DETERMINATION OF SPREADING PARAMETER IN MULTI-VALLEY SEMICONDUCTORS

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1. Introduction

In recent years the thermoelectric properties of materials (specifically solid solutions on the basis of lead [1, 2]), in which conduction band (in the case of n-type semiconductor) or valence band (in the case of p-type semiconductor) has a two-valley structure are often investigated. During the analyses of experimental findings of thermoelectric properties it is very important to have the value of parameter r -index of power in the dependence of the free path on the energy, which we'll briefly denominate spreading parameter.

2. Simulation model

In the case of one valley it is very easy to determine r. We consider a non-degenerated n-type semiconductor. For determination of the spreading parameter we use the Pisarenko formula for non-degenerated semiconductors

$$\alpha = -\frac{k}{e}\left[r + 2 + \ln\frac{2\left(2\pi m_0 kT_0\right)^{\frac{3}{2}}}{\hbar^3} + \frac{3}{2}\ln\left(\frac{m_e}{m_0}\right) + \frac{3}{2}\ln\left(\frac{T}{T_0}\right) - \ln n\right], \quad (1)$$

where m_0 is the rest mass of electron at $T_0 = 300\,\text{K}$. From (1), subject to the sign of thermoelectromotive, it is possible to determine the value of r:

$$r = \frac{\alpha}{k/e} - 2 - C - \frac{3}{2}\ln\left(\frac{m_e}{m_0}\right) - \frac{3}{2}\ln\left(\frac{T}{T_0}\right) + \ln n, \qquad C = \ln\frac{2\left(2\pi m_0 kT_0\right)^{\frac{3}{2}}}{\hbar^3}. \quad (2)$$

In the case of multi-valley semiconductor the problem is rather complicated, because the observed effective masses are non-constant and vary depending on temperature, in consequence of electron transitions from the light electrons valley to the valley of heavy electrons. It is shown in [3] that the conduction band of multi-valley semiconductor can be changed by equivalent one-valley band, parameters of which can be determined by parameters of one valley. In the same work it is proved that we can derive the following expression for the observed effective mass of equivalent band

$$(m^*)^{\frac{3}{2}} = \frac{M_j}{c_j}(m_j)^{\frac{3}{2}} \exp\left(\frac{\delta E_j}{kT}\right), \tag{3}$$

where δE_j is the energy distance between *j*-th valley and zero level, M_j, m_j, and c_j are, correspondingly, the number of equivalent minima, the effective mass of electrons, and the relative population of electrons of the *j*-th valley.

If the effective mass of electrons in any valley is known, then we can determine the observed effective mass in the equivalent band at each given temperature. If, specifically, we have the effective mass of electrons in the lowest valley ($\delta E = 0$), then in this case the observed effective mass in the equivalent band is determined by the expression, which follows from (3):

$$(m^*)^{\frac{3}{2}} = \frac{M}{c_1}(m_1)^{\frac{3}{2}}. \tag{4}$$

As in most cases the effective mass of electrons in the lowest valley is just known, so by substituting the value of observed effective mass of electrons from (4) instead of m_e in formula (2) we get

$$r = \frac{\alpha}{k/e} - 2 - C - \ln\left[\frac{M_1}{c_1(T)} \times \left(\frac{m_1}{m_0}\right)^{\frac{3}{2}}\right] - \ln\left(\frac{T}{T_0}\right)^{\frac{3}{2}} + \ln n, \tag{5}$$

where n is the total concentration of electrons, which we can determine based on the formula of the Hall coefficient for several types of conduction

$$R = \frac{\sum n_i \mu_i^2}{e\left(\sum n_i \mu_i\right)^2} = \frac{\sum c_i \mu_i^2}{en\left(\sum c_i \mu_i\right)^2}, \tag{6}$$

from which

$$n = \frac{\sum c_i \mu_i^2}{eR\left(\sum c_i \mu_i\right)^2}. \tag{7}$$

Formula (7) is written in the approximation that the Hall factor $r_{Hi} = 1$.

In more practical, two-valley case for n we have

$$n = \frac{c_1 \mu_1^2 + c_2 \mu_2^2}{eR(c_1 \mu_1 + c_2 \mu_2)^2} = \frac{c_1 b^2 + c_2}{eR(c_1 b_1 + c_2)^2}. \tag{8}$$

During determination of r in the case of multi-valley it is necessary to know relative populations of valleys too, which in case of two – valley are determined by the known formula [4]

$$\frac{n_2}{n_1} = \frac{c_2}{c_1} = M\left(\frac{m_2}{m_1}\right)^{\frac{3}{2}} e^{-\frac{\delta E}{kT}}. \tag{9}$$

If we take into account that in the case of two-valley $c_1 + c_2 = 1$, then we can determine relative populations of valleys c_1 and c_2.

In many cases necessity appears to determine the changing of spreading parameter by changing of temperature from T_1 to T_2 both in case of one valley and in the case of multi-valley semiconductor. For the case of one valley we use (2) for temperatures T_1 and T_2. Then

$$\Delta r = r(T_2) - r(T_1) = \frac{\alpha}{\frac{k}{e}} - \ln\left[\left(\frac{m(T_2)}{m(T_1)}\frac{T_2}{T_1}\right)^{\frac{3}{2}} \times \frac{n(T_1)}{n(T_2)}\right]. \tag{10}$$

But as in case of one valley the effective mass of electrons is constant, i.e. $m(T_1) = m(T_2)$, we find

$$\Delta r = \frac{\alpha}{k/e} - \ln\left[\left(\frac{T_2}{T_1}\right)^{\frac{3}{2}} \times \frac{n(T_1)}{n(T_2)}\right]. \tag{11}$$

Sometimes, for example, at change of phase, which takes place at defined temperature, from (10) we get

$$\Delta r = \frac{\alpha}{k/e} - \ln\left[\left(\frac{m(T_2)}{m(T_1)}\right)^{\frac{3}{2}} \times \frac{n(T_1)}{n(T_2)}\right]. \tag{12}$$

Note that component $\ln\left(\frac{m(T_2)}{m(T_1)}\right)^{\frac{3}{2}}$ is in (10). Since $m(T_2)$ and $m(T_1)$ are the observed effective masses of equivalent one valley band at temperatures T_1 and T_2, so by evaluating these values via the effective mass of the first valley, we have

$$[m(T_2)]^{\frac{3}{2}} = \frac{M_1}{c_1(T_2)}(m_1)^{\frac{3}{2}} \quad \text{and} \quad [m(T_1)]^{\frac{3}{2}} = \frac{M_1}{c_1(T_1)}(m_1)^{\frac{3}{2}}. \tag{13}$$

Consequently for $\left[\frac{m(T_2)}{m(T_1)}\right]^{\frac{3}{2}}$ we obtain

$$\left[\frac{m(T_2)}{m(T_1)}\right]^{\frac{3}{2}} = \frac{c_1(T_1)}{c_1(T_2)}. \tag{14}$$

Considering (14), from (10) we get

$$\Delta r = \frac{\alpha}{k/e} - \ln\left[\frac{c_1(T_1)}{c_1(T_2)} \times \left(\frac{T_2}{T_1}\right)^{3/2} \times \frac{n(T_1)}{n(T_2)}\right], \qquad (15)$$

which is more general formula, since in case of one valley, when $c_1(T_1) = c_1(T_2) = 1$, (15) is reduced to (11). Considering that

$$c_1(T_1) \times n(T_1) = n_1(T_1) \qquad \text{and} \qquad c_1(T_2) \times n(T_2) = n_1(T_2), \qquad (16)$$

and substituting these values into (15), finally we get

$$\Delta r = \frac{\alpha}{k/e} - \ln\left[\frac{n_1(T_1)}{n_1(T_2)} \times \left(\frac{T_2}{T_1}\right)^{\frac{3}{2}}\right]. \qquad (17)$$

Here $n_1(T_1)$ and $n_1(T_2)$ are concentrations of electrons in the first valley at appropriate temperatures. All said is true for the p -type semiconductors too.

3. Conclusion

Thus, by measurements of temperature dependences of the thermoelectromotive and Hall coefficients, it is possible to determine:

a) temperature dependence of $r(T)$ in case of one valley, if the value of effective mass of the electrons is known,

b) temperature dependence of $r(T)$ in case of multi-valley semiconductor, specifically in case of two valleys, if the band structure of semiconductor and values of effective masses in valleys are known,

c) change of parameters differences in case of one valley at change of temperature from T_1 to T_2,

d) change of spreading parameters differences in case of multi-valley semiconductor, if the band structure of semiconductor and values of effective masses in valleys at change of temperature from T_1 to T_2 are known.

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