Derivation of band model effective mass

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1 Derivation of single parabolic band

In single parabolic band, the energy dispersion relation is:

$$\varepsilon(k) = \hbar^2 k^2 / 2m^* \tag{1}$$

and velocity is given by:

$$v = \sqrt{2\varepsilon / m^*} \tag{2}$$

The energy dependent density of state $g(\varepsilon)$ is calculated, for a single spin state, according to

$$N_k(\varepsilon) = \frac{V}{8\pi^3}\frac{4}{3}\pi k^3$$

$$\frac{dN_k}{d\varepsilon} = \frac{dN_k}{dk}\frac{dk}{d\varepsilon} = \frac{V}{8\pi^3} 4\pi k^2 \frac{\sqrt{2m^*}}{\hbar}\frac{1}{2}\varepsilon^{-1/2} \tag{3}$$

$$\frac{dN_k}{d\varepsilon} = \frac{V}{2\pi^2}\frac{\sqrt{2}m^{*3/2}}{\hbar^3}\sqrt{\varepsilon} \tag{4}$$

$$g(\varepsilon) = \frac{V}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon} \tag{5}$$

The relationship between k points summation and energy integration is given by:

$$\lim_{V\to\infty}\sum_k F(\varepsilon(k)) = \int_{BZ}\frac{V dk}{8\pi^3}F(\varepsilon(k)) = V\int_{-\infty}^{\infty} d\varepsilon g(\varepsilon) F(\varepsilon) \tag{6}$$

The total number of carrier is therefore:

$$\begin{aligned} n &= \int_{-\infty}^{\infty} g(\varepsilon) f(\varepsilon) d\varepsilon \\ &= \frac{1}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\int_{-\infty}^{\infty}\frac{\sqrt{\varepsilon}}{e^{(\varepsilon-\mu)/k_bT}+1}d\varepsilon \end{aligned} \tag{7}$$

The Seebeck is given by:

$$S = \zeta/\sigma \tag{8}$$

with ζ and σ given by, taking account of spin factor 2:

$$\sigma = \frac{2e^2}{V}\int g(\varepsilon)\tau(\varepsilon)v^2(\varepsilon)\left(-\frac{\partial f}{\partial\varepsilon}\right)d\varepsilon \tag{9}$$

$$\zeta = \frac{2e}{VT}\int(\varepsilon-\mu)g(\varepsilon)\tau(\varepsilon)v^2(\varepsilon)\left(-\frac{\partial f}{\partial\varepsilon}\right)d\varepsilon \tag{10}$$

$$\tag{11}$$

Assuming the form of τ to be:

$$\tau = A\varepsilon^\eta \tag{12}$$

In the case of simplest acoustic phonon scattering, the coefficient is given by:

$$\tau = \frac{\hbar C_1 N_v}{\pi k_b T \Xi^2} g(\varepsilon)^{-1} f(\varepsilon) \tag{13}$$

We find the energy independent term in the integral can be moved out and get cancelled in the division. So we are left with:

$$S = \frac{1}{eT} \frac{\int \varepsilon^{3/2+\eta}(\varepsilon - \mu)\left(-\frac{\partial f}{\partial \varepsilon}\right) d\varepsilon}{\int \varepsilon^{3/2+\eta}\left(-\frac{\partial f}{\partial \varepsilon}\right) d\varepsilon} \tag{14}$$

2 Anisotropy of Effective mass

In the case of ellipsoid valleys, we can define anisotropic effective mass $m^*_\perp$ and $m^*_\parallel$. The DOS effective mass of such a valley can be averaged as:

$$m^*_{DOS} = ({m^*_\perp}^2 m^*_\parallel)^{1/3} \tag{15}$$

But for the mobility, the inertial effective mass can be given as

$$m^*_I = 3/(\frac{2}{m^*_\perp} + \frac{1}{m^*_\parallel}) \tag{16}$$

3 In the case of multivalley

For multivalley, we take the degeneracy to be N_v and the total DOS effective mass can be written using the single band value:

$$m^*_{total} = N_v^{2/3} m^* \tag{17}$$

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4 Some reference

Below is a table of seebeck coefficients of simple metal, for collaboration purpose:

Table 1: Parameter in simple metals

Elements	Z	$n(10^{22}cm^{-3})$	Seebeck $(\mu V/K)$
Na	1	2.65	-7
Ag	1	5.86	1.5
K	1	1.40	-14
Al	3	18.1	-1.5