**Notes on Effective Masses**

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Effective masses are obtained from a material's bandstructure. The effective mass tensor is a measure of the curvature in different directions near the bottom (or top) of a band. The effective mass tensor is given by

$$\frac{1}{m_{ij}^*} \equiv \frac{1}{\hbar^2} \frac{\partial^2 E\left(\vec{k}\right)}{\partial k_i \partial k_j} \tag{1}$$

In the simplest case of parabolic energy bands with spherical constant energy surfaces, the effective mass is a scalar, independent of energy and for the conduction band, we have

$$E\left(\vec{k}\right) = E_C + \frac{\hbar^2 k^2}{2m^*} . \tag{2}$$

For some semiconductors, the bands are parabolic, but the constant energy surfaces are ellipsoids. For example, in the conduction band of Si, the constant energy surfaces are six ellipsoids locates along the $k_x$, $k_y$, and $k_z$ axes (see Fig. 1) and (2) becomes

$$E\left(\vec{k}\right) = E_C + \frac{\hbar^2 \left(k_x - k_{x0}\right)^2}{2m_{xx}^*} + \frac{\hbar^2 \left(k_y - k_{y0}\right)^2}{2m_{yy}^*} + \frac{\hbar^2 \left(k_z - k_{z0}\right)^2}{2m_{zz}^*} . \tag{3}$$

For each of the six ellipsoids, two of the masses are the light, transverse effective mass, $m_t^*$ and the mass along the axis is the heavier, longitudinal effective mass, $m_\ell^*$.

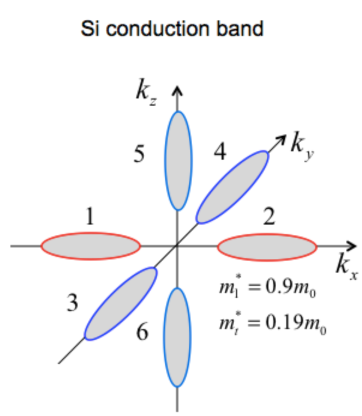


Fig. 1 Constant energy surfaces of silicon.

The **density-of-states** is an important quantity that can be derived from the bandstructure. For a parabolic band described by (2), the result in 3D is

$$D_{3D}\left(E\right)=\frac{\left(m^*\right)^{3/2}\sqrt{2\left(E-E_C\right)}}{\pi^2\hbar^3} \quad \left(E>E_C\right). \tag{4}$$

For ellipsoidal bands described by (3), the result is more complicated, but we can make it look simple by defining a "density-of-states effective mass" so that eqn. (4) becomes

$$D_{3D}\left(E\right)=\frac{\left(m^*_{DOS}\right)^{3/2}\sqrt{2\left(E-E_C\right)}}{\pi^2\hbar^3} \quad \left(E>E_C\right) \tag{5}$$

where for ellipsoidal bands

$$m^*_{DOS}=\left(g_V\right)^{2/3}\left(m^*_\ell m^{*2}_t\right)^{1/3}. \tag{6}$$

For the conduction band of Silicon, $g_V=6$ , so

$$m^*_{DOS}=\left(6\right)^{2/3}\left(m_t^2 m_\ell\right)^{1/3} \tag{7a}$$

For the conduction band of Ge, $g_V=4$, so

$$m^*_{DOS}=\left(4\right)^{2/3}\left(m_t^2 m_\ell\right)^{1/3} \tag{7b}$$

For other types of parabolic bandstructures, appropriate density-of-states effective masses could be defined to make the correct density-of-states look as simple as (5). For example, see R.F. Pierret (*Advanced Semiconductor Fundamentals*, 2nd Ed., 2003, p. 96) for the valence band density-of-state effective mass.

One can also define a **conductivity effective mass**. For a spherical, parabolic energy band, the conductivity is

$$\sigma=nq\frac{q\left\langle\left\langle\tau_m\right\rangle\right\rangle}{m^*}, \tag{8}$$

where $\left\langle\left\langle\tau_m\right\rangle\right\rangle$ is the average momentum relaxation time. For isotropic scattering, $\left\langle\left\langle\tau_m\right\rangle\right\rangle$, and $\left\langle\left\langle\tau_m\right\rangle\right\rangle$, so we use the density-of-state effective mass to determine $\left\langle\left\langle\tau_m\right\rangle\right\rangle$. The carrier density involves an integration of the density-of-states, for which we also use the density-of-state effective mass. But what should we use for the effective mass in the denominator of (8)?

Assume there is an electric field in the x-direction; we expect electrons to respond to the electric field with the effective mass in direction of the electric field. Near equilibrium, one sixth of the electrons are in each of the six ellipsoids. For ellipsoids one and two

$$\sigma_{1,2} = \frac{n}{6} q \frac{q\langle\langle \tau_m \rangle\rangle}{m_\ell^*} \tag{9a}$$

while for ellipsoids three through six,

$$\sigma_{3-6} = \frac{n}{6} q \frac{q\langle\langle \tau_m \rangle\rangle}{m_t^*} . \tag{9b}$$

The total conductivity is

$$\sigma = 2\sigma_1 + 4\sigma_3 \tag{9c}$$

or

$$\sigma = nq\left[\frac{1}{3m_\ell^*} + \frac{2}{3m_t^*}\right] q\langle\langle \tau_m \rangle\rangle . \tag{9d}$$

We can write (9d) in a simple form like (8) by defining a conductivity effective mass

$$\sigma = nq \frac{q\langle\langle \tau_m \rangle\rangle}{m_c^*} \tag{10a}$$

where

$$\frac{1}{m_c^*} = \frac{1}{3m_\ell^*} + \frac{2}{3m_t^*} . \tag{10b}$$

Now, what about the distribution of channels, $M_{3D}(E)$, which for spherical, parabolic bands is given by

$$M_{3D}\left(E\right)=\frac{m^*}{2\pi\hbar^2}\left(E-E_C\right) \qquad \left(E>E_C\right). \tag{11}$$

What effective mass do we use when the bands are ellipsoidal? The answer is $m^*_{DOM}$, the **distribution-of-modes** effective mass.

To compute, $m^*_{DOM}$, we begin with the general description of $M\left(E\right)$ for a general band:

$$M_{3D}\left(E\right)\equiv\frac{h}{2L}\sum_{\vec{k}}\left|\upsilon_x\right|\delta\left(E-E_k\right) \ . \tag{12}$$

(See: Jeong, Changwook; Kim, Raseong; Luisier, Mathieu; Datta, Supriyo; and Lundstrom, Mark S., "On Landauer versus Boltzmann and full band versus effective mass evaluation of thermoelectric transport coefficients*," J. Appl. Phys.*, **107**, 023707, 2010.)

When (12) is evaluated for ellipsoidal bands, we find fo each ellipsoid,

$$m^*_{DOM}=\sqrt{m^*_y m^*_z} \tag{13a}$$

where we have assumed transport in the x-direction. For Si, we add the channels in each ellipsoid to find

$$m^*_{DOM}=2m^*_t+4\sqrt{m^*_t m^*_\ell} \ . \tag{13b}$$

It is instructive to put numbers in. For Si, we find

$$m^*_{DOS}=\left(6\right)^{2/3}\left(m_t^2 m_\ell\right)^{1/3}=1.06m_0 \tag{14a}$$

$$m^*_c=\left[\frac{1}{3m^*_\ell}+\frac{2}{3m^*_t}\right]^{-1}=0.26m_0 \tag{14b}$$

$$m^*_{DOM}=2m^*_t+4\sqrt{m^*_t m^*_\ell}=2.04m_0\,, \tag{14c}$$

which shows that the numerical value of these masses can be quite different.

Now let's ask another question. We know that for a non-degenerate semiconductor, we can estimate the mean-free-path from the diffusion coefficient, which we obtain from the mobility with the Einstein relation.

$$D_n = \frac{k_B T}{q}\mu_n = \frac{\upsilon_T \lambda_0}{2} \qquad (15)$$

where the uni-directional thermal velocity is

$$\upsilon_T = \sqrt{\frac{2k_B T}{\pi m^*}} . \qquad (16)$$

What effective mass do we use? To answer this question, we should begin at the beginning.

$$\sigma = \frac{2q^2}{h}\lambda_0 \langle M_{3D} \rangle = \frac{2q^2}{h}\lambda_0 \frac{m^* k_B T}{2\pi\hbar^2}\mathcal{F}_0(\eta_F) \qquad (17a)$$

which is (A.34) in *Near-Equilibrium Transport* by Lundstrom and Jeong. The effective mass in (17) must be $m^*_{DOM}$

$$\sigma = \frac{2q^2}{h}\lambda_0 \frac{m^*_{DOM} k_B T}{2\pi\hbar^2}\mathcal{F}_0(\eta_F) = nq\mu_n . \qquad (17b)$$

We also know that

$$n = N_C \mathcal{F}_{1/2}(\eta_F) = 2\left[\frac{m^*_{DOS} k_B T}{2\pi\hbar^2}\right]^{3/2}\mathcal{F}_{1/2}(\eta_F), \qquad (18)$$

so from (18), we find

$$\begin{aligned}\mu_n &= \frac{1}{n}\frac{2q}{h}\lambda_0 \frac{m^*_{DOM} k_B T}{2\pi\hbar^2}\mathcal{F}_0(\eta_F) \\ &= \left[\frac{2\pi\hbar^2}{m^*_{DOS} k_B T}\right]^{3/2}\frac{2q}{h}\lambda_0 \frac{m^*_{DOM} k_B T}{2\pi\hbar^2}\frac{\mathcal{F}_0(\eta_F)}{\mathcal{F}_{1/2}(\eta_F)}\end{aligned} \qquad (19)$$

Assuming MB statistics and simplifying, we find

$$\mu_n = \frac{\lambda_0}{(k_B T/q)}\sqrt{\frac{2k_B T\left(m^*_{DOM}\right)^2}{\pi\left(m^*_{DOS}\right)^3}} \qquad (20)$$

Now let's re-write this as

$$\mu_n = \frac{1}{\left(k_B T/q\right)}\frac{\upsilon_T \lambda_0}{2} \tag{21}$$

$$\upsilon_T = \sqrt{\frac{2k_B T}{\pi \tilde{m}^*}} \tag{22}$$

$$\tilde{m}^* \equiv m^*_{DOS}\left(\frac{m^*_{DOS}}{2m^*_{DOM}}\right)^2 \tag{23}$$

Putting in numbers for Si, we find

$$\tilde{m}^* \equiv m^*_{DOS}\left(\frac{m^*_{DOS}}{2m^*_{DOM}}\right)^2 = 1.06m_0\left(\frac{1.06}{2\times 2.04}\right)^2 = 0.072m_0$$