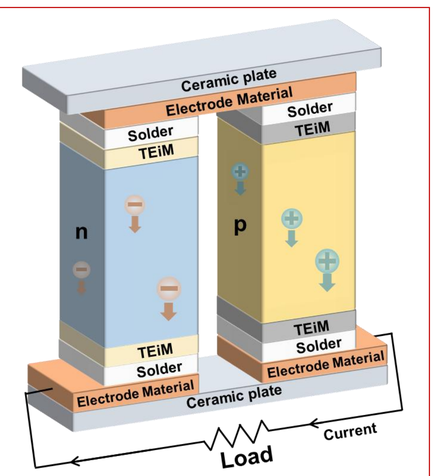
Sintering Process Optimization Promotes Grain Growth for Enhanced Thermoelectric Performance in $Mg_3(Sb, Bi)_2$

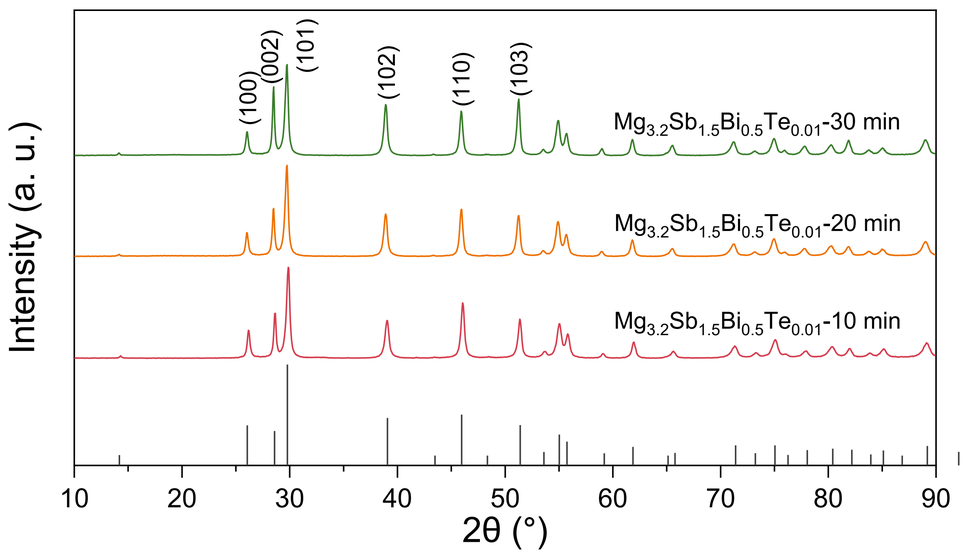
Liangjun Xie, Jonas Winkler, Kornelius Nielsch, and *Ran He*
Leibniz Institute for Solid State and Materials Research Dresden, Germany

Motivation

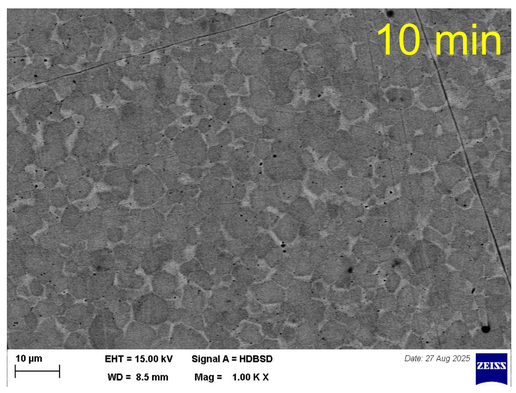
- $Mg_3(Bi, Sb)_2$-based thermoelectric materials have emerged as promising candidates for sustainable solid-state refrigeration and medium-temperature power generation, owing to their attractive thermoelectric properties and earth-abundant constituent elements.
- The room-temperature thermoelectric performance of polycrystalline $Mg_3(Bi, Sb)_2$ is strongly constrained by carrier scattering at grain boundaries. Enlarging the grain size could effectively reduce the density of grain boundaries and thereby mitigate carrier scattering, providing a promising strategy for further enhancing thermoelectric performance.

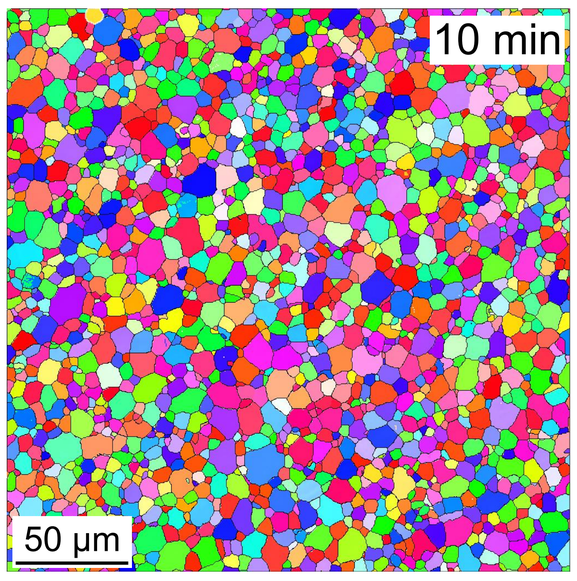


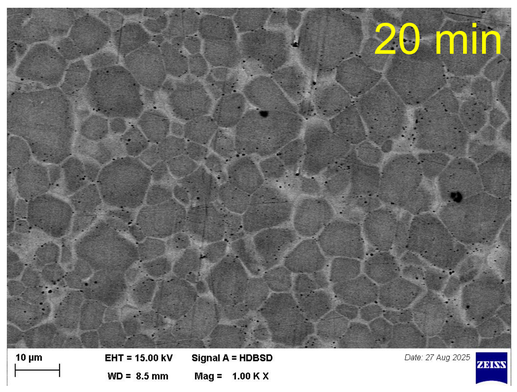
Microstructure

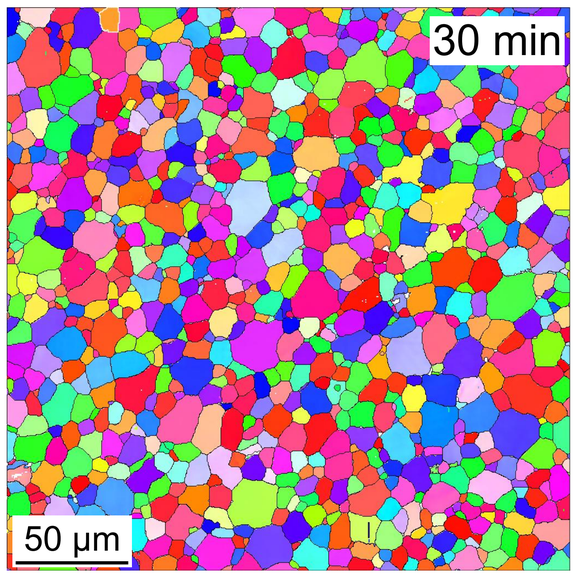


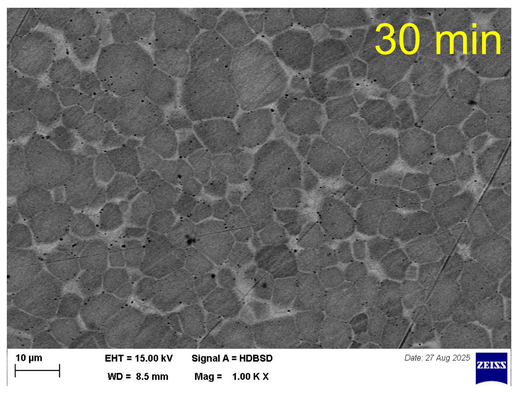
- No obvious impurity phases are detected in the XRD patterns, indicating high phase purity of the samples.
- The gradually increasing intensity of the (002) peak suggests enhanced crystallographic anisotropy.





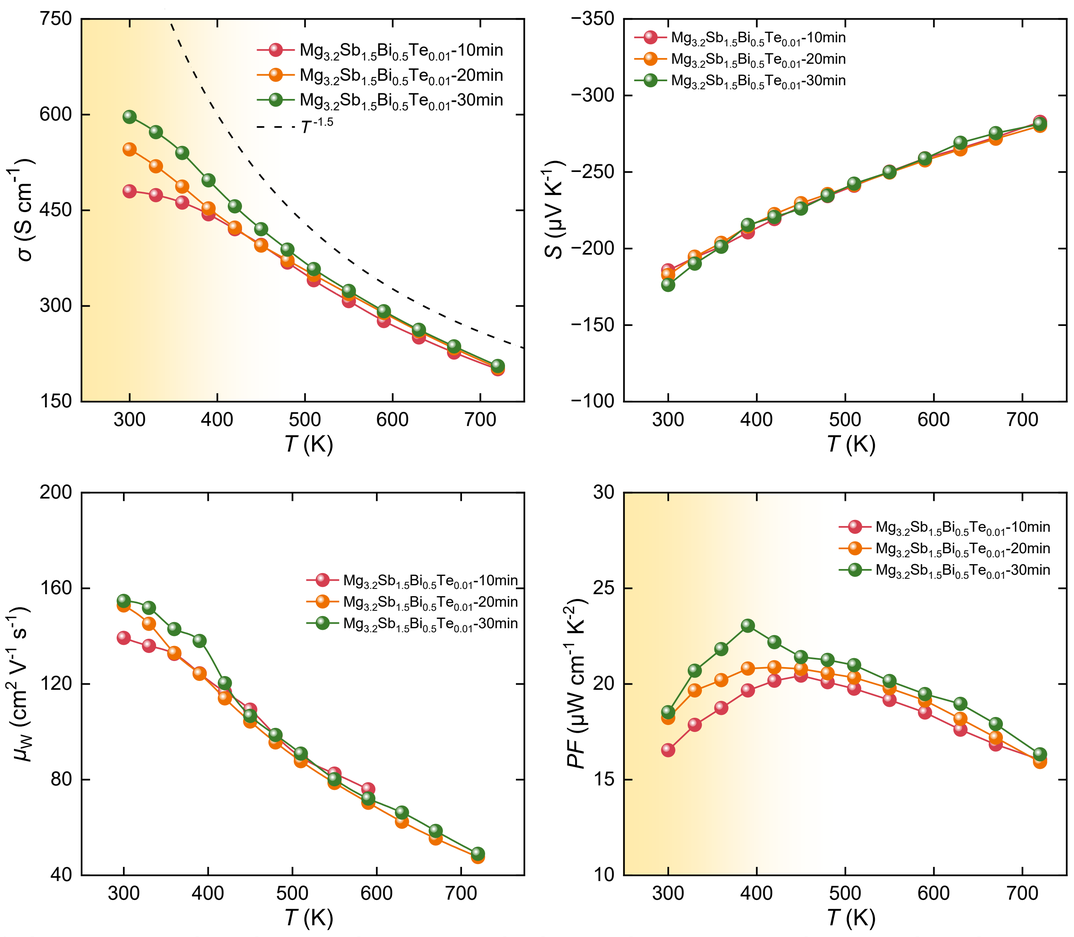




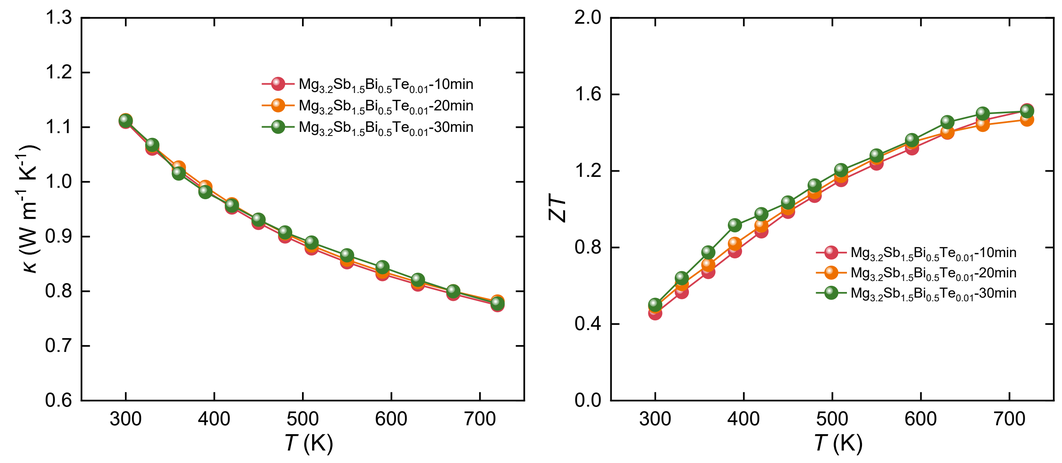


- Backscattered electron (BSE) images reveal evident phase separation in all samples.
- EBSD analysis demonstrates a significant increase in the equivalent area-weighted average grain size from ~8 to ~12 µm, indicating pronounced grain growth with optimized sintering.

TE performance



- Larger grain size reduces grain-boundary scattering and enhances electrical transport.
- The Seebeck coefficient remains nearly unchanged, indicating a consistent carrier concentration for the three samples.
- The *PF* increases across the entire temperature range for the 30-min sample due to the increased grain size.



- The thermal conductivity remains nearly unchanged with increasing sintering time.
- Owing to the enhanced power factor, the *ZT* value increases throughout the measured temperature range.

Conclusion

The enlarged grain size enhances weighted mobility by suppressing grain-boundary scattering, demonstrating the effectiveness of sintering optimization in $Mg_3(Bi, Sb)_2$ thermoelectric materials and highlighting their potential for broad thermoelectric applications.

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