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Thin Solid Films 302 (1997) 54–57

thin solid films

Indirect transitions caused by electron–dislocation interaction in size-quantized semiconductor film

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Received 27 June 1996; accepted 27 November 1996

Abstract

The light absorbtion coefficient of a semiconductor film caused by indirect electronic transitions is calculated under the assumption that the part of the third body plays a dislocation. There is obtained the frequency dependence of the absorbtion coefficient at various orientations of dislocations in the film. The comparison is carried out of the suggested mechanism with known mechanisms of indirect transititions. © 1997 Elsevier Science S.A.

Keywords: Germanium; Optical properties; Quantum effects; Semiconductors

1. Introduction

On considering the indirect interband electronic transitions in semiconductors in order to ensure the fulfillment of the momentum and energy conservation laws, a third body should necessarily be present. Usually, in solving such problems there has been taken, as a third body, either phonon or impurity center, or plasmon [1,2]. In this work we propose the new mechanism for the interband light absorption, namely it is assumed that the part of a third body is played by a dislocation [1]. In our opinion the consideration of the proposed mechanism of the indirect transition is particularly actual for quasi-two-dimensional (Q2D) semiconducting systems, for example, heterostructures, films, inversion layers, etc.

Indeed, the limitation of the charge carriers motion in one direction leads, as it is known, to the considerable changes of optical (the case of electromagnetic waves absorption included) properties of crystals [4–6].

On the other hand, in the two-dimensional electronic systems, under certain conditions, the dislocation mechanism of charge carriers scattering may become prevalent.

So, in earlier work [7], where the temperature dependence of the Hall mobility in heterostructures $In_xGa_{1-x}/GaAs$ on silicon was investigated, the authors point out the dislocation mechanism of the charge carriers absorption being effective already at temperatures below 200°C; the density of the formed dislocation network being 10^{12}–10^{13} m^{-2}. Such a state also is realized in heterostructures with the strained layers $Si–Si_{1-x}Ge_x$ on a silicon substrate, in which layer thickness being greater than some critical value [8].

2. Calculations

In the present work the optical edge in thin semiconductor films at the indirect transitions, with electron–dislocation interaction taken into account, is investigated.

Let us direct the z axis perpendicular to the film plane. We assume that in the direction of the z-axis electrons are bound in a potential well with infinitely high walls, and in the plane $x0y$ they are in the field of a two-dimensional lattice. According to this model the state of electron in a film is characterized by the order number of subbands (n) arising on account of the transversal motion by the two-dimensional band structure (assuming two values: c and v), and by the two-dimensional wave vector (**k**) characterizing the electronic state in the film plane.

Using the second approximation of the perturbation

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[1] In the work [3] the absorption coefficient of the plastically deformed direct-band semiconductors is calculated for the case when dislocation excitons are excited there.

PII S0040-6090(96)09572-7

theory the absorption coefficient stipulated by the indirect transitions can be represented in the form:

$$\alpha(\omega) = \frac{2\pi\hbar^2 c}{n_r \hbar\omega} \frac{N_D S}{|A_0|^2} \frac{2\pi}{\hbar V} \sum_{\substack{n'',\mathbf{k}' \\ n,\mathbf{k}}} \sum_{n'} \times \frac{|M^{phot}|^2 |M^{dis}|^2}{\left(E_g^0 + E_{c,n'}(\mathbf{k}) - E_{v,n}(\mathbf{k}) - \hbar\omega\right)^2} \times \delta\left(E_g + E_{c,n''}(\mathbf{k}') - E_{v,n}(\mathbf{k}) - \hbar\omega\right) \quad (1)$$

where the

$$E_{l,n}(k) = \frac{\pi^2\hbar^2 n^2}{2m_{l\perp}L_z^2} + \frac{\hbar^2 k^2}{2m_{l\parallel}}$$

is the energy of the charged particle in the band l ($m_{l\perp}$ and $m_{l\parallel}$ being the transversal and longitudinal effective masses respectively in the band l), ω and A_0 are the frequency and amplitude of the incident wave respectively, n_r is the refractive index of a medium, V and L_z are the specimen volume and thickness, respectively, S is the sectional area of the film placed perpendicular to the dislocation line, N_D is the concentration of dislocation in the mentioned area, E_g is the forbidden band width E_g^0 is the forbidden band width in the center of the Brillouin zone ($k = 0$).

The optical matrix element M^{phot} in (1) for the model we consider (provided the light falls perpendicular to the film plane) is of this form:

$$M^{phot} \equiv M_{n'n} = \frac{e}{m_0 c}|A_0|^2 m_0^{1/2} f_{cv}^{1/2} E_g^{01/2} |\chi_{n'n}(q_z L_z)| \quad (2)$$

$$|\chi_{n'n}(q_z L_z)| = \frac{4\pi^2 q_z L_z n' n |(-1)^{n'+n} e^{-iq_z L_z} - 1|}{\left[\pi^2(n'+n)^2 - (q_z L_z)^2\right]\left[\pi^2(n'-n)^2 - (q_z L_z)^2\right]}$$

and q_z is the z component of the incident light wave vector, f_{cv} is the oscillator force, m_0 is the free electron mass. The calculation of the matrix element of the charge carriers interaction with a dislocation M^{dis} has been done for two cases of the edge dislocation.

Let us take advantage of the expression for the electrostatic potential in the approximation [9]:

$$V(\rho) = v_0 K_0(\lambda\rho) \quad (3)$$

where $v_0 = 2e^2 f/\epsilon_S a$ and $f = a/d$ (ρ being the two-dimensional radius vector in the plane perpendicular to the dislocation line).

In formula (3) a is the distance between the dangling bonds (of the order of a lattice constant), d is the distance between the saturated bands, λ is the reverse value of the Debye screening radius, ϵ_s is the statistical dielectric constant of the medium, K_0 is the modified zero-order Bessel function of the second type.

Note that in addition to the electrostatic part of the potential a dislocation has also the deformation part, but, as it is shown by Bonch-Bruevich and Glasko [9], in the interaction of the charge carriers with the edge dislocation the main role is played by the electrostatic potential (3).

Below we consider two cases of dislocation orientation in the specimen. In the first case the dislocation is perpendicular to the film plane, and in the second one it lies in the plane. For the first case (the dislocation line is coincides with the z axis) it is necessary to have a condition when the Debye screening radius is much less than the film thickness $r_D = 1/\lambda \ll L_z$. This condition is fulfilled already at $T = 50$ K for example $L_z = 10^{-7}$ m and electron concentration $N = 10^{24}$ m^{-3}.

In the second case (the dislocation line coincides with the Y axis) this condition is weaker: ($r_D < L_z$). Then, for the matrix element of the electron–dislocation interaction it is not difficult to obtain expression

$$M^{dis} \equiv M_{n'n}^{\mathbf{k}'\mathbf{k}} = \frac{2\pi v_0}{S_1} \frac{1}{\lambda^2 + |\mathbf{k}' - \mathbf{k}|^2} \delta_{n'n} \quad (4)$$

and

$$M^{dis} \equiv M_{n'n}^{\mathbf{k}'\mathbf{k}} = \frac{4\pi^3 v_0}{S_2} \times \frac{L_z n' n}{\lambda^2 L_z^2 + (k_x' - k_x)^2 L_z^2 + \pi^2(n' - n)^2} \times \frac{1 - e^{-L_z\sqrt{\lambda^2 + (k_x' - k_x)^2}}}{\lambda^2 L_z^2 + (k_x' - k_x)^2 L_z^2 + \pi^2(n' + n)^2} \delta_{k_y' k_y} \quad (5)$$

in the first and the second case, respectively.

Here S_1 is the film area, S_2 is the cross-section of the film. Substituting (3) and (4) into (1) and performing the $\mathbf{k}$ and $\mathbf{k}'$ integration for the first absorption coefficient we obtain the expression:

$$\alpha^l(\omega) = \frac{8\pi^2 m_{l\parallel} m_L}{\hbar^4\left(\lambda^2 + k_L^2\right)^2} \frac{e^2}{m_0 c} f_{cv} \frac{v_0^2}{L_z} \frac{N_D^l r}{n_r \omega} E_g^0 \times \sum_{n'',n} |\chi_{n''n}(q_z L_z)|^2 \times \frac{a_{n''n}}{\left(E_g^0 + E_{c,n''}(\mathbf{0}) - E_{v,n}(\mathbf{0}) - \hbar\omega\right)^2} \times \Theta_{n''n}(a_{n''n}) \quad (6)$$

where m_L and $\mathbf{k}$ are the effective mass and wave vector of electron, respectively, at the point L (collateral minimum of the conduction band), N_D^l is the dislocations concentration in the film plane, the quantity $a_{n''n} = \hbar\omega - E_g - E_{c,n''}(\mathbf{k}_L) + E_{v,n}(\mathbf{0})$ defines the absorption edge, r is the

number of equivalent valleys in a semiconductor film (for example, in the case of Ge, $r = 3$).

Analogically for the second case we have:

$$\alpha^{II}(\omega) = \frac{(2\pi)^6}{L_z^2\hbar^2}\left\{1 - e^{-L_z\sqrt{\lambda^2+k_L^2}}\right\}\frac{m_{c\parallel}m_L}{m_{c\parallel}+m_L}\frac{e^2}{m_0 c} \times f_{cv}\frac{v_0^2 N_D^{II} r}{n_r \omega}E_\times^0 \sum_{n'',n} I_{n''n}^k(q_z L_z) \times \frac{\left(2\frac{m_{c\parallel}+m_L}{\hbar^2}a_{n''n} - k_{Ly}^2\right)^{1/2}}{\left(E_g^0 + E_{c,n''}(\mathbf{0}) - E_{v,n}(\mathbf{0}) - \hbar\omega\right)^2} \times \Theta_{n''n}(a_{n''n}) \quad (7)$$

where N_D^{II} is the dislocations concentration in the cross-section of the film, $I_{n''n}^k(q_z L_z)$ is a rather cumbersome expression dependent on k_L and $|\chi_{n''n}(q_z L_z)|^2$, etc. Note that in deriving (6) and (7) it was assumed that the energy containing denominators in (1) near the absorption edge do not depend on the integration variables and are approximately equal to $E_g^0 + E_{c,n''}(\mathbf{0}) - E_{v,n}(\mathbf{0}) - \hbar\omega$.

Making direct use out of the formulae $\chi_{n''n}(q_z L_z)$ it is not difficult to get convinced that the transitions with the same initial, intermediate and final indices $n'' = n' = n$ are the most probable ones.

In particular for $n'' = n' = n = 1$ by taking account of that $k_L^2 \gg L_z^2$, $L_z k_L \gg 1$ the expressions (6) and (7) get sufficiently simplified and assume, respectively, the form:

$$\alpha_{111}^I(\omega) = \frac{8\pi^2 m_{c\parallel}m_L}{\hbar^4 k_L^4}\frac{e^2}{m_0 c}f_{cv}\frac{v_0^2}{L_z}\frac{N_D^I r}{n_r\omega}E_g^0 \times |\chi_{11}(q_z L_z)|^2 \frac{a_{11}}{\left(E_g^0 + E_{c,1}(\mathbf{0}) - E_{v,1}(\mathbf{0}) - \hbar\omega\right)^2}\Theta_{11}(a_{11}) \quad (8)$$

where now $a_{11} = \hbar\omega - E_g - E_{c,1}(\mathbf{k}_L) + E_{v,1}(\mathbf{0})$

$$\alpha_{111}^{II}(\omega) = \frac{(2\pi)^6}{k_L^8\hbar^3}\frac{m_{c\parallel}+m_L}{(m_{c\parallel}+m_L)^{1/2}}\frac{e^2}{m_0 c}f_{cv}\frac{v_0^2 N_D^{II} r}{L_z^6 n_r\omega}E_g^0 \times |\chi_{11}(q_z L_z)|^2 \frac{(2a_{11})^{1/2}}{\left(E_g^0 + E_{c,1}(\mathbf{0}) - E_{v,1}(\mathbf{0}) - \hbar\omega\right)^2}\Theta_{11}(a_{11}) \quad (9)$$

3. Discussion of results

For simplicity we first study the limiting case when $q_z L_z \ll 1$ and α being so small that in the sum over n'' and n' in (6) and (7) only the first term with $n'' = n' = n = 1$ is not zero. As it is seen from (8) (the first case) under such condition near the edge there is a linear dependence of $\alpha_1(\omega)$ on $\hbar\omega - E_g - E_{c,1}(\mathbf{k}_L) + E_{v,1}(\mathbf{0})$.

The absorption in this range of energies corresponds to the transitions from the first subband of the valence band to the first subband of the conduction band through the first interstitial subband. In subsequent increase of energy because of the Θ function presence in (6) the transitions between other subbands become possible, for example at the transitions from $\hbar\omega - E_g > E_{c,1}(\mathbf{k}_L) - E_{v,1}(\mathbf{0})$ to the second subband of the valence band become already possible. Thus with the gradual increase in $\hbar\omega$ the absorption curve undergoes the jumps corresponding to the beginning of the transmission between energetically more remote subbands. Qualitatively the picture is not changed at $q_z L_z \neq 0$. In this case again the linear dependence is obtained with the jumps at the same points, the angles of the jumps will be different however.

In the second case near the edge, the dependence of α_2 on $\hbar\omega - E_g - E_{c,1}(\mathbf{k}_L) + E_{v,1}(\mathbf{0})$ is a square root one (9), what is the consequence of the presence of $\delta_{k'_y k_y}$ in the matrix element of the electron–dislocation interaction, which leads to alteration of the frequency dependence. As in the first case the dependence α_2 on $\hbar\omega$ is nonmonotonic.

As it follows from (8) and (9), because of the strong dependence of the absorption coefficient on the value of k_L ($\alpha^I \sim 1/k_L^4$; $\alpha^{II} \sim 1/k_L^8$), the indirect transitions are impeded because of necessity to transfer $\hbar\mathbf{k}_L$ quasi-momenta in the act of scattering. Let us compare the values of the absorption coefficients in scattering of the charge carriers by dislocation and by acoustic phonons in semiconducting films. For simplicity let us compare the expressions for $n'' = n' = n = 1$ transitions:

$$\frac{\alpha_1^{111}(\omega)}{\alpha_{FON}^{111}(\omega)} = \frac{2\pi^2}{3}\left(\frac{v_0^2}{C_1}\right)\frac{rN^D\rho L_z}{k_L^4 k_B T}C_s^2 \quad (10)$$

where C_1 is the constant of the deformation potential, ρ is the semiconductor density, C_s is the sound velocity in the specimen.

It is not difficult to get convinced that ratio (10) is of the order unity (for example for Ge) at $N^D \approx 10^{16}$ m^{-2}, $L_z \approx 10^{-8}$ m already at $T \leq T_b \approx 50K$ and consequently considered dislocation mechanism of the indirect absorption can compete with the conventional phonon mechanism.

Note also that in the work [10] there are considered, specific for a semiconducting the interband indirect transitions associated with the scattering by surface roughnesses (SR). For the completeness of conceivability let us give the ratio of the absorption coefficient for this case too:

$$\frac{\alpha_1^{111}(\omega)}{\alpha_{SR}^{111}(\omega)} = \frac{v_0^2 N^D}{2\pi\gamma^2 A(k_L\xi_0)}\frac{L_z^4}{\hbar^4 k_L^2}\frac{m_{c\perp}^2 m_{v\perp}^2}{(m_{c\perp}+m_{v\perp})^2} \quad (11)$$

where $\gamma \ll 1$ is a small parameter, ξ_0 is the correlation radius, $A(k_L\xi_0)$ is a function of k_L and $\xi 0$. This ratio at

the same conditions is of the order of $1/\gamma^2$, from which it follows that the dislocation mechanism of the indirect transition always prevails over the mechanism considered in [10].

As regards the second case of the dislocation mechanism, the numerical calculations show that $\alpha_1^{111}(\omega)/\alpha_2^{111}(\omega) \approx 10^5$ (for Ge), i.e. the contribution of α_2 to the absorption coefficient is negligible.

4. Conclusions

There are dicussed in detail the specificities of frequency dependence of partial and total absorption coefficients, caused by indirect transitions in a size quantized semiconductor film on scattering of electrons by dislocations. Account of size quantization leads to violation of monotonous behaviour of frequency dependence curve of absorption coefficient.

Numerical calculation carried out for Ge shows that this light absorbtion mechanism competes with phonon one at temperatures $T \leq 50$ K and dislocation density $N^D \approx 10^{16}$ m^{-2}.

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