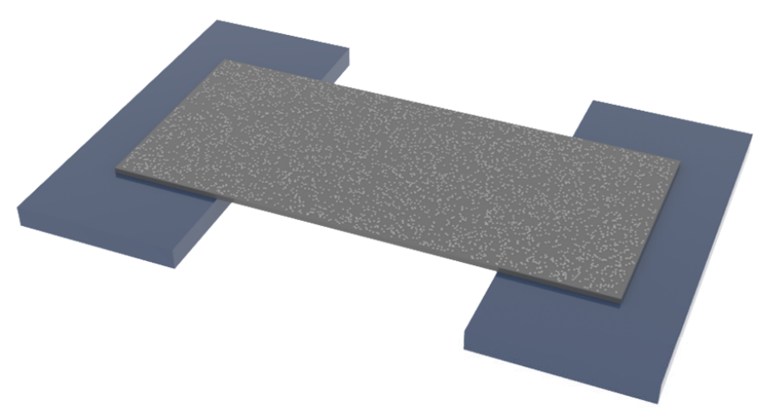
(i) As-grown material
Suspending Bi_2Te_3 flake on device



(ii) Dopant layer deposition
Deposition of thin (3 Å) Cr film

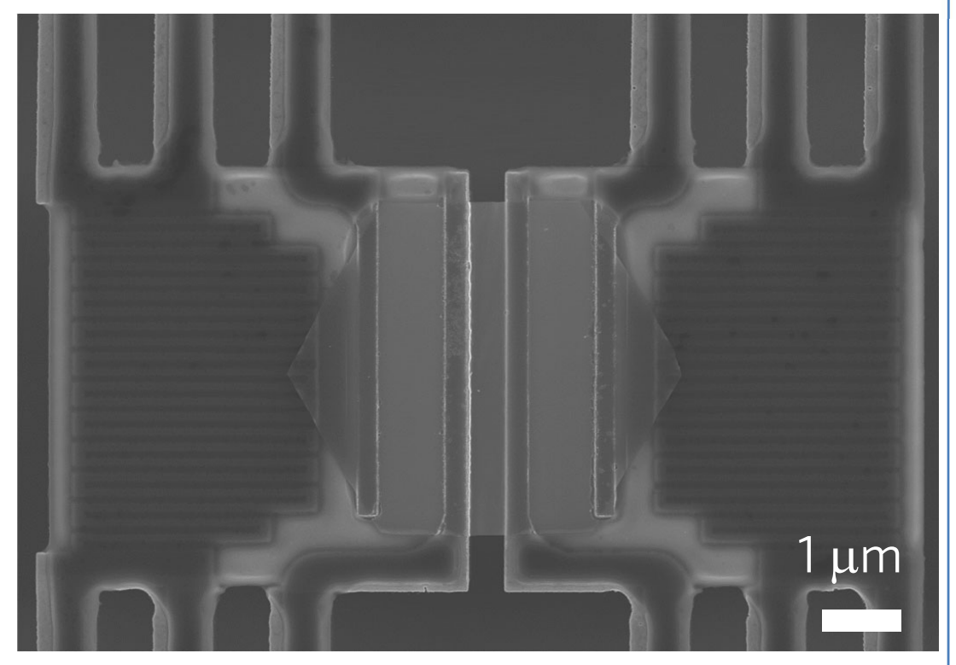


(iii) Thermal annealing
Deposition of thin (3 Å) Cr film

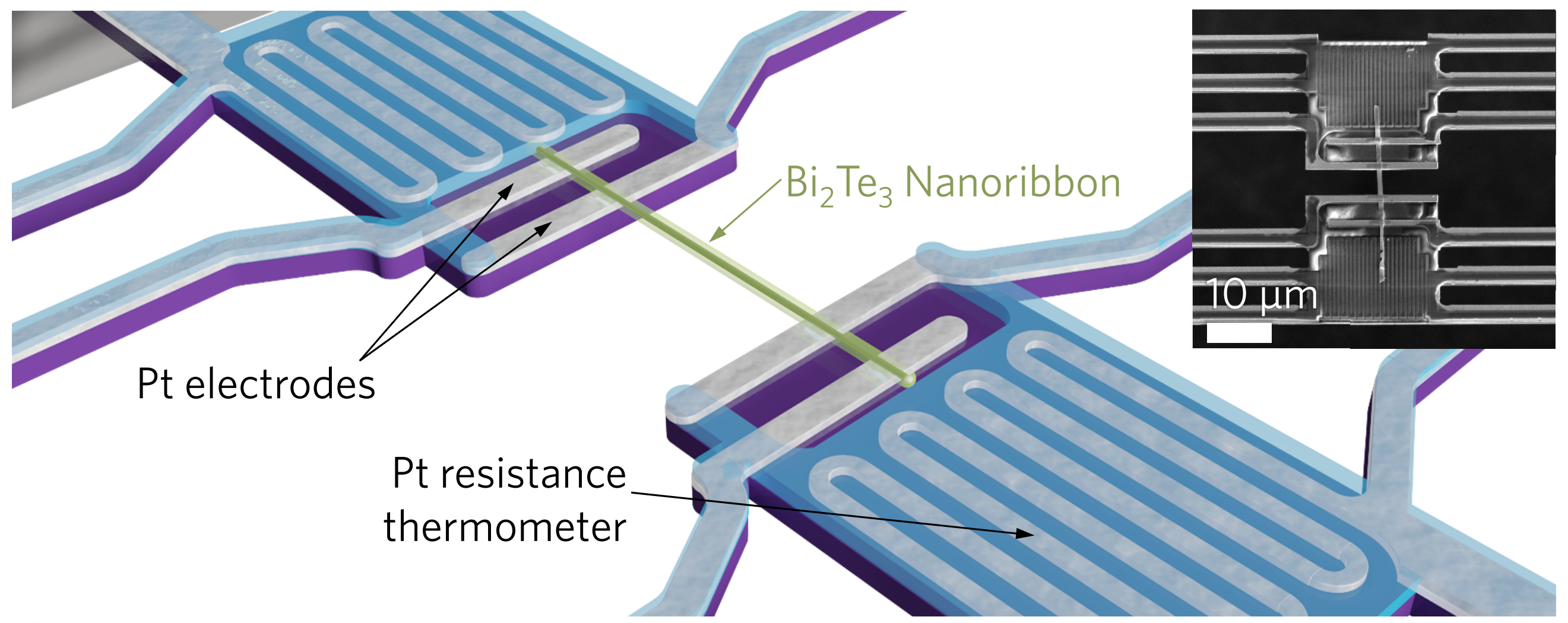


(i) Pure Bi_2Te_3 nanoribbon was transferred on a thermoelectric characterizing platform which separate both ends of suspended material.
(ii) Thin (~ 3 Å) Cr film was deposited onto upper side of nanoribbon, then annealed at 225 ˚C for 24 hrs in 15mTorr of Forming gas.

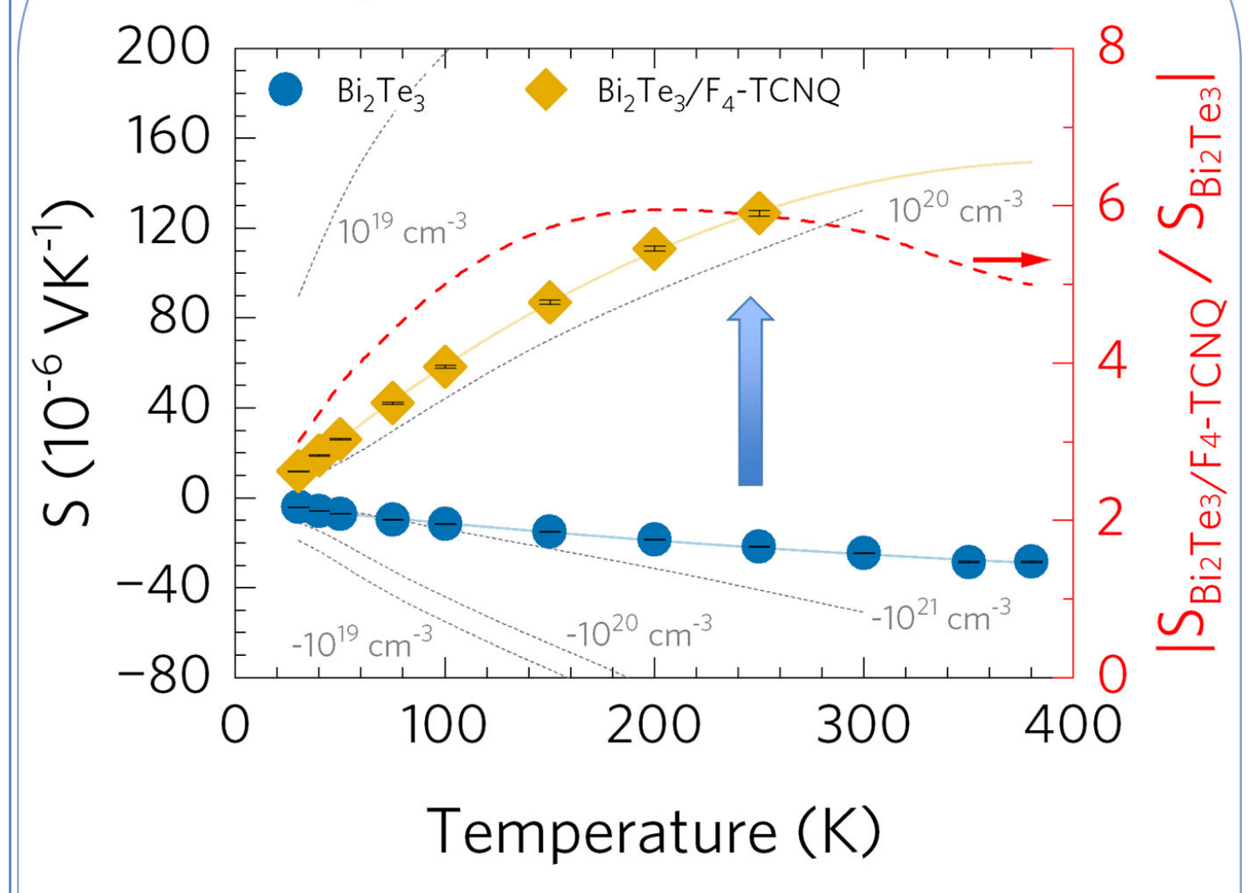
Device ready to measure

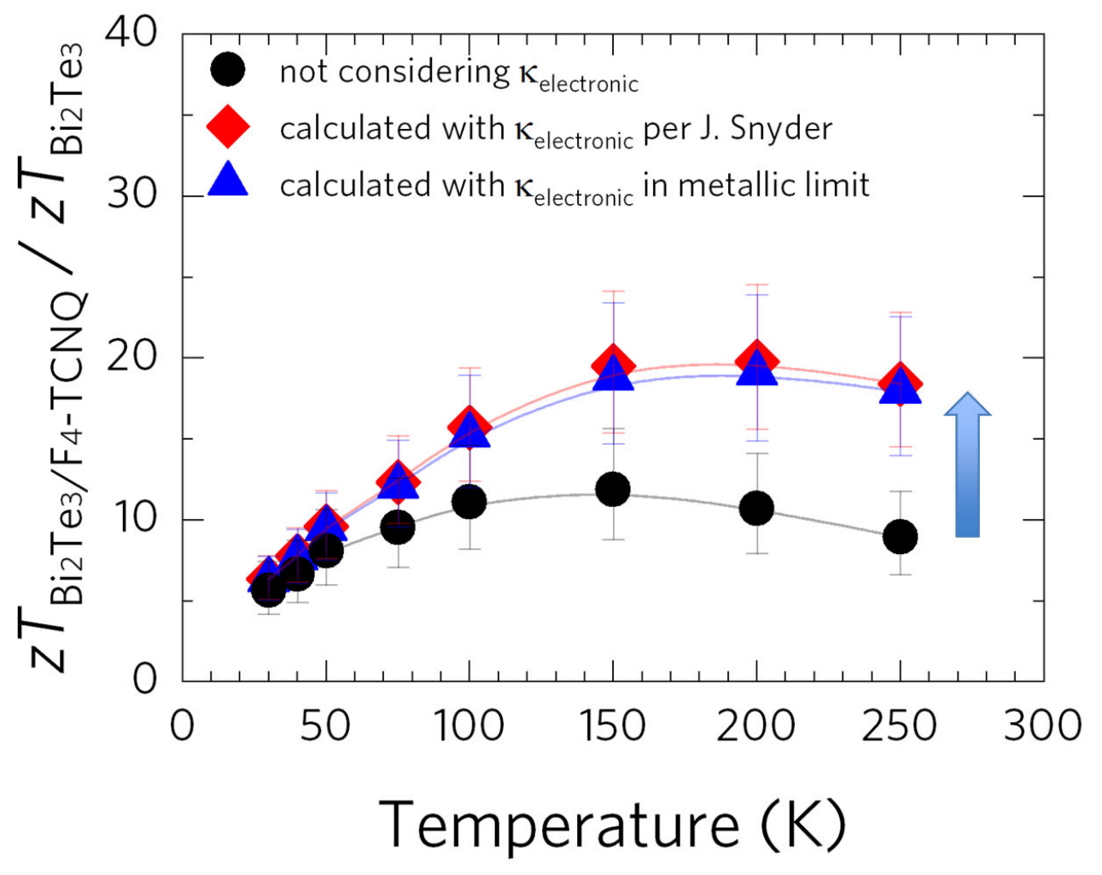


Device Characterization



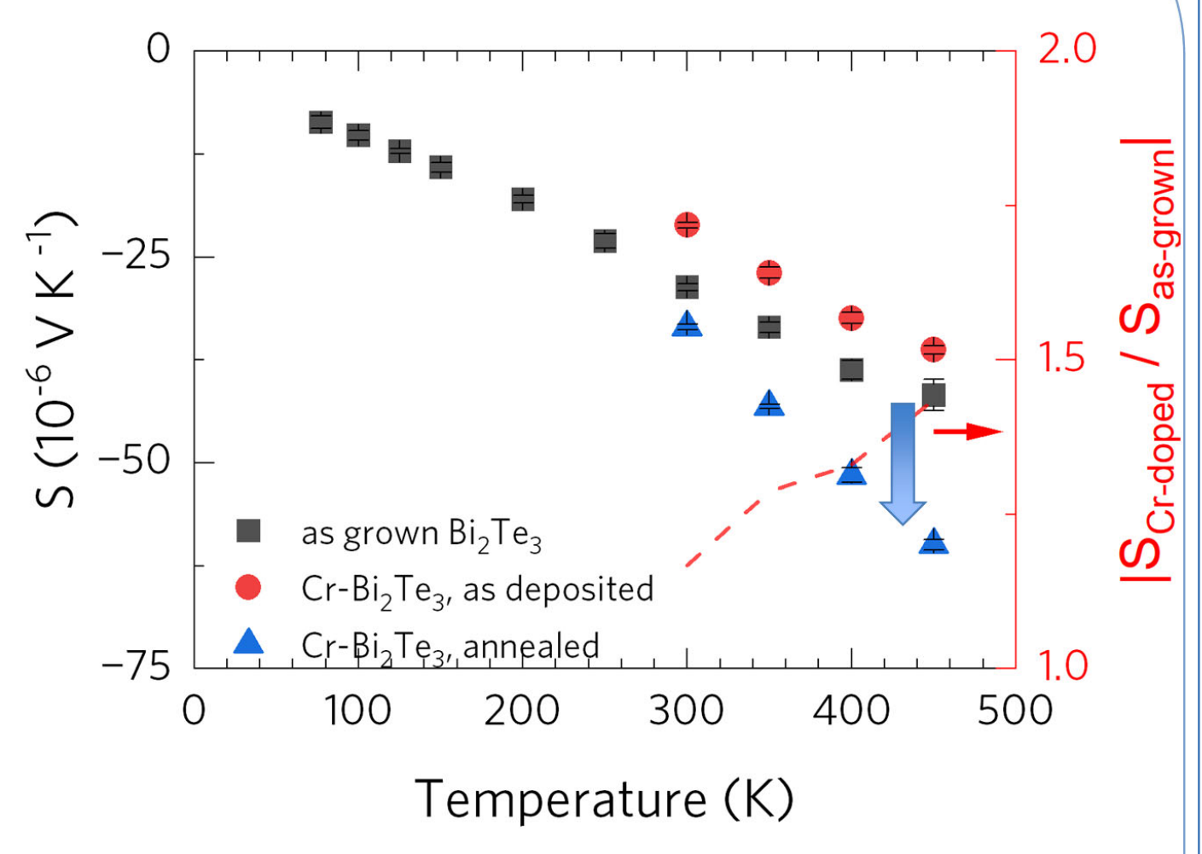
☐ *F_4-TCNQ doping*

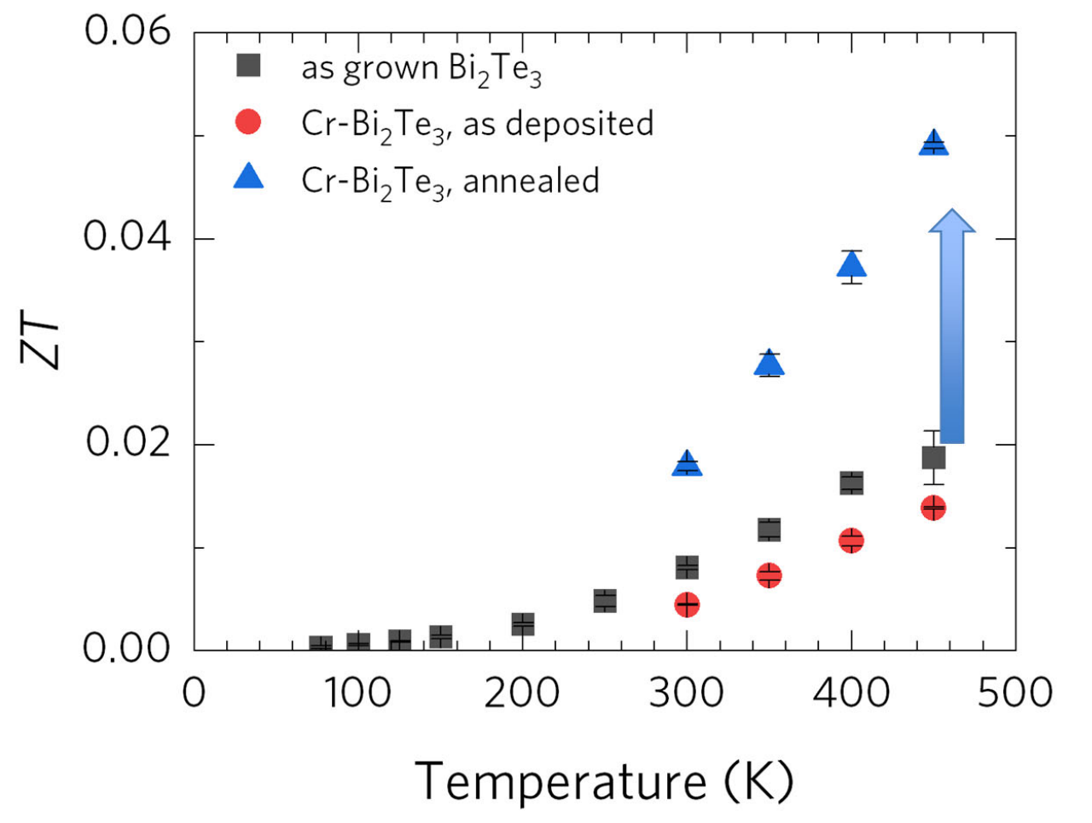




- change of major carrier type.
- 6-times enhanced Seebeck coefficient.

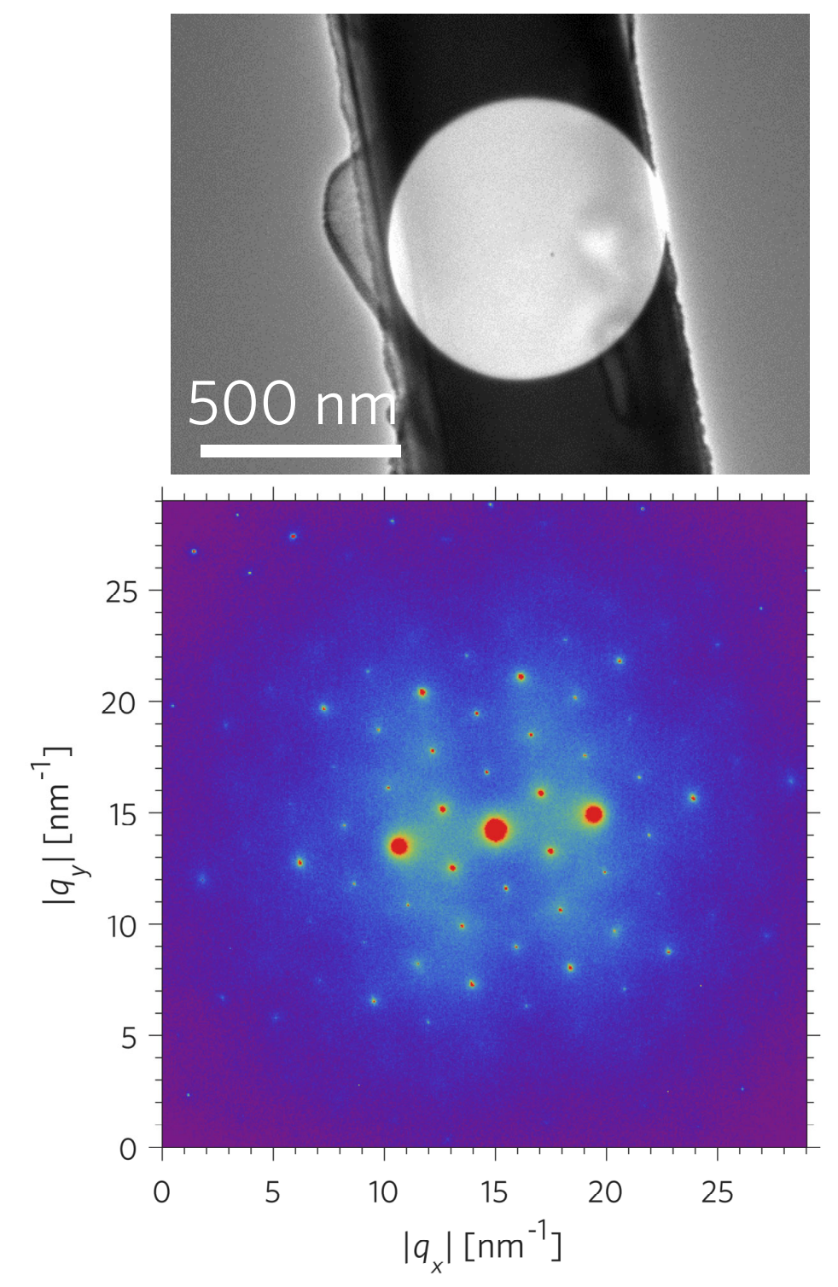
☐ *Cr-doping*

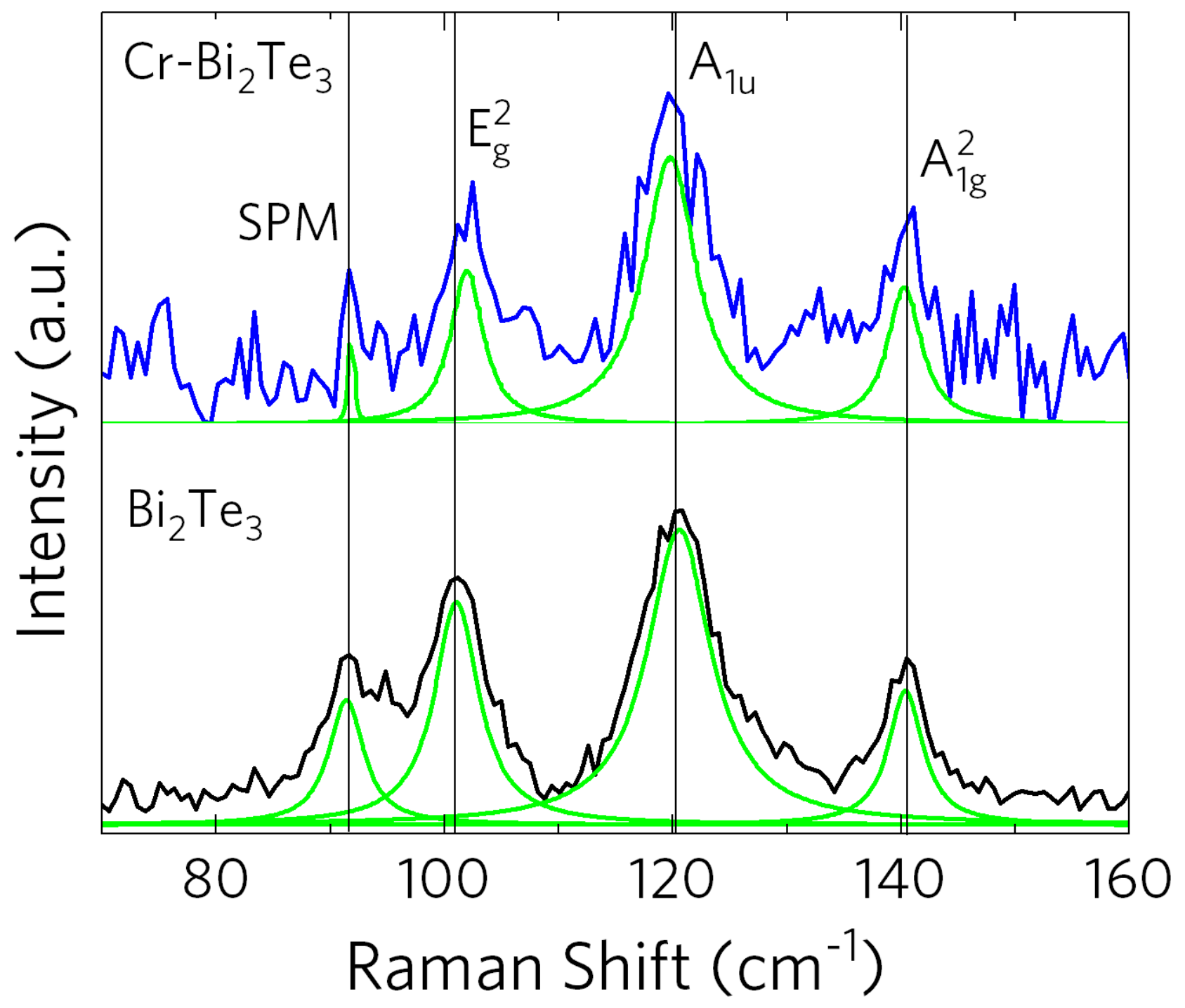




- Retaining major carrier type.
- 24% enhanced Sebeeck coefficient.

Structural Investigation





In-situ surface doping provides an epitaxial core-shell structure with a consistent thickness of the dopant layer, as confirmed through TEM investigation.

Ex-situ surface doping of Cr into the atomic structure of Bi_2Te_3 has been confirmed through Raman shift investigation, demonstrating shifts in the E_g and A_{1g} peaks.

Conclusion

- ✓ We present two strategies to enhance thermoelectric performance of Bi_2Te_3 nanoribbons; *in-situ* F_4-TCNQ layer and ex-situ Cr layer doping.
- ✓ The in-situ F_4-TCNQ layer transforms the major carrier from *n*-type to *p*-type, boosting the Seebeck coefficient by 6-fold and effectively protecting against oxidation for at least a month.
- ✓ The Cr layer increases the Seebeck coefficient by 24%, resulting in a 2-fold enhancement in thermoelectric figure of merit (zT).
- ✓ Structural analysis confirms the effectiveness of both doping methods at the atomic level..

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