Thermoelectrics:
A theoretical approach
to the search for better materials

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The devices

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

\[ T_1 \]

Bismuth Telluride
Elements with "N" & "P" type properties

\[ \sigma = \frac{\kappa}{\phi \cdot (T_2 - T_1)} \]

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

\[ \phi_{\text{MAX}} = \frac{T_1 \left[ \sqrt{1 + Z \bar{T}} - T_2 / T_1 \right]}{(T_2 - T_1) \left[ \sqrt{1 + Z \bar{T}} + 1 \right]} \quad \text{for} \quad Z \to +\infty \]

\[ Z = \frac{\sigma S^2}{\kappa} \]
Conductivity 101

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

\textit{Drude et al.}

![Diagram showing energy levels and wave vectors](image)
Conductivity 101

\[ J = e \sum_k f_0(\varepsilon_k) v_k = 0 \]

\[ J = e \sum_k f_k v_k \neq 0 \]
\[
\frac{\partial f_k}{\partial t} + \frac{\partial H}{\partial \vec{p}} \cdot \frac{\partial f_k}{\partial \vec{r}} - \frac{\partial H}{\partial \vec{r}} \cdot \frac{\partial f_k}{\partial \vec{p}} = \\
\frac{\partial f_k}{\partial t} - \{H, f_k\} = \left( \frac{\partial f_k}{\partial t} \right)_{\text{coll}}
\]

\[
\frac{d}{dt} \rho'(t) = \frac{1}{i\hbar} \left[ H + H'(t), \rho'(t) \right]
\]
\[ \frac{\partial f_k}{\partial t} + \frac{d\vec{r}}{dt} \cdot \frac{\partial f_k}{\partial \vec{r}} + \frac{d\vec{k}}{dt} \cdot \frac{\partial f_k}{\partial \vec{k}} = - \left( \frac{\partial f_k}{\partial t} \right)_{coll} \]
\[
\frac{\partial f_k}{\partial t} + \frac{d\vec{r}}{dt} \cdot \frac{\partial f_k}{\partial \vec{r}} + \frac{dk}{dt} \cdot \frac{\partial f_k}{\partial \vec{k}} = - \left( \frac{\partial f_k}{\partial t} \right)_{coll}
\]

\[
\frac{\partial f_k}{\partial t} = 0 \quad \frac{\partial f_k}{\partial \vec{r}} = 0
\]
\[ \frac{d\vec{k}}{dt} \cdot \frac{\partial f_{\vec{k}}}{\partial \vec{k}} = - \left( \frac{\partial f_{\vec{k}}}{\partial t} \right)_{\text{coll}} \]
\[ \frac{d\vec{k}}{dt} \cdot \frac{\partial f_{\vec{k}}}{\partial \vec{k}} = -\left( \frac{\partial f_{\vec{k}}}{\partial t} \right)_{\text{coll}} \]

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

\[
\frac{\partial f_0 (\varepsilon_k)}{\partial \vec{k}} = \frac{\partial f_0 (\varepsilon_k)}{\partial \varepsilon_k} \frac{\partial \varepsilon_k}{\partial \vec{k}} = \frac{\partial f_0 (\varepsilon_k)}{\partial \varepsilon_k} \hbar \nu \vec{k}
\]

\[
\frac{d\vec{k}}{dt} \cdot \frac{\partial f_\vec{k}}{\partial \vec{k}} = -\left( \frac{\partial f_\vec{k}}{\partial t} \right)_{\text{coll}}
\]
\[
\frac{dk}{dt} \cdot \frac{\partial f_k}{\partial k} = - \left( \frac{\partial f_k}{\partial t} \right)_{\text{coll}}
\]

\[
\left( \frac{\partial f_k}{\partial t} \right)_{\text{coll}} = - \left[ f_k - f_0(\varepsilon_k) \right] \frac{\tau_k}{\hbar}
\]

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

\[
\frac{\partial f_0(\varepsilon_k)}{\partial k} = \frac{\partial f_0(\varepsilon_k)}{\partial \varepsilon_k} \frac{\partial \varepsilon_k}{\partial k} = \frac{\partial f_0(\varepsilon_k)}{\partial \varepsilon_k} \hbar \nu_k
\]
\[
\frac{dk}{dt} = \frac{dp}{\hbar dt} = -\frac{eE}{\hbar}
\]

\[
\left( \frac{\partial f_k}{\partial t} \right)_{\text{coll}} = - \left[ f_k - f_0(\varepsilon_k) \right] \tau_k
\]

\[
\frac{\partial f_0(\varepsilon_k)}{\partial k} = \frac{\partial f_0(\varepsilon_k)}{\partial \varepsilon_k} \frac{\partial \varepsilon_k}{\partial k} = \frac{\partial f_0(\varepsilon_k)}{\partial \varepsilon_k} \hbar \nu_k
\]

\[
f_k = f_0(\varepsilon_k) + e \left( - \frac{\partial f_0(\varepsilon_k)}{\partial \varepsilon_k} \right) \tau_k \nu_k \cdot \vec{E}
\]
\[
\frac{dk}{dt} = \frac{1}{\hbar} \frac{dp}{dt} = -\frac{e\vec{E}}{\hbar}
\]

\[
\frac{\partial f_0}{\partial k} = \frac{\partial f_0}{\partial \epsilon_k} \frac{\partial \epsilon_k}{\partial k} = \frac{\partial f_0}{\partial \epsilon_k} \hbar \vec{v}_k
\]

\[
f_k = f_0(\epsilon_k) + e \left( -\frac{\partial f_0}{\partial \epsilon_k} \right) \tau_k \vec{v}_k \cdot \vec{E}
\]
\[ f_k = f_0(\varepsilon_k) + e \left( -\frac{\partial f_0}{\partial \varepsilon_k} \right) \tau_k \quad \vec{v}_k \cdot \vec{E} \]
\[ \vec{J} = e \sum_k f_k \vec{v}_k \]

\[ f_k = f_0(\vec{\varepsilon}_k) + e \left( -\frac{\partial f_0}{\partial \vec{\varepsilon}_k} \right) \tau_k \vec{v}_k \cdot \vec{E} \]
\[ \vec{J} = e \sum_{\vec{k}} f_{\vec{k}} \vec{v}_{\vec{k}} \]

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

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

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

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

$$\vec{J} = \vec{\sigma} \cdot \vec{E}$$
\[ \vec{J} = e \sum_k f_{\vec{k}} \vec{v}_{\vec{k}} \]

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

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

\[ \vec{J} = \vec{\sigma} \cdot \vec{E} \]

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

\[ \sigma = e^2 \sum_{\vec{k}} \left( - \frac{\partial f_0}{\partial \epsilon_{\vec{k}}} \right) \tau_{\vec{k}} \nu_{\vec{k}}^2 \]

\[ S = \frac{e k_B}{\sigma} \sum_{\vec{k}} \left( - \frac{\partial f_0}{\partial \epsilon_{\vec{k}}} \right) \tau_{\vec{k}} \nu_{\vec{k}}^2 \frac{\left( \epsilon_{\vec{k}} - \mu \right)}{k_B T} \]

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

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

\[ \kappa_{el}^0 = \kappa_{el} - \sigma S^2 T \]
\[ \sigma = e^2 \sum_{\tilde{k}} \left( -\frac{\partial f_0}{\partial \epsilon_{\tilde{k}}} \right) \tau_{\tilde{k}} v^2_{\tilde{k}} = e^2 \int d\epsilon \Sigma(\epsilon) \left( -\frac{\partial f_0}{\partial \epsilon} \right) \]

\[ S = \frac{ek_B}{\sigma} \sum_{\tilde{k}} \left( -\frac{\partial f_0}{\partial \epsilon_{\tilde{k}}} \right) \tau_{\tilde{k}} v^2_{\tilde{k}} \frac{(\epsilon_{\tilde{k}} - \mu)}{k_B T} = \frac{ek_B}{\sigma} \int d\epsilon \Sigma(\epsilon) \left( -\frac{\partial f_0}{\partial \epsilon} \right) \frac{(\epsilon - \mu)}{k_B T} \]

\[ \kappa_{el} = k_B^2 \sum_{\tilde{k}} \left( -\frac{\partial f_0}{\partial \epsilon_{\tilde{k}}} \right) \tau_{\tilde{k}} v^2_{\tilde{k}} \left[ \frac{(\epsilon_{\tilde{k}} - \mu)}{k_B T} \right]^2 = k_B^2 \int d\epsilon \Sigma(\epsilon) \left( -\frac{\partial f_0}{\partial \epsilon} \right) \left[ \frac{(\epsilon - \mu)}{k_B T} \right]^2 \]

\[ \Sigma(\epsilon) = \sum_{\tilde{k}} \tau_{\tilde{k}} v^2_{\tilde{k}} \delta(\epsilon_{\tilde{k}} - \epsilon) \]

\[ \sigma[\Sigma] \quad S[\Sigma] \quad \kappa_{el}[\Sigma] \]

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

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

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

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

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

\[
\varepsilon_0 \approx 2.4k_B T
\]

The “Best” Thermoelectric

\[
\Sigma(\varepsilon) = \sum_k \tau_k \vec{v}_k \vec{v}_k \delta(\varepsilon_k - \varepsilon) \\
= N(\varepsilon) v^2(\varepsilon) \tau(\varepsilon)
\]

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

\[
\varepsilon_0 \approx 2.4k_B T
\]
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.

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

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 1 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 coefficients

0031-9007/11/107(22)/226601(5) 22660
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.
Effect of quantum-well structures on the thermoelectric figure of merit

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

\[ Z_{2D} T \]

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

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

J. O. Sofo, G. D. Mahan, "Thermoelectric figure of merit of superlattices", 
\[ \epsilon_s(k_x, k_y, k_z) = \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} + E_s(k_z), \]

Limitations of the Boltzmann Equation Method

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

\[ \frac{\partial f_k}{\partial t} + \frac{d \vec{r}}{dt} \cdot \frac{\partial f_k}{\partial \vec{r}} + \frac{d \vec{k}}{dt} \cdot \frac{\partial f_k}{\partial \vec{k}} = -\left( \frac{\partial f_k}{\partial t} \right)_{\text{coll}} \]

\[ \frac{\partial f_k}{\partial t} + \frac{\partial H}{\partial \vec{p}} \cdot \frac{\partial f_k}{\partial \vec{r}} - \frac{\partial H}{\partial \vec{r}} \cdot \frac{\partial f_k}{\partial \vec{p}} = \frac{\partial f_k}{\partial t} - \{ H, f_k \} - \left( \frac{\partial f_k}{\partial t} \right)_{\text{coll}} \]

• 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.

Using Boltzmann with ab-initio

\[ \vec{\sigma} = e^2 \sum_k \left( -\frac{\partial f^0}{\partial \varepsilon} \right) \vec{\tau}_k \vec{\nu}_k \vec{v}_k \]

\[ \frac{1}{m} \frac{\partial \varepsilon_k}{\partial \vec{p}_k} = \frac{1}{m} \left\langle k \right| \hat{p} \]

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)*
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

<table>
<thead>
<tr>
<th>Type of scattering</th>
<th>Scattering potential energy, $\Delta V$</th>
<th>Matrix element excluding the overlap integral</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>1. Acoustic Phonon:</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>a) Deformation Potential</td>
<td>$E_1 v(r) S_C(q, \lambda)$</td>
<td>$E_1 \left( \frac{\hbar}{2V_{C\rho\omega q}} \right)^{1/2} S_C(q, \lambda) (\epsilon_0 \cdot q) \left( n_q + \frac{1}{2} \pm \frac{1}{2} \right)^{1/2}$</td>
</tr>
<tr>
<td>b) Piezoelectric [6.18]</td>
<td>$\frac{e h}{q \epsilon_0} v(r) S_C(q, \lambda)$</td>
<td>$\frac{e h}{\epsilon_0} \left( \frac{\hbar}{2V_{C\rho\omega q}} \right)^{1/2} S_C(q, \lambda) \left( n_q + \frac{1}{2} \pm \frac{1}{2} \right)^{1/2}$</td>
</tr>
<tr>
<td><strong>2. Optic Phonon:</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>a) Nonpolar [6.19]</td>
<td>$D_0 v(r) S_C(q, \lambda)$</td>
<td>$D_0 \left( \frac{\hbar}{2V_{C\rho\omega 0}} \right)^{1/2} S_C(q, \lambda) \left( n_0 + \frac{1}{2} \pm \frac{1}{2} \right)^{1/2}$</td>
</tr>
<tr>
<td>b) Polar [6.20]</td>
<td>$\frac{u(r) e \omega_k}{q} \left[ \frac{1}{V_{C\rho\omega 0}} \left( \frac{1}{K_{\omega 0}} - \frac{1}{K_S} \right) \right] S_C(q, \lambda)$</td>
<td>$\frac{e \omega_k}{q} \left( \frac{1}{K_{\omega 0}} - \frac{1}{K_S} \right)^{1/2} \left( \frac{\hbar \omega_k}{2V_{C\rho\omega 0}} \right)^{1/2} \left( n_0 + \frac{1}{2} \pm \frac{1}{2} \right)^{1/2}$</td>
</tr>
<tr>
<td><strong>3. Defect:</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>a) Ionised Impurity [6.21,22]</td>
<td>$\frac{Z e^2}{4 \pi \varepsilon r} \exp(-r/\lambda)$</td>
<td>$\frac{Z e^2}{\frac{c^e}{V_{C\rho\omega 0}} \left</td>
</tr>
<tr>
<td>b) Neutral Impurity [6.4a]</td>
<td>-</td>
<td>$\frac{2 \pi \hbar^2}{m^* V_c} \left( \frac{20 a_0}{4 \pi \kappa} \right)^{1/2}$</td>
</tr>
<tr>
<td>c) Dislocation:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(i) Charged type</td>
<td>$\frac{e f}{Z \pi a_D c} K_0(r/\lambda)$</td>
<td>-</td>
</tr>
<tr>
<td>(ii) Strain type [6.24]</td>
<td>$E_1 \frac{\lambda (1-2\nu)}{2 \pi (1-\nu)} \sin \theta \frac{r}{r}$</td>
<td>-</td>
</tr>
<tr>
<td>d) Alloy [6.25,Ref.6.2c]</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td><strong>4. Intervalltype Phonon</strong></td>
<td>$D_1 u(r) S_C(q, \lambda)$</td>
<td>$D_1 \left( \frac{\hbar}{2V_{C\rho\omega i}} \right)^{1/2} S_C(q, \lambda) \left( n_i + \frac{1}{2} \pm \frac{1}{2} \right)^{1/2}$</td>
</tr>
</tbody>
</table>

Ref. 6.1, p.107
### Meanings of symbols (Table 6.2):

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta V$</td>
<td>Potential energy of the electron due to the scattering potential</td>
</tr>
<tr>
<td>$E_1$</td>
<td>Acoustic phonon deformation potential constant</td>
</tr>
<tr>
<td>$u(r)$</td>
<td>Displacement due to a lattice wave</td>
</tr>
<tr>
<td>$q$</td>
<td>Wave vector of lattice wave</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Debye screening length</td>
</tr>
<tr>
<td>$V_C$</td>
<td>Volume of the crystal</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density of the material</td>
</tr>
<tr>
<td>$\omega_g$</td>
<td>Angular frequency of the lattice wave corresponding to the wave vector $q$</td>
</tr>
<tr>
<td>$\varepsilon \mathbf{e}_g$</td>
<td>Polarisation vector of the lattice wave</td>
</tr>
<tr>
<td>$n_g$</td>
<td>Occupation number of phonons with wave vector $q$</td>
</tr>
<tr>
<td>$h_{pz}$</td>
<td>Piezoelectric constant</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>Permittivity of the material</td>
</tr>
<tr>
<td>$D_0$</td>
<td>Nonpolar optic phonon deformation potential constant</td>
</tr>
<tr>
<td>$\omega_0$</td>
<td>Angular frequency of the nonpolar optic wave neglecting dispersion</td>
</tr>
<tr>
<td>$n_0$</td>
<td>Occupation number of optic phonons</td>
</tr>
<tr>
<td>$K_{oe}$</td>
<td>High-frequency dielectric constant</td>
</tr>
<tr>
<td>$K_S$</td>
<td>Static dielectric constant</td>
</tr>
<tr>
<td>$\omega_e$</td>
<td>Longitudinal frequency of vibration for polar optic wave</td>
</tr>
<tr>
<td>$\varepsilon_0$</td>
<td>Permittivity of free space</td>
</tr>
<tr>
<td>$n_e$</td>
<td>Occupation number of polar optic phonons</td>
</tr>
<tr>
<td>$Z$</td>
<td>Ionicity of an impurity atom</td>
</tr>
<tr>
<td>$k$</td>
<td>Wave vector of the electron in the original state</td>
</tr>
<tr>
<td>$k'$</td>
<td>Wave vector of the electron in the scattered state</td>
</tr>
<tr>
<td>$S_C(q,\lambda) = q^2(q^2 + \lambda^2)^{-1}$</td>
<td>Screening factor</td>
</tr>
<tr>
<td>$N_0$</td>
<td>Number of atoms in the crystal</td>
</tr>
<tr>
<td>$a_0$</td>
<td>Bohr radius</td>
</tr>
<tr>
<td>$r$</td>
<td>Distance from impurity centre, or distance from dislocation axis</td>
</tr>
<tr>
<td>$a_D$</td>
<td>Distance between dislocation centres</td>
</tr>
<tr>
<td>$f$</td>
<td>Probability of occupation of a dislocation centre by an electron</td>
</tr>
<tr>
<td>$K_0$</td>
<td>Modified Bessel function of zero order</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Poisson's ratio</td>
</tr>
<tr>
<td>$\lambda_S$</td>
<td>Unit crystallographic slip distance</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Angle measured from slip direction</td>
</tr>
<tr>
<td>$D_i$</td>
<td>Intervalley phonon deformation potential constant</td>
</tr>
<tr>
<td>$\omega_i$</td>
<td>Intervalley phonon angular frequency</td>
</tr>
<tr>
<td>$n_i$</td>
<td>Occupation number of intervalley phonons</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Fraction of atoms of type a</td>
</tr>
<tr>
<td>$(E_a - E_b)$</td>
<td>Difference between the band edge of atoms of type a and of type b constituting the alloy</td>
</tr>
<tr>
<td>±</td>
<td>The plus sign corresponds to emission and the minus sign to the absorption process.</td>
</tr>
</tbody>
</table>
Transport coefficients and thermoelectric figure of merit of $n$-Hg$_{1-x}$Cd$_x$Te

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\[ \text{Bi}_2\text{Te}_3 \]
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

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

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

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

• 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
Simulations describe complexity. Our theoretical work is to make it simple.
Thank you!

\[ Z = \frac{\sigma}{K^0_{el} + K_{ph}} = Z[\Sigma] \]

\[ \Sigma(\varepsilon) = \sum \tau_k v_k^2 \delta(\varepsilon_k - \varepsilon) \]

Transport distribution