Abstract Submitted
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Validity of Wiedemann-Franz law in thermoelectric half Heusler compounds[1] MAL-SOON LEE, University of New Orleans, S. D. MAHANTI, Michigan State University — There is renewed interest in the field of thermoelectrics for power generation. Several promising thermoelectrics are half-Heusler narrow band gap semiconductors. The efficiency of thermoelectric energy conversion depends on the transport coefficients through the figure of merit $ZT = \sigma S^2 T/\kappa$. For large ZT , it is necessary to decrease the total thermal conductivity ($\kappa = \kappa_l + \kappa_{el}$) as well as increase the Seebeck coefficient (S) and the electrical conductivity (σ)To determine κ_l experimentally, one usually subtracts the electronic thermal conductivity (κ_{el}) from measured κ, using the Wiedemann-Franz law ($\kappa_{el} = L_0 \sigma T$, $L_0 = 2.45 \times 10^{-8} W\Omega/K^2$). To examine the validity of this law in half-Heusler compounds, we have chosen HfCoS as an example. We have calculated the electronic transport coefficients by employing *ab-initio* electronic structure method and the Boltzmann transport equation in HfCoSb. We calculate κ_{el}at constant current **J** ($\kappa_{el,J}$) and constant electric filed **E** ($\kappa_{el,E}$) where $\kappa_{el,J} = \kappa_{el,E} - T\sigma S^2$ which shows a significant deviation from values obtained with Wiedemann-Franz law. $\kappa_{el,J}$ is much smaller than $\kappa_{el,E}$at low carrier concentrations (n) and/or at high temperatures (T) and the ratio $\kappa_{el,J}/\kappa_{el,E} \to 1$ at high n and/or low T.

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