Seebeck coefficient

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The j-th order Fermi integrals, $F_j(\eta)$, defined by

$$F_j(\eta) = \int_0^\infty \frac{\varepsilon^j}{1 + e^{\varepsilon - \eta}} d\varepsilon$$

here j is the order of integral, η is the reduced Fermi energy (chemical potential), ε is the reduced carrier energy.[1]

The experimental transport data can be analyzed using a common solution to the Boltzmann transport equation within the relaxation time approximation. It is assumed that electron conduction occurs within a single parabolic band (SPB) with a single scattering mechanism where the energy dependence of the carrier relaxation time can be expressed by a simple power-law $\tau = \tau_0 E^r$. The Seebeck coefficient derived from the Boltzmann transport equations within SPB model provided as follows[2]
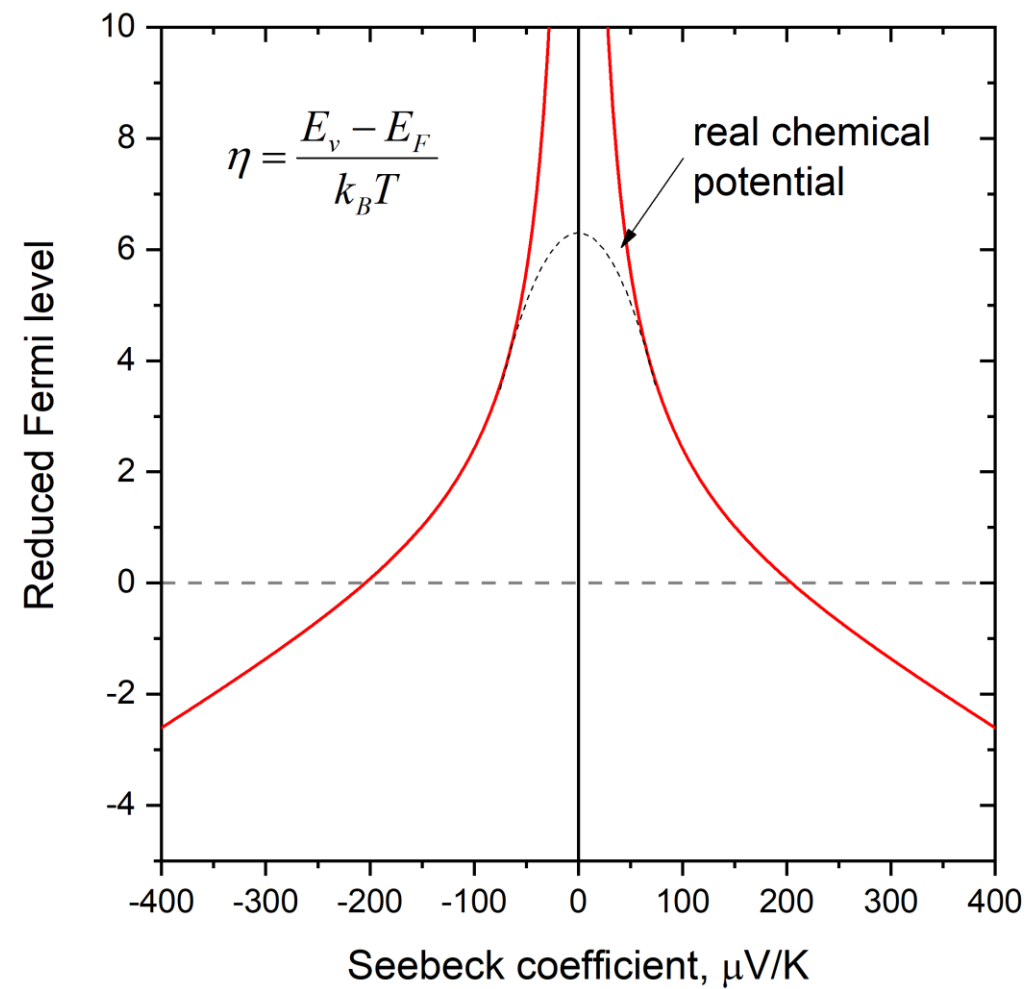
$$\alpha(\eta) = \pm \frac{k_B}{e} \left(\frac{(r + 5/2)F_{r+3/2}(\eta)}{(r + 3/2)F_{r+1/2}(\eta)} - \eta \right)$$

here k_B is the Boltzmann constant, r is the scattering parameter related to the energy dependence of the carrier relaxation time, τ. η could be obtained *via* analysis of the Seebeck coefficient data.

$$\alpha(\eta) = \pm \frac{k_B}{e}\left(\frac{(r+5/2)F_{r+3/2}(\eta)}{(r+3/2)F_{r+1/2}(\eta)} - \eta\right)$$

$$\eta = \frac{E_v - E_F}{k_B T}$$

real chemical potential

Reduced Fermi level

Seebeck coefficient, μV/K

$$\alpha(\eta) = \pm \frac{k_B}{e} \left(\frac{(r + 5/2)F_{r+3/2}(\eta)}{(r + 3/2)F_{r+1/2}(\eta)} - \eta \right)$$

degenerate limit

$\eta > 5$

non-degenerate limit

$\eta < -1$

The Fermi integral can be approximated for different regions of η. For example, for $F_{1/2}(\eta)$:

$$F_{1/2}(\eta) = \begin{cases} \dfrac{\sqrt{\pi}}{2} e^{\eta}, -\infty < \eta < -1 \\ \dfrac{\sqrt{\pi}}{2} \dfrac{1}{1/4 + e^{-\eta}}, -1 < \eta < 5 \\ \dfrac{2}{3} \eta^{3/2}, 5 < \eta < \infty \end{cases}$$

In the same manner, the Seebeck coefficient can be also approximated for two situations[3,4]

degenerate limit	non-degenerate limit

$$\alpha(\eta) = \pm \frac{\pi^2}{3} \frac{k_B}{e} \left(\frac{3}{2} + r\right) \frac{1}{\eta}$$

$$\alpha(\eta) = \pm \frac{k_B}{e} \left(\frac{5}{2} + r - \eta\right)$$

Thus

thus

$$\alpha = \pm \frac{8\pi^2 k_B^2 T}{3eh^2} m_S^* \left(\frac{\pi}{3n}\right)^{2/3} \left(\frac{3}{2} + r\right)$$

$$\alpha = \pm \frac{k_B}{e} \left(\frac{5}{2} + r + \ln\left[\frac{2\left(2\pi m_S^* k_B T / h^2\right)^{3/2}}{n}\right]\right)^*$$

*known as Pisarenko relation[2,5]

Reminder: for *p*-type semiconductors $\alpha > 0$, for *n*-type semiconductors $\alpha < 0$, when $r = -1/2$ (deformation scattering potential) $m_S^* \approx m_d^*$.

For metals $\alpha = \frac{\pi^2}{3} \frac{k_B^2 T}{e} \left\{\frac{\partial[\log_\sigma (E)]}{\partial E}\right\}_{E=E_F}$ and thus, in the neighborhood of $E = E_F$, $\sigma(E) = \text{const} \cdot E^r$, this

becomes $\alpha = \frac{\pi^2}{3} \frac{k_B^2 T}{e E_F} r$.[6] This formula is known as Mott relation and valid for all metals and alloys at $T > \theta_D$.
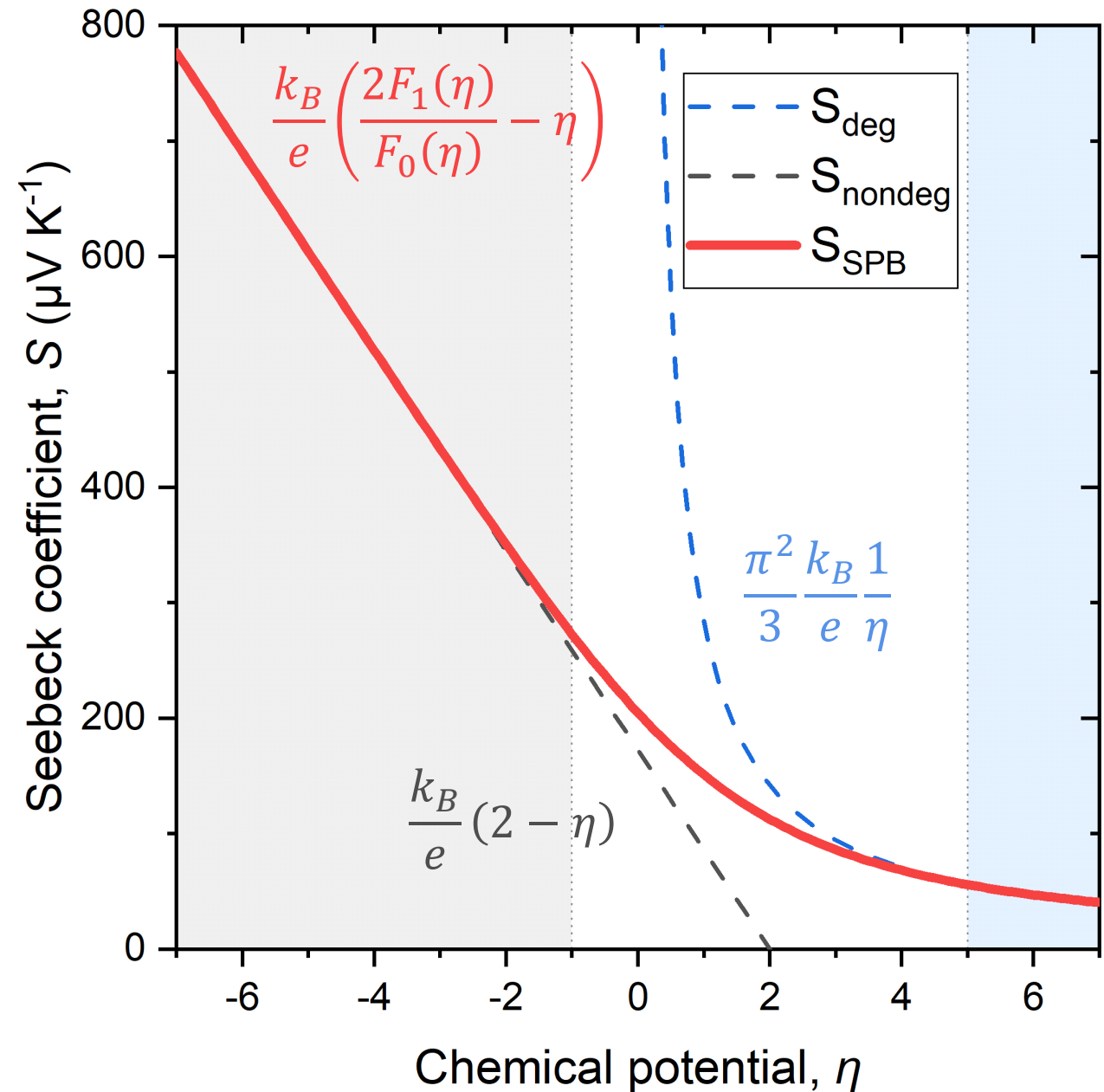
Seebeck coefficient

$$\alpha(\eta) = \pm \frac{k_B}{e}\left(\frac{(r+5/2)F_{r+3/2}(\eta)}{(r+3/2)F_{r+1/2}(\eta)} - \eta\right)$$

in the case of deformation potential (acoustic phonon scattering) $r = -1/2$

and thus, $\alpha(\eta) = \pm \frac{k_B}{e}\left(\frac{2F_1(\eta)}{F_0(\eta)} - \eta\right)$

degenerate limit: $\alpha(\eta) = \pm \frac{\pi^2}{3}\frac{k_B}{e}\frac{1}{\eta}$

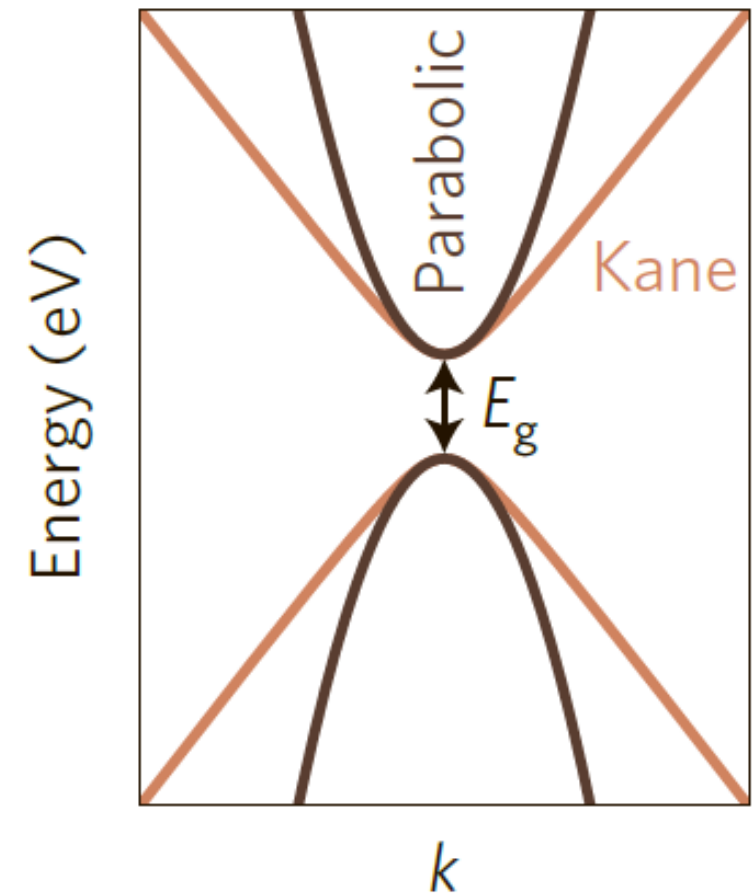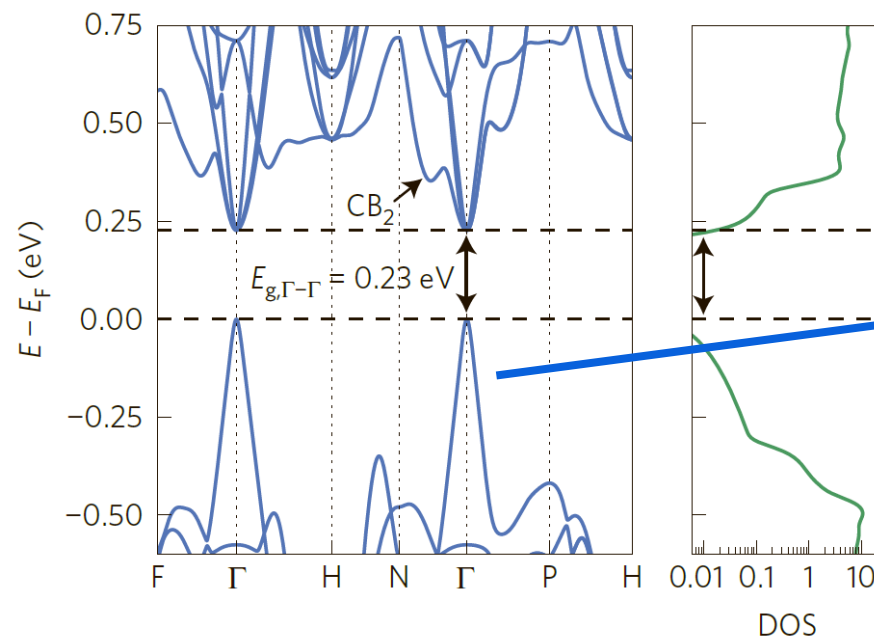non-degenerate limit: $\alpha(\eta) = \pm \frac{k_B}{e}(2 - \eta)$

Degenerate limit: $\alpha = \pm \frac{8\pi^2 k_B^2 T}{3eh^2} m_S^* \left(\frac{\pi}{3n}\right)^{2/3} \left(\frac{3}{2} + r\right)$

Degenerate limit for Kane dispersion: $\alpha = \pm \frac{8\pi^2 k_B^2 T}{3eh^2} m_S^* \left(\frac{\pi}{3n}\right)^{2/3} \left(\frac{3}{2} + r - \phi\right)$

correction factor: $\phi = \dfrac{\frac{4E}{E_g\left(1 + \frac{E}{E_g}\right)}}{\left(1 + \frac{2E}{E_g}\right)^2}$ and $m_S^* = m_0^* \left(1 + \frac{2E}{E_g}\right)$
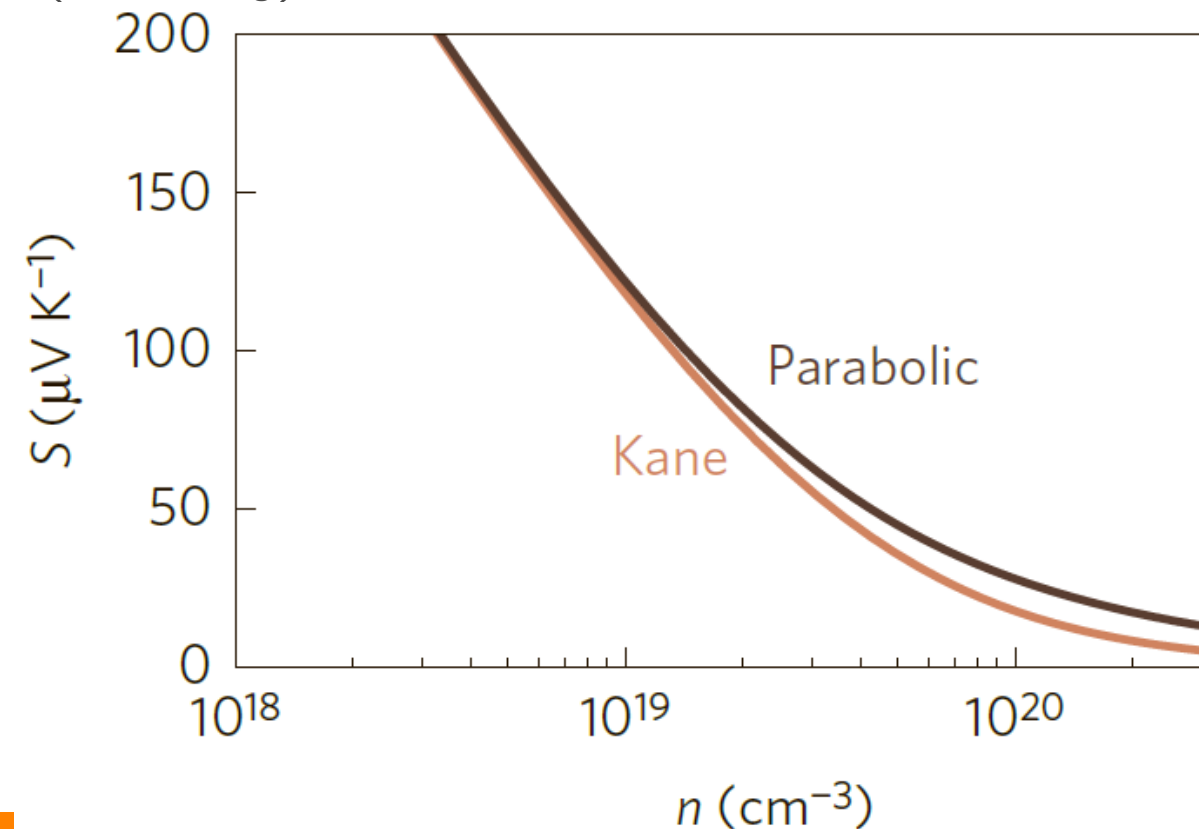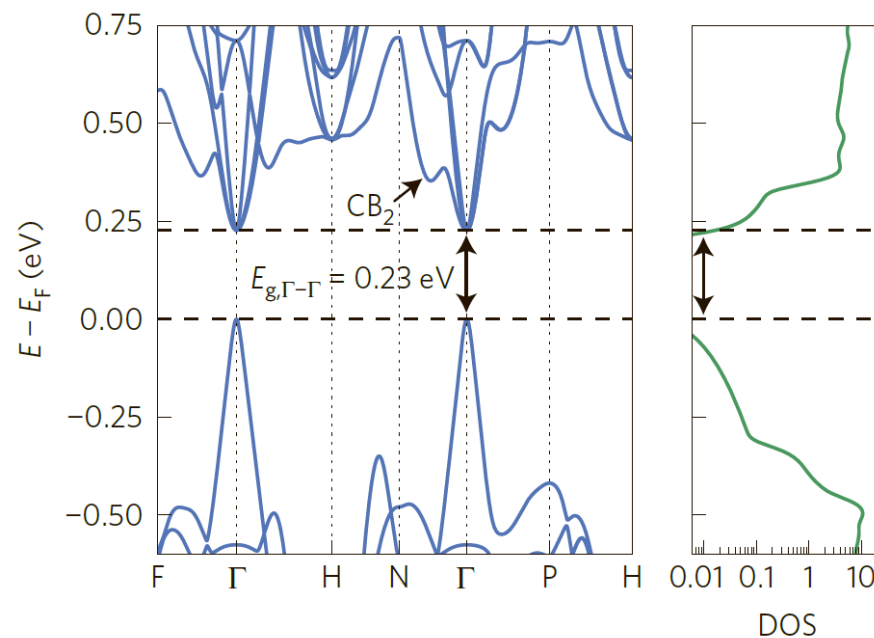

See Ref. [7]

Parabolic bands are not real?

Degenerate limit: $\alpha = \pm \dfrac{8\pi^2 k_B^2 T}{3eh^2} m_S^* \left(\dfrac{\pi}{3n}\right)^{2/3} \left(\dfrac{3}{2} + r\right)$

Degenerate limit for Kane dispersion: $\alpha = \pm \dfrac{8\pi^2 k_B^2 T}{3eh^2} m_S^* \left(\dfrac{\pi}{3n}\right)^{2/3} \left(\dfrac{3}{2} + r - \phi\right)$

correction factor: $\phi = \dfrac{4E \big/ E_g\left(1 + E/E_g\right)}{\left(1 + 2E/E_g\right)^2}$ and $m_S^* = m_0^* \left(1 + 2E/E_g\right)$

See Ref. [7]

Parabolic bands are not real?

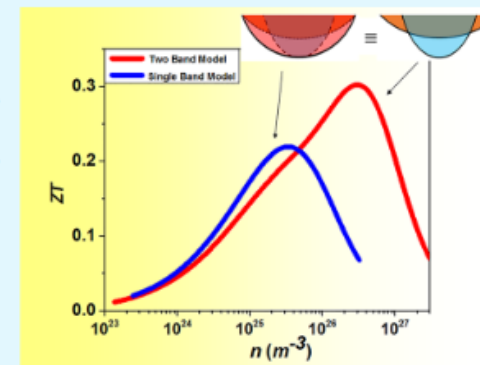## Critical Analysis of Single Band Modeling of Thermoelectric Materials

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Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai 400076, India

S Supporting Information

ABSTRACT: Study of the electronic band structure of thermoelectric (TE) materials is fundamental to both its understanding and further development. Currently theoretical models which assume a single-band-based charge transport are utilized due to their predictive capabilities and ease of implementation. However, most good thermoelectric materials have complex band structures with multiple bands near the band edge. The extent of applicability of single-band models in such systems is questionable and forms the objective of this study. To check this, we have chosen five well-known TE materials and modeled their room temperature properties using the single parabolic band (SPB) model and the single Kane band (SKB) model. The room temperature experimental data for these materials were extracted from literature reports, and the analysis was carried out on a relatively large sample set (with over 350 data points spread across the various materials). Our analysis indicates the failure of single-band models in situations where multiple near-degenerate bands are present close to the band extrema. The associated errors are in the estimated density of states effective mass (m_D^*), Lorenz number (L), and lattice thermal conductivity (κ_L), which in turn result in erroneous predictions of the optimum charge carrier concentration and zT values. We also find that identifying whether the band edge is parabolic is difficult from a visual comparison of the SPB and SKB Pisarenko plots since the observed variations are well within the acceptable limits of experimental error. To overcome this problem, we propose an error analysis technique which can be used to find the best fit model. The error analysis can also be useful in identifying the dominant charge carrier scattering mechanism as shown from our study. Overall, our work highlights the need for implementation of multiband modeling while working with materials with complex band structures.

KEYWORDS: single parabolic band model (SPB), single Kane band model (SKB), thermoelectric materials, Seebeck coefficient, Lorenz number, band mass

See Ref. [8]

Parabolic bands are not real?

Table 1. Single Band Expressions for Charge Carrier Concentration (n), Seebeck Coefficient (S), Hall Prefactor (r_H), Lorenz Number (L), Hall Mobility (μ_H), and Power Factor ($S^2\sigma$) for the SPB and SKB Models[a]

property	SPB	SKB
n	$\dfrac{(2m_D^* k_B T)^{3/2}}{3\pi^2 \hbar^3} F_{1/2}(\eta)$	$\dfrac{(2m_{D0}^* k_B T)^{3/2}}{3\pi^3 \hbar^3}\left({}^0F_0^{3/2}(\eta)\right)$
S	$\dfrac{k_B}{e}\left(\dfrac{2F_1(\eta)}{F_0(\eta)} - \eta\right)$	$\dfrac{k_B}{e}\left[\dfrac{{}^1F_{-2}^1(\eta)}{{}^0F_{-2}^1(\eta)} - \eta\right]$
r_H	$\dfrac{3}{4}F_{1/2}(\eta)\dfrac{F_{-1/2}(\eta)}{F_0^2(\eta)}$	$\dfrac{3K(K+2)({}^0F_0^{3/2})({}^0F_{-4}^{1/2})}{(2K+1)^2({}^0F_{-2}^1)^2}$
L	$\left(\dfrac{k_B}{e}\right)^2 \dfrac{3F_0(\eta)F_2(\eta) - 4F_1^2(\eta)}{F_0^2(\eta)}$	$\left(\dfrac{k_B}{e}\right)^2\left[\dfrac{{}^2F_{-2}^1(\eta)}{{}^0F_{-2}^1(\eta)} - \left(\dfrac{{}^1F_{-2}^1(\eta)}{{}^0F_{-2}^1(\eta)}\right)^2\right]$
μ_H	$\mu_0 \dfrac{F_{-1/2}(\eta)}{2F_0(\eta)}$	$r_H\mu_0 \dfrac{{}^0F_{-2}^1(\eta)}{{}^0F_0^{3/2}(\eta)}$
$S^2\sigma$	$\left(\dfrac{8\pi}{3e}\right)\mu_0 k_B^2\left(\dfrac{2m_D^* k_B T}{h^2}\right)^{3/2} F_0(\eta)\left(\dfrac{2F_1(\eta)}{F_0(\eta)} - \eta\right)^2$	$\left(\dfrac{8\pi}{3e}\right)\mu_0 k_B^2\left(\dfrac{2m_{D0}^* k_B T}{h^2}\right)^{3/2}{}^0F_{-2}^1(\eta)\left(\dfrac{{}^1F_{-2}^1(\eta)}{{}^0F_{-2}^1(\eta)} - \eta\right)^2$

[a]m_D^* represents the density of states effective mass of a parabolic band, while m_{D0}^* is the density of states effective mass at the band extremum ($E = 0$) of a nonparabolic band. μ_0 represents the mobility free parameter, and K is the ratio of the longitudinal to transverse effective mass.[3,4]

values. We also find that identifying whether the band edge is parabolic is difficult from a visual comparison of the SPB and SKB Pisarenko plots since the observed variations are well within the acceptable limits of experimental error. To overcome this problem, we propose an error analysis technique which can be used to find the best fit model. The error analysis can also be useful in identifying the dominant charge carrier scattering mechanism as shown from our study. Overall, our work highlights the need for implementation of multiband modeling while working with materials with complex band structures.

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n	$\dfrac{(2m_D^*k_BT)^{3/2}}{3\pi^2\hbar^3}F_{1/2}(\eta)$	$\dfrac{(2m_{D0}^*k_BT)^{3/2}}{3\pi^3\hbar^3}(^0F_0^{3/2}(\eta))$
S	$\dfrac{k_B}{e}\left(\dfrac{2F_1(\eta)}{F_0(\eta)}-\eta\right)$	$\dfrac{k_B}{e}\left[\dfrac{^1F_{-2}^1(\eta)}{^0F_{-2}^1(\eta)}-\eta\right]$
r_H	$\dfrac{3}{4}F_{1/2}(\eta)\dfrac{F_{-1/2}(\eta)}{F_0^2(\eta)}$	$\dfrac{3K(K+2)(^0F_0^{3/2})(^0F_{-4}^{1/2})}{(2K+1)^2(^0F_{-2}^1)^2}$
L	$\left(\dfrac{k_B}{e}\right)^2\dfrac{3F_0(\eta)F_2(\eta)-4F_1^2(\eta)}{F_0^2(\eta)}$	$\left(\dfrac{k_B}{e}\right)^2\left[\dfrac{^2F_{-2}^1(\eta)}{^0F_{-2}^1(\eta)}-\left(\dfrac{^1F_{-2}^1(\eta)}{^0F_{-2}^1(\eta)}\right)^2\right]$
μ_H	$\mu_0\dfrac{F_{-1/2}(\eta)}{2F_0(\eta)}$	$r_H\mu_0\dfrac{^0F_{-2}^1(\eta)}{^0F_0^{3/2}(\eta)}$
$S^2\sigma$	$\left(\dfrac{8\pi}{3e}\right)\mu_0k_B^2\left(\dfrac{2m_D^*k_BT}{h^2}\right)^{3/2}F_0(\eta)\left(\dfrac{2F_1(\eta)}{F_0(\eta)}-\eta\right)^2$	$\left(\dfrac{8\pi}{3e}\right)\mu_0k_B^2\left(\dfrac{2m_{D0}^*k_BT}{h^2}\right)^{3/2}{}^0F_{-2}^1(\eta)\left(\dfrac{^1F_{-2}^1(\eta)}{^0F_{-2}^1(\eta)}-\eta\right)^2$

$$^nF_k^m(\eta,\alpha)=\int_0^\infty\left(-\frac{\partial f}{\partial\varepsilon}\right)\varepsilon^n(\varepsilon+\alpha\varepsilon^2)^m(1+2\alpha\varepsilon)^k\,d\varepsilon \qquad (1)$$

Here the term "α" is known as the band nonparabolicity parameter and depends on the band gap of the material ($\alpha=\dfrac{kT}{E_G}$). The terms n, m, and k are indices of the integral whose values depend on the transport property and the charge carrier scattering mechanism.

[a]m_D^* represents the density of states effective mass of a parabolic band, while m_{D0}^* is the density of states effective mass at the band extremum ($E = 0$) of a nonparabolic band. μ_0 represents the mobility free parameter, and K is the ratio of the longitudinal to transverse effective mass.[3,4]
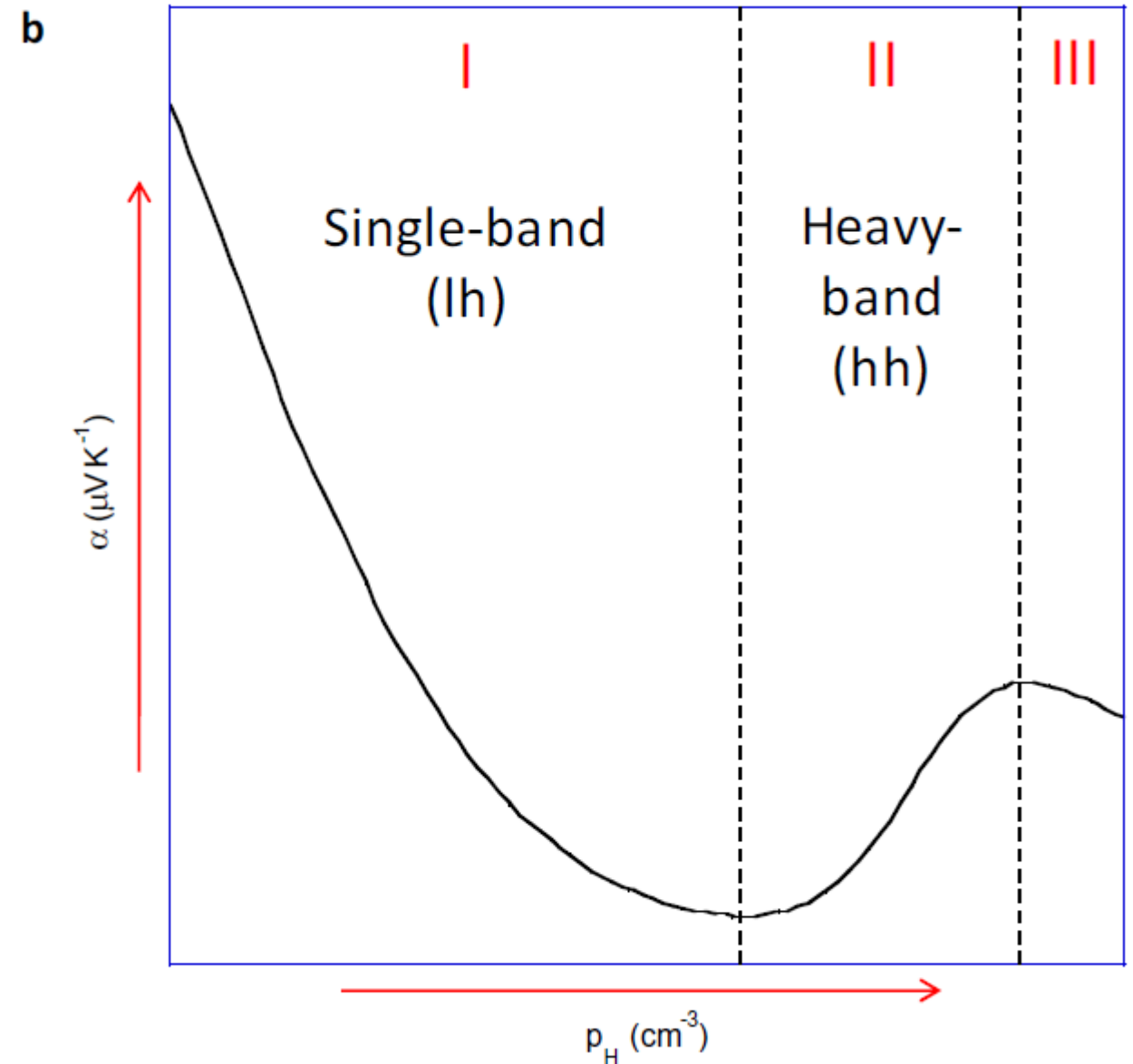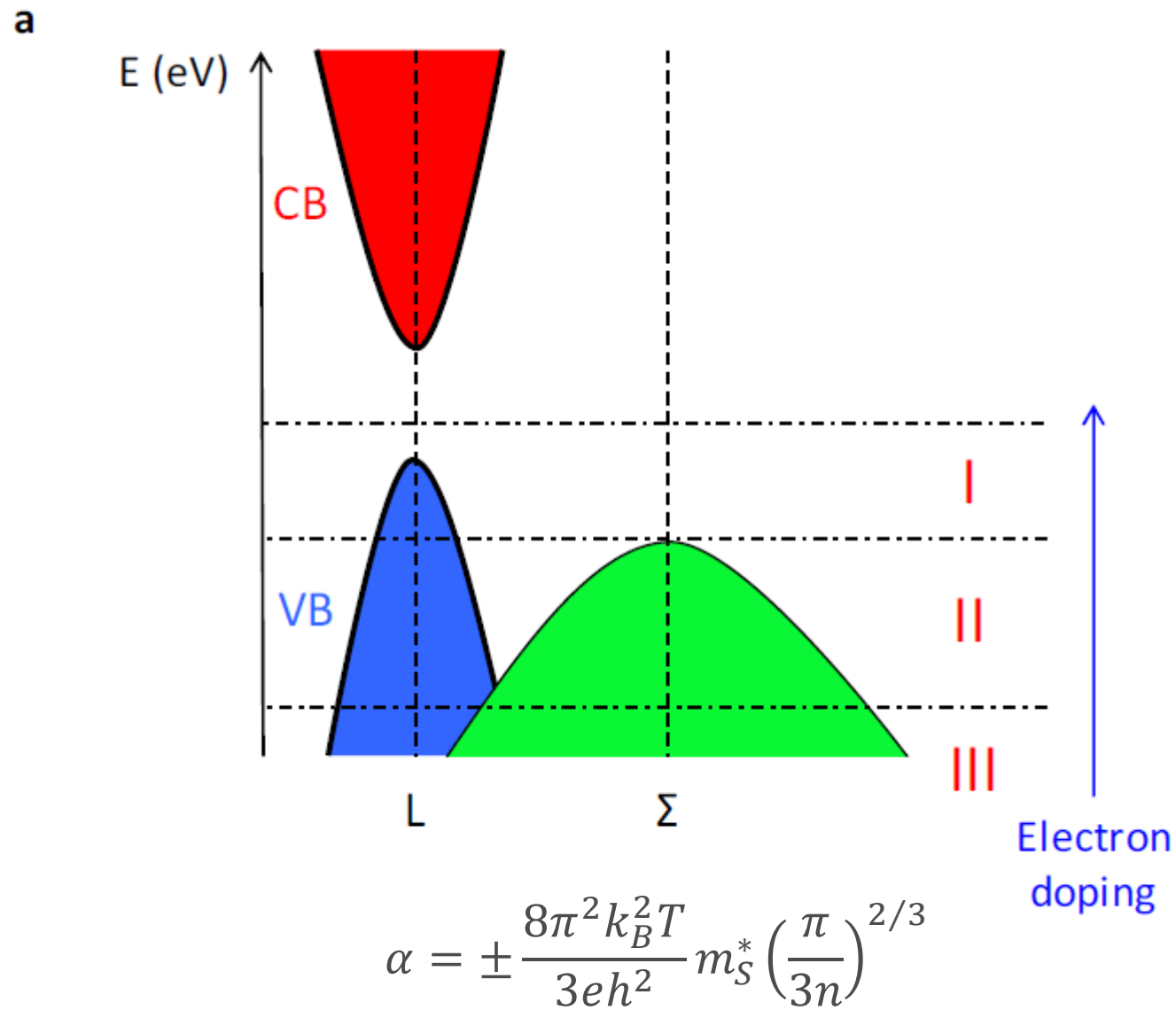
values. We also find that identifying whether the band edge is parabolic is difficult from a visual comparison of the SPB and SKB Pisarenko plots since the observed variations are well within the acceptable limits of experimental error. To overcome this problem, we propose an error analysis technique which can be used to find the best fit model. The error analysis can also be useful in identifying the dominant charge carrier scattering mechanism as shown from our study. Overall, our work highlights the need for implementation of multiband modeling while working with materials with complex band structures.

KEYWORDS: *single parabolic band model (SPB), single Kane band model (SKB), thermoelectric materials, Seebeck coefficient, Lorenz number, band mass*

See Ref. [8]

$$\alpha = \pm \frac{8\pi^2 k_B^2 T}{3eh^2} m_S^* \left(\frac{\pi}{3n}\right)^{2/3}$$

$$L(\eta) = \left(\frac{k_B}{e}\right)^2 \left(\frac{(r+7/2)F_{r+5/2}(\eta)}{(r+3/2)F_{r+1/2}(\eta)} - \left[\frac{(r+5/2)F_{r+3/2}(\eta)}{(r+3/2)F_{r+1/2}(\eta)}\right]^2\right)$$

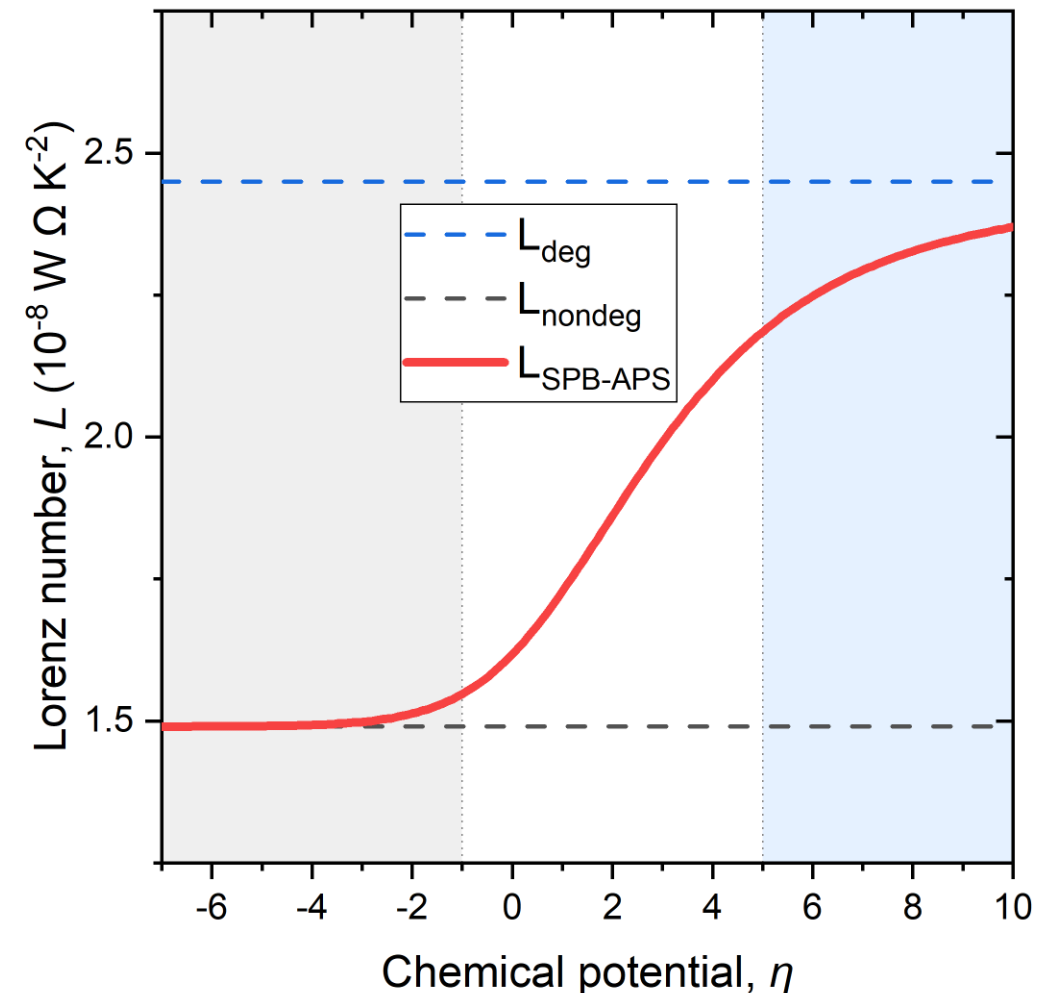Degenerate limit: $L = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 = 2.45 \cdot 10^{-8} \frac{V^2}{K^2}$

Non-degenerate limit: $L = 2\left(\frac{k_B}{e}\right)^2 = 1.49 \cdot 10^{-8} \frac{V^2}{K^2}$

Reasonable approximation $L = 1.5 + e^{-|\alpha|/116}$ (see Ref. [9])

Intrinsic region: $L = \left(\frac{k_B}{e}\right)^2 \left(r + \frac{5}{2} + \left[2\left(r + \frac{1}{2}\right) + \frac{eE_g}{k_B T}\right]^2 \frac{b}{(1+b)^2}\right)$,

$b = |\mu_n|/|\mu_p|$ and $(1+b) = \sigma_n + \sigma_p = \sigma$

at high temperatures $b = 1$

In the framework of the effective mass model (also called single parabolic band model) chemical (real) charge carrier concentration is defined as[1,2]

$$n(\eta) = 4\pi \left(\frac{2m_d^* k_B T}{h^2} \right)^{3/2} F_{1/2}(\eta)$$

It should be considered that the Hall charge carrier concentration is related to the chemical one *via* $n = n_H r_H$, where r_H is the Hall factor given by[1,2]

$$r_H(\eta) = \frac{3}{2} F_{1/2}(\eta) \frac{\left(\frac{3}{2} + 2r \right) F_{2r+1/2}(\eta)}{\left(\frac{3}{2} + r \right)^2 F_{r+1/2}^2(\eta)}$$

For complete degeneracy ($\eta > 5$) $r_H = 1$ regardless of the scattering mechanism. For non-degenerate semiconductors ($\eta < -1$) $r_H = 315\pi/512 = 1.93$ for ionized impurities scattering ($r = 3/2$), $r_H = 45\pi/128 = 1.13$ for polar optical phonon scattering ($r = 1/2$), $r_H = 1$ for charge-neutral impurity scattering ($r = 0$) and $r_H = 3\pi/8 = 1.18$ for a scattering of carries *via* acoustic phonons ($r = -1/2$).[2,10]

Hall factor

For non-degenerate region, the Hall factor can be approximated as follows
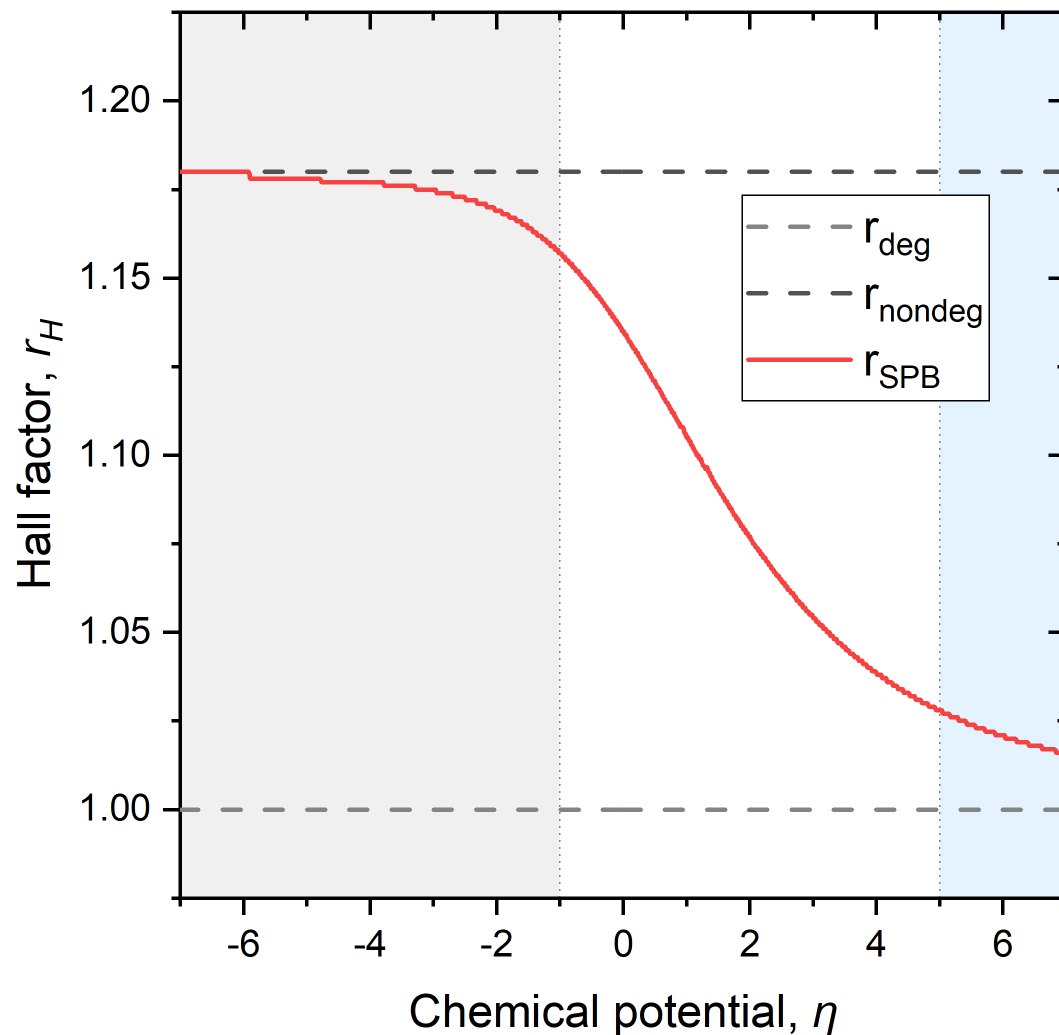
$$r_H = \Gamma\left(\frac{5}{2}\right)\frac{\Gamma\left(\frac{5}{2}+2r\right)}{\left[\Gamma\left(\frac{5}{2}+r\right)\right]^2}$$

For example, in the case of acoustic phonon scattering $\left(r = -\frac{1}{2}\right)$:

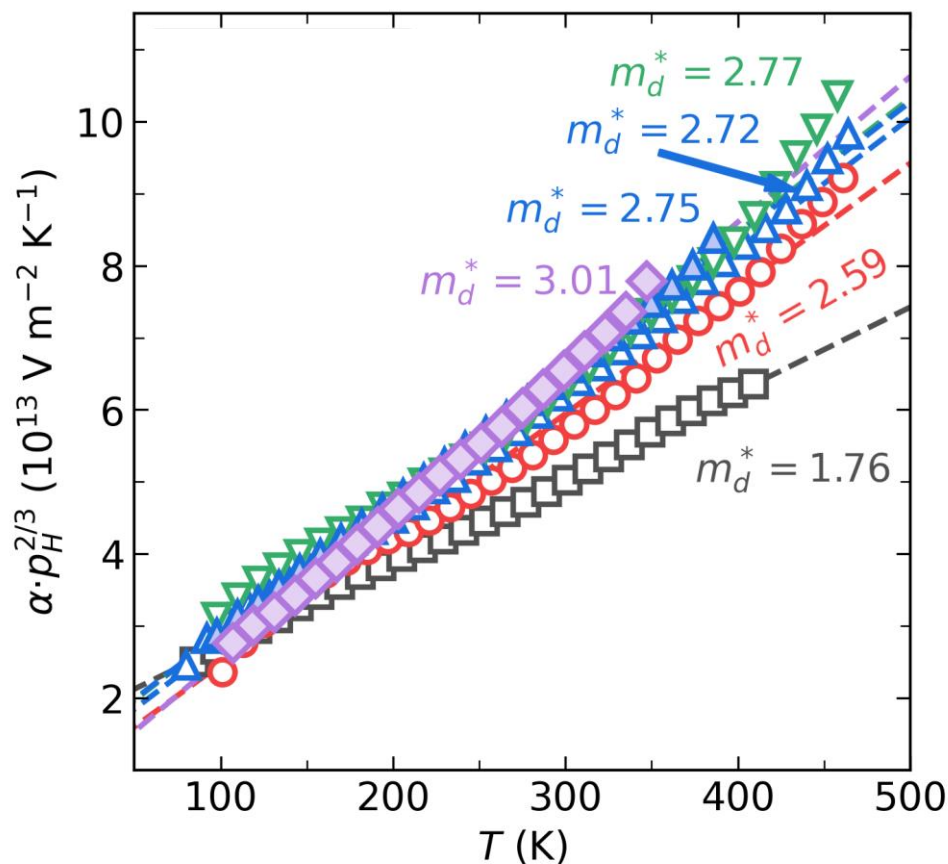$$r_H(\eta) = \frac{3}{4}F_{1/2}(\eta)\frac{F_{-1/2}(\eta)}{F_0^2(\eta)}$$

degenerate limit $r_H = 1$

non-degenerate limit $r_H = \Gamma\left(\frac{5}{2}\right)\frac{\Gamma\left(\frac{3}{2}\right)}{[\Gamma(2)]^2} = \frac{3\pi}{8} = 1.18$

If the Hall measurements were carried out, the effective mass can be calculated directly from

$n(\eta) = 4\pi \left(\frac{2m_d^* k_B T}{h^2}\right)^{3/2} F_{r+1}(\eta)$. Another possible trick is to calculate the effective mass by using

experimental values of the Seebeck coefficient: $\alpha = \pm \frac{8\pi^2 k_B^2 T}{3eh^2} m_S^* \left(\frac{\pi}{3n}\right)^{2/3} \left(\frac{3}{2} + r\right)$.

In the framework of the single parabolic band model (SPB) the effective mass is expected to be a constant with changes in carrier concentration or Fermi level. Thus, the plot of α as a function of n can be used to evaluate how well your data fit the SPB model.
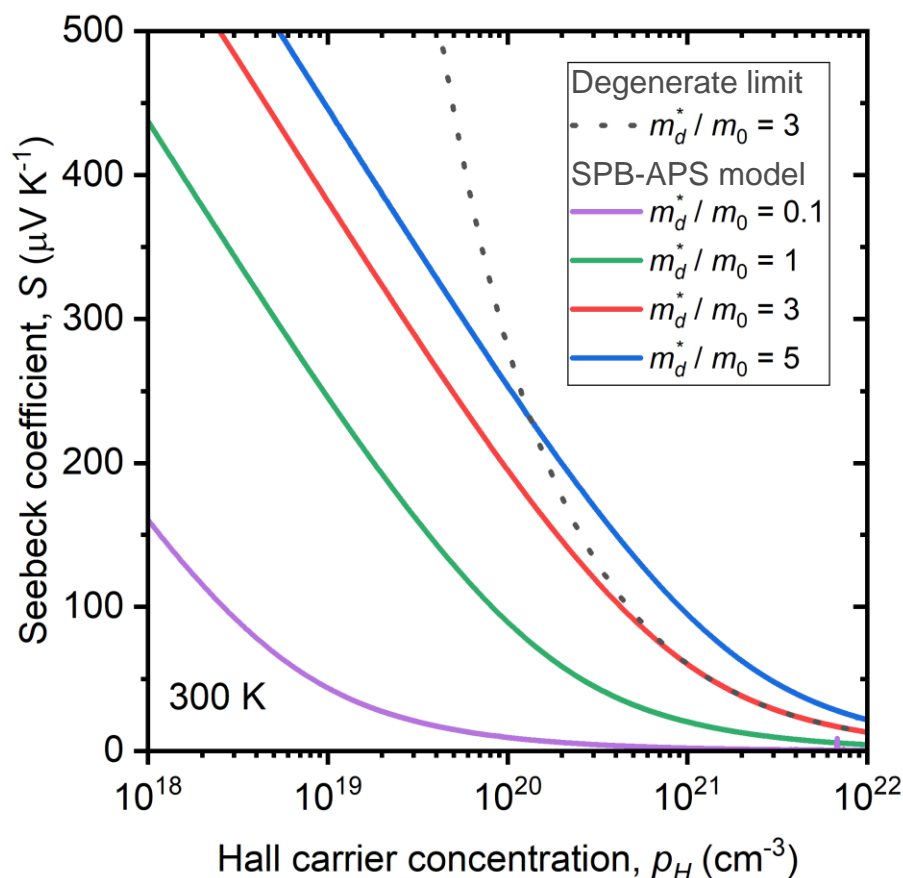

💡 If the measured Seebeck effective mass changes significantly with doping, chemical composition or temperature, it suggests there is something going on in the band's structure.

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Several common equations for the Seebeck coefficient assume the transport function has a narrow width, e.g., conducting electrons all have similar energy (band is narrower than $k_B T$). This means $f(E) \sim f(E_b)$ is a constant.
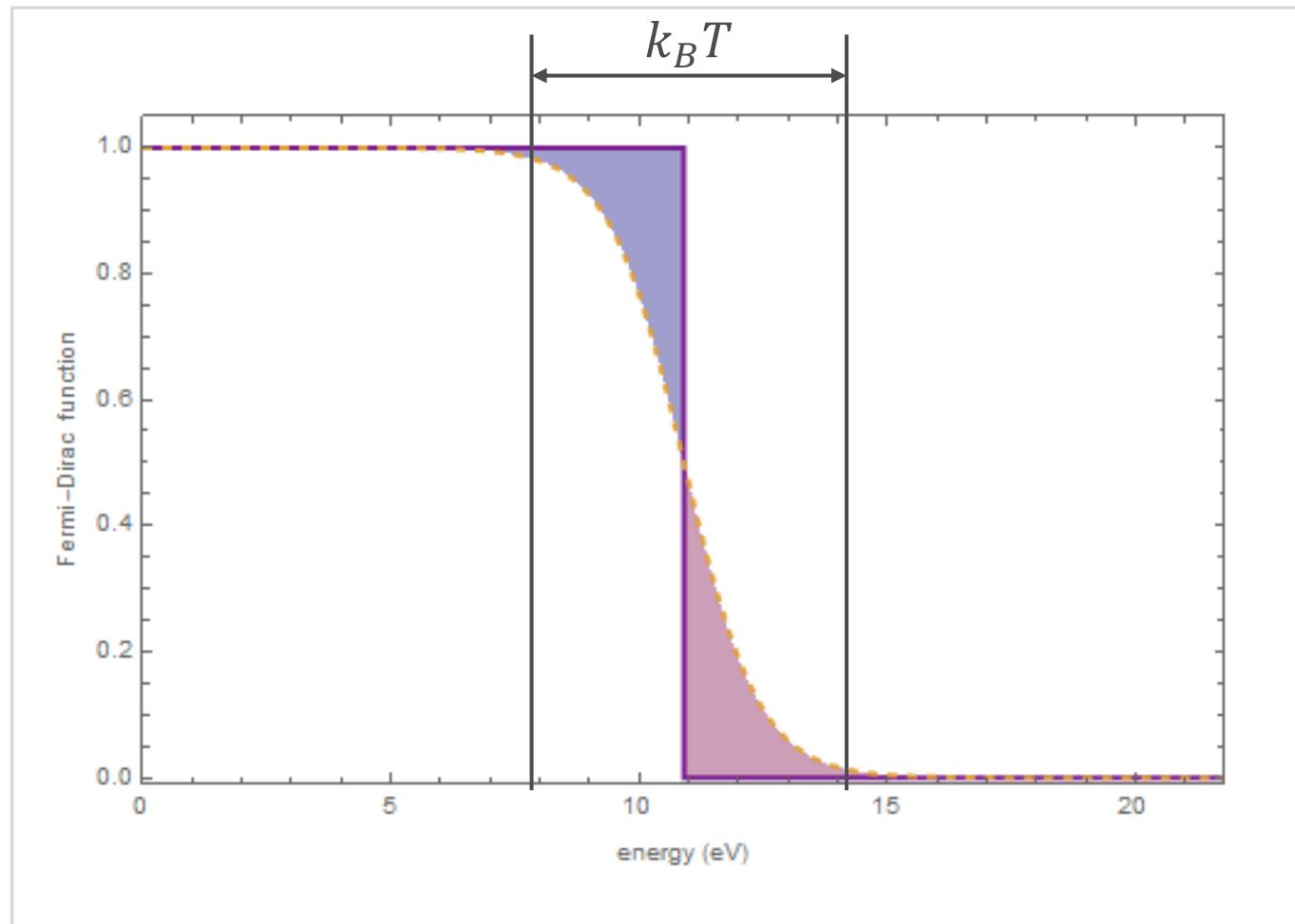
$$\alpha\sigma = -\frac{1}{eT}\int \sigma_e (E-F)\frac{\partial f}{\partial E}\,dE$$

$$f(E,T) = \frac{1}{e^{\frac{E-F}{k_B T}}+1}$$

$$\frac{\partial f(E,T)}{\partial E} = -f^2 e^{\frac{E-F}{k_B T}}\frac{1}{k_B T}$$

$$\boxed{\alpha = \frac{E_b - F}{eT}}$$

The narrow band formula is also often used for intrinsic semiconductors and amorphous materials even though the bands are not narrow.

$$\alpha = \frac{E_b - F}{eT} + A$$

where

$$A = \frac{\int (E - E_b)\sigma_E \frac{\partial f}{\partial E} dE}{eT \int \sigma_E \frac{\partial f}{\partial E} dE}$$

A contains all the difficult integration, so it is helpful only when A is reasonably small. In a normal band A is the Seebeck coefficient when $E_b = F$ at the band edge, approximately 200 µV·K⁻¹. This is not negligible for normal metals or semiconductors. A is small only in large band gap insulators, where the Fermi level is so far from the transport edge (many $k_B T$) that the $\alpha \gg 200$ µV·K⁻¹.
For intrinsic semiconductors:

$$\alpha \sim \ln \frac{1}{n} \text{ with } n = 2 \left(\frac{m^* k_B T}{2\pi\hbar^2} \right)^{3/2} e^{-\frac{E_b - F}{k_B T}}$$

The Heikes formula is commonly used to describe narrow band insulators, such as materials with localized d or f state electrons or other strongly correlated electron materials. As was shown already for carrier concentration: band at E_b has total states $N = \int g(E)dE$ and thus number of electrons or filled states $n = \int f(E,T)g(E)dE$. Then, fraction of filled states is equal to the Fermi function evaluated at the band:

$$c = f(E_b, T) = \frac{1}{e^{\frac{E_b - F}{k_B T}} + 1} = \frac{n}{N},$$

so, quite easy we can get that $\frac{E_b - F}{k_B T} = \ln\left(\frac{1-c}{c}\right)$.

Considering that $\alpha = \frac{E_b - F}{eT}$, the Seebeck can be represented as

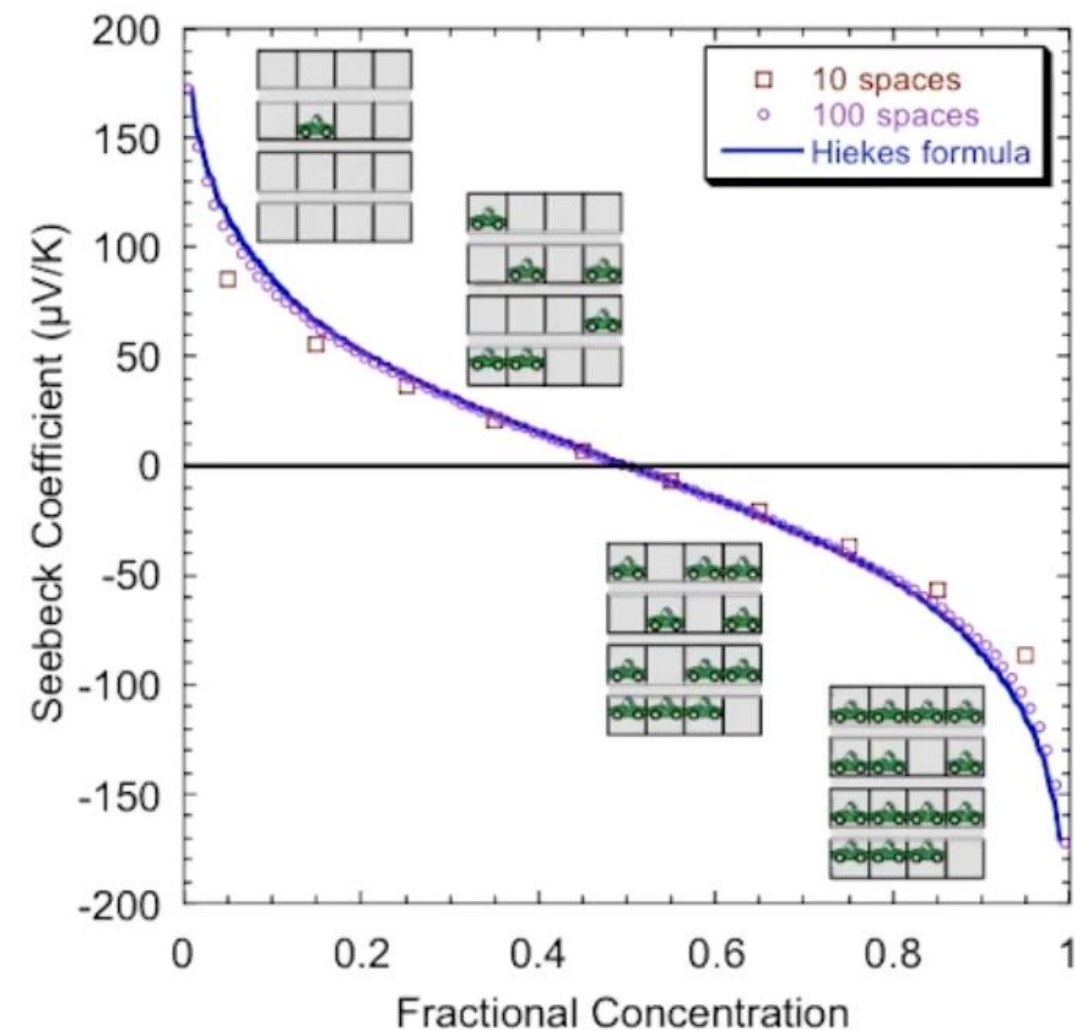$$\boxed{\alpha = \frac{k_B}{e} \ln\left(\frac{1-c}{c}\right)}$$
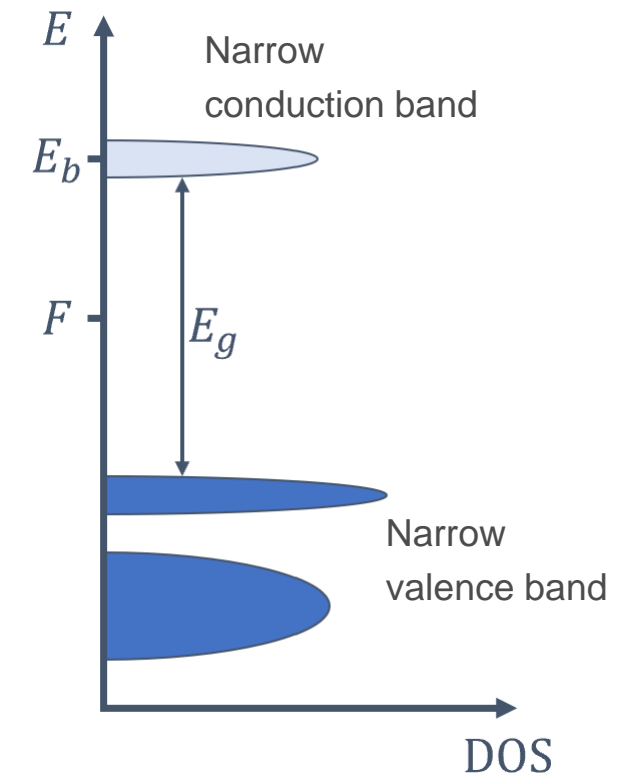
Considering that $\alpha = \frac{k_B}{e} \ln\left(\frac{1-c}{c}\right)$ and $c = \frac{n}{N}$, where n is the number of filled states, while N is the total number of states, the Seebeck coefficient may be related to the configurational entropy:

$$\alpha = \frac{k_B}{e} \frac{\partial \ln\Omega}{\partial n}$$

where $\Omega = \frac{N!}{(N-n)!n!}$ for n particles in N states.

Thus, the Seebeck coefficient can be considered as the change in entropy with number of particles:
small n and many more configurations → large α
over half full, Ω decrease, α sign change
larger n up to half full, less Ω increase, small α
(see Figure)

The Heikes formula is temperature independent because the Fermi level is adjusted at each temperature to make sure the fraction of filled states determined by the chemical composition is a constant.

For instance, to evaluate the contributions of spin orbital entropy, the Seebeck coefficient enhancement can be estimated *via* so-called modified Heikes formula:

$$\alpha = -\frac{k_B}{e}\ln\left(\frac{g_n}{g_{n+1}}\frac{x_{n+1}}{1-x_{n+1}}\right)$$

where g_n and g_{n+1} are the number the spin-orbital configurations of the M^{n+} and $M^{(n+1)+}$ ions, x is the concentration of $M^{(n+1)+}$ ions. For more details see Ref. [11,12].

Jonker-type analysis

For non-degenerate semiconductors Jonker proposed following relation between the Seebeck coefficient and the electrical conductivity:[13,14]

$$\alpha = \pm \frac{k_B}{e}(b - \ln\sigma)$$

here, parameter b involves $\mu_w T^{3/2}$ term, where μ_w is the weighted mobility (will be discussed in the next lecture). The Jonker plot (see Figure) with a constant slope of $\pm \frac{k_B}{e}$ describes the behavior of an ideal single-parabolic band semiconductor. Combined with the so-called Ioffe analysis can be used for $(\alpha^2\sigma)_{max}$ prediction.

For details see Ref. [15].

References
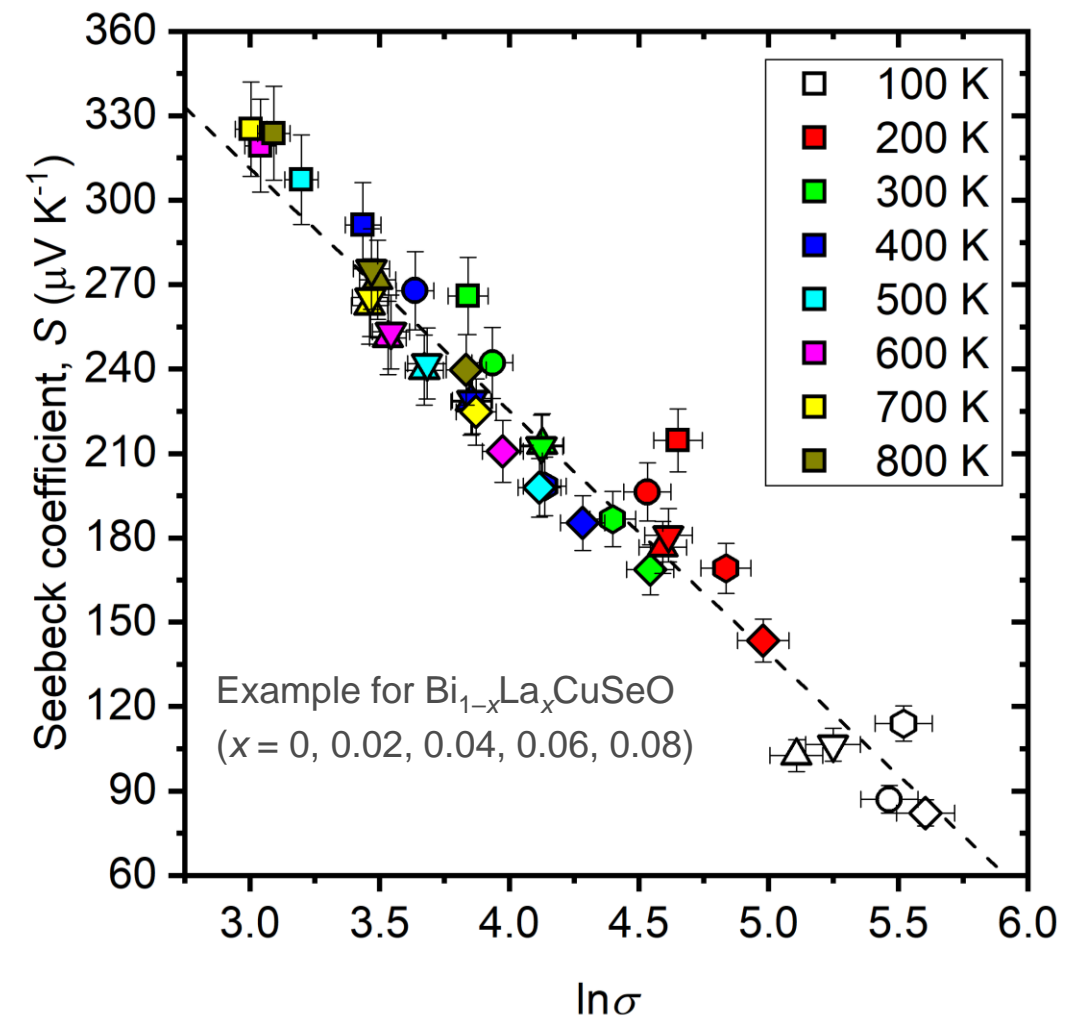
1. Kireev, P.S. *Semiconductor Physics*, 2nd ed.; Mir: Moscow, 1978.
2. Fistul', V.I. *Heavily Doped Semiconductors;* Springer New York: Boston, MA, 1995.
3. *Materials, Preparation, and Characterization in Thermoelectrics*; Rowe, D.M., Ed.; CRC Press, 2012.
4. Bonch-Bruevich, V.L.; Kalashnikov, S.G. *Semiconductor Physics*; Nauka: Moscow, 1977.
5. Ioffe, A.F. *Semiconductor Thermoelements, and Thermoelectric Cooling*; Infosearch: London, 1957.
6. Mott, N.F.; Jones, H. *The Theory of the Properties of Metals and Alloys*; Dover Publications: New York, 1958.
7. Tang, Y.; Gibbs, Z.M.; Agapito, L.A.; Li, G.; Kim, H.-S.; Nardelli, M.B.; Curtarolo, S.; Snyder, G.J. Convergence of Multi-Valley Bands as the Electronic Origin of High Thermoelectric Performance in $CoSb_3$ Skutterudites. *Nat. Mater.* 2015, 14 (12), 1223–1228.
8. Naithani, H.; Dasgupta, T. Critical Analysis of Single Band Modeling of Thermoelectric Materials. *ACS Appl. Energy Mater.* 2020, 3 (3), 2200–2213.
9. Kim, H.-S.; Gibbs, Z.M.; Tang, Y.; Wang, H.; Snyder, G.J. Characterization of Lorenz Number with Seebeck Coefficient Measurement. *APL Mater.* 2015, 3 (4), 041506.

References

10. Askerov, B.M. *Electron Transport Phenomena in Semiconductors*; World scientific, 1994.
11. Koshibae, W.; Tsutsui, K.; Maekawa, S. Thermopower in Cobalt Oxides. *Phys. Rev. B* 2000, 62 (11), 6869–6872.
12. Terasaki, I. High-Temperature Oxide Thermoelectrics. *J. Appl. Phys.* 2011, 110 (5), 053705.
13. Jonker, G.H. The Application of Combined Conductivity and Seebeck-Effect Plots for the Analysis of Semiconductor Properties (Conductivity vs Seebeck Coefficient Plots for Analyzing *n*-Type, *p*-Type and Mixed Conduction Semiconductors Transport Properties). *Philips Res. Reports* 1968, 23, 131–138.
14. Rowe, D.M.; Min, G. An Alpha-Ln Sigma Plot as a Thermoelectric Material Performance Indicator. *J. Mater. Sci. Lett.* 1995, 14 (9), 617–619.
15. Zhu, Q.; Hopper, E.M.; Ingram, B.J.; Mason, T.O. Combined Jonker and Ioffe Analysis of Oxide Conductors and Semiconductors. *J. Am. Ceram. Soc.* 2011, 94 (1), 187–193.