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Landauer approach to thermoelectric transport across grain boundaries in Si MICHAEL SHAUGHNESSY, DOUG MEDLIN, FRANCOIS LEONARD, CATALIN SPATARU, Sandia National Laboratories — Thermoelectric transport is strongly influenced by electron and phonon scattering from defects, grain boundaries, and nano structuring. While scattering from point defects is relatively well understood, the impact of the detailed structure of grain boundaries is still poorly understood. We use a Landauer approach based on ab initio Density Functional Theory and classical Molecular Dynamics simulations to compute electron and phonon transport coefficients in the presence of grain boundaries. The approach allows the calculation of all the thermoelectric quantities, including thermal conductivity, electrical conductivity, Seebeck coefficient, and the overall figure of merit, ZT. The method is applied to grain boundaries in Si, focusing on the {111}twin in the high and low density regimes. For ordered arrays of {111}twins in Si a small change in ZT is predicted because of compensating differences between thermal conductivity on the one hand and electrical conductivity and Seebeck coefficient on the other.

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