Semiconductors

Jiinyuan Wu

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1 Two-band model

At $T = 0$ there is strictly no such thing as a semiconductor: there are just band metals or band insulators. When $T > 0$, however, the following two mechanisms happen. The first is that electrons jump from the valence band to the conduction band. The second is if there are energy levels near the highest point of the valence band (E_v) or the lowest point of the conduction band (E_c), thermally excited electrons will jump to them. (From another point of view we may say doped atoms eat electrons or give electrons, so some electrons are missing if we only look at Bloch states in the spectrum.) In both mechanisms, we have electrons in the conduction band and holes in the valence band, which are **carriers** of electric current.

In the discussion below, we assume that the band gap is *larger* compared with $k_B T$, and this means when $E \geq E_c$,

$$n_{\text{electron}} = e^{-(E-\mu)/k_B T}, \tag{1}$$

and when $E \leq E_v$

$$n_{\text{hole}} = e^{-(\mu-E)/k_B T}. \tag{2}$$

In semiconductor physics we usually use the following abbreviations: p (positive), v (valence), h (hole) mean holes in the valence band, and n (negative), c (conduction), e (electron) mean electrons in the conduction band. Thus the density of electrons and holes are given by

$$n = \int_{E_c}^{\infty} D_c(E)\, dE\, e^{-(E-\mu)/k_B T}, \tag{3}$$

and

$$p = \int_{-\infty}^{E_v} D_v(E)\, dE\, e^{-(\mu-E)/k_B T}. \tag{4}$$

Consider the simplest case, where we have a band gap (possibly indirect)

$$E_g = E_c - E_v \tag{5}$$

between the highest valence band the the lowest conduction band. The $\Delta E \gg k_B T$ condition also means there should be electrons or holes with very high energy, and therefore the hyperbolic approximation works, and the conduction band is completely characterized by its effective mass and the momentum with lowest energy, and so is the case for the valence band. We have

$$D(E) = \frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right) \sqrt{E - E_{\text{max/min}}} \tag{6}$$

for hyperbolic bands, and therefore we have (note that in the valence band, the effective mass of the electron is negative, so the effective mass of the hole is positive)

$$n = 2 \left(\frac{m_e^* k_B T}{2\pi \hbar^2} \right)^{3/2} e^{-(E_c-\mu)/k_B T}, \tag{7}$$

$$p = 2 \left(\frac{m_h^* k_B T}{2\pi \hbar^2} \right)^{3/2} e^{-(\mu-E_v)/k_B T}. \tag{8}$$

Note that if there is doping, electrons donated or attracted by the doped atoms are not included in the above equations.

2 The intrinsic semiconductor limit

In the **intrinsic semiconductor limit**, there is no doping, and only the first mechanism – thermal excitation in the conduction band and the valence band – works. This limit is useful when T is very high so the effect of doping can be ignored. (So in the opposite, when T is low enough, even materials that are very clean can't be described well by the intrinsic semiconductor limit, because in this case, if the material has any semiconductor property, then it has to come from doping.) Since there is no doping, we have $n = p$ because of charge neutrality, and we have $n = \sqrt{np}$, and solving this equation we find

$$\mu = E_{\mathrm{v}} + \frac{1}{2}E_{\mathrm{g}} + \frac{3}{4}k_{\mathrm{B}}T\ln\left(\frac{m_{\mathrm{h}}^*}{m_{\mathrm{e}}^*}\right). \tag{9}$$

Here we can see that when $T = 0$, actually $\mu \neq E_{\mathrm{F}} = E_{\mathrm{v}}$, but it doesn't matter: when T is zero and we are working with an insulator, putting μ anywhere between E_{c} and E_{v} is acceptable.

Here Drude model works, because the density of electrons and holes is small (TODO: why no strong correlation, like Wigner crystal?), and the quantum nature of electrons isn't apparent. So we have

$$\sigma_{\mathrm{e}} = n\mu_{\mathrm{e}}, \quad \sigma_{\mathrm{H}} = p\mu_{\mathrm{H}}, \tag{10}$$

and the mobilities are

$$\mu_{\mathrm{e}} = -\frac{\tau e}{m_{\mathrm{e}}^*}, \quad \mu_{\mathrm{h}} = \frac{\tau e}{m_{\mathrm{h}}^*}. \tag{11}$$

Usually the mobility of holes isn't as good as electrons because in general $m_{\mathrm{h}}^* > m_{\mathrm{e}}^*$, and for large effective mass we expect low mobility. This can be found by looking at (11), and (11) comes from the semiclassical EOM of electrons and holes, so we can also explain the fact from a quantum perspective. Suppose a hole is stuck in the lattice (it may slightly distort the lattice, so what is stuck is actually a hole and some phonons, or a polaron). It may still tunnel away because x is localized and p is uncertain, which may give it a kinetic energy large enough to escape, but if m_{h}^* is large enough, the kinetic energy fluctuation can be ignored, so the hole is safely localized.

When the anisotropy of the lattice is strong, we have

$$n = 2\left(\frac{k_{\mathrm{B}}T}{2\pi\hbar^2}\right)^{3/2}(\tilde{m}_{\mathrm{e}}^*\tilde{m}_{\mathrm{h}}^*)^{3/4}\mathrm{e}^{-E_{\mathrm{g}}/k_{\mathrm{B}}T}, \tag{12}$$

where $\tilde{m}$ means $(\det \boldsymbol{M})^{1/3} = \sqrt[3]{m_1^* m_2^* m_3^*}$, with the three m^*'s being the eigenvalues of the mass matrix, which is defined as

$$E = E \pm \frac{1}{2}\boldsymbol{k} \cdot \boldsymbol{M}^{-1} \cdot \boldsymbol{k}. \tag{13}$$

3 Doping

The overall effect of doping is to introduce

$$\Delta n = n - p \neq 0. \tag{14}$$

Still we have

$$n \cdot p = n_{\mathrm{i}}^2 = p_{\mathrm{i}}^2, \tag{15}$$

where n_{i} is the n given by (7) and (9). This gives

$$n = \frac{\Delta n + \sqrt{4n_{\mathrm{i}}^2 + \Delta n^2}}{2}, \quad p = \frac{-\Delta n + \sqrt{4n_{\mathrm{i}}^2 + \Delta n^2}}{2}. \tag{16}$$

And then the chemical potential can be found by (7).