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Kinetics of the Intraband Absorption and Magnetoabsorption Coefficients in Mixed Semiconductors with Composition Fluctuations

By

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The influence of short-range ordering in a mixed semiconductor on the intraband absorption and magnetoabsorption coefficients is determined. The coefficients are shown to be temperature-dependent. Their time-evolution after changing the temperature is calculated. An experiment, permitting measurements of the degree of ordering (non-ideality) in alloys is proposed, and a numerical example for HgTe-CdTe is given.

On détermine l'effet d'ordre proche dans un semiconducteur mixte sur les coefficients d'absorption intrabande et de magnéto-absorption. On montre que ceux-ci dépendent de la température, et on calcule leur évolution dans le temps provoquée par des variations thermiques. L'auteur propose une expérience ayant pour de mesurer le degré d'ordre (d'imperfection) des alliages. A titre d'exemple, on donne des calculs numériques pour le système HgTe-CdTe.

1. Introduction

The interest in mixed semiconductor crystals has increased steadily over the past few years. They differ essentially from other semiconductors in that the distribution of atoms in their lattice is, to a higher or lesser degree, random, leading to local deviations in compositions $v = v(\mathbf{r})$ from the average v_0 . These fluctuations can be expected to lead to various new, interesting effects unobserved in ideal structures. Alloy scattering [1], which occurs in mixed crystals in addition to the normal scattering mechanisms specific to non-mixed ones, is an effect of this kind. Recently, composition fluctuations have been shown to affect magnetoabsorption [2] and absorption [3] on the free carriers.³⁾

Studies on fluctuational effects in mixed semiconductors are commonly based on the assumption of a strictly random distribution of atoms in the lattice. However, numerous results for metal alloys point to the presence, usually, of some degree of ordering in mixed crystals. The deviations from strict randomness (the so-called non-ideality of the alloy) are related with differences in interaction and atomic radii of the components of the alloy. Recent papers by Bublik et al. [4, 5] appear to provide evidence of short-range ordering in semiconducting alloys as well.

In the present paper, we shall be dealing with the influence of fluctuations in composition on absorption and magnetoabsorption in mixed crystals, exhibiting a tendency to short-range order. Our considerations will also include non-equilibrium states, i.e. when the short-range ordering evolves in time.

2. Mixed Semiconducting Crystals

We shall concentrate on triple substitutional II-VI, III-V, IV-VI compounds of the $A_vB_{1-v}C$ type in which one of the elements (denoted as C) is shared by both

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³⁾ In equation (39) of [2] the factor 8 in the denominator should be replaced by 16. In equation (3.18) of [3] in line 4 the factor $\zeta^2/12$ should be replaced by $\zeta^2/12$.

components of the crystal. In this situation, a C-atom can have, as all its nearest neighbours, atoms A or atoms B or a mixture of the ones and others. Thus the crystal can be divided into primitive cells of the type A (containing atoms C and A) and of the type B (with atoms C and B). As we shall have to deal with the statistical thermodynamics of mixed crystals, we proceed to give a definition of the lattice model:

1. We assume the potential energy of the crystal as the sum of the interaction energies of pairs AA, BB, and AB (configurational term) and a constant term, equal for all atomic configurations.

2. We shall be neglecting all pairwise (AA, BB, AB) interactions unless the partners are nearest neighbours (nearest neighbour model). This assumption is roughly correct for crystals in which long-range forces are unessential.

3. We assume the lattice parameters as independent of composition, and the thermal dilatation of the lattice as negligible.

On the above assumptions, we write the configurational part U_C of the energy in the form

$$U_C = N_{AA}\epsilon_{AA} + N_{AB}\epsilon_{AB} + N_{BB}\epsilon_{BB}, \quad (1)$$

where N_{AA} , N_{BB} , and N_{AB} are, respectively, the numbers of nearest neighbours AA, BB, and AB, whereas ϵ_{AA} , ϵ_{BB} , ϵ_{AB} are the respective interaction energies.

By assumption 3, we shall omit volume effects (differences in volume of primitive cells). However, these effects should, in some cases, be taken into account (Guggenheim [6]).

We now introduce the following quantity, providing a measure of the degree of non-ideality of the crystal:

$$\mathcal{E} = \epsilon_{AB} - \frac{1}{2}(\epsilon_{AA} + \epsilon_{BB}). \quad (2)$$

The change in configurational energy induced by the transposition $A \rightleftharpoons B$ amounts to

$$\Delta U_C = \Delta N_{AB}\mathcal{E}. \quad (3)$$

The parameter $\mathcal{E}$ has a simple physical meaning. If $\mathcal{E} = 0$, an interchange of A and B does not affect the configurational energy of the crystal. We refer to this case as that of an ideal solid solution. An ideal alloy exhibits no tendency to atomic ordering. If $\mathcal{E} \neq 0$, we deal with a non-ideal alloy which exhibits a tendency to short-range ordering.

A binary alloy arises as the result of mixing of its two components. Often, it is desirable to compare the properties of the mixture to those of the pure components. To this aim, we define the following thermodynamical mixing functions:

$$\Delta_m X = X(p, T, n_1, n_2) - X_A(p, T, n_1) - X_B(p, T, n_2), \quad (4)$$

where n_1 and n_2 are the numbers of moles of A and B, respectively, whereas X is a thermodynamical potential. In order to separate mixing effects from those due to variations in temperature and pressure, we shall compare the mixture and its components at the same values of T and p .

Dealing with non-ideal solutions, we shall consider the simplest model of a deviation from ideality. We define the concept of a regular solution as follows. The entropy of mixing is the same as for an ideal crystal, and the energy of mixing is different from zero. An interchange of sites by the atoms of the alloy leads to a variation of internal energy. This description is justified provided $\mathcal{E}$ is small. Using the assumptions 1 to 3, we obtain the following expression for the Gibbs free energy:

$$\Delta_m G = Nzv(1-v)\mathcal{E} + NkT[v \ln v + (1-v) \ln(1-v)], \quad (5)$$

where N is the number of lattice points and z is a coordination number.

Moreover, we calculate the derivative $\partial^2 \Delta_m G / \partial v^2$:

$$\frac{\partial^2 \Delta_m G}{\partial v^2} = -2zN\varepsilon + \frac{NkT}{v(1-v)}. \quad (6)$$

One notes that in the case of an ideal or weakly non-ideal solution the curve of $\Delta_m G$ versus v is always concave ($\partial^2 \Delta_m G / \partial v^2 > 0$). Henceforth, we shall deal with weakly non-ideal solutions.

Formula (5) was derived in the approximation of a regular solution and on the assumptions 1 to 3. Irrespective of these restrictions, formula (5) is found to be most useful in the description of a wide class of phenomena in solids, e.g. processes of nucleation [7], the kinetics of short-range ordering [8], critical scattering in alloys [9], and others.

3. Intraband Absorption and Magnetoabsorption in Mixed Semiconductors

The present section is devoted to a discussion of the formulae for the magnetoabsorption [2] and absorption [3] coefficients of mixed semiconductors.

We restrict our analysis to a non-degenerate, parabolic and spherical conduction band edge and neglect spin effects. If $|v(\mathbf{r}) - v_0|$ is small and $v(\mathbf{r})$ varies slowly on the dimension of the unit cell, the position-dependent inverse effective mass and band edge may be written in the form [10]

$$\frac{1}{m_0^*(\mathbf{r})} = \frac{1}{m_0^*} + \frac{1}{m_0^*} \alpha_0 [v(\mathbf{r}) - v_0], \quad (7)$$

$$U(\mathbf{r}) = U_0 + \beta_0 [v(\mathbf{r}) - v_0] + \gamma_0 \nabla^2 [v(\mathbf{r}) - v_0], \quad (8)$$

where m_0^{*-1} and U_0 are the average values of the inverse effective mass and band edge, respectively, α_0 , β_0 , and γ_0 are macroscopic constants of the material defined for composition v_0 . On expanding the function $v(\mathbf{r})$ in a Fourier series we obtain

$$v(\mathbf{r}) = v_0 + \sum_{\mathbf{q}}' \varrho(\mathbf{q}) \exp(i\mathbf{q}\mathbf{r}). \quad (9)$$

The sum denoted $\sum'$ excludes vectors with $\mathbf{q} = 0$. Since $v(\mathbf{r})$ is real, we have

$$\varrho(-\mathbf{q}) = \varrho^*(\mathbf{q}). \quad (10)$$

In the presence of the magnetic field we restrict our considerations to the quantum limit [2], i.e. we assume that the electrons occupy states with $n = 0$ only and that $k_z < k_{zF}$, where k_{zF} is given by

$$k_{zF} = \pi^2 \lambda^2 N_e \quad (11)$$

with N_e being the electron concentration and λ the magnetic length:

$$\lambda = \left(\frac{c\hbar}{eH} \right)^{1/2}, \quad (12)$$

where H is the magnetic field.

The quantum limit condition can be written in the form

$$\hbar\omega_{co} > \frac{\hbar^2 k_{zF}^2}{2m_0^*}, \quad (13)$$

where ω_{co} is the cyclotron frequency

$$\omega_{co} = \frac{eH}{m_0^* c}. \quad (14)$$

For incident light linearly polarized along the z -axis and taking into consideration only transitions permitted in the presence of concentration fluctuations, i.e. at $\omega > \omega_{co}$, where ω is the frequency of the incident light, the formula for the magneto-absorption coefficient takes the following form:

$$\begin{aligned}
 K_{n' ||} = \varepsilon \left(\omega \geq \omega_{co} n' - \frac{\hbar k_{zF}^2}{2m_0^*} \right) (e^2 \omega_{co} / 2\pi^3 n'! \kappa^{1/2} c \hbar \omega^3) \times \\
 \times \int d^2 q_{\perp} \left(\frac{1}{2} \lambda^2 q_{\perp}^2 \right)^{n'} \exp \left(-\frac{1}{2} \lambda^2 q_{\perp}^2 \right) \int_{q_{z1}}^{q_{z2}} dq_z q_z \left\{ \frac{1}{\hbar^2} (\beta_0 - \gamma_0 q^2)^2 + \right. \\
 \left. + \frac{1}{\hbar} \left[\omega_{co} \left(\frac{1}{4} \lambda^2 q_z^2 + n' + 1 \right) - \frac{m_0^*}{\hbar q_z^2} (\omega^2 - \omega_{co}^2 n'^2) \right] \alpha_0 (\beta_0 - \gamma_0 q^2) + \right. \\
 \left. + \frac{1}{4} \left[\omega_{co} \left(\frac{1}{4} \lambda^2 q_z^2 + n' + 1 \right) - \frac{m_0^*}{\hbar q_z^2} (\omega^2 - \omega_{co}^2 n'^2) \right] \alpha_0^2 \right\} \langle |\varrho(\mathbf{q})|^2 \rangle, \quad (15)
 \end{aligned}$$

where

$$\varepsilon(a \leq b) = \begin{cases} 1 & \text{for } a \leq b, \\ 0 & \text{for } a > b, \end{cases} \quad (16)$$

and $n' \geq 2$ is the Landau level; we have, moreover, used the following notations:

$$q_{z1} = \left| k_{zF} - \left[k_{zF}^2 + 2 \frac{m_0^*}{\hbar} (\omega - \omega_{co} n') \right]^{1/2} \right|, \quad (17)$$

$$q_{z2} = k_{zF} + \left[k_{zF}^2 + 2 \frac{m_0^*}{\hbar} (\omega - \omega_{co} n') \right]^{1/2}, \quad (18)$$

$$\langle |\varrho(\mathbf{q})|^2 \rangle = V \cdot \overline{|\varrho(\mathbf{q})|^2}, \quad (19)$$

with: V the volume of the crystal, $\overline{|\varrho(\mathbf{q})|^2}$ the average over all possible configurations, and κ the dielectric constant.

In the absence of magnetic field and when the electrons are contained within the Fermi sphere of the radius $k_F = (3\pi^2 N_e)^{1/3}$, i.e. at strong degeneracy of the electron gas [3], the formula for absorption coefficient on free carriers takes the form

$$\begin{aligned}
 \eta = (e^2 \hbar / 12 m_0^{*2} \omega \pi^2 \kappa^{1/2} c) \left(\int_{k_F \zeta^{1/2}}^{k_F [(1+\zeta)^{1/2} + 1]} q dq \int_{-\frac{m_0^* \omega}{\hbar q} + \frac{q}{2}}^{k_F} k dk + \int_{k_F \zeta^{1/2}}^{k_F \zeta^{1/2}} q dq \int_{\frac{m_0^* \omega}{\hbar q} - \frac{q}{2}}^{k_F} k dk \right) \times \\
 \times \left\{ \alpha_0^2 \left[\frac{\hbar}{m_0^* \omega^2} q^2 k^2 \left(k^2 + \frac{2m_0^* \omega}{\hbar} \right) \right] + \alpha_0 (\beta_0 - \gamma_0 q^2) \frac{4}{\hbar} \left[-\frac{2m_0^{*2}}{\hbar^2} + \right. \right. \\
 \left. \left. + \frac{1}{\omega^2} q^2 \left(k^2 + \frac{m_0^* \omega}{\hbar} \right) \right] + (\beta_0 - \gamma_0 q^2)^2 \frac{4m_0^*}{\hbar^3 \omega^2} q^2 \right\} \langle |\varrho(\mathbf{q})|^2 \rangle, \quad (20)
 \end{aligned}$$

where E_F is the Fermi energy, $\zeta = \hbar \omega / E_F$ and $E_F < \hbar \omega$ is assumed.

In both cases (absorption and magnetoabsorption), since we consider intraband transitions, the energy $\hbar \omega$ of the incident light has to be less than the energy gap,

$$\hbar \omega < E_g. \quad (21)$$

The formulae (15) and (20) were derived in the "virtual crystal approximation" using the effective-mass Hamiltonian which was derived in Leibler's [10] paper.

By (15) and (20), in order to calculate the absorption coefficients, the dependence of $\langle |\varrho(\mathbf{q})|^2 \rangle$ on $\mathbf{q}$ has to be given in explicit form. In [2, 3] the calculations were performed assuming a strictly random distribution of atoms A and B in the sublattice. However, with regard to the differences between the compounds AC and BC (the components of the alloy), the distribution can be expected to be not strictly random. A procedure permitting in general the calculation of $\langle |\varrho(\mathbf{q})|^2 \rangle$ can be found in the thermodynamic theory of fluctuations.

Hitherto, when referring to the mean value, we had in mind the one over various configurations of atoms at thermodynamic equilibrium. However, considerations on systems not at equilibrium and their mean values can lead to interesting results, as it will be shown in the next sections.

4. The Absorption Coefficients for Non-Ideal Semiconductors

To calculate $\langle |\varrho(\mathbf{q})|^2 \rangle$, we have recourse to the thermodynamical fluctuation theory [11]. A macroscopic theory of this kind can be applied to volumes large as compared with the atomic volume. We thus have to restrict our considerations to fluctuations with large wavelengths. This restriction is consistent with the assumptions made when deriving formulae (15) and (20).

In order to determine the fluctuation wave probability, we have to consider the variation in concentration in the entire volume of the crystal. In the macroscopic approximation, the concentration fluctuations from one point in the alloy to another are characterized by the continuous function

$$\delta v(\mathbf{r}) = v(\mathbf{r}) - v_0. \quad (22)$$

It should be noted that, in our case, the fluctuations lead to a re-grouping of the atoms in various parts of the crystal, i.e. $\int \delta v(\mathbf{r}) dV = 0$. By the thermodynamic theory, the probability density for the occurrence of a fluctuation in concentration is

$$w \propto \exp\left(-\frac{\Delta F}{kT}\right), \quad (23)$$

ΔF being the difference in total Helmholtz free energy in the presence and absence of the fluctuation,

$$\Delta F = \int (f - \bar{f}) dV \quad (24)$$

with f the Helmholtz free energy per unit volume and $\bar{f}$ the average of f over the whole crystal.

It can be shown ([11, 12]) by expanding $\delta f = f - \bar{f}$ in a series in powers of $v(\mathbf{r})$ and using the Fourier expansion (9) of the concentration, that

$$\overline{|\varrho(\mathbf{q})|^2} = \frac{kT}{V} \left(\frac{d^2 f}{dv^2} + Kq^2 \right)^{-1}. \quad (25)$$

As shown by Cahn and Hilliard [13], for a regular solution K is of the order of $\mathcal{E}/r_0$, where $\mathcal{E}$ is given by (2) and r_0 characterizes the dimensions of the primitive cell. Since $(qr_0)^2 \ll 1$, we obtain using (6) (in the present case, there is no need to distinguish between ΔF and ΔG) that the second term of (25) can be omitted.

Finally, using (25) and applying (6) and introducing the notations $N_v = N/V$ and $L(T) = (1 - v_0(1 - v_0) 2z\mathcal{E}/kT)^{-1}$, we obtain

$$\langle |\varrho(\mathbf{q})|^2 \rangle = \frac{v_0(1 - v_0)}{N_v} L(T). \quad (26)$$

We now proceed to a discussion of formula (26). At high temperatures one has

$$\langle |\varrho(\mathbf{q})|^2 \rangle = \frac{v_0(1-v_0)}{N_v}. \quad (27)$$

An identical result has been obtained [2] on the assumption of a strictly random distribution. This could have been expected, since at high temperatures the atoms tend to be distributed randomly. Formula (27) is also obtained on making $\bar{\varepsilon}$ go over to zero, i.e. on assuming the alloy to be an ideal one. The mean value (27) is independent of temperature and $\mathbf{q}$. Temperature does not affect the magnitude of the fluctuations. If $\bar{\varepsilon} \neq 0$, $\langle |\varrho(\mathbf{q})|^2 \rangle$ depends on temperature significantly. At the limiting concentrations ($v_0 = 0$ and $v_0 = 1$) both (26) and (27) vanish, as could be expected.

As stated, the absorption coefficients (15) and (20) were calculated in [2] and [3] on the assumption of a random distribution of atoms in the sublattice. Since (26) is independent of the wave vector $\mathbf{q}$, it is easily shown that if short-range order in the crystal is taken into account within the framework of the regular solution approximation, the magneto-absorption coefficient $K_{n\parallel}$ and the absorption coefficient η calculated in [2] and [3] are modified by the factor $L(T)$:

$$K_{n\parallel}(T) = L(T) K_{n\parallel}, \quad (28)$$

$$\eta(T) = L(T) \eta. \quad (29)$$

The new coefficients $K_{n\parallel}(T)$ and $\eta(T)$ depend explicitly on temperature.

5. The Kinetics of Absorption Coefficients

Hitherto, we dealt with situations of equilibrium. In solids, however, with regard to the relatively low mobility of the atoms, non-equilibrium situations can be expected to occur more commonly than in other media. Such a situation can be created, e.g. by subjecting the crystal to a sudden change of temperature. Phenomenological theories of kinetics of ordering in mixed crystals show that in such a case

$$\langle |\varrho(\mathbf{q}, t)|^2 \rangle = [\langle |\varrho(\mathbf{q}, 0)|^2 \rangle - \langle |\varrho(\mathbf{q}, \infty)|^2 \rangle] e^{-2\tilde{D}q^2 t} + \langle |\varrho(\mathbf{q}, \infty)|^2 \rangle, \quad (30)$$

where $\tilde{D}$ is the interdiffusion coefficient [14]. $\langle |\varrho(\mathbf{q}, 0)|^2 \rangle$ and $\langle |\varrho(\mathbf{q}, \infty)|^2 \rangle$ are equilibrium mean values at the initial temperature T_0 and final temperature T_∞ , respectively. By (26), we finally obtain

$$\langle |\varrho(\mathbf{q}, t)|^2 \rangle = \frac{v_0(1-v_0)}{N_v} [L(T_0) - L(T_\infty)] e^{-2\tilde{D}q^2 t} + \frac{v_0(1-v_0)}{N_v} L(T_\infty). \quad (31)$$

A description of this kind was introduced by Cahn [15] basing on Fick's equation and is at present extensively developed in application to metal alloys [8]. A strict treatment in terms of statistical physics based on the master equation is due to Langer [16]. With regard to metal alloys, various experiments aimed at checking the theory [17], including numerical ones [18], have been carried out.

We start from formula (15) for the magnetoabsorption coefficient in the quantum limit. We put $\gamma_0 = 0$, thus neglecting in (8) the term proportional to the Laplacian of δv as compared with the one proportional to δv , and we use (31). Denoting

$$E_F = \frac{\hbar^2 k_{zF}^2}{2m_0^*} \quad \text{and} \quad X = \frac{\hbar\omega}{n'\hbar\omega_{co}}, \quad Y = \frac{E_F}{n'\hbar\omega_{co}}, \quad P = \frac{4\tilde{D}}{\lambda^2},$$

we obtain, after some algebra

$$\begin{aligned}
 K_{n' ||}(t) = & \frac{e^2 v_0 (1 - v_0)}{\pi^2 c \hbar N_{\nu} n'^{1/2} \lambda^4} \frac{1}{n'^2 (1 + Pt)^{n'+1}} [L(T_0) - L(T_\infty)] \varepsilon(X \geq 1 - Y) \times \\
 & \times \frac{\alpha_0^2}{X^3} \left\{ -\frac{1}{Ptn'} F_0(X, t) \left[\left(\frac{\beta_0}{\alpha_0 \hbar \omega_{co}} \right)^2 + \frac{\beta_0}{\alpha_0 \hbar \omega_{co}} (n' + 1) + \frac{1}{4} (n' + 1)^2 - \frac{1}{8} n'^2 (X^2 - 1) \right] - \right. \\
 & - \left[\frac{1}{Ptn'} F_1(X, t) + \frac{1}{(Ptn')^2} F_0(X, t) \right] \left[\frac{1}{2} n' \frac{\beta_0}{\alpha_0 \hbar \omega_{co}} + \frac{1}{4} n' (n' + 1) \right] - \\
 & - \left[\frac{1}{Ptn'} F_2(X, t) + \frac{2}{(Ptn')^2} F_1(X, t) + \frac{2}{(Ptn')^3} F_0(X, t) \right] \frac{1}{16} n'^2 + \\
 & + [E_1(Ptn'A) - E_1(Ptn'B)] \left[-\frac{\beta_0}{\alpha_0 \hbar \omega_{co}} \frac{n'}{2} - \frac{1}{4} n' (n' + 1) \right] (X^2 - 1) + \\
 & + Ptn' [E_2(Ptn'A) - E_2(Ptn'B)] \left[\frac{1}{16} n'^2 (X^2 - 1)^2 \right] \left. \right\} + L(T_\infty) K_{n' ||}, \quad (32)
 \end{aligned}$$

where

$$\begin{aligned}
 A &= [Y^{1/2} - (X + Y - 1)^{1/2}]^{1/2}, \quad B = [Y^{1/2} + (X + Y - 1)^{1/2}]^{1/2}, \\
 F_n(X, t) &= B^n \exp(-Ptn'B) - A^n \exp(-Ptn'A) \quad (n = 0, 1, \dots).
 \end{aligned}$$

We have, moreover

$$E_n(X) = \int_X^\infty \frac{\exp(-t)}{t^n} dt, \quad n = 1, 2, \dots \quad (33)$$

and for $n = 0$

$$E_0(X) = \frac{\exp(-X)}{X}. \quad (34)$$

It can be shown that $E_1 = -\text{Ei}(-X)$ and $E_2(X) = E_0(X) - E_1(X)$.

Obviously, at $t = 0$, $K_{n' ||}(t)$ is equal to its equilibrium value at the initial temperature T_0 , whereas at $t \rightarrow \infty$, $K_{n' ||}(t)$ tends to its equilibrium value at the temperature T_∞ :

$$K_{n' ||}(t = 0) = K_{n' ||}(T_0), \quad (35)$$

$$K_{n' ||}(t = \infty) = K_{n' ||}(T_\infty) \quad (36)$$

with $K_{n' ||}(T)$ defined by (28).

We proceed to consider the time evolution of the absorption coefficient $\eta(t)$. Formula (20), after changing the variables

$$\varepsilon = \frac{\hbar^2 q^2}{2m_0^*}, \quad E = \frac{\hbar^2 k^2}{2m_0^*}, \quad E_F = \frac{\hbar^2 k_F^2}{2m_0^*} \quad \text{and} \quad \zeta = \frac{\hbar \omega}{E_F},$$

$$y = \frac{E}{E_F}, \quad z = \frac{\varepsilon}{E_F},$$

using (31) and integrating over y , takes the form

$$\eta(t) = \frac{2e^2 E_F^2 m_0^{*2} v_0 (1 - v_0)}{3 \hbar^5 \kappa^{1/2} c \pi^2 N_v} \frac{\alpha_0^2}{\zeta^3} [L(T_0) - L(T_\infty)] \times$$

$$\times \int_{[(1+\zeta)^{1/2}-1]^*}^{[(1+\zeta)^{1/2}+1]^*} dz \exp(-2Rzt) \left\{ Y_2(z) z + Y_1(z) \left[z\zeta + \frac{2\beta_0}{\alpha_0 E_F} z \right] + \right.$$

$$\left. + Y_0(z) \left[\frac{\beta_0}{\alpha_0 E_F} (-\zeta^2 + z\zeta) + \left(\frac{\beta_0}{\alpha_0 E_F} \right)^2 z \right] \right\} + L(T_\infty) \eta, \quad (37)$$

where

$$Y_n(z) = \int_{z/4(1-\zeta/z)^2}^1 y^n dy, \quad R = \tilde{D} k_F^2.$$

The analytical form of (37), though easy to obtain, is bulky and algebraically inconvenient.

We now propose the following experiment. A mixed crystal at thermodynamic equilibrium at temperature T_0 is suddenly cooled (or heated) to temperature T_∞ and annealed at the latter during the time t . Next, the crystal is placed in a low-temperature region (when diffusion is extremely slow) and the absorption coefficients are measured. This may be done for different times t . Then, we can obtain the time evolution of absorption coefficients.

6. Numerical Example

For a numerical example of magnetoabsorption we assume material parameters close to those for n-Hg_{0.75}Cd_{0.25}Te [2] at low temperatures: $v_0 = 0.25$, $N_v = 1.5 \times 10^{22} \text{ cm}^{-3}$, $\kappa = 10$, $m_0^* = 0.02m_0$, $\alpha_0 = -10$, $\beta_0 = 0.5 \text{ eV}$, $N_e = 6.8 \times 10^{16} \text{ cm}^{-3}$, $H = 50 \text{ kG}$, $E_F = 14.8 \text{ meV}$, $\hbar\omega_{co} = 29 \text{ meV}$, $E_g = 200 \text{ meV}$, and proceed to consider the case $n' = 2$. Moreover we have $\lambda = 115 \text{ \AA}$, $Y = 0.25$. The energy range of incident radiation corresponds to X -values from the interval (0.75 to 1.3). We note that the quantum limit condition $\hbar\omega_{co} > \hbar^2 k_{zF}^2 / 2m_0^*$ is fulfilled, as well as the assumptions $\hbar\omega$, $n'\hbar\omega_{co} < E_g$.

The cell dimensions in HgTe-CdTe are almost equal ($a_{\text{CdTe}} = 6.48 \text{ \AA}$, $a_{\text{HgTe}} = 6.46 \text{ \AA}$). Hence, in solid solutions of these compounds correlations due to the volume effect can be thought to be negligible, in agreement with our lattice model assumption 3. According to results of Bublik et al. [4, 5] for crystals of Hg_{0.73}Cd_{0.27}Te and

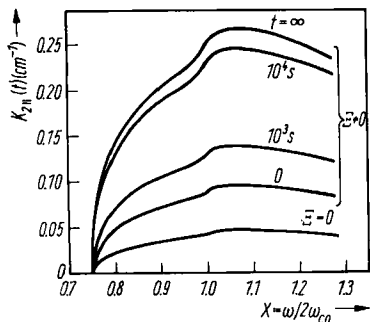


Fig. 1. Time evolution of magnetoabsorption coefficient

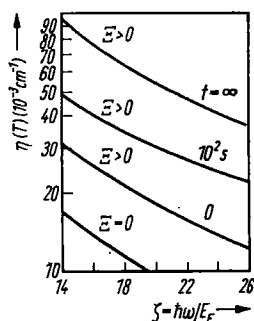


Fig. 2. Absorption coefficient versus time, for $E > 0$. (Read $\eta(t)$ instead of $\eta(T)$)

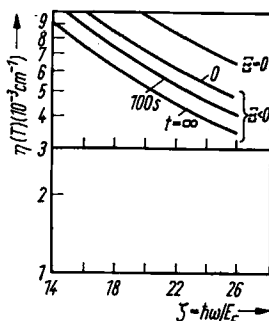


Fig. 3. Absorption coefficient versus time, for $E < 0$. (Read $\eta(t)$ instead of $\eta(T)$)

$\text{Hg}_{0.66}\text{Cd}_{0.34}\text{Te}$ (i.e. for crystals similar to that considered by us), the alloy HgTe-CdTe exhibits a tendency to clustering. We take $E = 0.0075$ eV, which is of the order of Bublik's results. Also HgTe-CdTe has been shown to comply to the regular solution approximation.

The data for the interdiffusion and selfdiffusion coefficients are fragmentary [19]. In our work, we assumed $\tilde{D} = 10^{-16} \text{ cm}^2\text{s}^{-1}$. Finally, we take $T_0 = 650^\circ\text{C}$ and $T_\infty = 300^\circ\text{C}$. $K_{21}(t)$ calculated with the preceding parameters is plotted in Fig. 1 for various annealing times t .

For a numerical example of absorption we assume the same material parameters except for N_v , which we now take as equal to $N_v = 2 \times 10^{15} \text{ cm}^{-3}$. The latter value presents the advantage that the composition fluctuation effects are comparable with effects due to ionized impurities. The range of the incident radiation energy corresponds to ζ from the interval (14, 27). Obviously, $(1 - \zeta) < 0$. Likewise, the condition $\hbar\omega < E_g$ is fulfilled. For the above values the time dependence of the absorption coefficient is plotted in Fig. 2.

Were our crystal endowed with a tendency to ordering ($E < 0$), the evolution in time of its absorption coefficient would have the shape of the curves plotted in Fig. 3.

7. Conclusions

If $E > 0$, the factor $L(T)$ is larger than unity. Hence, the absorption coefficients for all values of time are larger than those of the ideal crystal. Magnetoabsorption and absorption increase from a minimum value at the higher temperature T_0 to a maximum value at the temperature T_∞ . Similar time-dependent curves as those of Fig. 1 and 2 are obtained assuming $E < 0$. However, in this case the absorption coefficients decrease from a maximum value at T_0 to a minimum value at T_∞ . This behaviour of the absorption coefficients can provide the basis for experimental determinations of the type of ordering in the alloy. On inspection of (32) and Fig. 1 as well as (37) and Fig. 2 and 3 it is apparent that the distance between the curves for $t = 0$ and $t = \infty$ is completely defined by the quantity $L(T_0) - L(T_\infty)$, and, thus, by E . Some information about the diffusion coefficient can also be obtained from the kinetics of the absorption and magnetoabsorption coefficients.

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