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ABSTRACT:

Distinguishing the Role of Structure and Chemistry on Thermal Transport at Grain Boundaries

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Microstructural defects such as grain boundaries offer a powerful route to control thermal transport across materials and applications. Grain boundaries exist in diverse configurations and often differ from adjoining grains in local composition and atomic arrangement. Yet how these chemical and structural features govern grain-boundary thermal response remains unclear. Here, Mn-doped SnTe serves as a model system to elucidate the mechanisms governing thermal resistance at individual grain boundaries. Solidification-induced chemical gradients are promoted within the material resulting in Mn-poor micro-segregations around grain boundaries. Correlative imaging of local thermal conductivity and chemical composition are performed, enabling a high-throughput and spatially-resolved probing of thermal conductivity as a function of chemistry. Regions around grain boundaries show up to 30% lower thermal conductivity than grain interiors of the same composition. Electron microscopy investigations reveal residual strain and dislocation accumulation along boundaries, which are attributed to the solidification process. These results indicate that structural strain and associated defects play a greater role in grain-boundary thermal resistance than local compositional variations. Together, these findings provide crucial new insights into how grain boundary structure contributes to thermal resistance, pointing to new defect-engineering strategies for controlling thermal transport in materials.