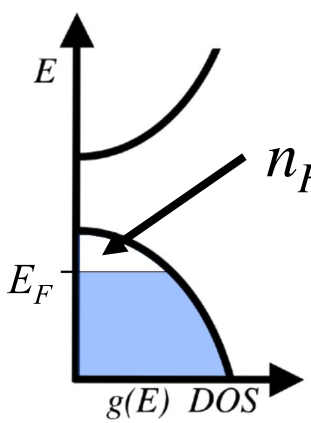
Electron Engineering of Thermoelectric Materials

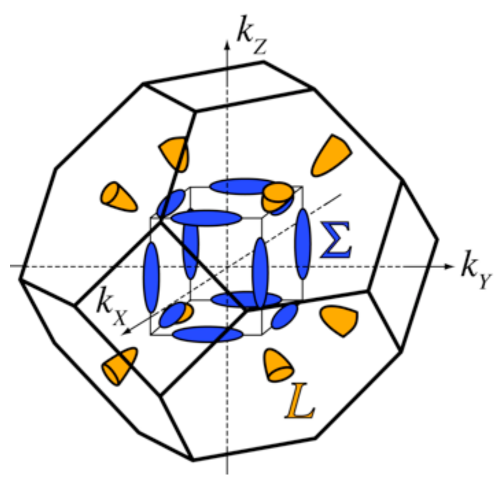
G. Jeffrey Snyder

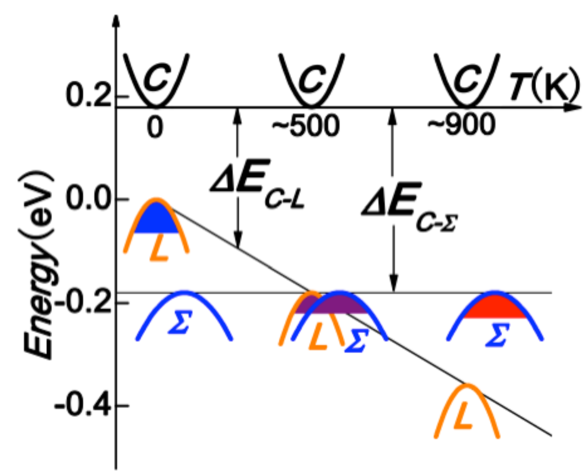
Northwestern University

Evanston IL, USA

http://thermoelectrics.matsci.northwestern.edu







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Pei, Snyder, ***Advanced Materials,*** **24**, 6125 (2012)
May, Snyder CRC Handbook (2012)

Thermoelectric Device

Thermoelectrics
Convert Heat into Electricity

Heat Flow drives free
electrons and holes
from hot to cold

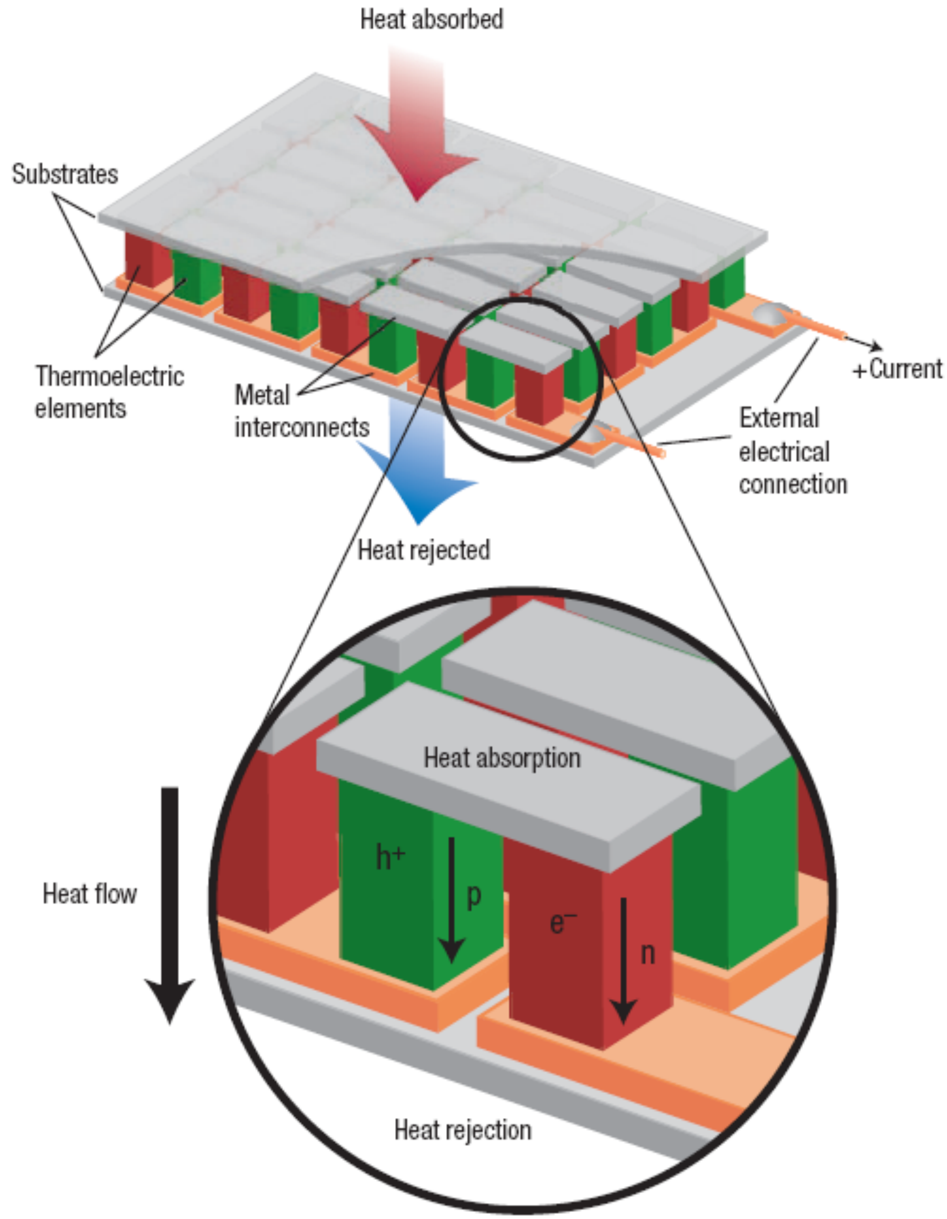
Voltage Produced
Seebeck effect
or Thermoelectric Power

$$V = \alpha \Delta T = S \Delta T$$

Seebeck Coefficient α (or S)

Efficiency ~ zT

$$zT = \frac{\alpha^2 \sigma T}{\kappa}$$



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Snyder, Toberer Nature Materials ***7,*** *105 (2008)*

Carrier Concentration

Desire High *zT* Figure of Merit

$$zT = \frac{\alpha^2 \sigma T}{\kappa}$$

Conflicting Materials Requirements

S, α Seebeck Coefficient

Need small *n*, large *m**

- Semiconductor (Valence compound)

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

σ Electrical Conductivity

Need large *n*, high *μ*

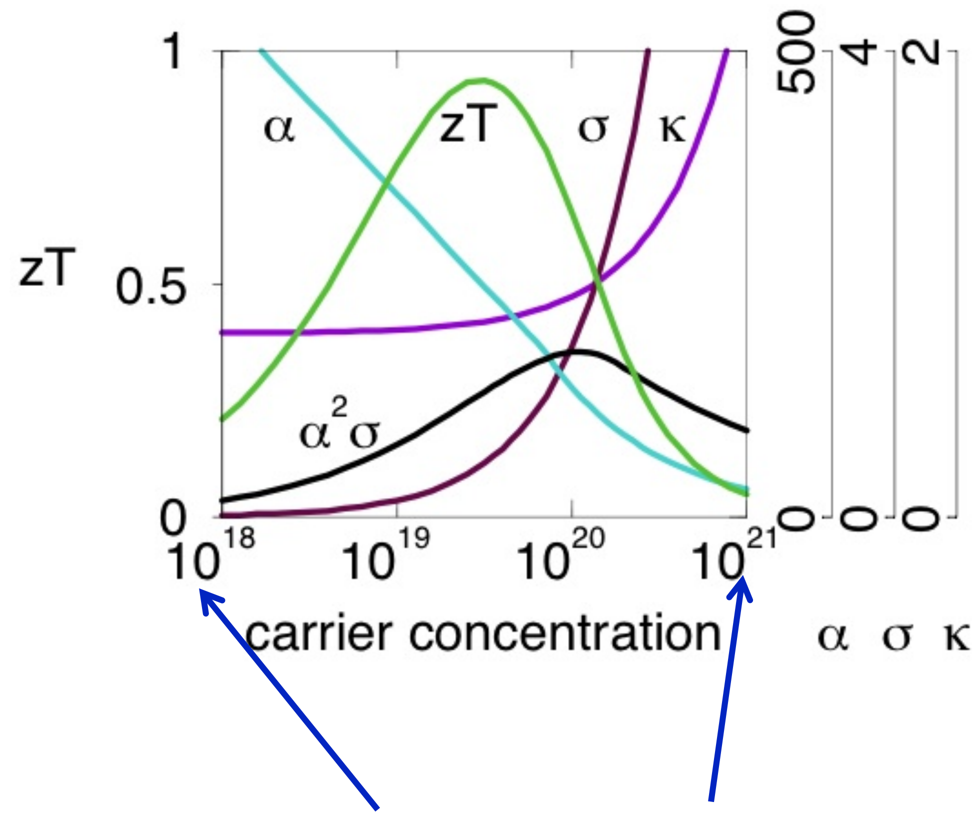
- Metal

$$\sigma = ne\mu$$

κ Thermal Conductivity

Desire small κ_l, small *n*

$$\kappa \approx \kappa_l + LTne\mu$$



Optimum between Insulator and Metal

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TE: Valence Metals with Band Gap

Thermoelectric materials are typically:

Nearly Valence Balance compounds with band gap (Usint Zintl concept of Valence)

- Band Gap < 0 is *Semi-Metal* = bad for Thermoelectrics

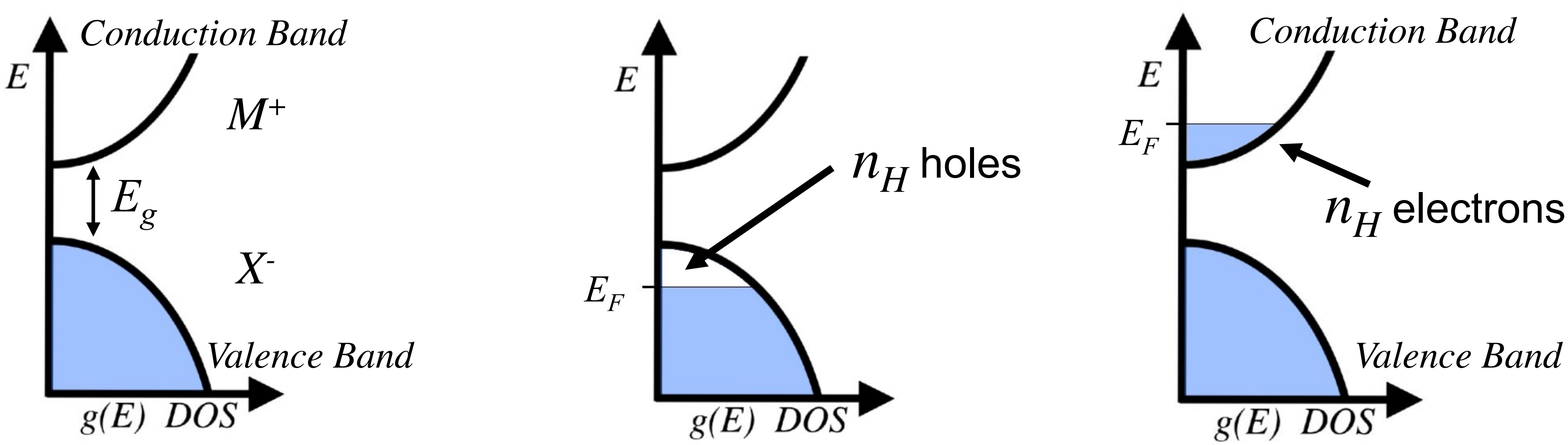
Where ***concentration of valence imbalance = free carrier concentration***

- free Carrier Concentration measured by Hall Effect n_H

Transport properties are metallic

- Heavily doped, degenerate semiconductors

Valence Balanced Semi-conductor | p-type Thermoelectric | n-type Thermoelectric

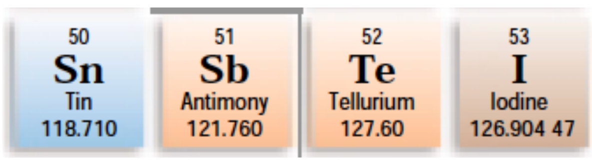


Toberer, May, Snyder ***Chem. Mat., 22,*** *p. 624 (2010)*

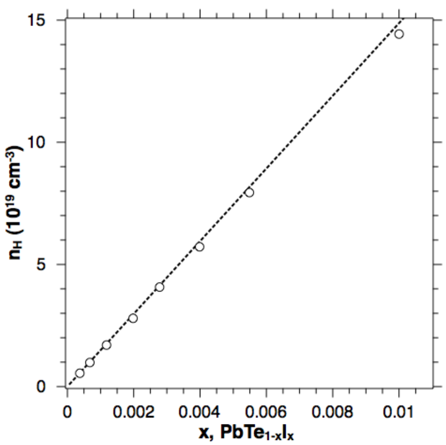
Carrier Concentration Tuning

$PbTe_{1-x}I_x$

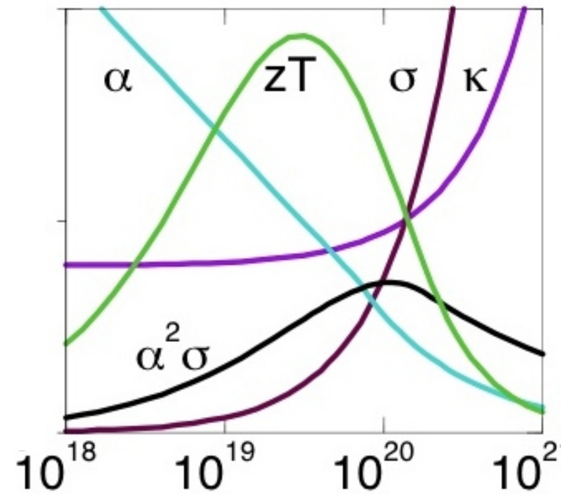
Iodine (I) supplies one more electron than Tellerium (TE)



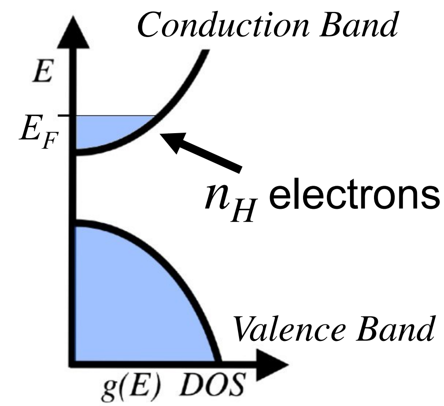
Iodine (I^-) replaces Te^{2-} producing 1 e^-



From Room Temperature Hall Effect



10^{18} - 10^{20} e^-/cm^3



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Hall Effect

Hall Effect

Magnetic Field deflects mobile charges

Hall Effect measurements give:

Sign of Charge Carrier

- n (electron) or p (hole) type

Carrier concentration

- $n_H = 1/R_H e$

Mobility

- $\mu_H = \sigma/n_H e$

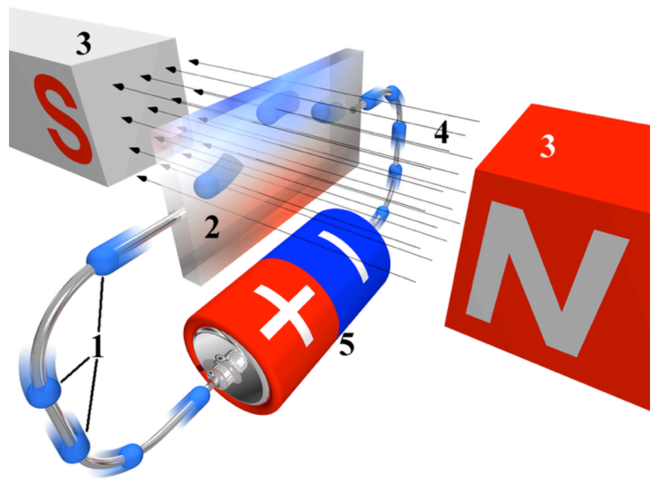
Hall Effect of Extrinsic Semicond.

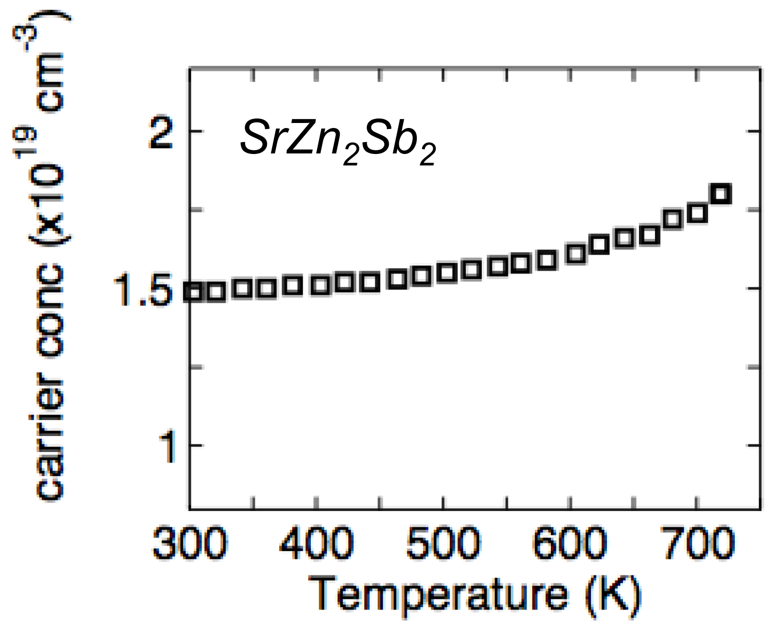
Constant n_H at low temp

- n_H = dopant concentration

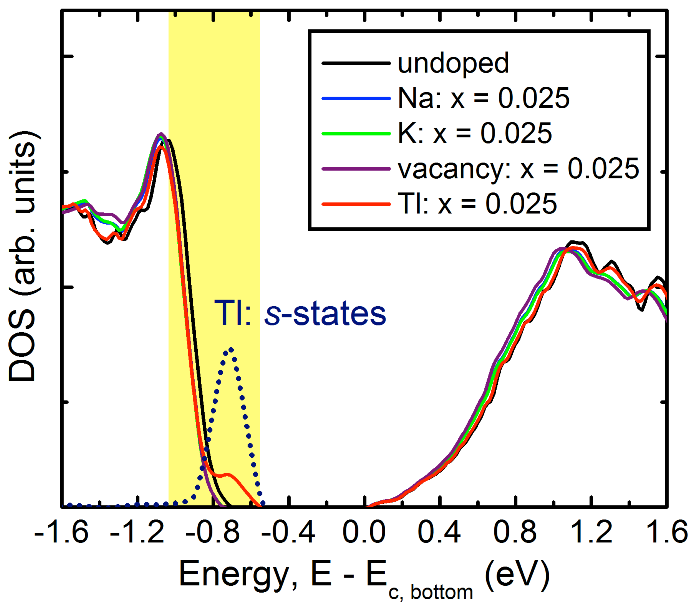
Rises at high temp

- minority carriers activated across Band Gap



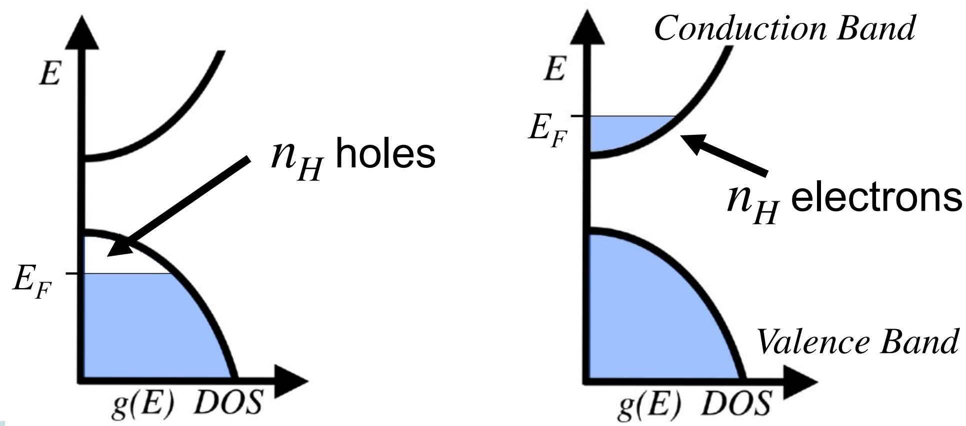


Rigid Bands



Band structure of PbTe unchanged by typical p-type doping (KKR-CPA)

Tl – resonant doping is exception

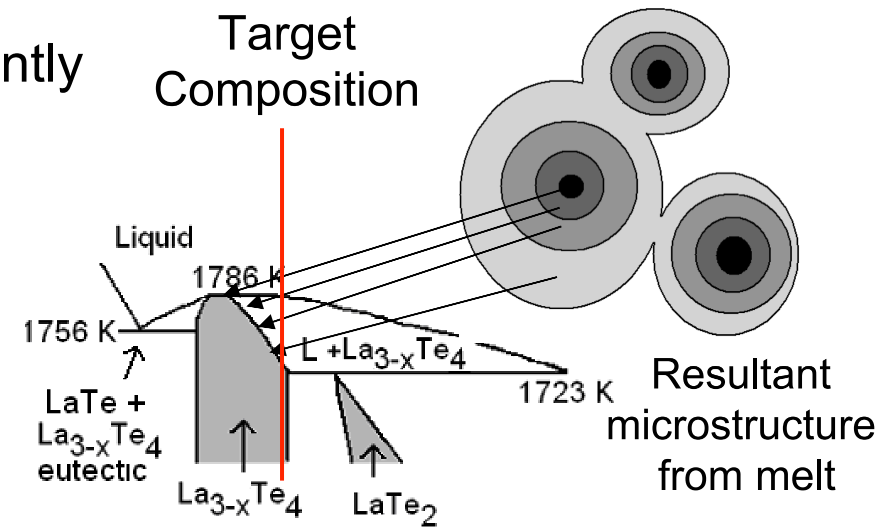


Takagiwa, Snyder, et al. *APL Materials* **1**, 011101 (2013).

Solid-State Synthesis

Complex alloys typically melt incongruently

- Synthesis from melt produces inhomogeneous materials
- inhomogeneities = Seebeck variations



Solid-state reaction diffusion limited

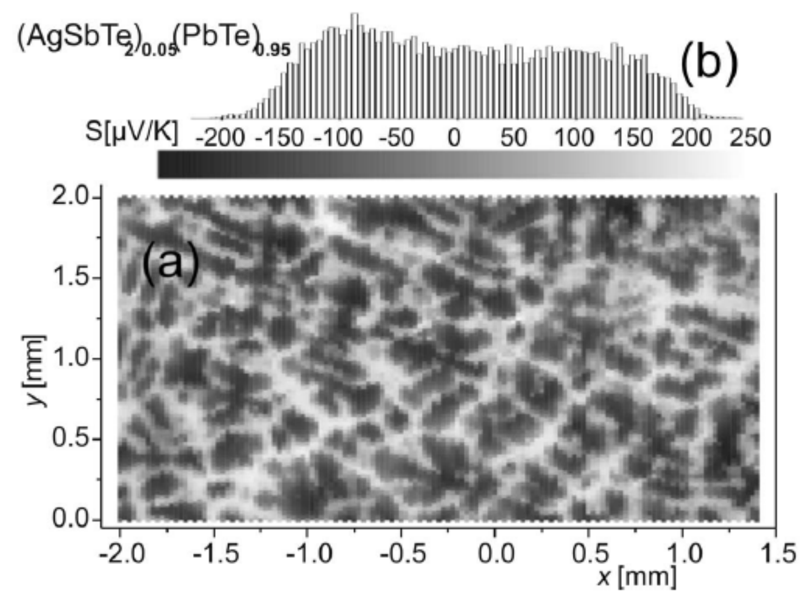
- reaction time t
- particle size l
- diffusion coefficient D

$$t \approx \frac{l^2}{D}$$

Mechanical Alloying - Ball Milling

- Reduce particle size l to 10-100nm

re

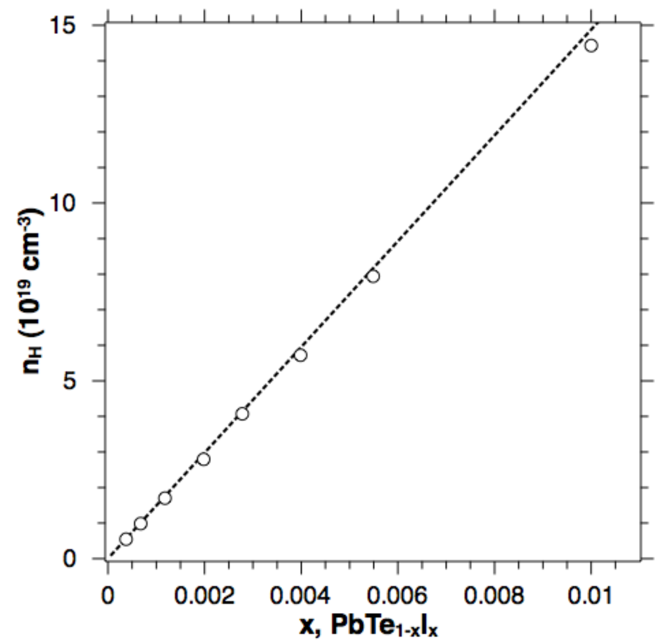


Snyder, Müller et al., ***Appl. Phys. Lett., 87,*** p. 171903 (2005)

Homogeneous n-type $PbTe_{1-x}I_x$

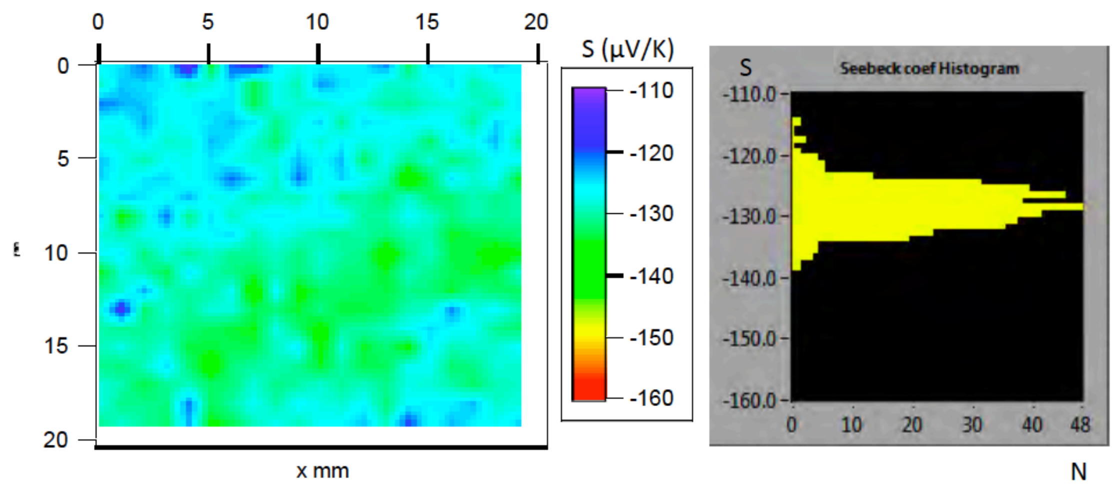
$PbTe_{1-x}I_x$
Iodine (I^-) replaces Te^{2-} producing 1 e^-

10^{18} - 10^{20} e^-/cm^3



Caltech sample

Area (mm^2)	2 x2
Interval (mm)	0.1
Sbk_ave (μV/K)	-128.817
Sbk_stdev (μV/K)	3.42
T_ave (C)	~ 40
ΔT (C)	~15



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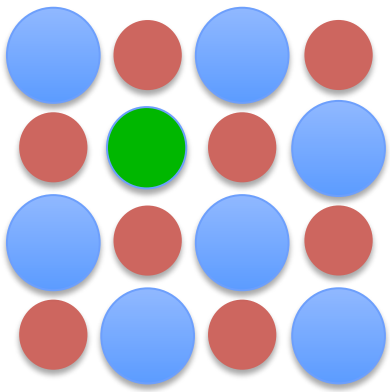
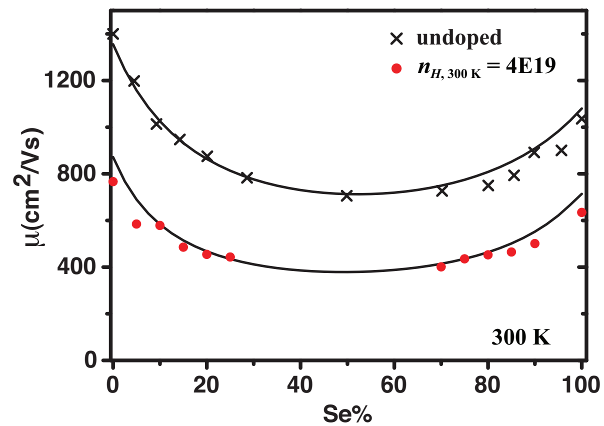
Lalonde, Pei, Snyder *Energy and Environmental Science* **4**, *2090* (2011)

Impurities reduce Mobility

Similar case – isovalent substitution (solid solutions)





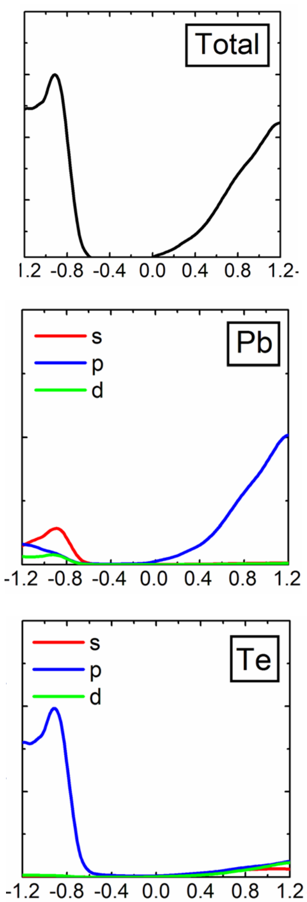
Mobility reduced due to alloy scattering (disorder scattering)

Relaxation time:

$$\tau_{alloy} = \frac{8\hbar^4}{3\sqrt{2}\pi\Omega C_A(1-C_A)U^2 m_b^{*3/2}(k_B T)^{1/2}}(\varepsilon+\varepsilon^2\alpha)^{-1/2}(1+2\varepsilon\alpha)^{-1}$$

Doping on Cation vs Anion site

Same substitution has different influence on n- and p- alloys

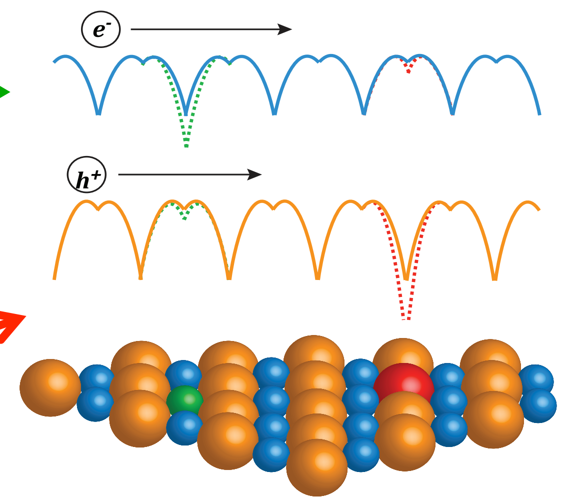


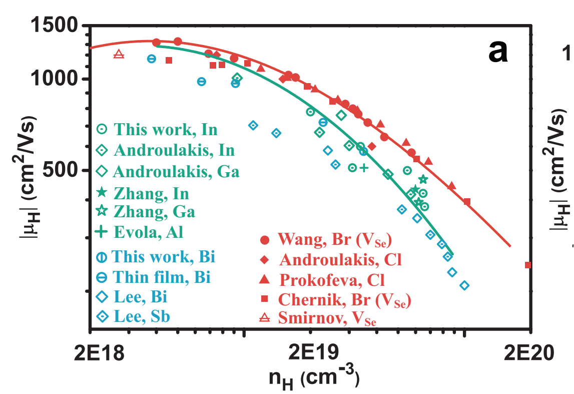
Cation site donor (green) perturbs conduction band

which is primarily formed of cations

Anion site donor (red) perturbs valence band

leading to higher conduction band mobility





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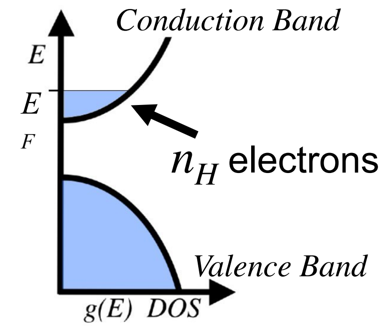
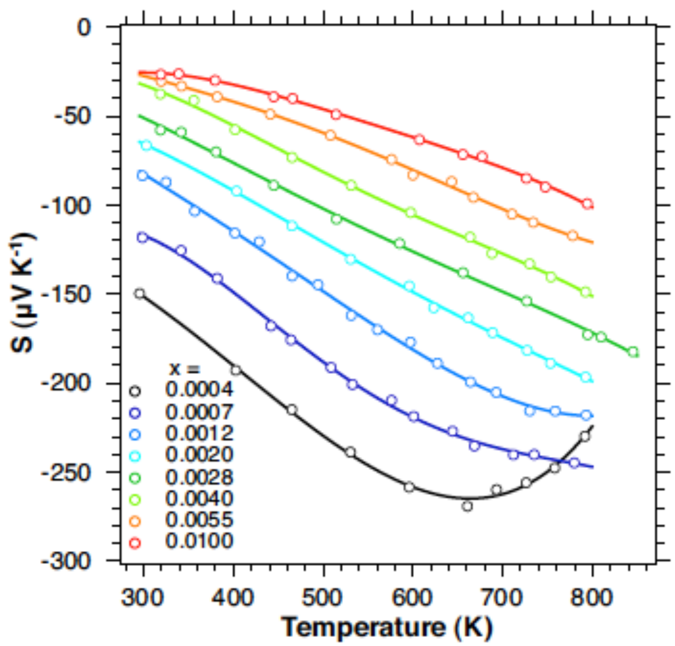
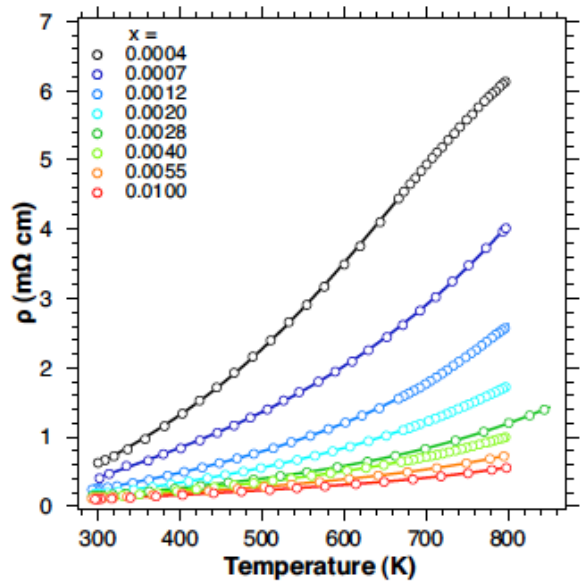
Heng Wang, G. Jeffrey Snyder *Materials Horizons* 2, 10.1039/C5MH00021A (2015)
Takagiwa et al., *APL* 101, 092102 (2012)

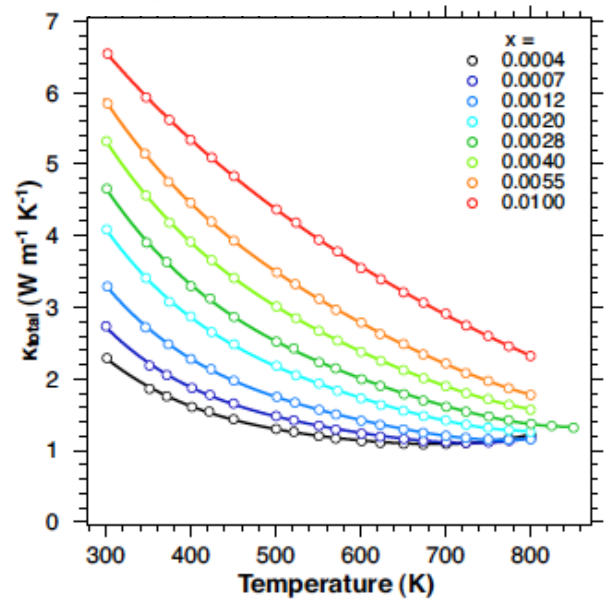
Degenerate Semiconductor Behavior

1. linear Seebeck $E_g = 2e\alpha_{max}T_{max}$
2. Linear Resistivity
3. 1/T + Constant thermal conductivity









Non-Degenerate Resistivity
(Intrinsic Semiconductor)

$$\ln\left(\frac{1}{\rho}\right) = \frac{-E_g}{2k_B T}$$

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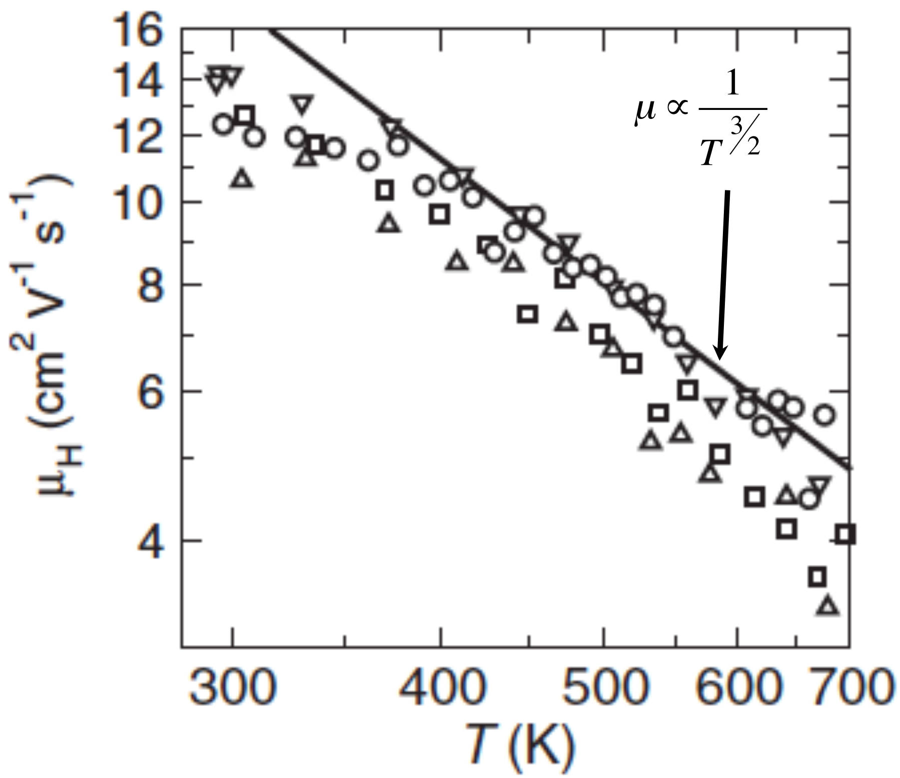
1. Scattering Mechanism

1. Scattering Mechanism

Acoustic Phonon Scattering at High Temperatures

$$\frac{1}{\rho} = \sigma = ne\mu$$



Degenerate (Metals)

$$\mu \propto \frac{1}{T}$$

Non Degenerate (Semiconductors)

$$\mu \propto \frac{1}{T^{3/2}}$$

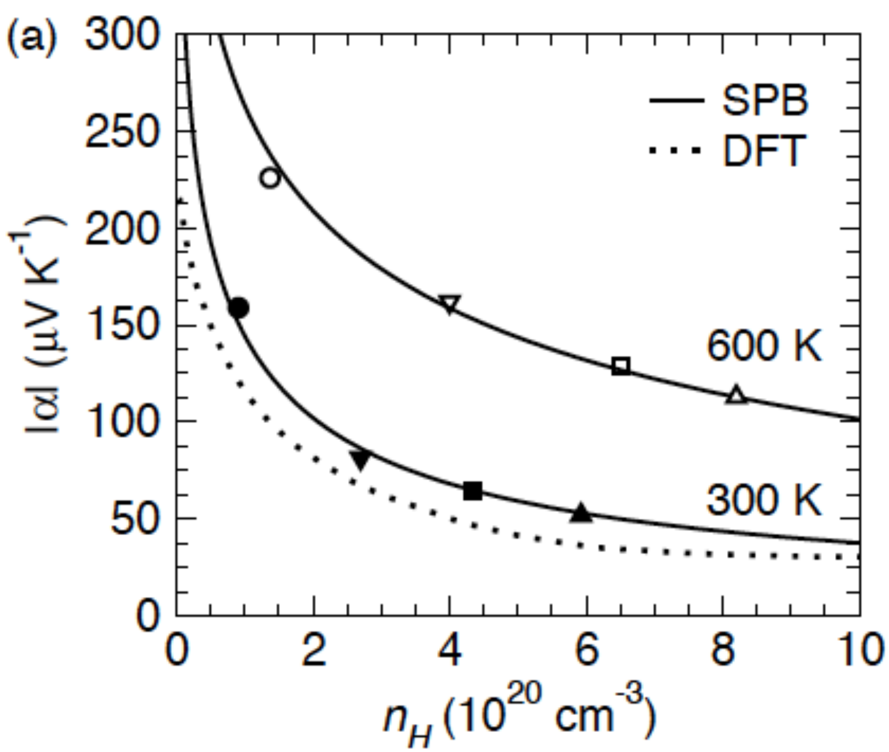
2. Effective Mass

2. Effective Mass (e.g. at 300K)

Pisarenko Plot of Seebeck vs Carrier Concentration

indicates quality of band model

- parabolic, Kane (linear), multiple bands



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

Degenerate (Metals)

3. Mobility Parameter μ_0

3. Mobility parameter μ_0 (near temp of max zT)

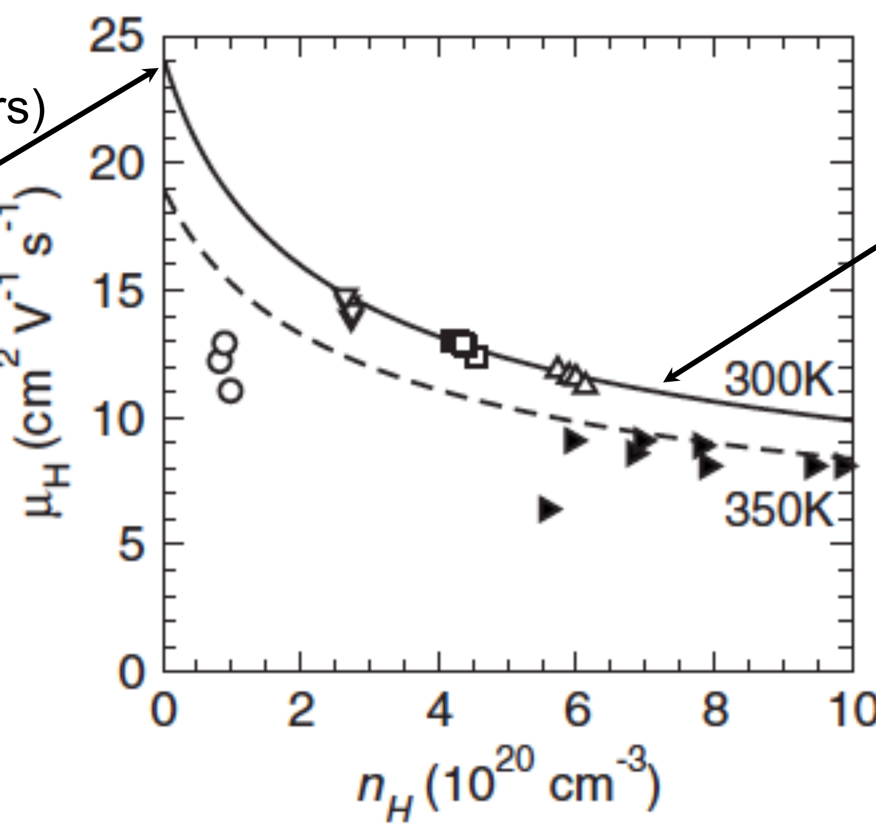
Plot of Mobility vs Carrier Concentration

also indicates quality of band model

- parabolic, Kane (linear), multiple bands

Non Degenerate limit
(small n semiconductors)

$$\mu_{H,0} = \frac{\sqrt{\pi}}{2}\mu_0$$



Degenerate
(Metals)

$$\mu \propto \frac{\mu_0}{m^{*2} T n^{1/3}}$$

4. Electronic Thermal Conductivity

4. Lorenz factor from Seebeck only

independent of carrier concentration or Temperature

subtract to get lattice thermal conductvity

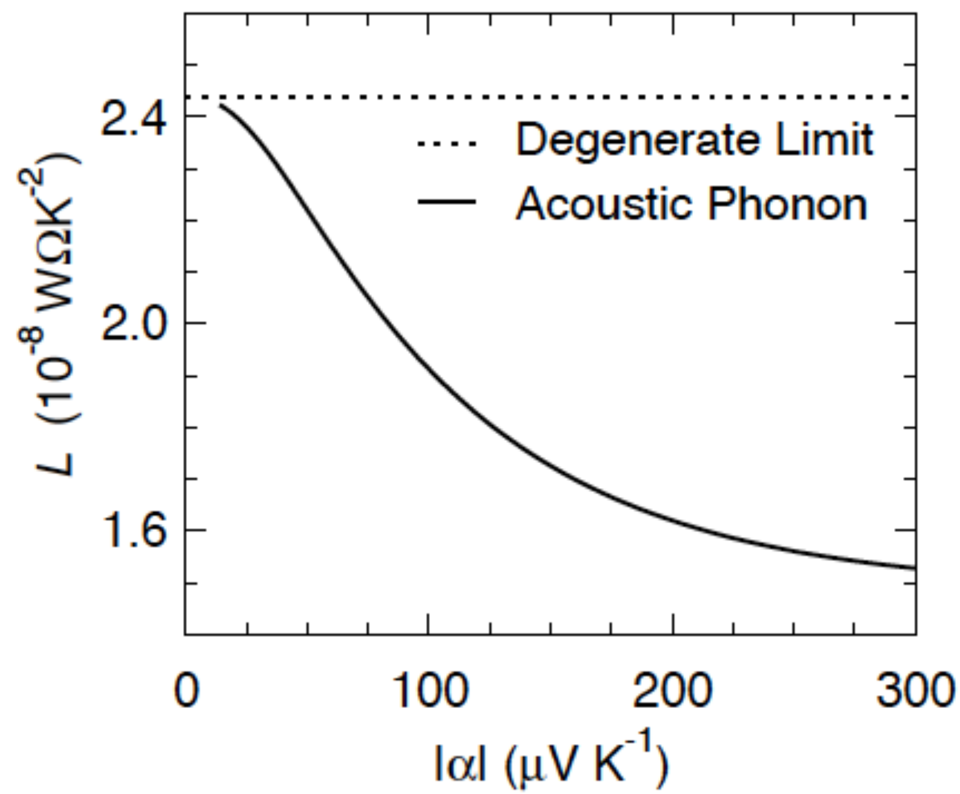
$$\kappa_e = L\sigma T \qquad \kappa = \kappa_e + \kappa_l$$

Degenerate (Metals)

$$L = \frac{\pi^2 k_B^2}{3e^2} = 2.45\times10^{-8}\,\mathrm{W\Omega K^{-2}}$$

$$L = 1.5 + Exp\left[-\frac{|S|}{116}\right]$$

$$\times10^{-8}\,\mathrm{W\Omega K^{-2}}$$



H-S Kim, Snyder et. al. *APL Materials,* **3**, 041506 (2015)

Optimum Carrier Concentration

Maximum zT depends on Quality Factor

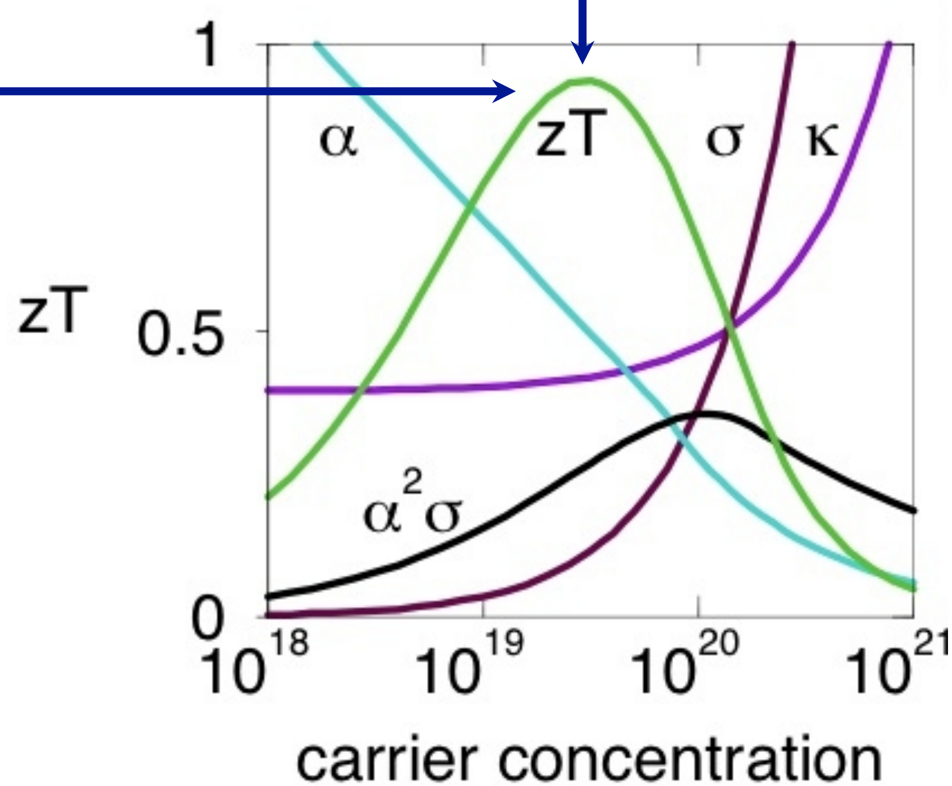
$$B = \frac{\mu m^{*3/2}}{\kappa_L}$$

Density of States
effective mass m^*

But μ decreases with transport (inertial) mass m_I^*

$$\mu = \frac{e\tau}{m_I^*}$$

Optimized carrier concentration
$n \sim m^* \, T^{3/2}$



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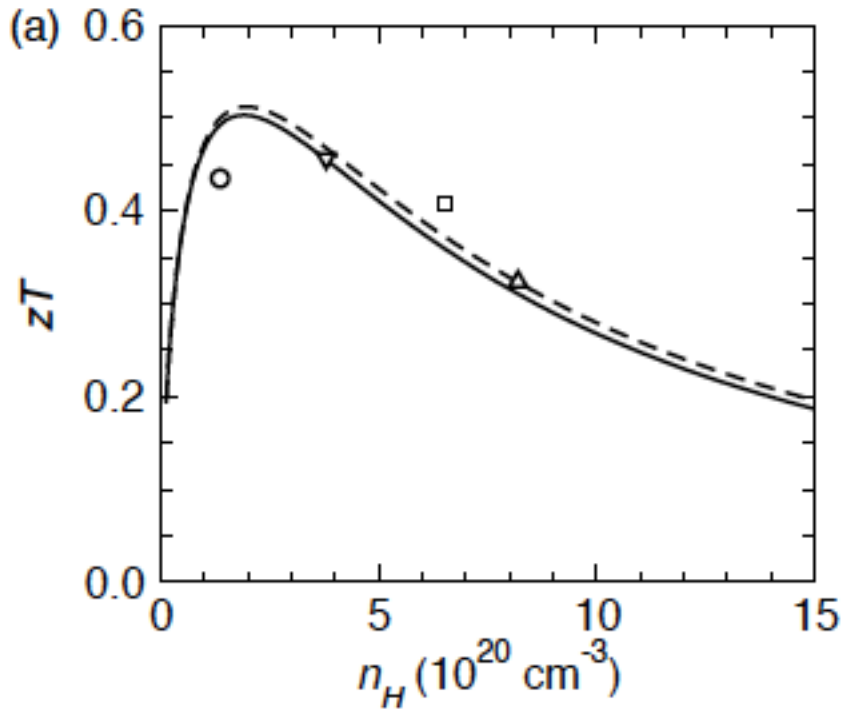
5. Predict *zT* and Doping

5. *zT* as function of doping

Predicts peak *zT*

predicts optimum carrier concentration

$$zT = \frac{\alpha^2}{L + (\psi\beta)^{-1}}$$



$$\beta = \frac{\mu_0 \left(\frac{m^*}{m_e}\right)^{3/2}}{\kappa_l} T^{5/2}$$

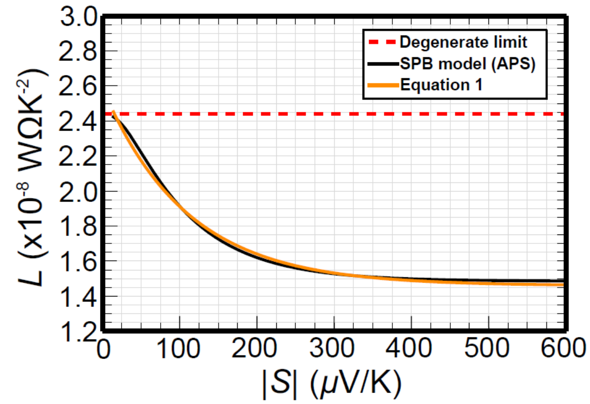
Quality factor parameter

Seebeck Coefficient

Thermopower (Abs. of Seebeck Coefficient) is a good measure of E_F/kT

Lorenz Factor

$$L = 1.5 + Exp\left[-\frac{|S|}{116}\right]$$



H-S Kim, Snyder et. al. *APL Materials*, **3**, 041506 (2015)

Effective Mass

$$S = \frac{2k_B^2}{3e\hbar^2}T\left(\frac{\pi}{3n}\right)^{2/3}(1+r)m^*_{Seebeck}$$

Band Gap

$$E_g = 2eS_{\max}T_{\max}$$

Snyder et. al. *J12.00004*, 3:06pm Room: 007C

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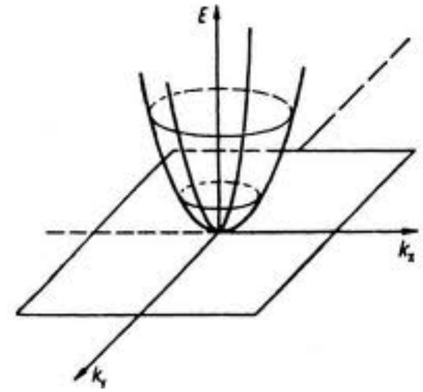
Gibbs, Snyder et. al. *Materials Horizons*, **2**, 68 (2015)
Applied Physics Letters **106**, 022112 (2015)

Free Electron –like Effective Mass

with Free electron-like (single parabolic) band (SPB)

mass has analogy to classical mechanics

$$E = \frac{mv^2}{2} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m^*}$$



and is commonly used for

electrical conductivity DOS, n, cyclotron

$$\sigma = \frac{ne^2\tau}{m^*} \qquad \mu = \frac{e\tau}{m^*}$$

a common definition is effective mass tensor

$$\frac{1}{m^*_{ij}} = \frac{\partial^2 E}{\hbar^2 \partial k_i \partial k_j}$$

but how is it related to measurements ?

σ = conductivity

f = Fermi function

ζ = chemical potential

g = DOS

v = velocity

τ = relaxation time

E = energy

T = temperature

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Wilson The Theory of Metals (1954)

Seebeck Effective Mass

In Thermoelectrics we measure thermopower |Seebeck coefficient|

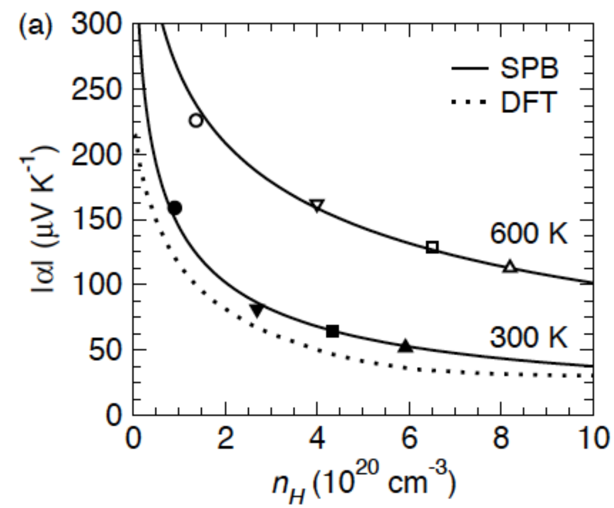
gives reduced chemical potential (reduced Fermi level) = chemical potential / kT

and Hall Effect for carrier concentration

$S_{exp} \rightarrow$ $$S = \frac{k_B}{e}\left(\frac{(2+\lambda)F_{\lambda+1}}{(1+\lambda)F_\lambda} - \eta\right)$$ $\rightarrow \eta_{SPB}$

$n_{exp} \rightarrow$ $$n = \frac{1}{4\pi^2}\left(\frac{2m_d^* k_B T}{\hbar^2}\right)^{3/2} F_{1/2}$$

$\rightarrow m^*_{d,Seeb}$



Need to have scattering parameter r and band shape

For Parabolic bands in degenerate limit (metals):

$$S = \frac{2k_B^2}{3e\hbar^2} T \left(\frac{\pi}{3n}\right)^{2/3} (1+r) m^*_{Seebeck}$$

σ = conductivity
$\alpha = S$ = Seebeck coefficient
r = scattering parameter
f = Fermi function
ζ = chemical potential
g = DOS
v = velocity
τ = relaxation time
E = energy
T = temperature

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Wilson The Theory of Metals (1954)

Thermoelectrics Effective Mass

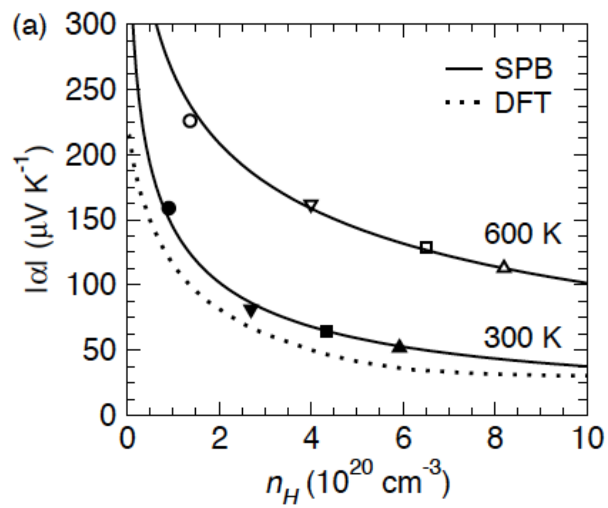
In Thermoelectrics we measure electrical conductivity and Hall Effect

$$\sigma = \frac{ne^2\tau}{m_I{*}} \qquad \mu = \frac{e\tau}{m_I{*}}$$

Even for Parabolic bands we need to distinguish band degeneracy N_V

$$S = \frac{2k_B^2}{3e\hbar^2} T \left(\frac{\pi}{3n}\right)^{2/3} (1+r) m^*_{Seebeck}$$

$$m^*_{DOS} = m^*_{band} N_V^{2/3}$$



σ = conductivity

$\alpha = S$ = Seebeck coefficient

r = scattering parameter

f = Fermi function

ζ = chemical potential

g = DOS

v = velocity

τ = relaxation time

E = energy

T = temperature

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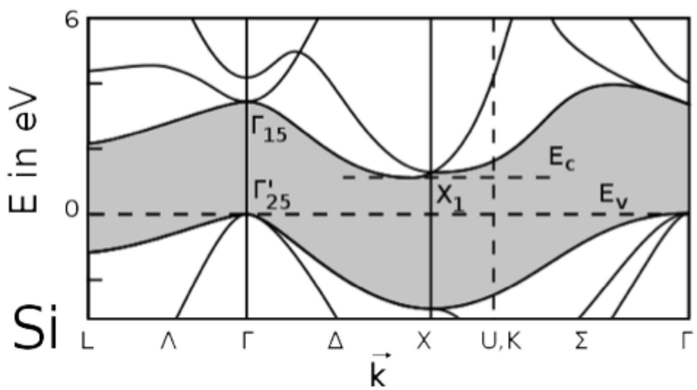
Wilson The Theory of Metals (1954)

Valley Degeneracy N_v

N_v is number of carrier pockets (valleys)

Spherical Fermi Surface

- free-electron model

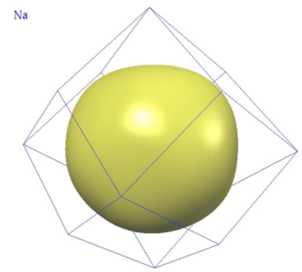


Multiple valley when:

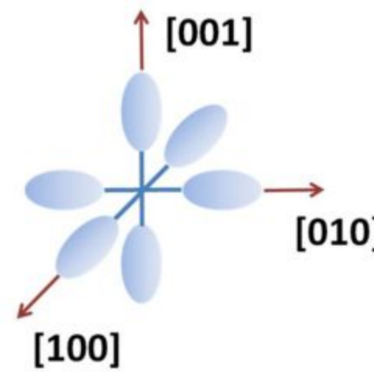
- Symmetrically equivalent (not at Γ)
- Different bands at band gap (orbital degeneracy)

Fermi Surfaces

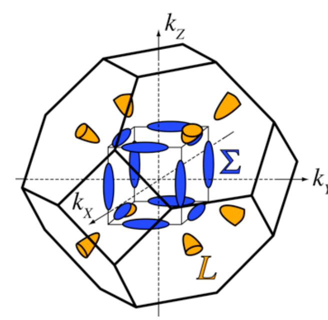
Na
$N_v = 1$



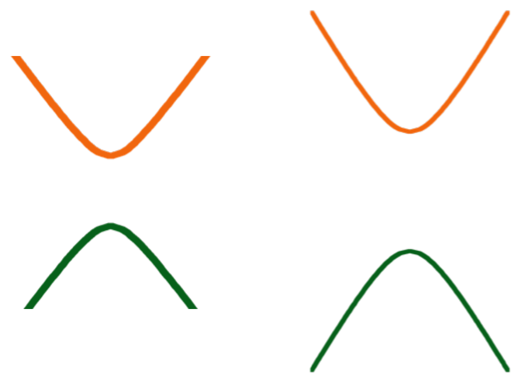
Si
v: $N_v = 3$
c: $N_v = 6$



PbTe
v: $N_v = 4, 12$
c: $N_v = 4$



Band Gap



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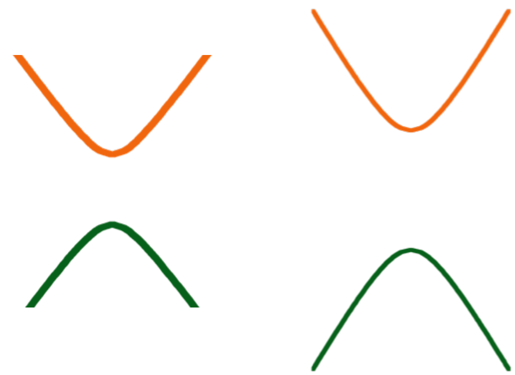
Band Gap

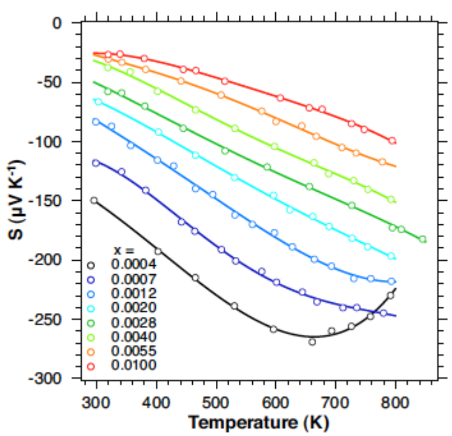
Excitation of minority carriers across band gap

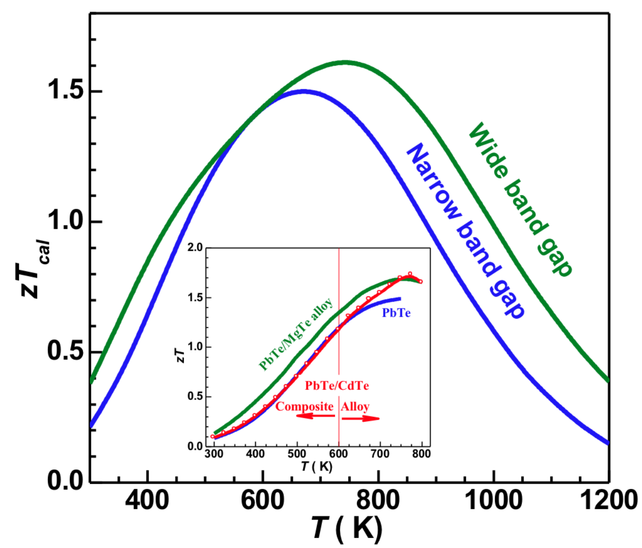
reduces Seebeck

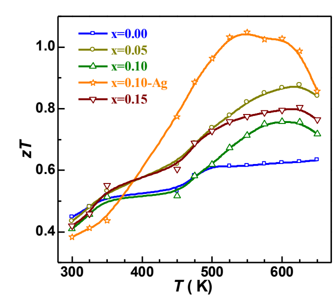
leads to peak in zT



$$E_g = 2e\alpha_{\max}T_{\max}$$







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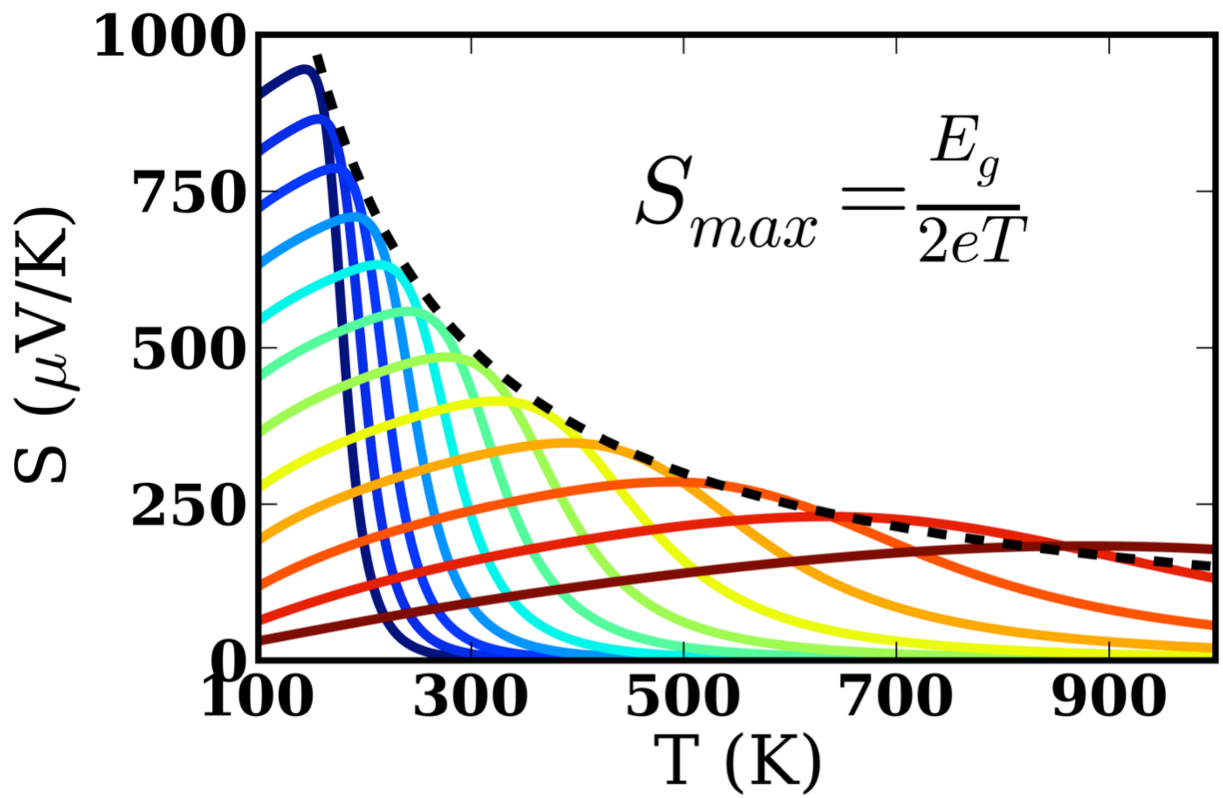
Gibbs, H-S Kim, GJS *Applied Physics Letters* 106, 022112 (2015)

Goldsmid-Sharp Maximum Seebeck

Doping changes S vs T

But peak S is limited by E_g

$$E_g = 2eS_{\max}T_{\max}$$



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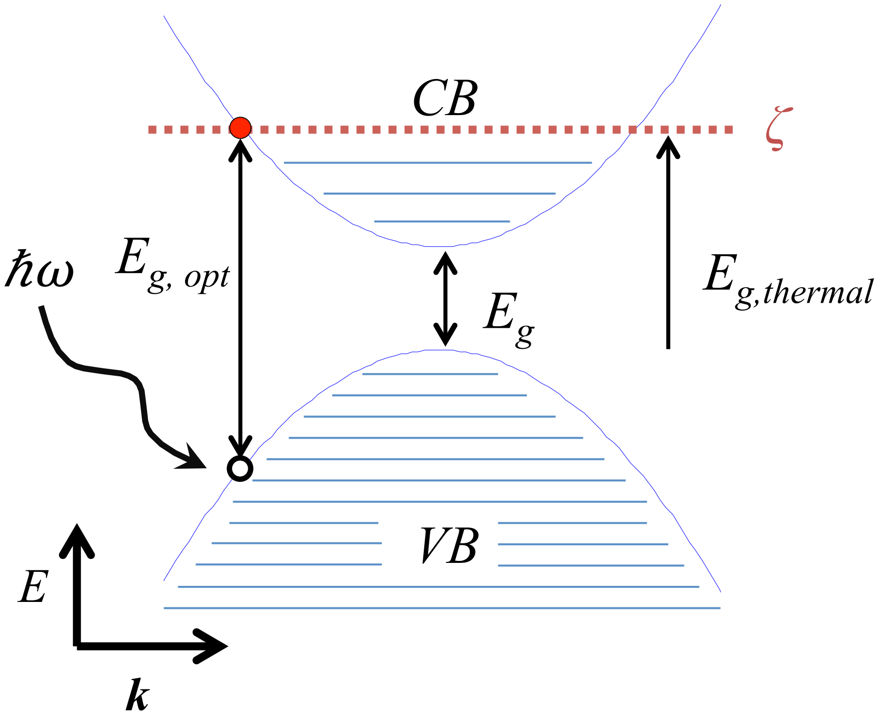
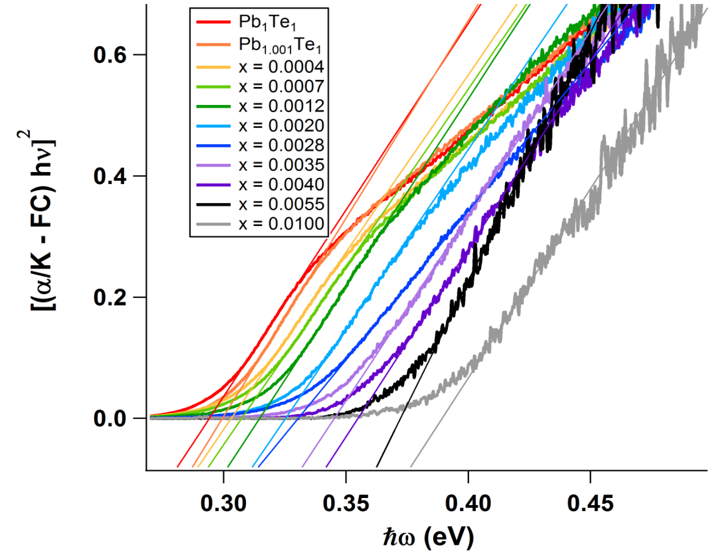
Gibbs, H-S Kim, GJS *Applied Physics Letters* 106, 022112 (2015)

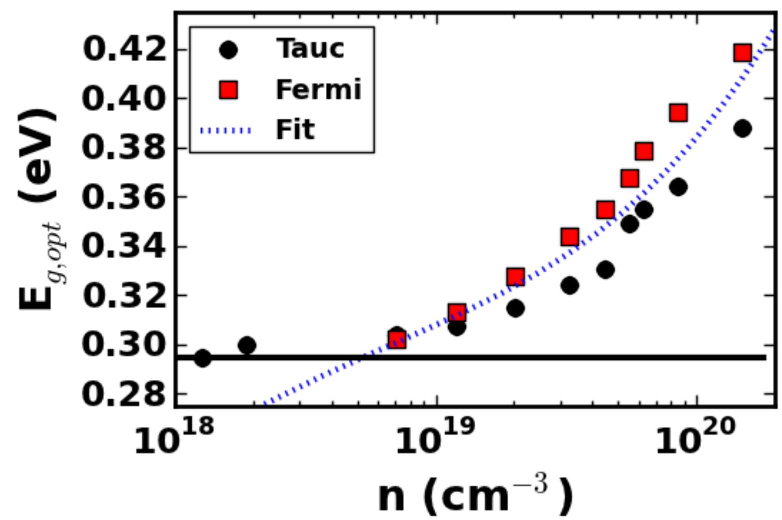
Optical Band gap





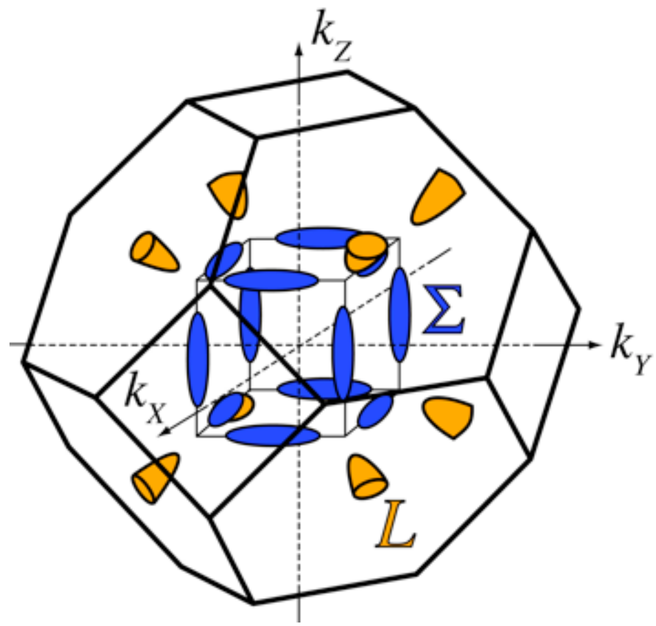
Optical band gap appears larger with doping

but may actually decrease



Gibbs, Snyder, et al. *New Journal Physics* **15,** 075020 (2013).

Band Engineering



Seebeck Mass

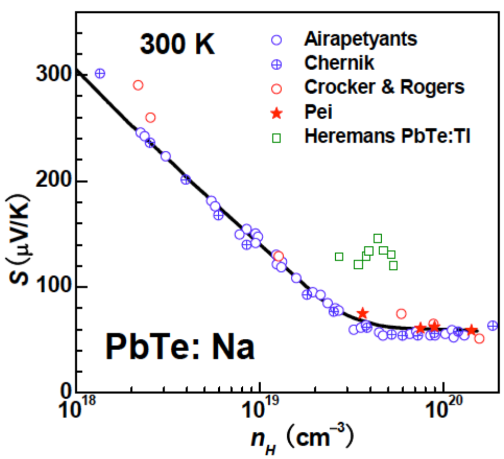
Want to Know: is Seebeck changing because of

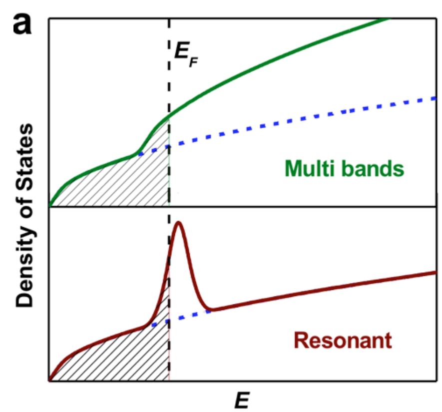
m^* DOS effective mass (scattering r doesn't change) or

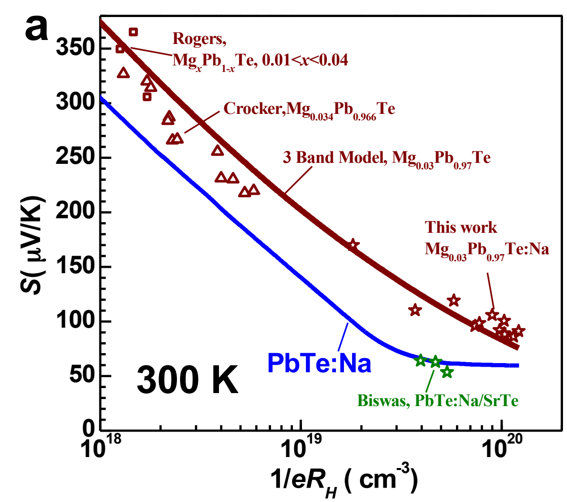
n simply carrier concentration

for degenerate (heavily doped semiconductors, metals):

$$S = \frac{2k_B^2}{3e\hbar^2} T \left(\frac{\pi}{3n}\right)^{2/3} (1+r) m^*_{Seebeck}$$







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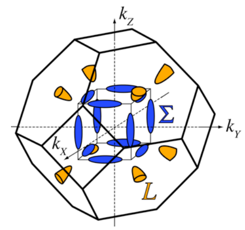
J. P. Heremans, Snyder et al. *Science* **321**, p 554 (2008)
Pei, Snyder et al *NPG Asia Materials* **4,** e28 (2012)

Quality Factor

Multi Valley Fermi Surface
with Valley Degeneracy N_v

$$m^* = m_b^* N_V^{2/3}$$



Optimized
carrier concentration

$$n \sim N_v (m_b^* T)^{3/2}$$

Maximum zT depends on
Quality Factor

$$B = \frac{\mu N_v m_b^{*3/2}}{\kappa_L}$$

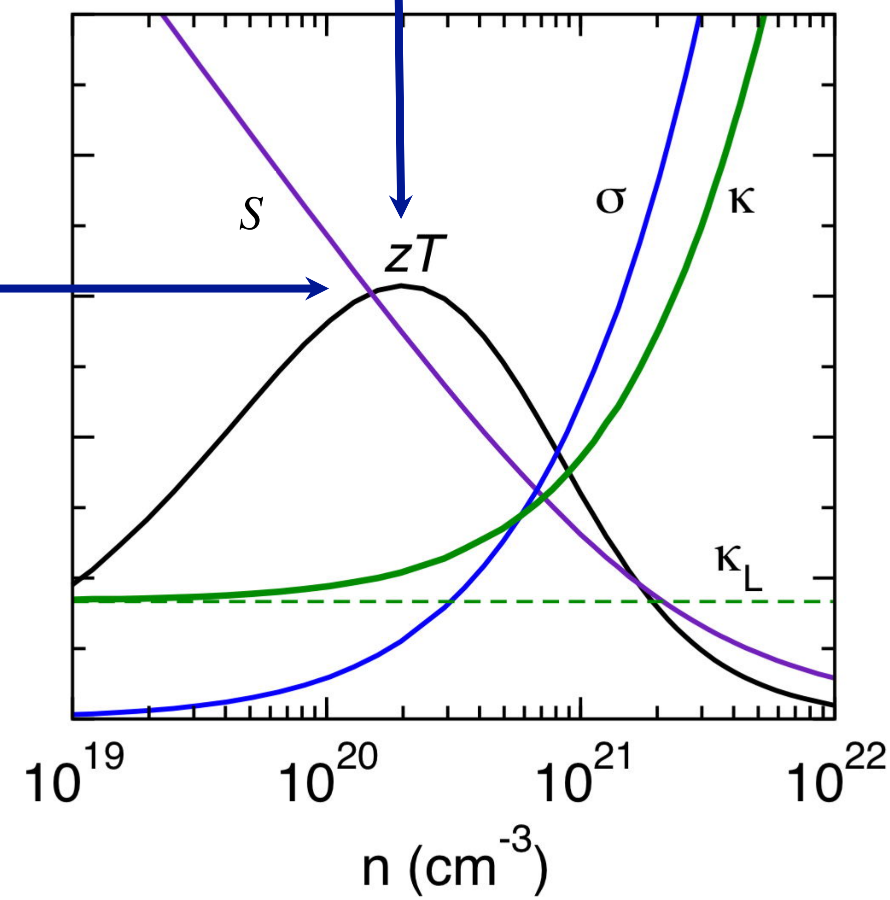
But μ decreases with m^*

$$\mu = \frac{e\tau}{m_I^*}$$

Acoustic Phonon Scattering

$$\tau \propto \frac{1}{m_b^{*3/2}}$$

$$B \sim \frac{N_V C_l}{m_I^* \Xi^2 \kappa_L}$$



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Pei, Wang, Snyder *Advanced Materials* **24**, 6125 (2012).

High N_V in PbTe

Valence Band Maximum is at L point

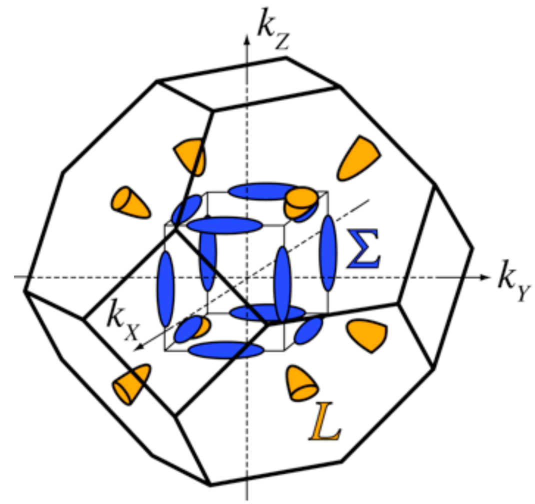
- "Light Band" $N_V = 4, \quad m_b{}^* = 0.14\, m_e$

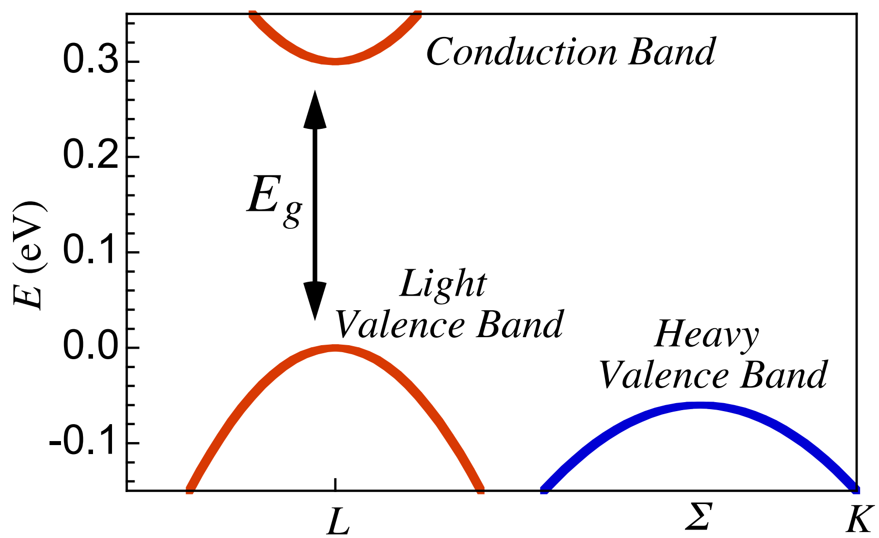
Second valence band occurs at Σ line

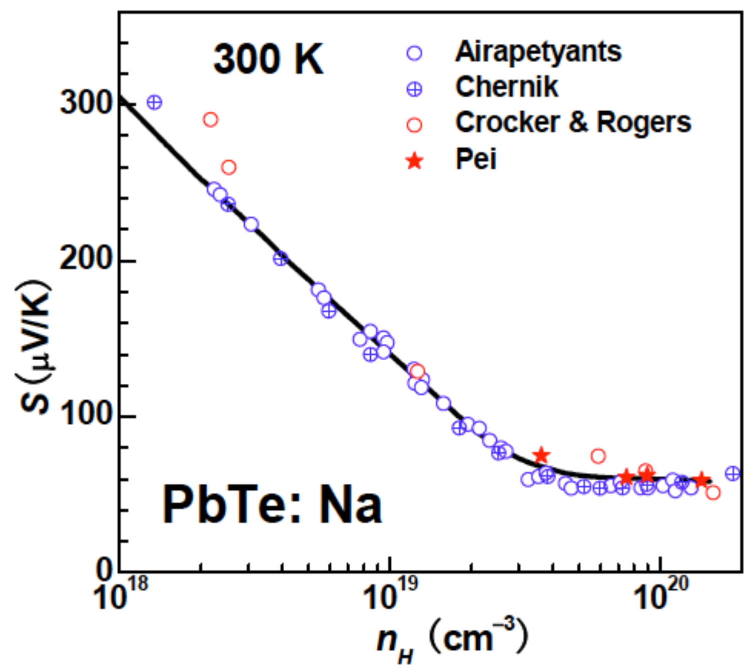
- "Heavy Band" $N_V = 12\ , \quad m_b{}^* = 0.28\, m_e$

$$m^* = m^*_{band} N_V^{2/3}$$

Transition from single to multiple band occurs at $n_H \sim 3 \times 10^{19}$ holes/cm^3





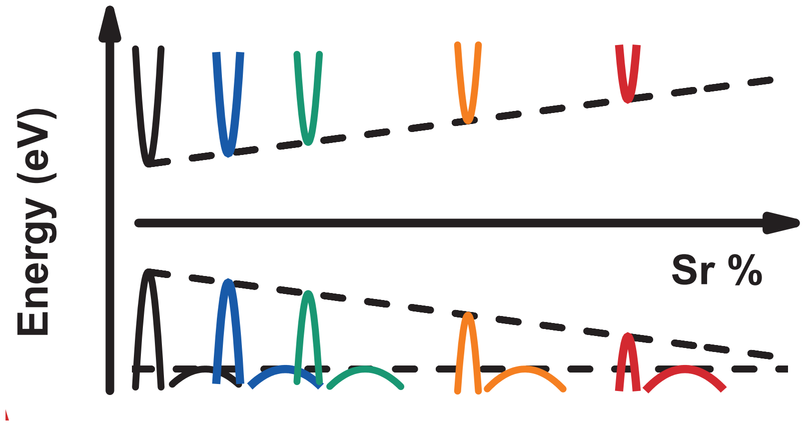


Pei, Snyder, et al.. *Energy Environ. Sci.* **4**, 2085 (2011).

Band Convergence with Alloying

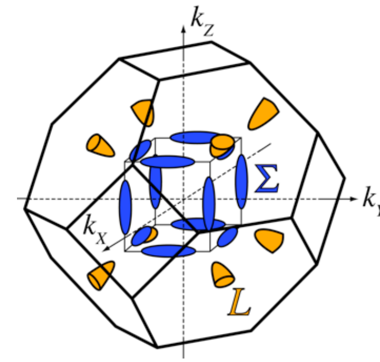
PbSe

$N_v \approx 4$

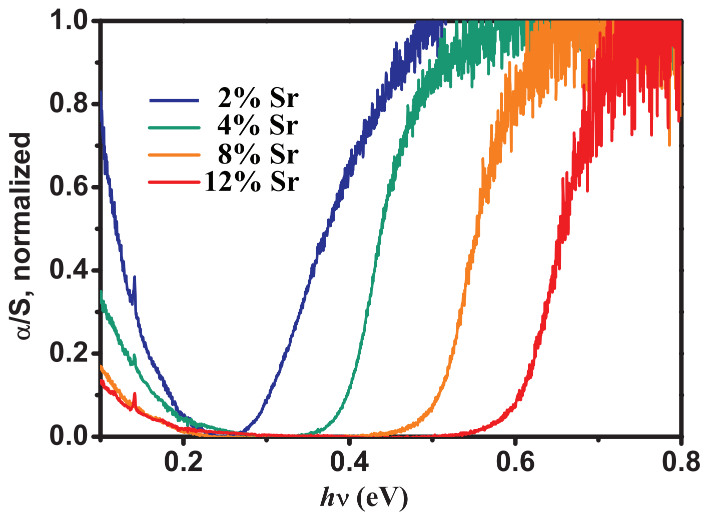


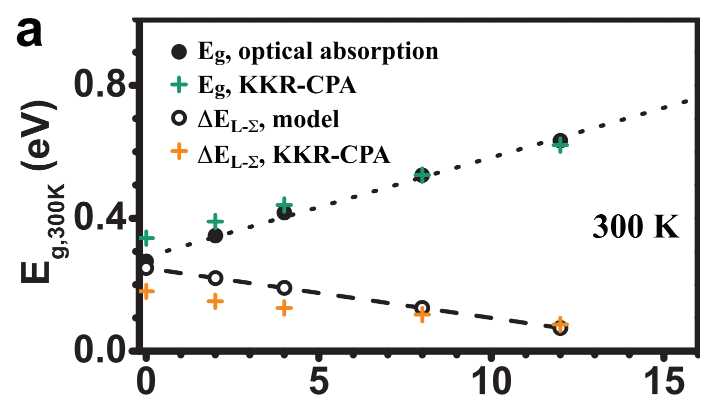
(Pb,Sr)Se

$N_v \approx 16$



Optical Band Gap





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Wang, Gibbs, Snyder et. al. *Energy Env. Sci.* **7**, 804 (2014)

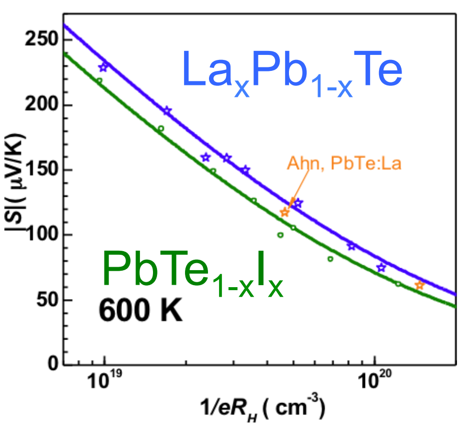
Single Band Mass

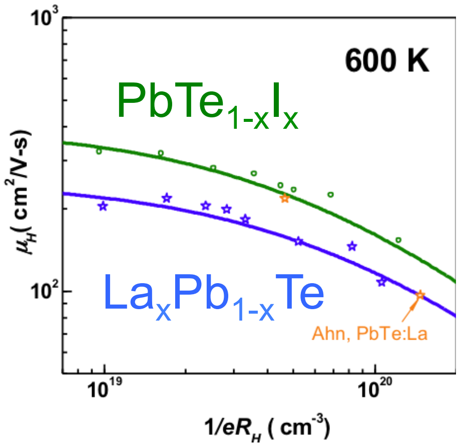
small Effective mass

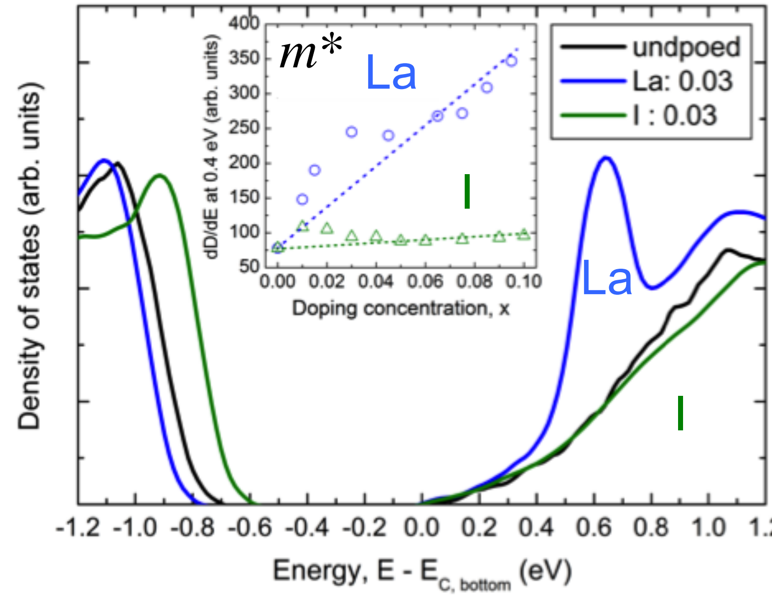
$La_xPb_{1-x}Te$ vs. $PbTe_{1-x}I_x$

Both n-type L-band

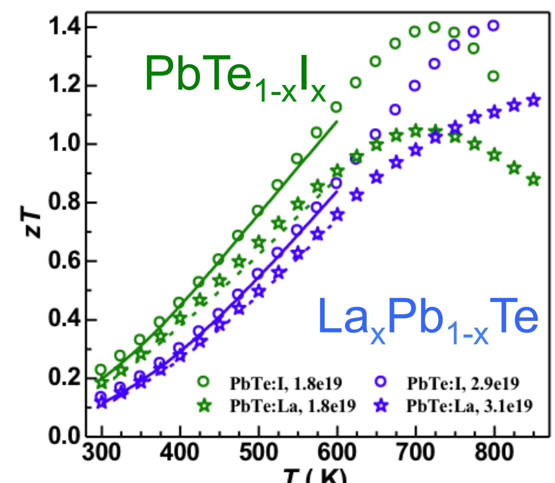
20% lower m^* 30% higher μ







20% Higher zT



$$\mu \propto \frac{1}{m^*_I \, m^{*3/2}_b} \qquad B \sim \frac{N_V}{m_I^* \kappa_L}$$

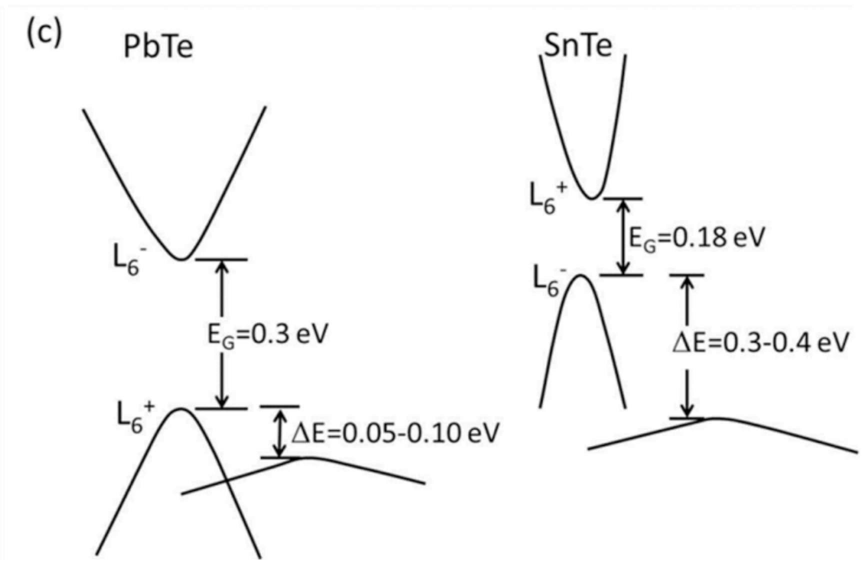
Pei, Snyder, et al. *Energy and Environmental Science* **5**, 7963 (2012)

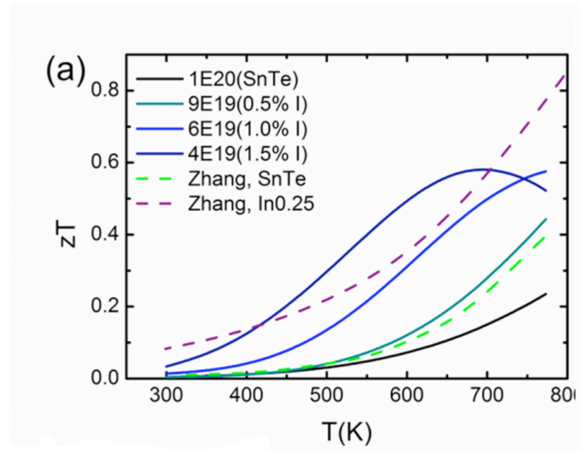
Takagiwa, Snyder, et al. *Applied Physics Letters* **91**, 092102(2012).

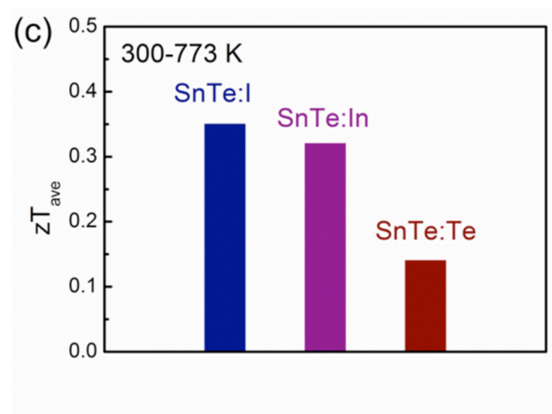
SnTe Small Effective Mass

Light band 0.14me in SnTe

better than high Nv band







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Zhou, Snyder, et al, *Physical Chemistry Chemical Physics* (2014)

Non-Parabolic Bands effect on Mass

non parabolic Bands

Band edge should be parabolic but

Deep into bands they are complex

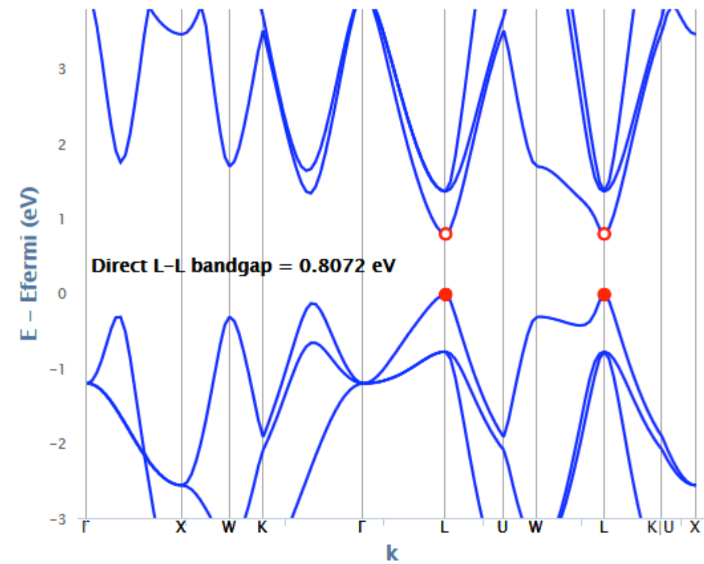
- non parabolic shape
- may change curvature (mixed n- p-type)

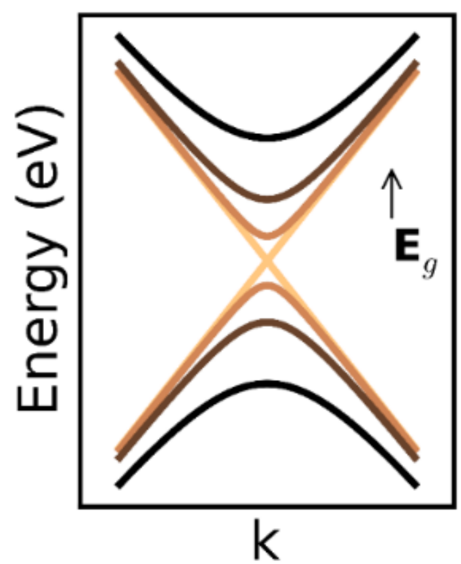
Light, low E_g Bands often linear

- parabolic at band extrema
  - physical – no cusps
- linear at high E like Dirac cone band

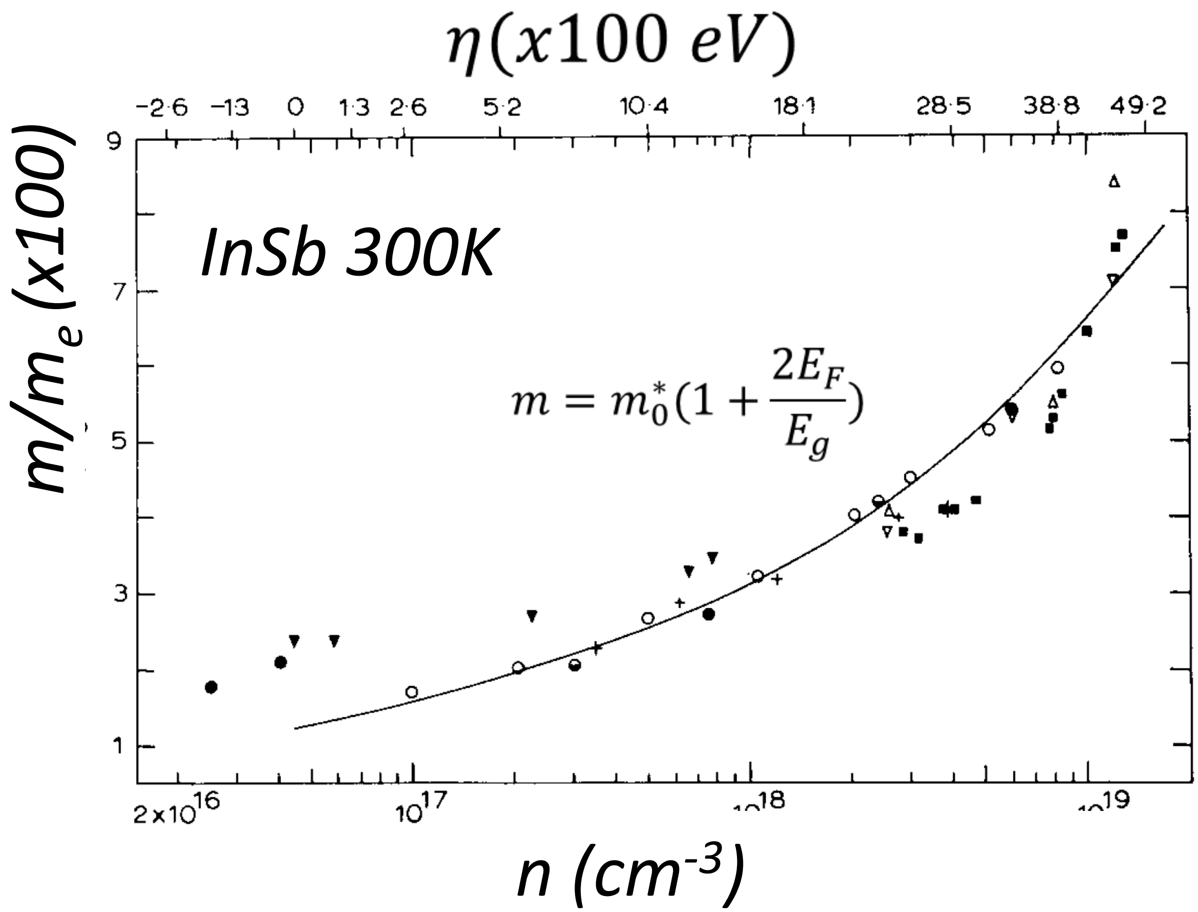
What is effect on transport, effective mass?

PbTe





Increasing m^* in Kane Band

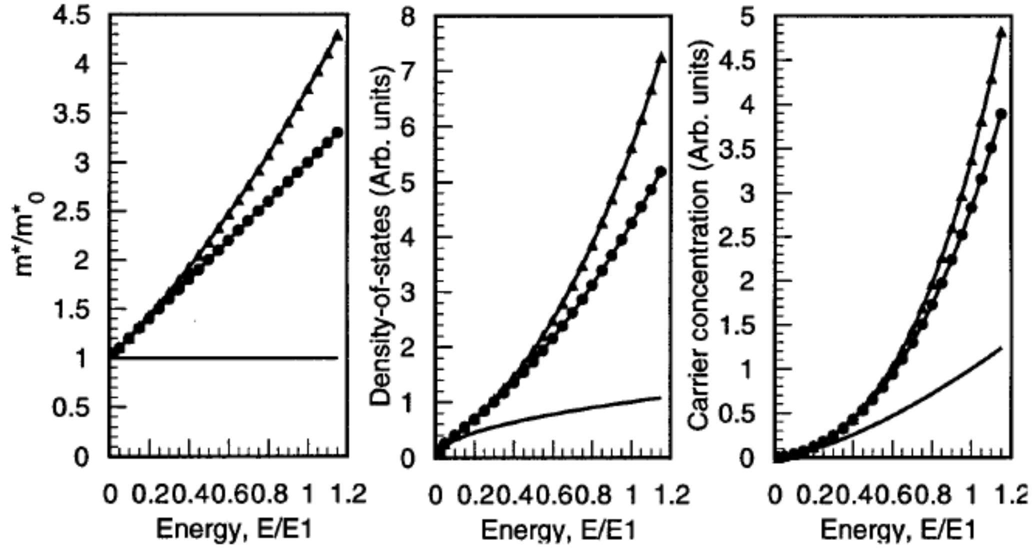


Variety of measurement Techniques:

Faraday Rotation, Thermomagnetic (Seebeck, Nernst), Optical Reflectivity

W. Zawadzki *Advances in Physics* **23**, 435 (1974).

Increasing m^* in Kane Band



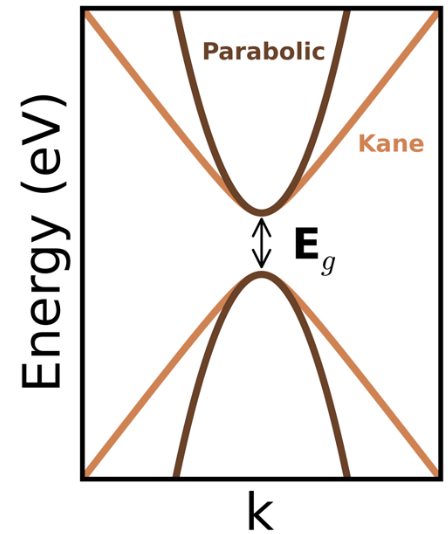


Figure 1. Influence of non-parabolicity on effective mass, density-of-states and carrier concentration. The solid lines in each of the three figures show the variation for a parabolic band, for which $m^*(E) = m_0 = \text{const.}$, $D(E)\ \alpha\ E^{1/2}$, and $n\ \alpha\ E^{3/2}$. Two cases of non-parabolicity are considered. The symbols ●, indicate first-order non-parabolicity, which is given by $\gamma = E(1+E/E_1)$. The ▼ symbols indicate second-order non-parabolicity, which is given by $\gamma = E\,(1 + E/E_1 + E^2/E_2^2)$. In the latter calculation, E_2 was taken as equal to 2 E_1. In both of the non-parabolic band calculations, $m^*(E) = m_0^*\, d\gamma/dE$, $D(E) \propto (m_0^*)^{3/2}[\gamma(E_F)]^{1/2}(d\gamma/dE)$, and $n \propto (m_0^*)^{3/2}[\gamma(E_F)]^{3/2}$.

Variety of measurement Techniques:

Faraday Rotation, Thermomagnetic (Seebeck, Nernst), Optical Reflectivity

W. Zawadzki *Advances in Physics* **23**, 435 (1974)
Kaydanov, Young, Coutts, *MRS* (2000)

Energy dependent $m^*(E)$

For nonparabolic dispersion, e.g. Kane-like

$$E + \frac{E^2}{E_g} = \frac{\hbar^2 k_B^2}{2m_0^*}$$

'energy dependent mass' often defined as

$$m^*(E) = m_P^* \equiv \frac{p}{v} \qquad m_P^*(E) = m_0^*\left(1 + \frac{2E}{E_g}\right)$$

but properties are not simply a function of $m^*(E)$

$$g(E) = \frac{4\pi\left(2m_P^*\right)^{3/2} E^{1/2}}{h^3}\left(\frac{1+\frac{E}{E_g}}{1+\frac{2E}{E_g}}\right)^{1/2} \qquad n = \frac{8\pi\left(2m_P^*\right)^{3/2} E^{3/2}}{3h^3}\left(\frac{1+\frac{E}{E_g}}{1+\frac{2E}{E_g}}\right)^{3/2}$$

Do all properties at least increase with increasing $m^*(E)$?

$$S = \frac{2k_B^2}{3e\hbar^2} T\left(\frac{\pi}{3n}\right)^{2/3}(1 + r - \lambda)m_P^* \qquad \lambda = \frac{4E}{E_g}\left(1 + \frac{E}{E_g}\right)$$

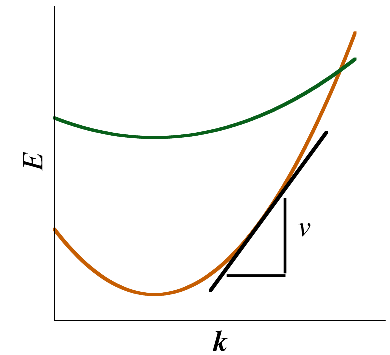
W. Zawadzki *Advances in Physics* **23**, 435 (1974)
Young, Coutts, Kaydanov *American Vacuum Society* (1999)

Linear or Parabolic

For r = 0, τ and DOS (g) cancel each other

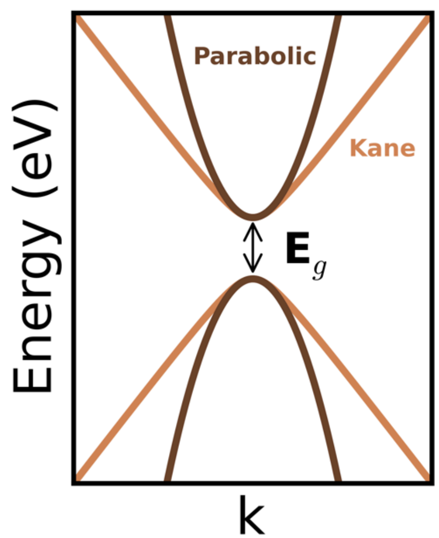
$$S = \frac{\pi^2}{3}\frac{k_B^2 T}{e}\left(\frac{2\partial v}{v\partial E} + \frac{\partial \tau}{\tau \partial E} + \frac{\partial g}{g\partial E}\right)$$

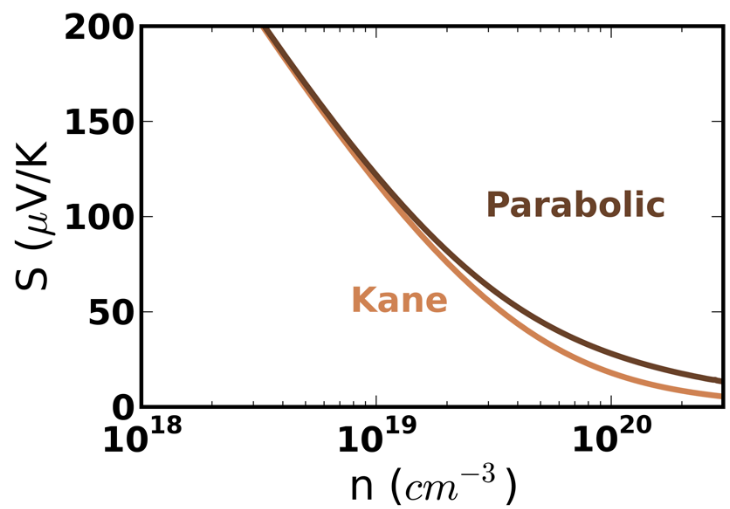
$$v \equiv \frac{dE}{\hbar dk}$$



so S depends on dv/dE

linear dv/dE = 0





Constant m_0*

parabolic is definitely better

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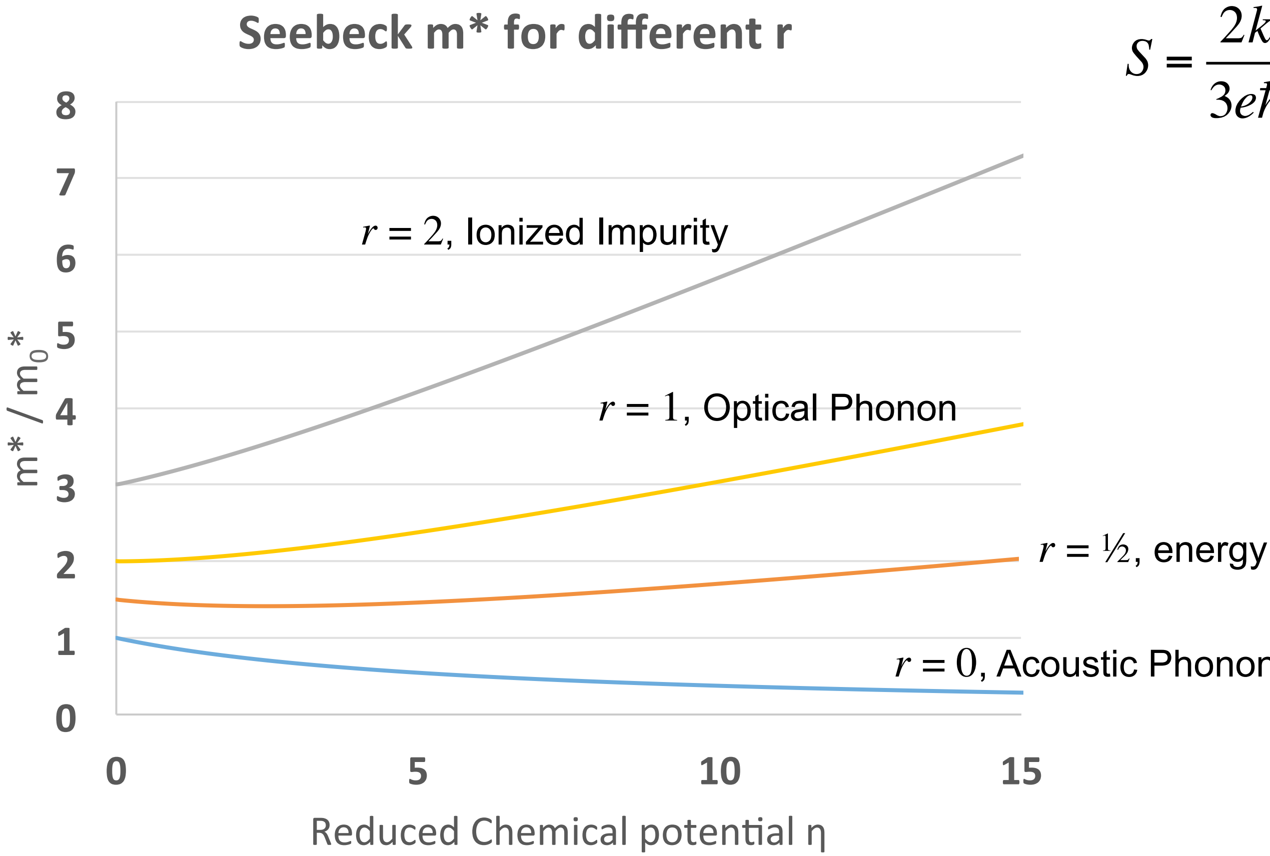
Non parabolic Seebeck m^*



$$S = \frac{2k_B^2}{3e\hbar^2} T \left(\frac{\pi}{3n}\right)^{2/3} (1 + r - \lambda) m_P^*$$

$$\lambda = \frac{4E}{E_g}\left(1 + \frac{E}{E_g}\right)$$

$$m_P^*(E) = m_0^* \left(1 + \frac{2E}{E_g}\right)$$

$m^*(E)$ depends on scattering – decreases for $r = 0, ½$!

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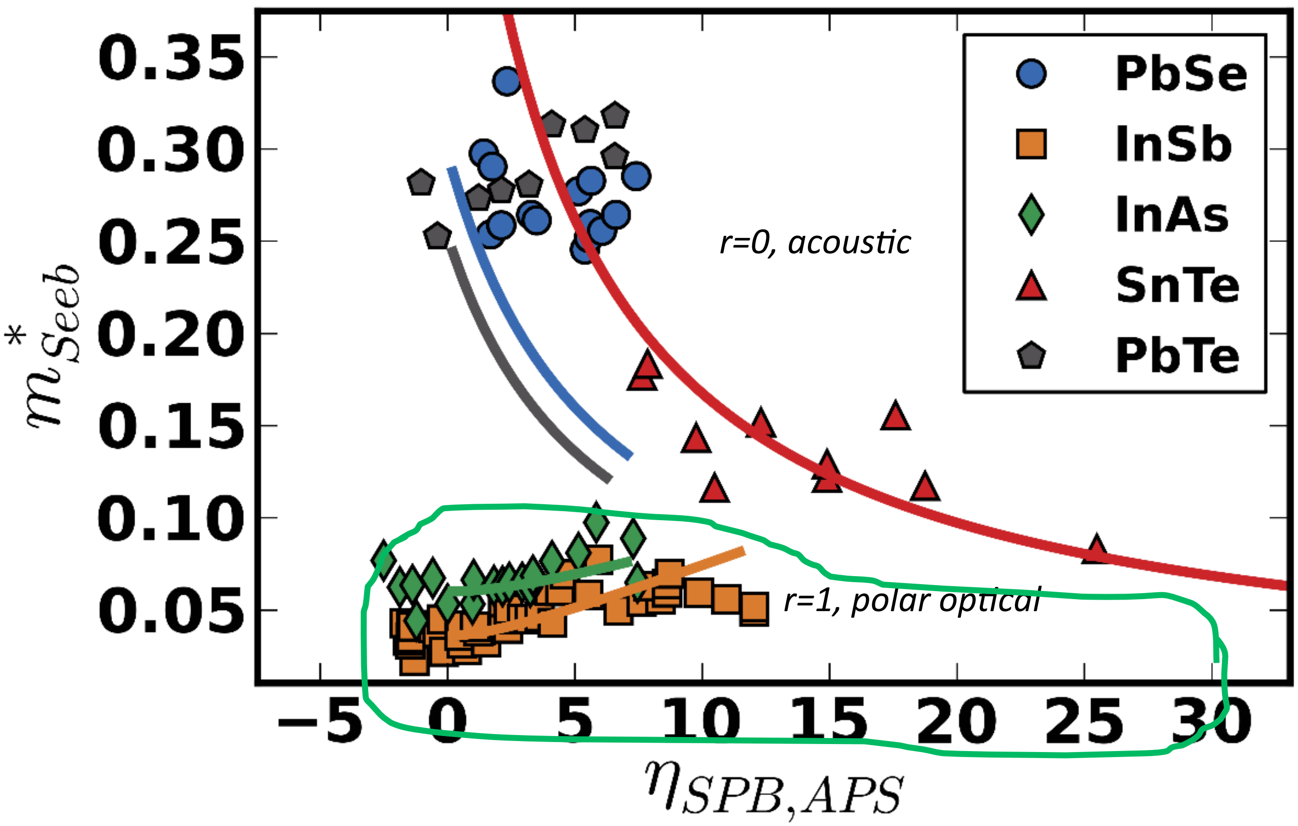
W. Zawadzki *Advances in Physics* **23**, 435 (1974)
Young, Coutts, Kaydanov *American Vacuum Society* (1999)

Experiment of Kane Band $m^*_{Seebeck}$



SnTe – the only one with some evidence of decreasing m*
Zhou, Gibbs 2014

InSb/InAs – Different Scattering mechanism, not fair to compare

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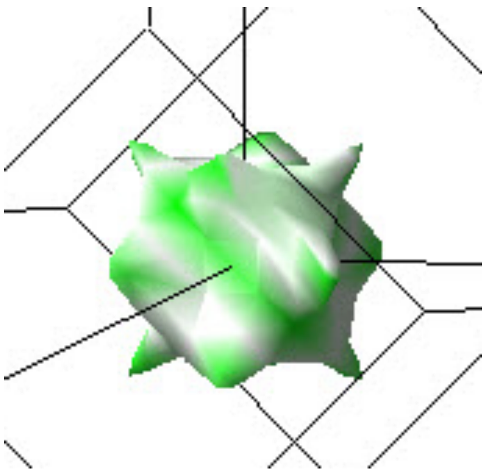
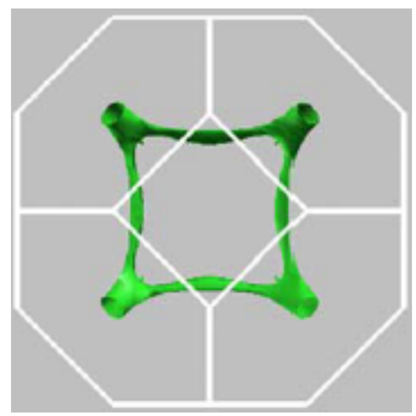
Zhou, Gibbs, et al. *Phys.Chem.Chem.Phys.* 16, 20741 (2014)

Non-spherical Fermi Surface



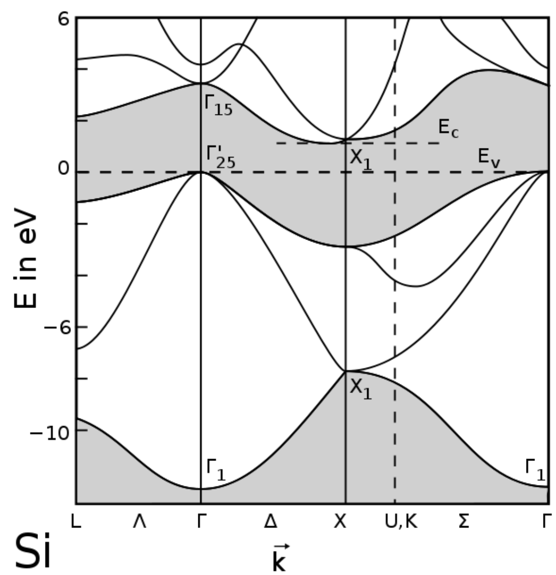


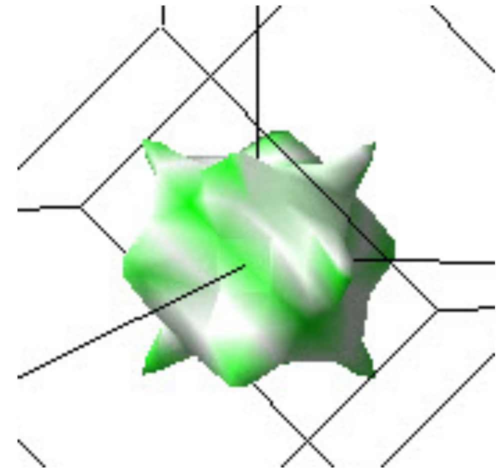
Spherical, Ellipsoidal, non-Elipsiodal

Parabolic Bands may not be isotropic

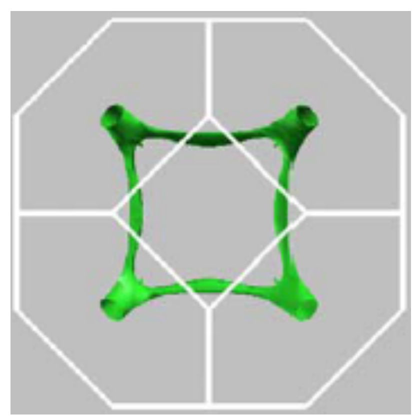
$$E = \frac{\hbar^2 k_x^2}{2m_x^*} + \frac{\hbar^2 k_y^2}{2m_y^*} + \frac{\hbar^2 k_z^2}{2m_z^*}$$

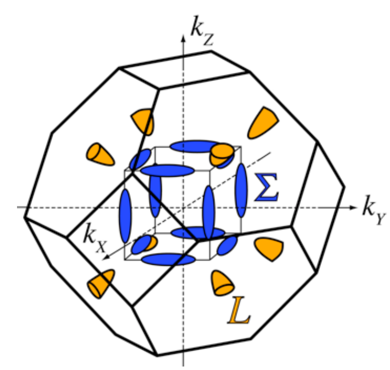
Ellipsoid
e.g conduction band
Fermi Surface of Si





Fermi Surface Threads
in p-PbTe





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This is just cubic materials …

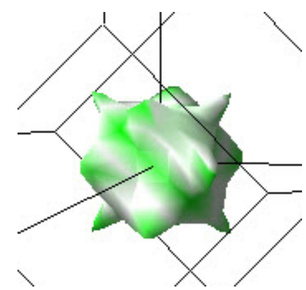
Fermi Surface Area m^*

Boltzmann Transport integral over all k space

$$\sigma_{ij} = \frac{e^2}{4\pi^3} \iiint v_i v_j \tau \frac{-\partial f}{\partial E} d\vec{k} \qquad S\sigma_{ij} = \frac{e^2}{4\pi^3} \iiint v_i v_j \tau (E - \zeta) \frac{-\partial f}{\partial E} d\vec{k}$$

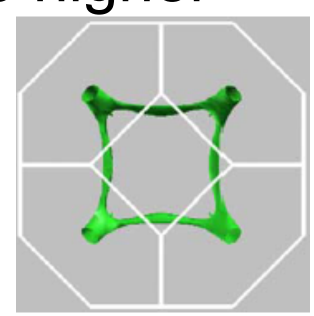
Transform to integrate over Fermi Surface S first than Energy

$$\sigma = \frac{e^2}{4\pi^3} \int \left(\oint_E v\tau \, dS \right) \frac{-\partial f}{\partial E} dE$$



Fermi Surface volume is number of electrons, n

Larger Fermi Surface due to complexity should give higher conductivity and Thermopower



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X Chen, Parker, Singh *Sci. Reports* **3**, 3168 (2013)
Singh *PRB* **81**, 195217(2010)