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Electronic transport simulations in nano-crystalline materials for enhanced thermoelectric power factors NEOPHYTOS NEOPHYTOU, University of Warwick, MISCHA THESBERG, Technical University of Vienna — Nanocrystalline thermoelectric materials have shown the potential to provide much larger Seebeck coefficients compared to pristine materials. In this work we perform electronic transport simulations to study thermoelectric transport through 2D nanocrystalline channels. In these channels, the grain boundaries act as barriers for energy filtering, which provides large improvements to the Seebeck coefficient. On the other hand, the grain geometry, doping, and the underlying electrostatic potential can be engineered in such a way as to compensate for the reduction of the electrical conductivity that the barriers on the grain boundaries cause. Thus, optimal designs can be achieved, in which the power factor is improved compared to pristine materials. We discuss in addition the influence that the variation in the local thermal conductivity of the grains compared to that of the grain boundaries has on providing further improvements to the Seebeck coefficient, as well as the influence of parameter variations on degrading the power factor.

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