6-10 JULY 2026
NANOSMAT
RHODES ▪ GREECE

17th International Conference of Surfaces, Coatings
and Nanostructured Material | **NANOSMAT2026**
RHODES-GREECE | 6-10 JULY 2026
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ABSTRACT:

Towards Grain Boundary Phase Engineering Via High Resolution Microstructure and Transport Property Imaging

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Engineering the microstructure of materials offers superior control over transport properties, critically impacting the thermoelectric performance. One such example is grain boundary (GB) engineering. GBs can exist in a variety of structural configurations and can adopt chemical compositions that differ from those of the neighboring grains. For this reason, GBs can sometimes be described as distinct two-dimensional phases, called complexions or defect-phases, characterized by their own thermodynamic equilibrium.1 In thermoelectrics, GBs have traditionally been employed to suppress the thermal conductivity (κ). However, boundaries can also accumulate charged defects, resulting in an energy barrier for charge carriers that detrimentally affects the electrical conductivity. As such, maximizing the thermoelectric performance requires a comprehensive understanding of how specific GB features influence thermoelectric transport.

In this talk, we will discuss recent efforts to capture the individual properties of GBs in several thermoelectrics, including SnTe, silicon, Bi2Te3 and Mg3(Sb,Bi)2. Microscale thermal conductivity imaging using thermoreflectance-based techniques are employed to characterize the thermal transport properties of individual boundaries.2,3 Experimental observations reveal a κ suppression localized in the vicinity of GBs, quantified in terms of an excess thermal boundary resistance.4 Remarkably, boundaries show order-of-magnitude variations in behavior, with both structural parameters, including misorientation angle and interface morphology, and local changes in the chemical composition exerting strong and distinct influence on the boundary resistance. We also illustrate how this methodology is capable of detecting local variations in κ that arise from other types of heterogeneity, including crystal anisotropy,5 as well as presence of secondary phases and micro segregations. Finally, we provide an outlook for extending local investigations to other thermoelectric properties, granting a comprehensive picture for a rational design of GBs.

Extracting the transport properties of individual microstructures offers a powerful route to clarifying the interaction of heat and charge carriers with defects, enabling the establishment of local structure-chemistry-property correlations. This understanding can guide the rational engineering of microstructure for superior performance in thermoelectrics.

Acknowledgment: This work is supported by the European Research Executive Agency, under Marie Skłodowska-Curie Actions, project 101150912 — MetaSCT, as well as by the Italian Ministry of University and Research according to the D.D. n.18010 November 12th 2025 – BANDO FIS 3, project 'HEAT', FIS-2024-05016 (CUP E53C25002220001).

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