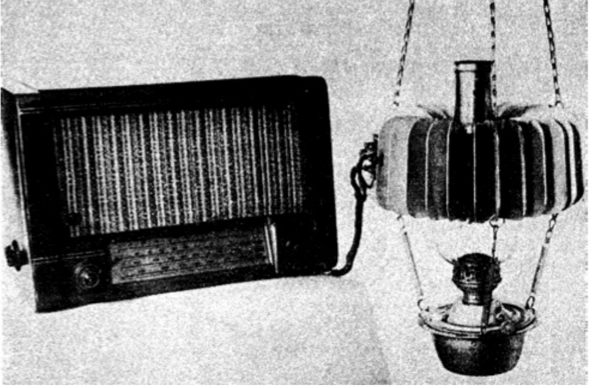

Thermoelectrics:
A theoretical approach
to the search for better materials

Jorge O. Sofo
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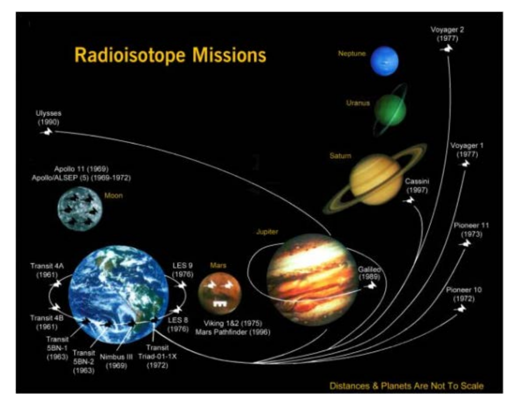
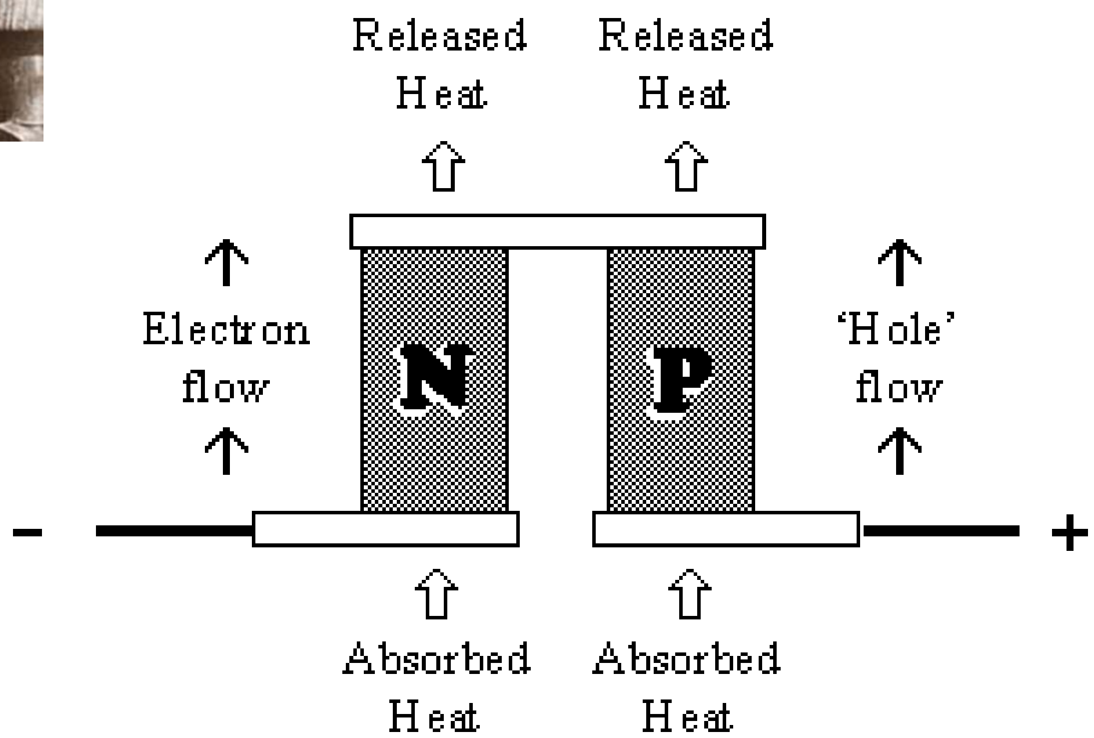
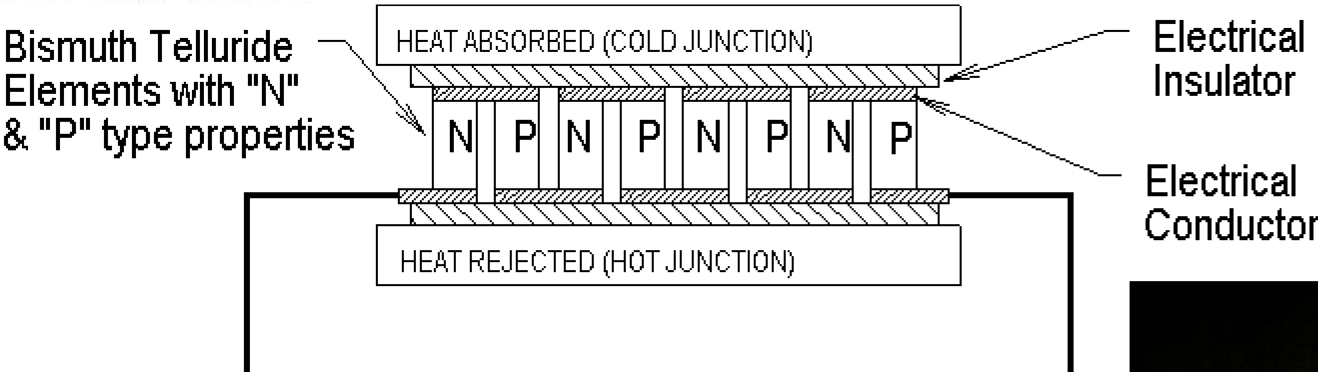


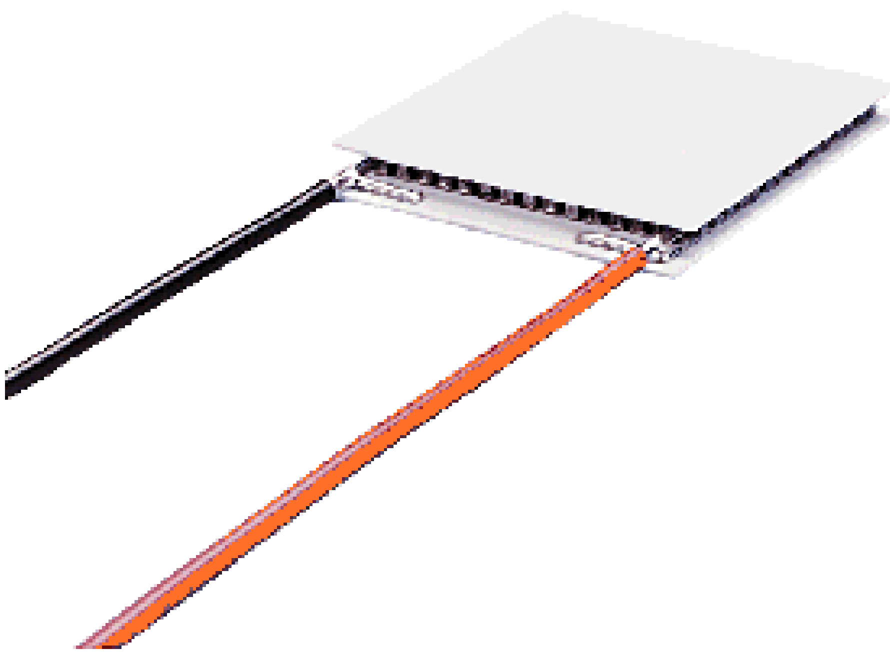
The basics

Abram F. Ioffe



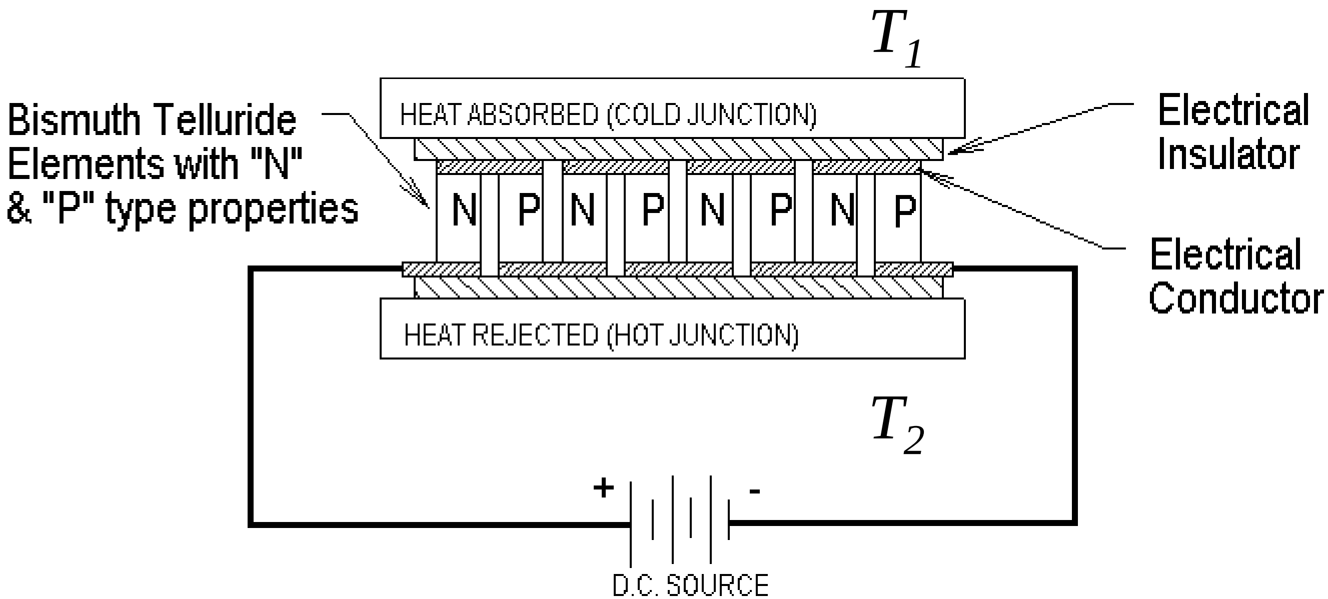
The devices





Raymond Marlow
Sept. 24, 1931 - Oct. 11, 2013

The performance



Elements Electrically in series & thermally in parallel

$$\phi = \frac{\dot{Q}}{W} = \frac{SIT_1 - (T_2 - T_1)\kappa - I^2 R/2}{SI(T_2 - T_1) + I^2 R}$$

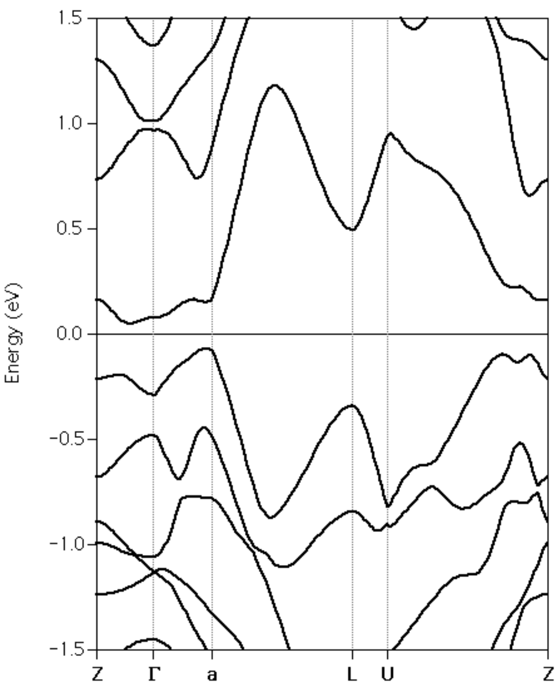
$$\phi_{\mathrm{MAX}} = \frac{T_1\left[\sqrt{1+Z\overline{T}} - T_2/T_1\right]}{(T_2 - T_1)\left[\sqrt{1+Z\overline{T}} + 1\right]} \xrightarrow[Z \to +\infty]{} \frac{T_1}{(T_2 - T_1)}$$

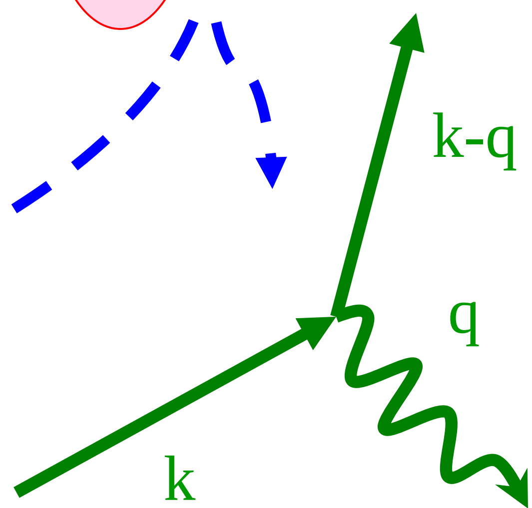
$$Z = \frac{\sigma S^2}{\kappa}$$

Conductivity 101

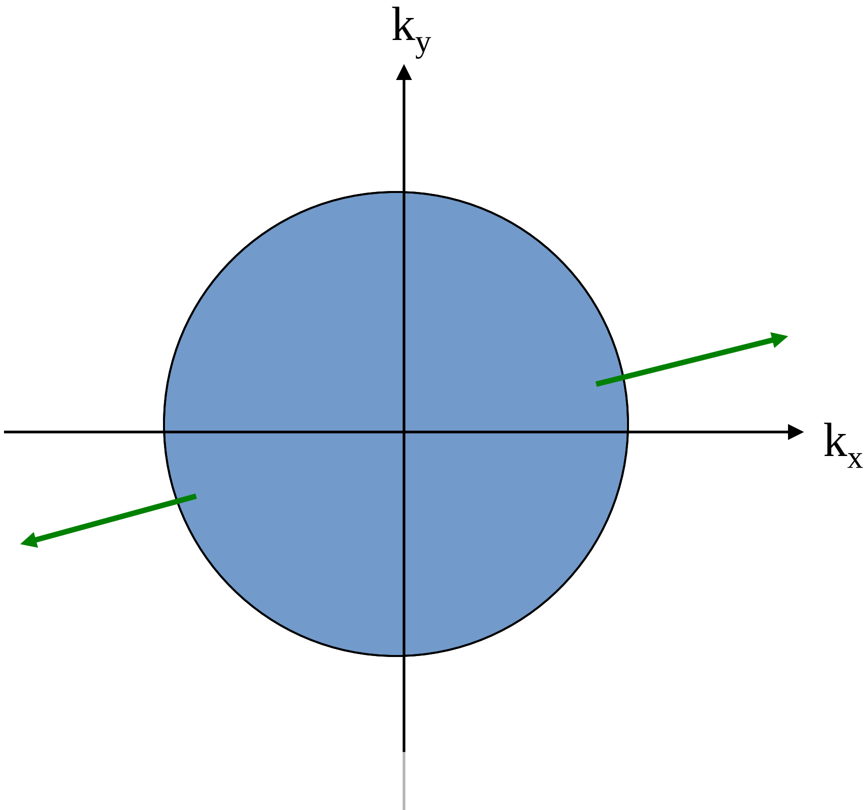
Drude et al.

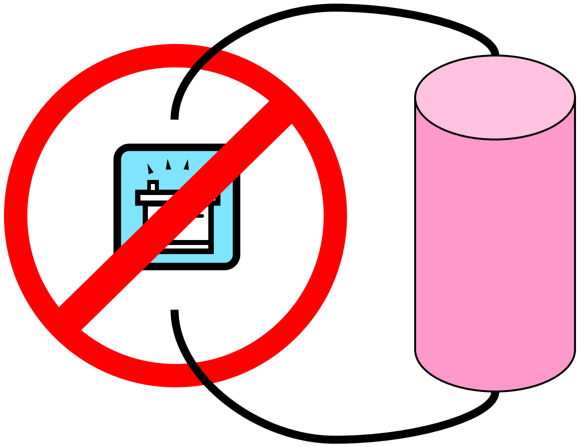
$$\sigma = e^2 \frac{n}{m} \tau$$





Conductivity 101





$$J = e\sum_k f_0(\varepsilon_k)\, v_k = 0$$

$$J = e\sum_k f_k\, v_k \neq 0$$

$$\frac{\partial f_{\vec{k}}}{\partial t}+\frac{\partial H}{\partial \vec{p}}\cdot\frac{\partial f_{\vec{k}}}{\partial \vec{r}}-\frac{\partial H}{\partial \vec{r}}\cdot\frac{\partial f_{\vec{k}}}{\partial \vec{p}}=$$

$$\frac{\partial f_{\vec{k}}}{\partial t}-\left\{H, f_{\vec{k}}\right\}=\left(\frac{\partial f_{\vec{k}}}{\partial t}\right)_{coll}$$

$$\frac{d}{dt}\rho'(t)=\frac{1}{i\hbar}\left[H+H'(t),\rho'(t)\right]$$

$$\frac{\partial f_{\vec{k}}}{\partial t} + \frac{d\vec{r}}{dt} \cdot \frac{\partial f_{\vec{k}}}{\partial \vec{r}} + \frac{d\vec{k}}{dt} \cdot \frac{\partial f_{\vec{k}}}{\partial \vec{k}} = -\left(\frac{\partial f_{\vec{k}}}{\partial t} \right)_{coll}$$

$$\boxed{\frac{\partial f_{\vec{k}}}{\partial t}} + \frac{d\vec{r}}{dt}\cdot\boxed{\frac{\partial f_{\vec{k}}}{\partial \vec{r}}} + \frac{d\vec{k}}{dt}\cdot\frac{\partial f_{\vec{k}}}{\partial \vec{k}} = -\left(\frac{\partial f_{\vec{k}}}{\partial t}\right)_{coll}$$

$$\boxed{\frac{\partial f_{\vec{k}}}{\partial t} = 0}$$

$$\boxed{\frac{\partial f_{\vec{k}}}{\partial \vec{r}} = 0}$$

$$\frac{d\vec{k}}{dt} \cdot \frac{\partial f_{\vec{k}}}{\partial \vec{k}} = -\left(\frac{\partial f_{\vec{k}}}{\partial t} \right)_{coll}$$

$$\boxed{\frac{d\vec{k}}{dt}} \cdot \frac{\partial f_{\vec{k}}}{\partial \vec{k}} = -\left(\frac{\partial f_{\vec{k}}}{\partial t}\right)_{coll}$$

$$\boxed{\frac{d\vec{k}}{dt} = \frac{1}{\hbar}\frac{d\vec{p}}{dt} = -\frac{e\vec{E}}{\hbar}}$$

$$\boxed{\frac{d\vec{k}}{dt}}\cdot\boxed{\frac{\partial f_{\vec{k}}}{\partial \vec{k}}} = -\left(\frac{\partial f_{\vec{k}}}{\partial t}\right)_{coll}$$

$$\boxed{\frac{d\vec{k}}{dt} = \frac{1}{\hbar}\frac{d\vec{p}}{dt} = -\frac{e\vec{E}}{\hbar}}$$

$$\boxed{\frac{\partial f_0\left(\varepsilon_{\vec{k}}\right)}{\partial \vec{k}} = \frac{\partial f_0\left(\varepsilon_k\right)}{\partial \varepsilon_{\vec{k}}}\frac{\partial \varepsilon}{\partial \vec{k}} = \frac{\partial f_0\left(\varepsilon_k\right)}{\partial \varepsilon_{\vec{k}}}\hbar\vec{v}_{\vec{k}}}$$

$$\frac{d\vec{k}}{dt}\cdot\frac{\partial f_{\vec{k}}}{\partial\vec{k}} = -\left(\frac{\partial f_{\vec{k}}}{\partial t}\right)_{coll}$$

$$\left(\frac{\partial f_{\vec{k}}}{\partial t}\right)_{coll} = -\frac{\left[f_{\vec{k}} - f_0\left(\varepsilon_{\vec{k}}\right)\right]}{\tau_{\vec{k}}}$$

$$\frac{d\vec{k}}{dt} = \frac{1}{\hbar}\frac{d\vec{p}}{dt} = -\frac{e\vec{E}}{\hbar}$$

$$\frac{\partial f_0\left(\varepsilon_{\vec{k}}\right)}{\partial\vec{k}} = \frac{\partial f_0\left(\varepsilon_k\right)}{\partial\varepsilon_{\vec{k}}}\frac{\partial\varepsilon}{\partial\vec{k}} = \frac{\partial f_0\left(\varepsilon_k\right)}{\partial\varepsilon_{\vec{k}}}\hbar\vec{v}_{\vec{k}}$$

$$\boxed{\frac{d\vec{k}}{dt}}\cdot\boxed{\frac{\partial f_{\vec{k}}}{\partial \vec{k}}} = -\boxed{\left(\frac{\partial f_{\vec{k}}}{\partial t}\right)_{coll}}$$

$$\left(\frac{\partial f_{\vec{k}}}{\partial t}\right)_{coll} = -\frac{\left[f_{\vec{k}} - f_0\left(\varepsilon_{\vec{k}}\right)\right]}{\tau_{\vec{k}}}$$

$$\frac{d\vec{k}}{dt} = \frac{1}{\hbar}\frac{d\vec{p}}{dt} = -\frac{e\vec{E}}{\hbar}$$

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$$\boxed{f_{\vec{k}} = f_0(\varepsilon_{\vec{k}}) + e\left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}}\right)\tau_{\vec{k}}\,\vec{v}_{\vec{k}}\cdot\vec{E}}$$

$$\frac{d\vec{k}}{dt}\cdot\frac{\partial f_{\vec{k}}}{\partial \vec{k}} = -\left(\frac{\partial f_{\vec{k}}}{\partial t}\right)_{coll}$$

$$\left(\frac{\partial f_{\vec{k}}}{\partial t}\right)_{coll} = -\frac{\left[f_{\vec{k}} - f_0\left(\varepsilon_{\vec{k}}\right)\right]}{\tau_{\vec{k}}}$$

$$\frac{d\vec{k}}{dt} = \frac{1}{\hbar}\frac{d\vec{p}}{dt} = -\frac{e\vec{E}}{\hbar}$$

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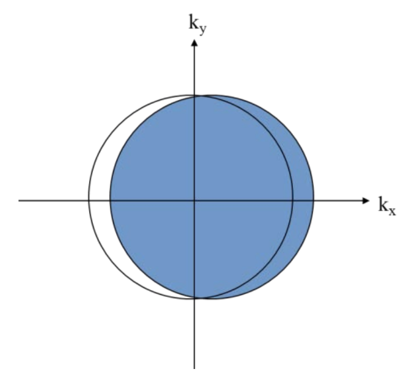
$$\boxed{f_{\vec{k}} = f_0(\varepsilon_{\vec{k}}) + e\left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}}\right)\tau_{\vec{k}}\,\vec{v}_{\vec{k}}\cdot\vec{E}}$$



$$f_{\vec{k}} = f_0(\varepsilon_{\vec{k}}) + e\left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}}\right)\tau_{\vec{k}}\ \vec{v}_{\vec{k}} \cdot \vec{E}$$

$$\vec{J} = e \sum_{\vec{k}} f_{\vec{k}} \, \vec{v}_{\vec{k}}$$

$$f_{\vec{k}} = f_0(\varepsilon_{\vec{k}}) + e\left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}}\right)\tau_{\vec{k}} \, \vec{v}_{\vec{k}} \cdot \vec{E}$$

$$\vec{J} = e \sum_{\vec{k}} f_{\vec{k}} \, \vec{v}_{\vec{k}}$$

$$f_{\vec{k}} = f_0(\varepsilon_{\vec{k}}) + e\left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}}\right)\tau_{\vec{k}} \, \vec{v}_{\vec{k}} \cdot \vec{E}$$

$$\vec{J} = \left[e^2 \sum_{\vec{k}} \left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}}\right) \tau_{\vec{k}} \, \vec{v}_{\vec{k}} \vec{v}_{\vec{k}} \right] \cdot \vec{E}$$

$$\vec{J} = e \sum_{\vec{k}} f_{\vec{k}} \, \vec{v}_{\vec{k}}$$

$$f_{\vec{k}} = f_0(\varepsilon_{\vec{k}}) + e\left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}}\right)\tau_{\vec{k}} \, \vec{v}_{\vec{k}} \cdot \vec{E}$$

Ω

$$\boxed{\vec{J} = \overleftrightarrow{\sigma} \cdot \vec{E}}$$

$$\vec{J} = \left[e^2 \sum_{\vec{k}} \left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}}\right)\tau_{\vec{k}} \, \vec{v}_{\vec{k}} \vec{v}_{\vec{k}} \right] \cdot \vec{E}$$

$$\vec{J} = e \sum_{\vec{k}} f_{\vec{k}} \, \vec{v}_{\vec{k}}$$

$$f_{\vec{k}} = f_0(\varepsilon_{\vec{k}}) + e\left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}}\right)\tau_{\vec{k}} \, \vec{v}_{\vec{k}} \cdot \vec{E}$$

Ω

$$\vec{J} = \overleftrightarrow{\sigma} \cdot \vec{E}$$

$$\vec{J} = \left[e^2 \sum_{\vec{k}} \left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}}\right)\tau_{\vec{k}} \, \vec{v}_{\vec{k}} \vec{v}_{\vec{k}} \right] \cdot \vec{E}$$

$$\boxed{\overleftrightarrow{\sigma} = e^2 \sum_{\vec{k}} \left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}}\right)\tau_{\vec{k}} \, \vec{v}_{\vec{k}} \vec{v}_{\vec{k}}}$$

$$J = \sigma E$$

$$Z = \frac{\sigma S^2}{\kappa_{el}^0 + \kappa_{ph}}$$

$$\sigma = e^2 \sum_{\vec{k}} \left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}} \right) \tau_{\vec{k}} \, v_{\vec{k}}^2$$

$$S = \frac{e k_B}{\sigma} \sum_{\vec{k}} \left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}} \right) \tau_{\vec{k}} \, v_{\vec{k}}^2 \, \frac{\left(\varepsilon_{\vec{k}} - \mu \right)}{k_B T}$$

$$\kappa_{el}^0 = \kappa_{el} - \sigma S^2 T$$

$$\kappa_{el} = k_B^2 \sum_{\vec{k}} \left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}} \right) \tau_{\vec{k}} \, v_{\vec{k}}^2 \left[\frac{\left(\varepsilon_{\vec{k}} - \mu \right)}{k_B T} \right]^2$$

$$\sigma = e^2 \sum_{\vec{k}} \left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}} \right) \tau_{\vec{k}}\, v_{\vec{k}}^2 = e^2 \int d\varepsilon\, \Sigma(\varepsilon) \left(-\frac{\partial f_0}{\partial \varepsilon} \right)$$

$$S = \frac{ek_B}{\sigma} \sum_{\vec{k}} \left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}} \right) \tau_{\vec{k}}\, v_{\vec{k}}^2 \frac{\left(\varepsilon_{\vec{k}} - \mu\right)}{k_B T} = \frac{ek_B}{\sigma} \int d\varepsilon\, \Sigma(\varepsilon) \left(-\frac{\partial f_0}{\partial \varepsilon} \right) \frac{\left(\varepsilon - \mu\right)}{k_B T}$$

$$\kappa_{el} = k_B^2 \sum_{\vec{k}} \left(-\frac{\partial f_0}{\partial \varepsilon_{\vec{k}}} \right) \tau_{\vec{k}}\, v_{\vec{k}}^2 \left[\frac{\left(\varepsilon_{\vec{k}} - \mu\right)}{k_B T} \right]^2 = k_B^2 \int d\varepsilon\, \Sigma(\varepsilon) \left(-\frac{\partial f_0}{\partial \varepsilon} \right) \left[\frac{\left(\varepsilon - \mu\right)}{k_B T} \right]^2$$

$$\Sigma(\varepsilon) = \sum_{\vec{k}} \tau_{\vec{k}}\, v_{\vec{k}}^2\, \delta\left(\varepsilon_{\vec{k}} - \varepsilon\right)$$

Transport distribution

$$\boxed{\sigma[\Sigma] \qquad S[\Sigma] \qquad \kappa_{el}[\Sigma]}$$

$$\sigma = e^2 \int \left(-\frac{\partial f_0}{\partial \varepsilon} \right) \Sigma(\varepsilon)\, d\varepsilon$$

$$S = \frac{k_B}{\sigma} \int \left(-\frac{\partial f_0}{\partial \varepsilon} \right) \Sigma(\varepsilon) \left[\frac{(\varepsilon - \mu)}{k_B T} \right] d\varepsilon$$

$$\kappa_{el} = k_B^2 \int \left(-\frac{\partial f_0}{\partial \varepsilon} \right) \Sigma(\varepsilon) \left[\frac{(\varepsilon - \mu)}{k_B T} \right]^2 d\varepsilon$$

$$Z = \frac{\sigma S^2}{\kappa_{el}^0 + \kappa_{ph}} = Z[\Sigma] \qquad \Sigma_{best} \Big/ \max_{\Sigma} Z[\Sigma] = Z[\Sigma_{best}]$$

$$\boxed{\Sigma_{best}(\varepsilon) = C\delta(\varepsilon - \varepsilon_0)} \qquad \boxed{\varepsilon_0 \approx 2.4 k_B T}$$

"The best thermoelectric," G. D. Mahan and J. O. Sofo
Proc. Nat. Acad. Sci. USA, **93**, 7436 (1996)

The "Best" Thermoelectric

$$\Sigma(\varepsilon) = \sum_k \tau_k \vec{v}_k \vec{v}_k \delta(\varepsilon_k - \varepsilon)$$

$$N(\varepsilon) = \int dS \frac{1}{|\nabla \varepsilon_k|}$$

$$= N(\varepsilon) v^2(\varepsilon) \tau(\varepsilon)$$

$$v(\varepsilon) = \nabla \varepsilon_k$$

$$\Sigma_{best}(\varepsilon) = C\delta(\varepsilon - \varepsilon_0)$$

$$\varepsilon_0 \approx 2.4 k_B T$$

Optimal Bandwidth for High Efficiency Thermoelectrics

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(Received 31 August 2011; published 22 November 2011)

The thermoelectric figure of merit (ZT) in narrow conduction bands of different material dimensionalities is investigated for different carrier scattering models. When the bandwidth is zero, the transport distribution function (TDF) is finite, not infinite as previously speculated by Mahan and Sofo [Proc. Natl. Acad. Sci. U.S.A. **93**, 7436 (1996)], even though the carrier density of states goes to infinity. Such a finite TDF results in a zero electrical conductivity and thus a zero ZT. We point out that the optimal ZT cannot be found in an extremely narrow conduction band. The existence of an optimal bandwidth for a maximal ZT depends strongly on the scattering models and the dimensionality of the material. A nonzero optimal bandwidth for maximizing ZT also depends on the lattice thermal conductivity. A larger maximum ZT can be obtained for materials with a smaller lattice thermal conductivity.

miniband formation [1,19].

Although mathematically rigorous, Mahan and Sofo also noted in their original paper [9] that the exact delta-shaped TDF cannot be found in real materials due to the energy-dependent relaxation time and carrier velocity. It is therefore very meaningful to reinvestigate what is the best electronic structure of materials to maximize ZT when the

0031-9007/11/107(22)/226601(5) 2266(

Let us look at the case for an extremely narrow band first. When $W_\alpha \to 0$, the DOS is infinite, since $N_\alpha(E) \sim 1/W_\alpha$. However, the TDF $\Xi_\alpha(E)$ in Table I is always finite when we consider different carrier scattering possibilities, even though the DOS is infinite. This is very different from the Mahan-Sofo hypothesis [9] which assumes an infinite delta-shaped TDF. Such an infinite delta-shaped TDF can never hold in nature, since it requires $\tau_\alpha(E) \sim 1/W_\alpha^2$ [24], which cannot be found with known scattering models. Mathematically, for finite $\Xi_\alpha(E)$, all the transport coeffi-

Proc. Natl. Acad. Sci. USA
Vol. 93, pp. 7436–7439, July 1996
Applied Physical Sciences

This contribution is part of a special series of
elected on April 25, 1995.

The best thermoelectric

G. D. MAHAN*† AND J. O. SOFO‡

In summary, we have written the thermoelectric figure of merit as a functional of the transport distribution. This function must be a Dirac delta function to maximize the figure of merit. Of course, this exact situation is not found in nature. However, our results indicate that we have to search for materials where the distribution of energy carriers is as narrow as possible, but with high carrier velocity in the direction of the applied electric field.

PHYSICAL REVIEW B VOLUME 47, NUMBER 19 15 MAY 1993-I

Effect of quantum-well structures on the thermoelectric figure of merit

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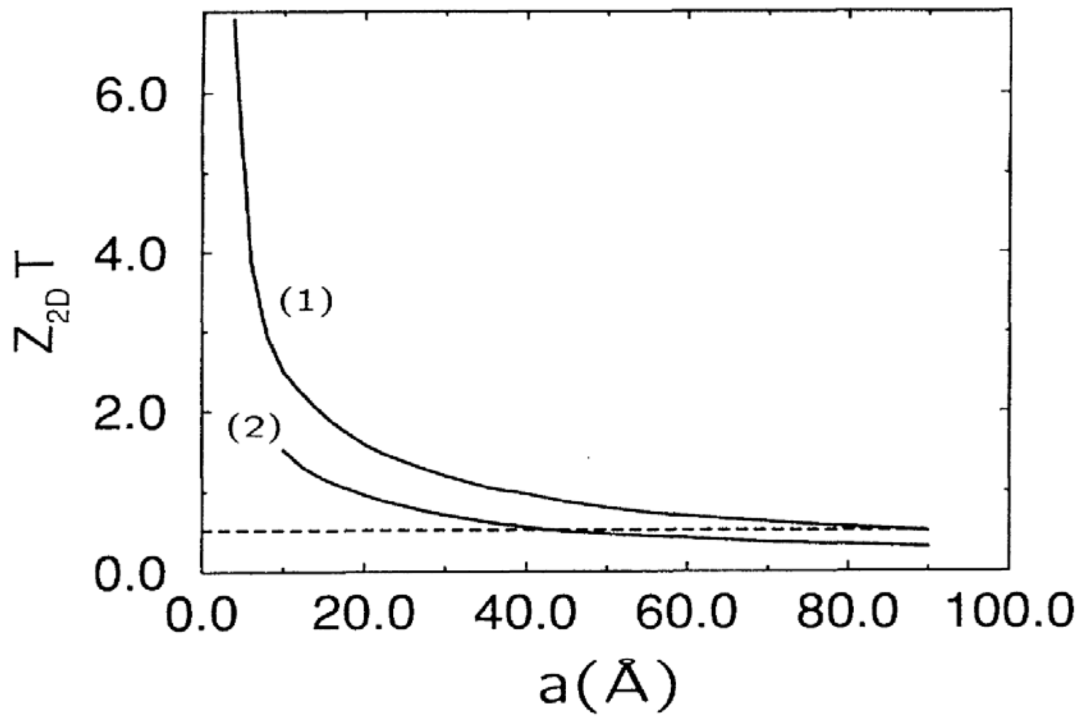
(Received 3 December 1992)

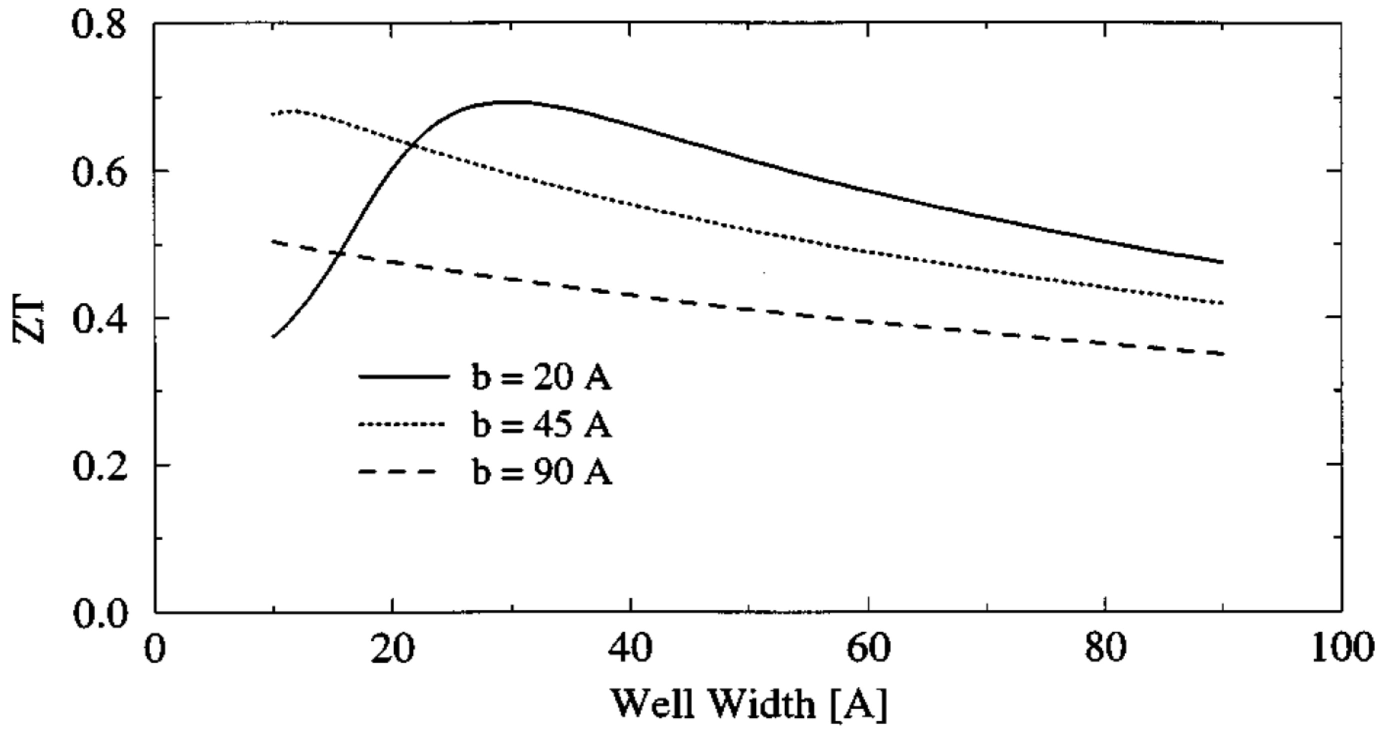
$$\varepsilon(k_x, k_y) = \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} + \frac{\hbar^2 \pi^2}{2m_z a^2},$$



$$\varepsilon(k_x, k_y) = \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} + \frac{\hbar^2 \pi^2}{2m_z a^2},$$

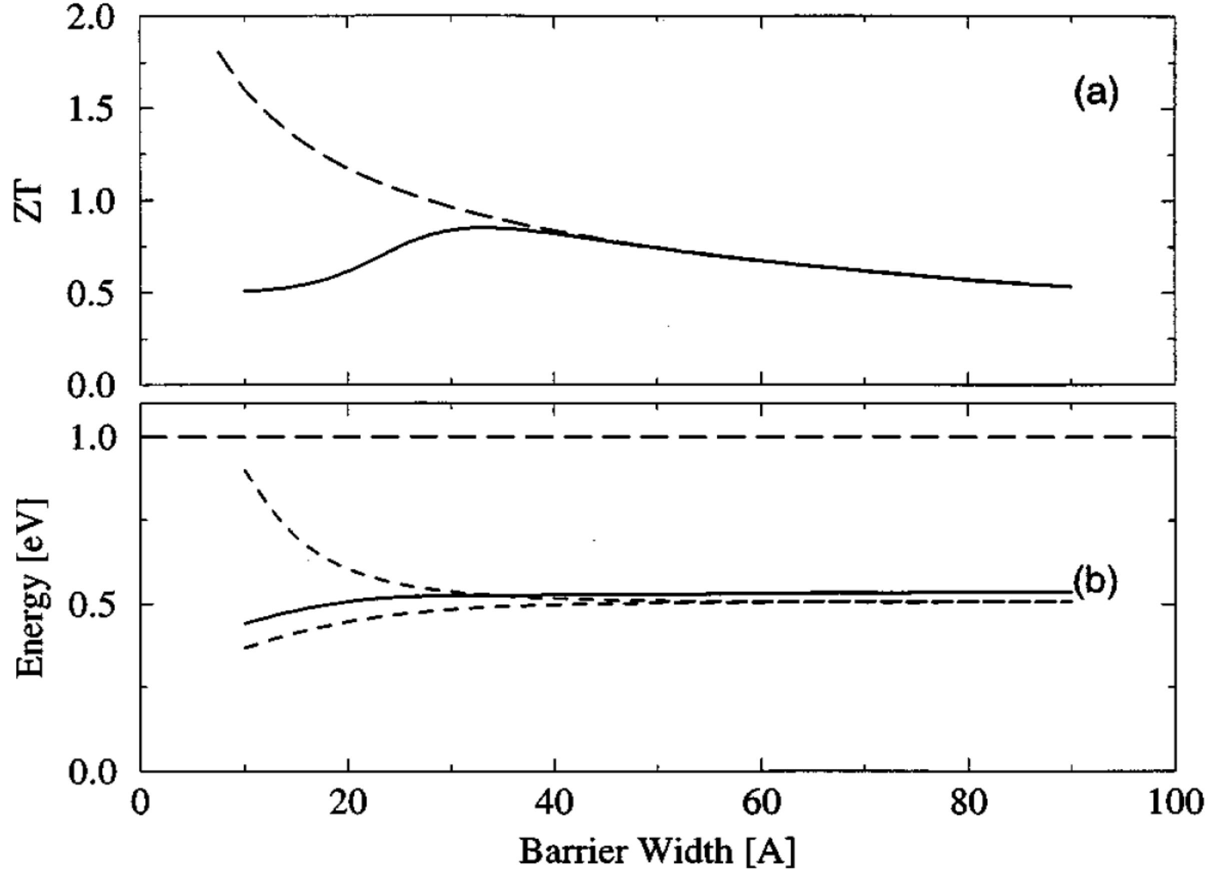
$$\epsilon_s(k_x, k_y, k_z) = \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} + E_s(k_z),$$

$$\epsilon_s(k_x, k_y, k_z) = \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} + E_s(k_z),$$



J. O. Sofo, G. D. Mahan, “Thermoelectric figure of merit of superlattices”, *Appl. Phys. Lett.* **65**, 2690 (1994).

$$\epsilon_s(k_x, k_y, k_z) = \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} + E_s(k_z),$$



J. O. Sofo, G. D. Mahan, "Thermoelectric figure of merit of superlattices", *Appl. Phys. Lett.* **65**, 2690 (1994).

Limitations of the Boltzman Equation Method

- Also known as the Kinetic Method because of the relation with classical kinetic theory

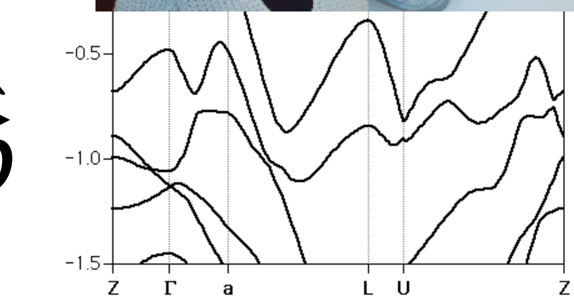
$$\frac{\partial f_{\vec{k}}}{\partial t}+\frac{d\vec{r}}{dt}\cdot\frac{\partial f_{\vec{k}}}{\partial \vec{r}}+\frac{d\vec{k}}{dt}\cdot\frac{\partial f_{\vec{k}}}{\partial \vec{k}}=-\left(\frac{\partial f_{\vec{k}}}{\partial t}\right)_{coll} \qquad \frac{\partial f_{\vec{k}}}{\partial t}+\frac{\partial H}{\partial \vec{p}}\cdot\frac{\partial f_{\vec{k}}}{\partial \vec{r}}-\frac{\partial H}{\partial \vec{r}}\cdot\frac{\partial f_{\vec{k}}}{\partial \vec{p}}=\frac{\partial f_{\vec{k}}}{\partial t}-\left\{H, f_{\vec{k}}\right\}-\left(\frac{\partial f_{\vec{k}}}{\partial t}\right)_{coll}$$

- According to Kubo, Toda, and Hashitsume(1) cannot be applied when the mean free path is too short (e.g., amorphous semiconductors) or the frequency of the applied fields is too high.
- However, it is very powerful and can be applied to non linear problems.

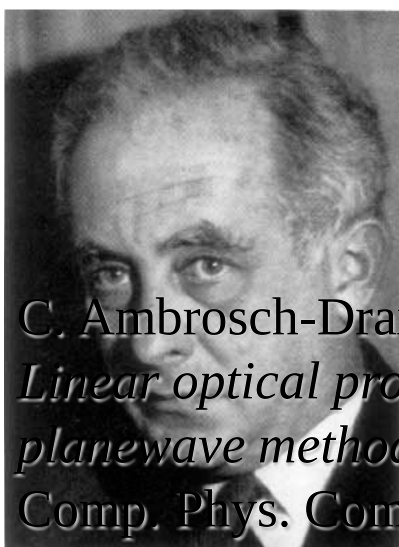
(1) R. Kubo, M. Toda, and N. Hashitsume, Statistical Physics II: Non-equilibrium Statistical Mechanics (Springer-Verlag, Berlin, 1991) p. 197

Using Boltzman with ab-initio

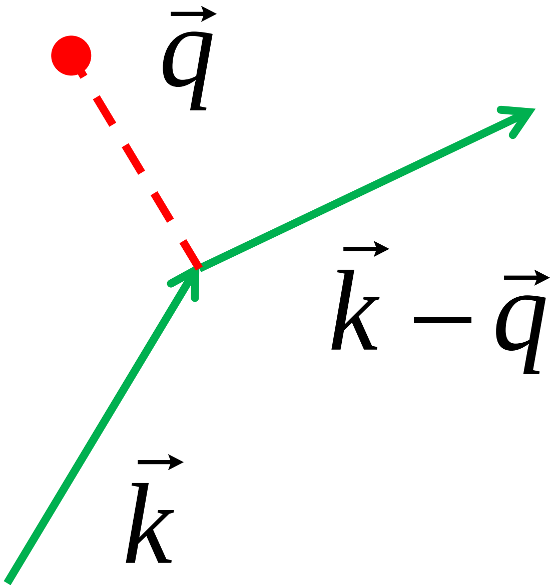
$$\overleftrightarrow{\sigma} = e^2 \sum_k \left(-\frac{\partial f^0}{\partial \varepsilon} \right) \tau_k \vec{v}_k \vec{v}_k$$



$$\frac{1}{\hbar}\frac{\partial \varepsilon_k}{\partial \vec{k}} = \frac{\vec{p}_k}{m} = \frac{1}{m}\left\langle k \middle| \hat{\vec{p}} \right.$$



C. Ambrosch-Draxl and J. O. Sofo
Linear optical properties of solids within the full-potential linearized augmented planewave method
Comp. Phys. Commun. **175**, 1-14 (2006)



τ_k

First Born Approximation

- Defect scattering
  - Crystal defects
  - Impurities
    - Neutral
    - Ionized
  - Alloy
- Carrier-carrier scattering
- Lattice scattering
  - Intravalley
    - Acoustic
      - Deformation potential
      - Piezoelectric
    - Optic
      - Non-polar
      - Polar
  - Intervalley
    - Acoustic
    - Optic

Table 6.2. Matrix elements for different kinds of scattering

Type of scattering	Scattering potential energy, ΔV	Matrix element excluding the overlap integral
1. Acoustic Phonon:		
a) Deformation Potential [Ref.6.1,Chap.2;6.17]	$E_1 \nabla u(\underline{r}) S_c(q,\lambda)$	$E_1\left(\frac{\hbar}{2V_c\rho\omega_q}\right)^{1/2} S_c(q,\lambda)(\underline{e}_q\cdot\underline{q})\left(n_q+\frac{1}{2}\pm\frac{1}{2}\right)^{1/2}$
b) Piezoelectric [6.18]	$\frac{eh_{pz}}{q\epsilon}\nabla u(\underline{r})S_c(q,\lambda)$	$\frac{\lvert e\rvert h_{pz}}{\epsilon}\left(\frac{\hbar}{2V_c\rho\omega_q}\right)^{1/2}S_c(q,\lambda)\left(n_q+\frac{1}{2}\pm\frac{1}{2}\right)^{1/2}$
2. Optic Phonon:		
a) Nonpolar [6.19]	$D_0 u(\underline{r})S_c(q,\lambda)$	$D_0\left(\frac{\hbar}{2V_c\rho\omega_0}\right)^{1/2}S_c(q,\lambda)\left(n_0+\frac{1}{2}\pm\frac{1}{2}\right)^{1/2}$
b) Polar [6.20]	$\frac{u(\underline{r})e\omega_\ell}{q}\left[\frac{\rho}{V_c\epsilon_0}\left(\frac{1}{K_\infty}-\frac{1}{K_S}\right)\right]S_c(q,\lambda)$	$\frac{\lvert e\rvert}{q}\left(\frac{1}{K_\infty}-\frac{1}{K_S}\right)^{1/2}\left(\frac{\hbar\omega_\ell}{2V_c\epsilon_0}\right)^{1/2}\left(n_\ell+\frac{1}{2}\pm\frac{1}{2}\right)^{1/2}S_c(q,\lambda)$
3. Defect:		
a) Ionised Impurity [6.21,22]	$\frac{Ze^2}{4\pi\epsilon r}\exp(-r/\lambda)$	$\frac{Ze^2}{V_c\epsilon}\frac{1}{\lvert\underline{k}-\underline{k}'\rvert^2+\lambda^{-2}}$
b) Neutral Impurity [6.4a]	—	$\frac{2\pi\hbar^2}{m^*V_c}\left(\frac{20a_0}{4\pi k}\right)^{1/2}$
c) Dislocation:		
(i) Charged type [Ref.6.2d,p.232;6.23]	$\frac{ef}{2\pi a_D\epsilon}K_0(r/\lambda)$	—
(ii) Strain type [6.24]	$\frac{E_1\lambda_S(1-2\nu)}{2\pi(1-\nu)}\frac{\sin\theta}{r}$	—
d) Alloy [6.25,Ref.6.2c]	—	$\frac{N_0^{1/2}\alpha^{1/2}(1-\alpha)^{1/2}(E_a-E_b)}{V_c^{1/2}}$
4. Intervalley Phonon [Ref.6.1,p.107]	$D_i u(\underline{r})S_c(q,\lambda)$	$D_i\left(\frac{\hbar}{2\rho V_c\omega_i}\right)^{1/2}S_c(q,\lambda)\left(n_i+\frac{1}{2}\pm\frac{1}{2}\right)^{1/2}$

Meanings of symbols (Table 6.2):

ΔV - Potential energy of the electron due to the scattering potential
E_1 - Acoustic phonon deformation potential constant
$u(\underline{r})$ - Displacement due to a lattice wave
$\underline{q}$ - Wave vector of lattice wave
λ - Debye screening length
V_c - Volume of the crystal
ρ - Density of the material
$\omega_{\underline{q}}$ - Angular frequency of the lattice wave corresponding to the wave vector q
$\underline{e}_{\underline{q}}$ - Polarisation vector of the lattice wave
$n_{\underline{q}}$ - Occupation number of phonons with wave vector $\underline{q}$
h_{pz} - Piezoelectric constant
ε - Permittivity of the material
D_0 - Nonpolar optic phonon deformation potential constant
ω_0 - Angular frequency of the nonpolar optic wave neglecting dispersion
n_0 - Occupation number of optic phonons
K_∞ - High-frequency dielectric constant
K_S - Static dielectric constant
ω_ℓ - Longitudinal frequency of vibration for polar optic wave
ε_0 - Permittivity of free space
n_ℓ - Occupation number of polar optic phonons
Z - Ionicity of an impurity atom
$\underline{k}$ - Wave vector of the electron in the original state
$\underline{k}'$ - Wave vector of the electron in the scattered state
$S_c(\underline{q},\lambda)=q^2(q^2+\lambda^{-2})^{-1}$ - Screening factor
N_0 - Number of atoms in the crystal
a_0 - Bohr radius
r - Distance from impurity centre, or distance from dislocation axis
a_D - Distance between dislocation centres
f - Probability of occupation of a dislocation centre by an electron
K_0 - Modified Bessel function of zero order
ν - Poisson's ratio
λ_S - Unit crystallographic slip distance
θ - Angle measured from slip direction
D_i - Intervalley phonon deformation potential constant
ω_i - Intervalley phonon angular frequency
n_i - Occupation number of intervalley phonons
α - Fraction of atoms of type a
(E_a-E_b) - Difference between the band edge of atoms of type a and of type b constituting the alloy
$\pm$ - The plus sign corresponds to emission and the minus sign to the absorption process.

B. R. Nag - 1980 - Electron Transport in Compound Semiconductors

Transport coefficients and thermoelectric figure of merit of n-$Hg_{1-x}Cd_xTe$

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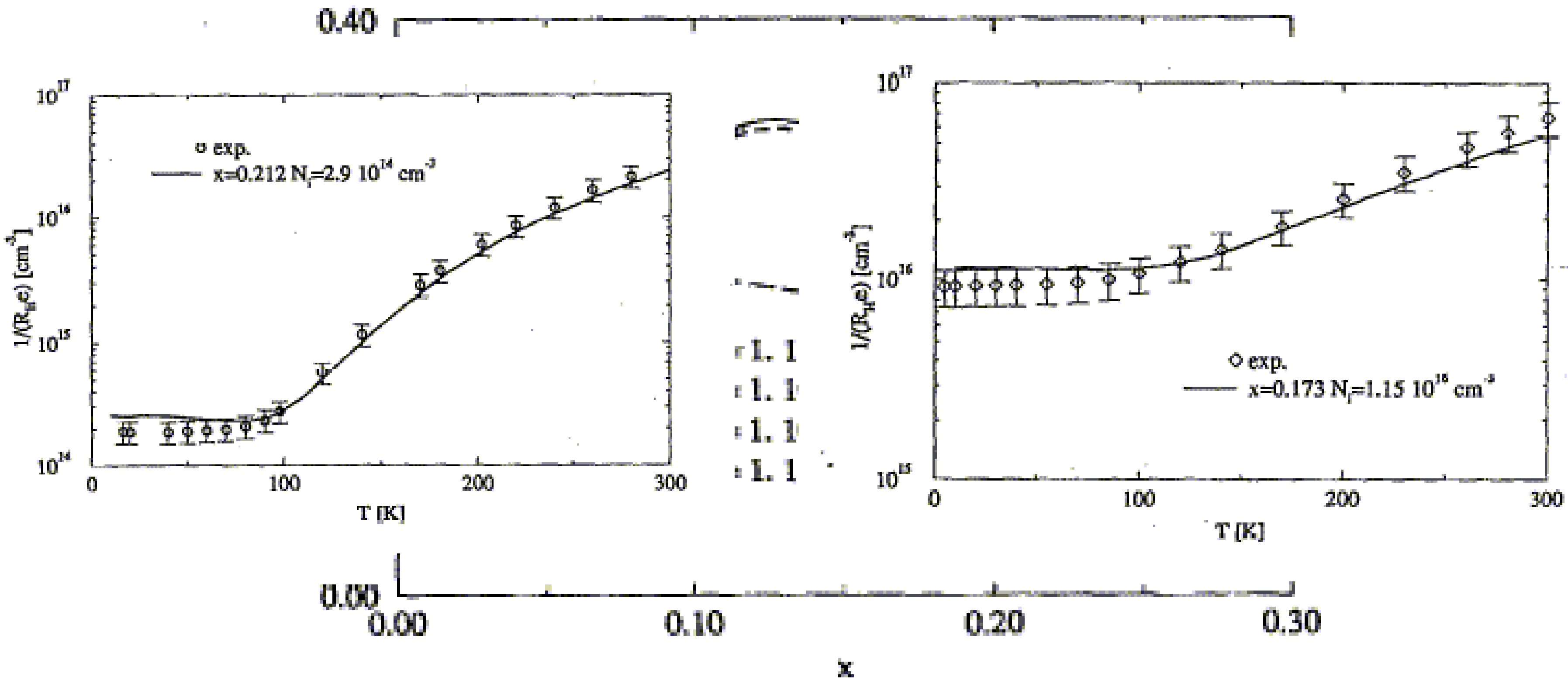
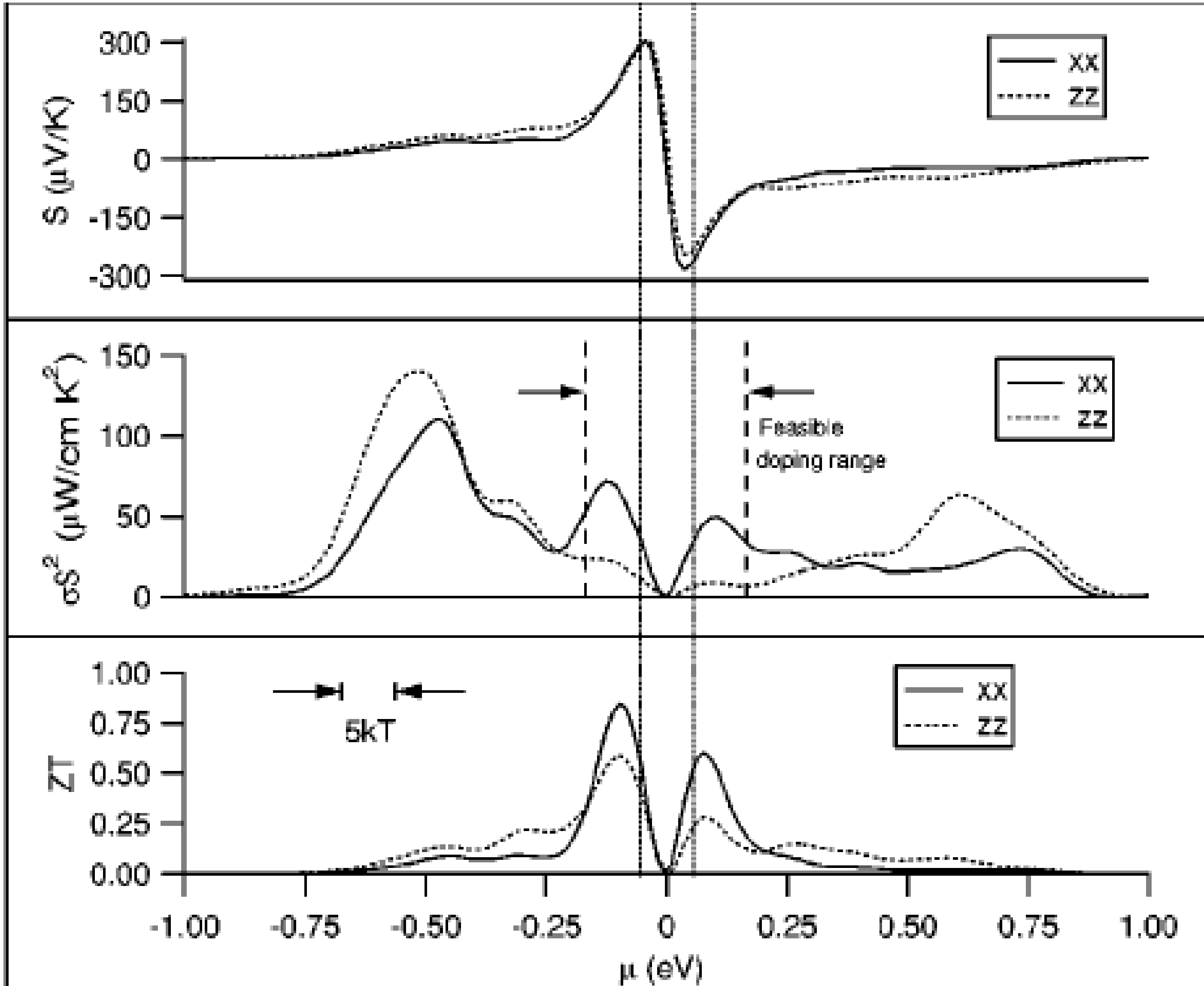


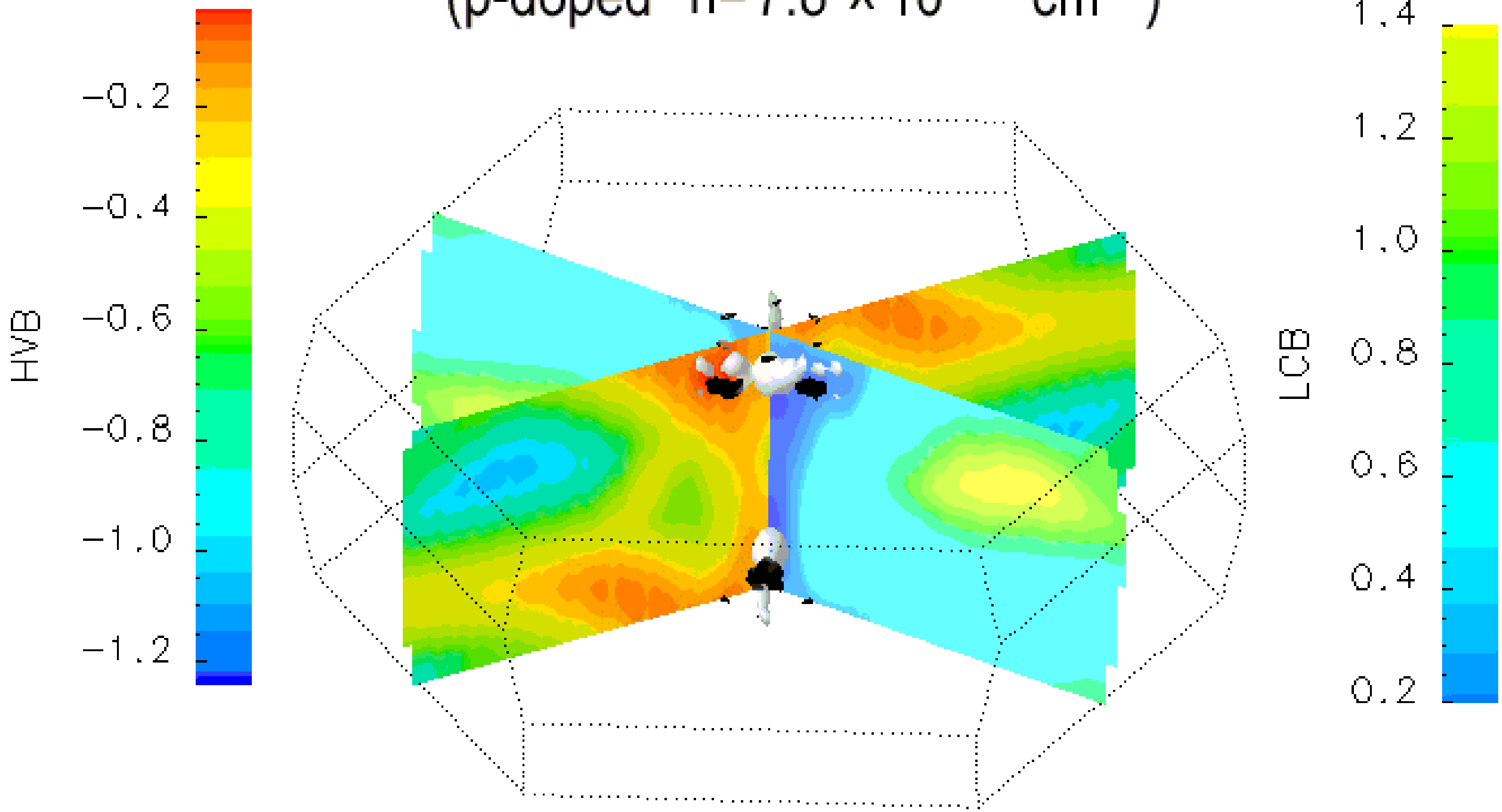
T. J. Scheidemantel, C. Ambrosch-Draxl, T. Thonhauser, J. V. Badding, and J. O. Sofo. “Transport Coefficients from First-principles Calculations.” *Phys. Rev. B* **68**, 125210 (2003)

Bi_2Te_3



Bismuth Telluride

(p-doped $n = 7.8 \times 10^{18}$ cm^{-3})



- Positive contribution to S
- Negative contribution to S

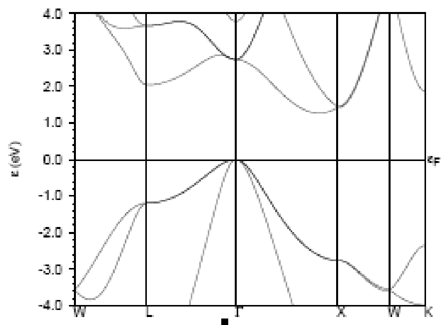
Georg Madsen's
The Grand Search

L/APW+lo, DFT

Spin orbit coupling (incl. $p_{1/2}$)

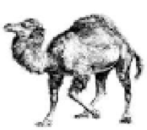
Efficient

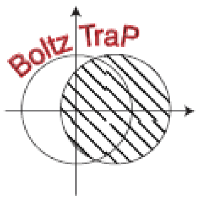
All space groups



DCSC, SDU Odense

960 node PIV cluster





Semiclassic equations

Efficient: FFT, blas

Full conductivity tensors

Inorganic Crystal Structure Database

All known inorganic crystal structures

Careful…

- Doping: rigid band
- Gap problem
- Temperature dependence of the electronic structure.
- Alloys. Single site approximations do not work.
- Many k-points
- Correlated materials?
- Connection with magnetism and topology?

Linear Response Theory (Kubo)

- Valid only close to equilibrium

$$\sigma_{\alpha\beta}(\vec{q},\omega) = \frac{i}{\omega}\left[\delta_{\alpha\beta}\frac{n_0 e^2}{m} + \Pi_{\alpha\beta}\left(\vec{q},\omega+0^+\right)\right]$$

$$\Pi_{\alpha\beta}(\vec{q},i\omega_n) = -\frac{1}{V}\int_0^\beta d\tau e^{i\omega_n\tau}\left\langle T_\tau j_\alpha^\dagger(\vec{q},\tau)\, j_\beta(\vec{q},\tau)\right\rangle$$

- However
  - Does not need well defined energy “bands”
  - It is easy to incorporate most low energy excitations of the solid
  - Amenable to diagrammatic expansions and controlled approximations
  - Equivalent to the Boltzmann equation when both are valid.

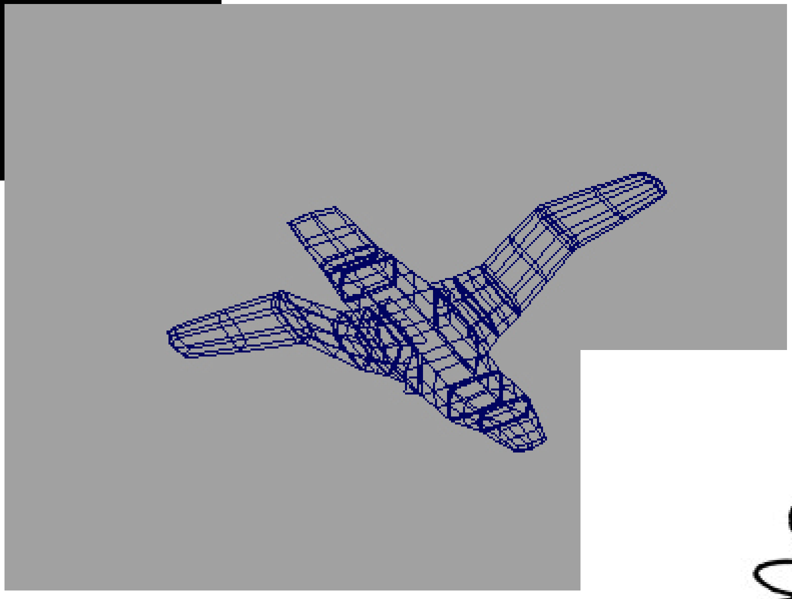
Summary

- Look for narrow transmission channels with high velocity…
- Tool to explore new compounds, pressure, “negative” pressure.
- Prediction of a new compound by G. Madsen.
- Easy to expand adding new Scattering Mechanisms
- Limited to applications on “non-correlated” semiconductors.
- Magneto-Thermoelectric effects are beginning to be explored.

A final comment:

EXPERIMENT<-> SIMULATION<->THEORY

PENNSTATE



Simulations describe complexity. Our theoretical work is to make it simple

Thank you!

$$Z = \frac{\sigma S^2}{\kappa_{el}^0 + \kappa_{ph}} = Z[\Sigma]$$

$$\Sigma(\varepsilon) = \sum_{\vec{k}} \tau_{\vec{k}} v_{\vec{k}}^2 \delta(\varepsilon_{\vec{k}} - \varepsilon)$$

Transport distribution