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Calculation of the mobility of pure non-polar semiconductors by a new method

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Abstract. The mobility formula recently derived by us has been applied to pure non-polar semiconductors and detailed mobility calculations have been carried out for Ge. The optic deformation potential and acoustic phonon scatterings together give a value of $\mu = 0.43 \times 10^4$ $cm^2\ V^{-1}\ s^{-1}$ at room temperature which agrees reasonably with experiment.

1. Introduction

For a pure non-polar semiconductor such as Ge, the presence of phonons results in carrier scattering which essentially determines the mobility. When we examine the variation of electron mobility μ as a function of temperature T we have a continuously falling curve between 10 K and 500 K. By dividing the T axis into a few parts, this experimental curve may be fitted to a curve of the form $\sim T^{-n}$ in each region. In the region $T = 10$–77 K the power n is approximately equal to 1.50 thus confirming the predominant effect of acoustic phonons (Nag 1972) predicted by classical and quantum mechanical theories. From around 77 K to above room temperature the power n of the fitted curve changes (Morin 1954, Seeger 1989) to a value of approximately 1.67, showing that in this region acoustical phonons alone are not the only effect. To explain the observed mobility, therefore, the contribution of optical deformation potential scattering should be considered. It is known that when there is more than one scattering effect at the same time, for example μ_1 and μ_2, their combined mobility is given by $1/\mu = 1/\mu_1 + 1/\mu_2$ so the smaller of μ_1 and μ_2 determines the dominant effect (Van Der Ziel). This means that we need an accurate expression of mobility for each of the above scattering cases in order to interpret the results. In this context there are available the classical theories using the momentum relaxation time concept and there is also the more rigorous Kubo formula (Kubo 1957) of conductivity. In practice, calculations cannot be done with the direct use of the Kubo formula because it is difficult to obtain from it a term in g^{-2} where g is the coupling constant. This is important because for weak scattering this would give the leading term. In a previous study (Ünal *et al* 1992) the problem of putting the Kubo formula into a suitable form was discussed and the mobility formula of Milinski (1991) was corrected.

The new mobility formula

$$\mu = \frac{1}{2} eN \frac{\alpha_r''}{(\alpha_r')^2} \frac{1}{3} \tag{1.1}$$

has essentially kept the form given by Milinski. Here e is the electronic charge, N is the total number of carriers in the conduction band and α_r', α_r'' are respectively the first

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and second derivatives, with respect to frequency ω, of force–force correlation function $\alpha = \alpha_r(\omega) + i\alpha_i(\omega)$. This formula is based entirely on quantum mechanical concepts; besides it is valid also for the stronger-scattering case provided that α_r', α_r'' are evaluated correctly. In the applications (Ünal *et al* 1992) of equation (1.1) to acoustic and polar optic phonons, it was shown to have given good agreement with the known results whereas before its correction Milinski's application (Milinski and Nettel 1988) showed a singular character. In order to show the usefulness of the new formula, applications were made also to pseudopotential scattering in liquid metals (Ünal and Alkan 1993) and to the completely disordered lattice (Aktaş *et al* 1993) all giving satisfactory results. Transport properties of carriers in Ge crystals were subject to intensive work in the 1950s (Morin 1954). At that time, it was believed generally that the classical Boltzmann transport equation treatment of the problem gave (Morin and Maita 1954) sufficiently good results to compare with experiment. Later it was shown that (Paige 1964) as T increases, scattering from optic phonons becomes more effective and the effects of all the other sources which may cause temperature variation of μ, e.g effective mass m, deformation potential D, elastic constant and inter-valley phonons, are insignificant. Paige used adjustable constants in order to make the calculated μ values as close as possible to the measured ones. Therefore one cannot say that his calculations are absolutely theoretical. This point will be discussed more fully in later sections. Here in this work we wanted to do a pure theoretical calculation; our results obtained from equation (1.1) agreed satisfactorily with the experiment. Section 2 concerns the model system and writing the derivatives of the real part of the correlation function α_r', α_r''. In section 3 we have carried out the calculation of mobility by evaluating α_r' and α_r'' and by using equation (1.1). The appendix concerns the evaluation of I_1 and I_2 integrals which appear in the definition of correlation functions. In section 4 the calculations of section 3 are repeated by considering the tensor character of effective mass. Finally in section 5 the results are discussed.

2. Optical deformation potential model

In pure semiconductors we can describe the coupling between the carriers and the rest of the many-particle system by the optical deformation potential U:

$$U = \sum_{k,q} U_q a_{k+q}^{\dagger} a_k (b_q + b_{-q}^{\dagger}) \tag{2.1}$$

where $a_{k+q}^{\dagger}$ and a_k are creation and annihilation operators of carriers with wave vectors $k+q$ and k respectively. $b_{-q}^{\dagger}$ and b_q are also creation and annihilation operators for the longitudinal phonon with frequency ω_q. U_q is the interaction matrix element as follows (Seeger 1989):

$$U_q = \frac{D\hbar}{(2\rho V)^{1/2}} \frac{1}{(\hbar\omega_0)^{1/2}} \tag{2.2}$$

where D is the optical deformation constant of the band edge (in units of eV cm^{-1}), $\hbar\omega_0$ is the optical phonon energy, ρ is the density of the solid and V is the volume per atom. The effect of the spin factor will be taken into account during calculations. The energy spectrum of the considered system is first assumed to be simply parabolic

$$E(k) = \frac{\hbar^2 k^2}{2m} \tag{2.3}$$

with effective mass m; later the effect of different effective masses in the constant energy surface are considered. In the new formula (1.1), $\alpha_\tau'(0)$ and $\alpha_\tau''(0)$ are given, in the $\omega \to 0$ limit, by

$$\alpha_\tau'(0) = \frac{4\pi}{3}\sum_{k,q}\hbar^2 q^2 |U_q|^2 n_k(1-n_{k+q})\{(N_q+1)\delta''(\Delta E) + N_q\delta''(\Delta E')\} \tag{2.4}$$

$$\alpha_\tau''(0) = -\frac{4\pi}{3}\hbar\sum_{k,q}\hbar^2 q^2 |U_q|^2 n_k(1-n_{k+q})\{(N_q+1)\delta'''(\Delta E) + N_q\delta'''(\Delta E')\} \tag{2.5}$$

where $\Delta E = E_{k+q} - E_k + \hbar\omega_0$, $\Delta E' = E_{k+q} - E_k - \hbar\omega_0$. These expressions have been taken from equations (2.19) and (2.20) of our first study (Ünal *et al* 1992). Here n_k, N_q are electron and phonon occupation numbers respectively, $\delta'(\Delta E)$ is the derivative of the usual Dirac delta function whith respect to ΔE and the other deltas have similar meanings. By changing indices in the first terms in curly brackets in equations (2.4) and (2.5) and using $\beta = 1/kT$ with T temperature and k the Boltzmann constant we have

$$n_{k+q}(N_q+1) = n_k N_q \, \mathrm{e}^{-\beta\,\Delta E'}. \tag{2.6}$$

By using the general relation

$$g(x)\delta^{(k)}(x) = \sum_{j=0}^{k}(-1)^j\binom{k}{m}g^{(j)}(0)\delta^{(k-j)}(x) \tag{2.7}$$

together with $1 - n_k \simeq 1$, we have

$$\alpha_\tau' = \frac{D^2\hbar^2}{2\rho V}\frac{1}{\hbar\omega_0}\frac{4\pi}{3}\sum_{k,q}\hbar^2 q^2 n_k N_q[2\delta''(\Delta E') + 2\beta\delta'(\Delta E') + \beta^2\delta(\Delta E')] \tag{2.8}$$

$$\alpha_\tau'' = \frac{D^2\hbar^2}{2\rho V\hbar\omega_0}\frac{4\pi}{3}\hbar\beta\sum_{k,q}\hbar^2 q^2 n_k N_q[3\delta''(\Delta E') + 3\beta\delta'(\Delta E') + \beta^2\delta(\Delta E')]. \tag{2.9}$$

These expressions will be evaluated in the next section by turning the sums over k, q into integrations in the usual way (Ünal *et al* 1992) and then they will be used in the mobility equation (1.1).

3. Calculation of mobility

In order to calculate mobility, first we have to evaluate α_τ' and α_τ'' and since the process is lengthy but straightforward it will be described briefly. In equation (2.8) we define two terms such that $\alpha_\tau'(1)$ contains $\delta''(\Delta E')$ and $\alpha_\tau'(23)$ contains $\delta'(\Delta E')$, $\delta(\Delta E')$ together, which are evaluated separately. The integration is carried out in the order $\mathrm{d}q \longmapsto \mathrm{d}\nu \longmapsto \mathrm{d}k$ because with this order, during the transformation of the delta function into simpler forms the Jacobians never become zero; otherwise nothing fixes the order of integration

Table 1. The values of I_1, I_2 obtained by numerical calculation.

$a = T_D/T$	I_1	I_2
0.1	277.62	379.34
0.2	102.03	133.38
0.3	56.17	70.37
0.4	36.85	44.25
0.5	26.75	30.79
0.6	20.76	22.92
0.7	16.90	17.92
0.8	14.28	14.57
0.9	12.41	12.21
1.0	11.04	10.50
1.1	10.01	9.23
1.2	9.22	8.26
1.3	8.60	7.52
1.4	8.11	6.94
1.5	7.72	6.48
2.0	6.64	5.27
2.5	6.28	4.91
3.0	6.20	4.87
3.3	6.22	4.93

and the result will be the same irrespective of order. Related integrals are evaluated in the appendix; using the notation $\alpha_r' = \alpha_r'(1) + \alpha_r'(23)$, α_r'' they are given by

$$\alpha_r' = \frac{D^2 m^4 N_q V}{3\rho\pi^3\hbar^4} I_1 \tag{3.1}$$

$$\alpha_r'' = \frac{D^2 m^4 N_q V}{3\rho\pi^3\hbar^4} \hbar\beta I_2. \tag{3.1a}$$

The integrals I_1, I_2 depend on T through the parameter $a = T_D/T$ and values of I_1, I_2 obtained by numerical calculation are shown in table 1. Through the inspection of this table it is seen that change of I_1, I_2 integrals with T is not very fast, so the temperature dependence of μ is mainly due to the factor N_q involved in equation (1.1).

Using this table, shortly it will be shown that the μ versus T curve is smooth and asymptotic to the vertical axis at $T = 0$ (see equation (4.2) and figure 1). In the calculations the Debye temperature for Ge is taken (Sze 1981) to be $T_D = 429$ K, the effective mass $m = 0.2m_0$ and the density is $\rho = 5.3267$ g cm^{-3}. The deformation potential constant, as calculated from $D = d_{lo}(\text{con})/2a$, has the value $D = -2.45 \times 10^8$ eV cm^{-1} when we take (Potz and Vogl 1981) $d_{lo}(\text{con}) = -27.7$ eV and lattice constant $a = 5.646$ Å. The mobility equation is obtained by using α_r', α_r'' given by equations (3.1), (3.1a) in equation (1.1); then we have

$$\mu = \frac{4(2\pi)^{1/2} e\hbar^2 \rho (kT_D)^{1/2}}{3m^{5/2} D^2} f(T/T_D) \tag{3.2}$$

where the function $f(T/T_D)$ is given by

$$f(T/T_D) = \left(\frac{T}{T_D}\right)^{1/2} \frac{3\pi I_2}{16 N_q I_1^2} \tag{3.2a}$$

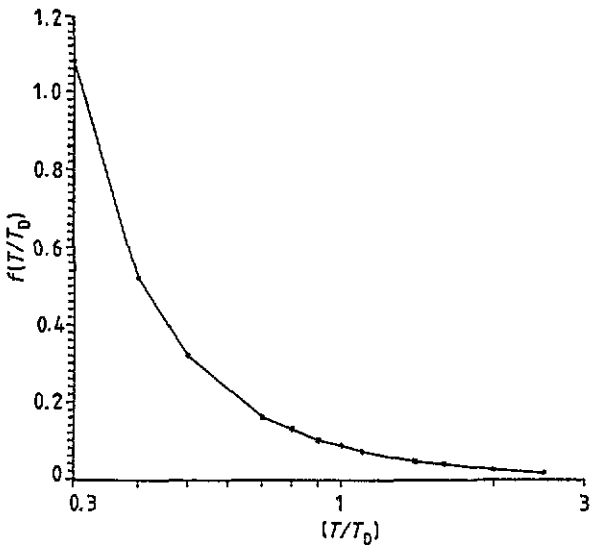

Figure 1. Variation of the function $f(T/T_D)$ with T/T_D.

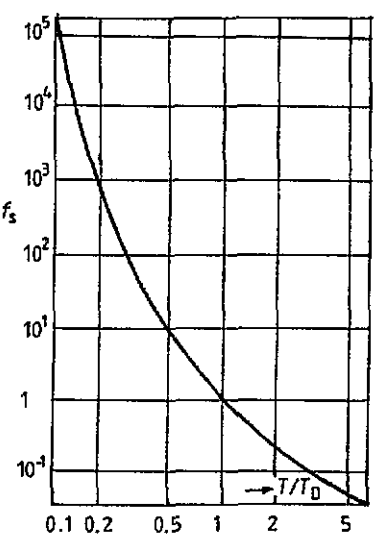

Figure 2. Variation of the function $f_s(T/T_D)$ with T/T_D.

with $N_q = (e^a - 1)^{-1}$ and T_D/T. This function is shown in figure 1. The T dependence of $f(T/T_D)$ contains factors like the root and exponential, therefore it is not a simple function. Its curve (figure 1) shows an imperceptible structure around 400–600 K.

Morin and Maita (1954) assumed lattice scattering by optical modes to be $\mu_{op} = BT^{-0.5}(e^{T_D/T} - 1)$ with B an adjustable constant. They combined this with the acoustical phonon scattering mobility μ_{ac} and equated the result to the measured mobility between 100 and 300 K. By this means they obtained the value of constant B and the result was an excellent agreement with experiment. For the reasons below this assumption cannot be accepted. In actual fact one cannot take B to be constant, because mobility formulas

derived from pure theory show that B contains T-dependent integrals (Nag 1972). The mobility expression obtained from the Boltzmann equation in the momentum relaxation time approximation is

$$\mu_s = \frac{4(2\pi)^2 e\hbar^2 \rho (kT)^2}{3m^5 D^2} f_s(T/T_D) \tag{3.3}$$

where the function $f_s(T/T_D)$ is given by (Seeger 1989)

$$f_s(T/T_D) = \left(\frac{T_D}{T}\right)^{1/2} (e^{T_D/T} - 1) \int_0^\infty \frac{x^{3/2} e^{-x} dx}{(x+a) + e^a \operatorname{Re}\{(x-a)^2\}}. \tag{3.3a}$$

When we compare this with the expression of Morin and Maita (1954) we can see that their B cannot be taken to be constant. We checked that B values change about 20 times between 100 K and 400 K. Since Seeger (1989) has taken this variation into account, we thought that comparison of our μ values with his would be appropriate. We include his f_s curve in figure 2 for comparison.

4. Calculation of mobility using effective mass tensor

In the previous section a single effective mass was assumed for each of the conduction band minima which is usually done when preliminary results are required. It is known that the Ge crystal has eight minima in the conduction band; constant energy surfaces in k space around these minima have ellipsoidal shapes rather than being spherical. To be more realistic one has to consider different values for longitudinal and transverse effective masses m_L, m_T respectively. Taking this fact into account we cannot use the spherical coordinates of section 3; here we have to use cylindrical coordinates whose k_z axis is in the direction of the applied field. We take one constant energy ellipsoid in k space and find longitudinal μ_L by considering the external field to be applied longitudinally; afterwards the external field is turned to the transverse direction and the corresponding μ_T value is calculated in turn. These mobilities are averaged by adding them together and dividing by two. In fact the averaging procedure should not be as simple as this because, in Ge, the longitudinal axes of equivalent ellipsoids in k space are not perpendicular to each other; if they were so, as in the case of Si, then our averaging would be exact. Since our aim is to estimate the order of mobility and to provide an alternative basis for mobility calculations we preferred the simple averaging process. Evaluation of α_t', α_t'' is carried out by using similar mathematical techniques as used in section 3. For longitudinal mobility we have

$$\mu_L = \frac{m^{3/2} e\hbar^2 \rho (kT)^{1/2}}{m_L^3 m_T D^2} \frac{(2\pi)^{1/2}}{6N_q} \frac{I_2}{I_1^2} \tag{4.1}$$

$$I_1 = a\, e^{a/2} K_2(a) - 2\, e^{a/2} K_1(a) + a\, e^{a/2} K_0 \tag{4.1a}$$

$$I_2 = \frac{a}{2} e^{a/2} K_2(a) - 3a\, e^{a/2} K_1(a) + \frac{3a}{2} e^{a/2} K_0 \tag{4.1b}$$

where K_0, K_1, K_2 are Bessel functions. For transverse mobility we have

$$\mu_T = \frac{(m)^{3/2} e\hbar^2 \rho (kT)^{1/2}}{(m_T m_L)^{1/2} m_T^3 D^2} \frac{(\pi)^{3/2}}{3(2)^{1/2} N_q} \frac{I_2}{I_1^2} \tag{4.2}$$

$$I_1 = a\, e^{a/2} K_2(a) - 2\, e^{a/2} K_1 + 4a\, e^{a/2} K_0(a) \tag{4.2a}$$

$$I_2 = \frac{a}{2} e^{a/2} K_2(a) - 3\, e^{a/2} K_1(a) + 6a\, e^{a/2} K_0(a). \tag{4.2b}$$

Taking $m_L = 1.64m_0$, $m_T = 0.082m_0$ we calculated μ_L, μ_T values at room temperature to be $\mu_L = 317.2$ cm^2 V^{-1} s^{-1} and $\mu_T = 19.35 \times 10^4$ cm^2 V^{-1} s^{-1}. The average mobility $\mu = (\mu_L + \mu_T)/2$ is $\mu = 9.7 \times 10^4$ cm^2 V^{-1} s^{-1} which has the expected order of magnitude. As will be discussed in section 5, this value of mobility is not very different from the value $\mu = 1.8 \times 10^4$ cm^2 V^{-1} s^{-1} obtained for the homogeneous mass case studied in the previous section. For this reason we have not drawn any curves in this section.

5. Conclusions

We have carried out mobility calculations for both the homogeneous mass and inhomogeneous mass cases. Let us first look at section 3 and compare its results with experiment and also with other results in the literature. If we look at equations (3.3) and (3.2), we can see that apart from the function $f(T/T_D)$, the prefactors are the same. So the difference between the two mobility equations comes from the function $f(T/T_D)$. At $T = 300$ K, by using equation (3.2) we obtained the mobility μ_{op} to be 1.8×10^4 cm^2 V^{-1} s^{-1}. This value is reasonably close to the experimental value 0.39×10^4 cm^2 V^{-1} s^{-1} given by Price (1953). If we combine optic and acoustic phonon scattering mobilities we obtain still a better result $\mu = 0.43 \times 10^4$ cm^2 V^{-1} s^{-1}. The acoustic phonon scattering mobility μ_{ac} obtained from equation (1.1) has been shown to be $\mu_{ac} = (9\pi/32)\mu_0$ where μ_0 is the classical result (Ünal *et al* 1992) and we have used this formula in calculating the acoustic phonon contribution, while, at the same temperature, the mobility formula (3.3) introduced in Seeger's book (1989) gives a value of order 10^6 cm^2 V^{-1} s^{-1}. This difference between two mobility values obtained from two different formulas is very important. As mentioned earlier in the introduction, in intrinsic semiconductors like Ge, we expect that optical phonons should be dominant in determining the mobility. If we consider another scattering, in order to obtain the mobility of the system we have to sum the reciprocals of the mobilities, as $1/\mu = 1/\mu_1 + 1/\mu_2$. So the smaller mobility determines the mobility of the system. In our work, we considered only the contribution of the optical phonons to the mobility. Our result is about 10^2 times smaller than the value obtained from Seeger's formula (3.3), and therefore is closer to experiment. From this closeness we can say that optical phonons determine the mobility at room temperature and above. This conclusion entirely obeys our expectations. On the other hand Seeger's results are very far from satisfying such an expectation. The behaviour of theoretical mobility is determined by our f versus $1/a$ curve (figure 1) which extends far beyond the temperature interval covered by the experimental curve. Therefore we did not draw the theoretical and experimental curves together; we only compared the two at one point corresponding to room T. Now we can explain why our result is 4.6 times greater than the experimental value. In our calculation,

we assumed a parabolic band, neglecting the dependence on T of effective masses and the band gap. It is known that both of these quantities do depend on T significantly (Sze 1981). The largest effect comes from the optical deformation constant D which appears in the prefactor of the mobility formula. Several different values are given for it (Renucci *et al* 1974, Richter *et al* 1978), and each of them differs from the others by a factor of three or five. This shows that various theoretical methods used for the estimation of D disagree to a great extent (Potz and Vogl 1981). To obtain a mobility comparable with experiment, above all, it is necessary that we should know the true value of D as far as possible. We believe that uncertainties in the value of D prevent us from getting any closer to experiment. The results of section 4 are not far from that of section 3; taking a single homogeneous mass gives $\mu = 1.8 \times 10^4$ cm^2 V^{-1} s^{-1} and taking two different masses in the inhomogeneous case gives $\mu = 9.7 \times 10^4$ cm^2 V^{-1} s^{-1}. The calculations of section 3 alone are sufficient for comparison purposes with the experiment as neither a new nor a better approximation appears from section 4. However the outcomes of section 4 do show that changes in the effective mass would influence the value of μ to a great extent. Owing to the difficulties encountered when we try to average mobilities for different directions, as mentioned in section 4, it is better to employ a single homogeneous mass for Ge.

Appendix

In this appendix we show how to evaluate the three terms of equation (2.8) by writing α_r' in the form $\alpha_r' = \alpha_r'(1) + \alpha_r'(23)$ where $\alpha_r'(1)$ is the contribution of the first term which reads

$$\alpha_r'(1) = \frac{D^2\hbar^2}{\rho V \hbar\omega_0}\frac{2\pi}{3}N_q\sum_{k,q}\hbar^2q^2 2n_k\delta''(\Delta E') \tag{A.1}$$

where $\delta''(\Delta E')$ is given by, with $\nu = \cos\theta$

$$\delta''(\Delta E') = \delta''\left(-\frac{\hbar^2kq}{m}\nu + \frac{\hbar^2q^2}{2m} - c\hbar\omega_0\right). \tag{A.2}$$

If we consider the following expression (Ünal *et al* 1992):

$$\delta''\{f(x)\} = \sum_{x_0}\frac{1}{|f'(x_0)|^3}\left\{\delta''(x-x_0) + 3\frac{f''(x_0)}{f'(x_0)}\delta'(x-x_0) + \frac{7(f''(x_0))^2 - f'''(x_0)f'(x_0)}{(f'(x_0))^2}\delta(x-x_0)\right\} \tag{A.3}$$

we obtain

$$\alpha_r'(1) = (.)\frac{V}{8\pi^3}\frac{2\pi}{\hbar}\sum_k 2n_k\int_{-1}^{+1}\frac{m^3\,d\nu}{(\hbar^2k^2\nu^2 + A^2)^{3/2}}\int_0^\infty\left[\delta''(\hbar q - \hbar q_2) + \frac{3\delta'(\hbar q - \hbar q_2)}{(\hbar^2k^2\nu^2 + A^2)^{1/2}} + \frac{7\delta(\hbar q - \hbar q_2)}{\hbar^2k^2\nu^2 + A^2}\right]\hbar^4q^4\,d(\hbar q) \tag{A.4}$$

where $A^2 = 2m\hbar\omega_0$ has been defined and the notation (.) shows all the prefactors before the summation sign in (A.1). From two roots $\hbar q_1 = \hbar k\nu - (\hbar^2k^2\nu^2 + 2m\hbar\omega_0)^{1/2}$,

$\hbar q_2 = \hbar k v + (\hbar^2 k^2 v^2 + 2m\hbar\omega_0)^{1/2}$ the negative root $\hbar q_1$ has been dropped out as being unphysical. The effect of the derivative delta function on $\hbar^4 q^4$ may be considered by using equation (2.7) and equation (A.4) becomes

$$\alpha_r'(1) = \frac{D^2 m^3}{3\rho\hbar\omega_0}\frac{N_q}{2\pi\hbar}\frac{1}{3}\sum_k \frac{n_k}{\hbar k}\int_{-1}^{+1}\frac{\hbar k\,\mathrm{d}v}{(\hbar^2k^2v^2+A^2)^{3/2}}\left[12\hbar^2q_2^2 - \frac{12\hbar^3q_2^3}{(\hbar^2k^2v^2+A^2)^{1/2}} + \frac{7\hbar^4q^4}{(\hbar^2k^2v^2+A^2)}\right] \tag{A.5}$$

$$\alpha_r'(1) = \frac{D^2m^3}{3\rho\hbar\omega_0}\frac{N_qV}{2\pi^3\hbar^4}\int_0^\infty n_k\hbar^2k^2\,\mathrm{d}(\hbar k)\left\{\frac{12}{\hbar k}\int_{-1}^{+1}\frac{\hbar k\,\mathrm{d}v[\hbar kv+(\hbar^2k^2v^2+A^2)^{1/2}]^2}{(\hbar^2k^2v^2+A^2)^{3/2}} - \frac{12}{\hbar k}\int_{-1}^{+1}\frac{\hbar k\,\mathrm{d}v[\hbar kv+(\hbar^2k^2v^2+A^2)^{1/2}]^3}{(\hbar^2k^2v^2+A^2)^{3/2}(\hbar^2k^2v^2+A^2)^{1/2}} + \frac{7}{\hbar k}\int_{-1}^{+1}\frac{\hbar k\,\mathrm{d}v[\hbar kv+(\hbar^2k^2v^2+a^2)^{1/2}]^4}{(\hbar^2k^2v^2+A^2)^{3/2}(\hbar^2k^2v^2+A^2)}\right\}. \tag{A.6}$$

Integration over v is carried out easily, and to do the $\mathrm{d}(\hbar k)$ integral we replace it as usual by the energy integral $\mathrm{d}E$,

$$\alpha_r'(1) = \frac{D^2m^4}{3\rho\hbar\omega_0}\frac{N_qV}{\pi^3\hbar^4}\int_0^\infty \mathrm{e}^{-E/kT}(E)^{1/2}\,\mathrm{d}E\left\{-\frac{25}{(E+\hbar\omega_0)^{1/2}} + \frac{16}{(E)^{1/2}}\ln\frac{(E+\hbar\omega_0)^{1/2}+(E)^{1/2}}{(E+\hbar\omega_0)^{1/2}-(E)^{1/2}} - \frac{7}{3}\frac{E}{(E+\hbar\omega_0)(E+\hbar\omega_0)^{1/2}}\right\} \tag{A.7}$$

$$\alpha_r'(1) = \frac{D^2m^4N_qV}{3\rho\pi^3\hbar^4}I(1) \tag{A.8}$$

where $I(1)$ is the dimensionless integral

$$I(1) = \frac{1}{a}\int_0^\infty \mathrm{e}^{-x}\mathrm{d}x\left\{-25x^{1/2}(x+a)^{-1/2} - \frac{7}{3}x^{3/2}(x+a)^{-3/2} + 16\ln\frac{(x+a)^{1/2}+x^{1/2}}{(x+a)^{1/2}-x^{1/2}}\right\}. \tag{A.8a}$$

a is given by $a = T_D/T$ and T_D is the lattice temperature defined as $T_D = \hbar\omega_0/k$. The contribution of second plus third terms of equation (2.8) is calculated in a similar way:

$$\alpha_r'(23) = \frac{D^2\hbar^2}{2\rho V}\frac{1}{\hbar\omega_0}\frac{4\pi}{3}\sum_{k,q}\hbar^2q^2n_kq^2N_q[2\beta\delta'(\Delta E') + \beta^2\delta(\Delta E')] \tag{A.9}$$

$$\alpha_r'(23) = \frac{D^2m^4N_qV}{3\rho\pi^3\hbar^4}I(23) \tag{A.10}$$

where

$$I(23) = \frac{1}{a}\int_0^\infty e^{-x}dx\left\{\left(\frac{3a}{4}-6\right)x^{1/2}(x+a)^{1/2} + 2x^{3/2}(x+a)^{1/2} - 2x^{3/2}(x+a)^{-1/2} + \frac{3}{2}x^{1/2}(x+a)^{3/2} + \frac{3a^2}{8}\ln\frac{(x+a)^{1/2}+x^{1/2}}{(x+a)^{1/2}-x^{1/2}}\right\}. \tag{A.10a}$$

We may evaluate α_r'' in equation (2.9) similarly, and the results are

$$\alpha_r' = \frac{D^2m^4N_qV}{3\rho\pi^3\hbar^4}I_1 \tag{A.11}$$

$$\alpha_r'' = \frac{D^2m^4N_qV}{3\rho\pi^3\hbar^4}\hbar\beta I_2 \tag{A.12}$$

$$I_1 = \frac{1}{a}\int_0^\infty e^{-x}dx\left\{-25x^{1/2}(x+a)^{-1/2} - \frac{7}{3}x^{3/2}(x+a)^{-3/2} + \left(\frac{3a}{4}-6\right)x^{1/2}(x+a)^{1/2} + 2x^{3/2}(x+a)^{1/2} - 2x^{3/2}(x+a)^{-1/2} + \frac{3}{2}x^{1/2}(x+a)^{3/2} + \left(\frac{3a^2}{8}+16\right)\ln\frac{(x+a)^{1/2}+x^{1/2}}{(x+a)^{1/2}-x^{1/2}}\right\} \tag{A.11a}$$

$$I_2 = \frac{1}{a}\int_0^\infty e^{-x}dx\left\{-\frac{75}{2}x^{1/2}(x+a)^{-1/2} - \frac{7}{2}x^{3/2}(x+a)^{-3/2} + \left(\frac{3a}{4}-9\right)x^{1/2}(x+a)^{1/2} - 3x^{3/2}(x+a)^{-1/2} + 2x^{3/2}(x+a)^{1/2} + \frac{3}{2}x^{1/2}(x+a)^{3/2} + \left(\frac{3a^2}{8}+24\right)\ln\frac{(x+a)^{1/2}+x^{1/2}}{(x+a)^{1/2}-x^{1/2}}\right\}. \tag{A.12a}$$

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