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The Role of Minority Carriers in Thermoelectrics: Why Half Heusler ZrNiSn is a good n-type but poor p-type Thermoelectric

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The bipolar excitation of minority carriers limits the maximum zT of a typical thermoelectric material. This is because the thermopower (absolute value of the Seebeck coefficient) of a typical heavily doped semiconductor rises with temperature until it reaches a maximum value, and then decreases due to the activation of minority carriers of opposite sign. The temperature of the thermopower roll-over is determined largely by the band gap which acts as the activation energy of the minority carriers. Julian Goldsmid and Jeff Sharp showed that the a simple relationship, $E_g = 2 S_m T_m$, between the maximum thermopower (S_m) the temperature where the maximum occurs (T_m) and the band gap (E_g , measured in eV) is a good approximation for many materials, particularly when both types of carriers have similar mobilities. The (Ti, Zr, Hf)NiSn half Heusler compounds, however, demonstrate the limits of this relationship. The Goldsmid-Sharp band-gap for n-type ZrNiSn is several times greater than that for p-type ZrNiSn that ultimately results in high thermopower at high temperature and therefore high zT for the n-type material but the p-type is not useful. We have explained this phenomena using optical band gap measurements and transport modeling. The greater mobility of the conduction band compared to the valence band suppresses the bipolar effect of the holes that enables the n-type material to retain high thermopower to high temperature. The models give quantitative guide to the accuracy of Goldsmid-Sharp band-gap by providing a correction factor that works well for Bi₂Te₃, and can be used to guide strategies for suppression of bipolar effects to increase the maximum zT .