Numerical extraction of TE coefficients of complex bandstructure materials with full energy/momentum scattering dependences – the example of half-Heusler alloys

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We present an approach for the numerical extraction of charge transport coefficients considering the full band energy/momentum dependence of the scattering rates and relaxation times in the framework of the Boltzmann Transport Equation.

We investigate the impact of different treatment of carrier scattering, specifically, the commonly employed constant relaxation time, versus energy dependent elastic and inelastic phonon scattering and ionized impurity scattering on the thermoelectric power factors of Co-based half-Heusler alloys. Typically, thermoelectric transport calculations employ the constant relaxation carrier scattering time to reduce computational complexity[1,2]. However, such simplifications fail to capture the details of bandstructure features such as band anisotropy and manifold band and valley degeneracies and therefore fail to give accurate results, especially for complex bandstructures [3,4]. In this work, we have developed an advanced simulator to go beyond this simple approximation and consider all the energy, momentum and band dependent details of the scattering process.

We show that depending on the scattering treatment, different material performance rankings, different optimal doping regimes, and different temperature dependent trends are found. We also give an indication of single relaxation time values that are valid for different Fermi levels/doping concentrations, which both experimentalists and theorists would find useful in interpreting measured/simulated data. We present simulation results of ranking the performance of number of half-Heuslers, as well as the possibility of further improving their thermoelectric powers factors by strain induced band alignment. The work points out the importance of detailed scattering physics in electronic transport, and provides understanding and optimization directions in the performance of complex bandstructure materials,

References

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