
POLARIZATION-RELATED PECULIARITIES OF LIGHT ABSORPTION SPECTRA IN DIRECT-GAP SEMICONDUCTORS WITH SCREW DISLOCATIONS NEAR THE FUNDAMENTAL ABSORPTION EDGE

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The spectrum of interband absorption of light in direct-gap semiconductors with randomly distributed parallel screw dislocations is calculated in the region of the quasicontinuous spectrum of dislocation states near the fundamental absorption edge. It is shown that the mechanism of dislocational absorption is related to a local change of the gap width caused by the long-range deformation potential of dislocations. The comparison to the corresponding results for edge dislocations reveals a series of common features as well as essential distinctions. The spectral dependence of dislocational absorption was found to be different for the different polarizations of light. This presents additional possibilities for experimental investigation.

Introduction

Dislocations are linear structural defects which are always present in crystals affecting the electronic structure of crystals. There is a steady interest in the bound electronic states related to dislocations, because a permanent improvement of experimental methods opens new possibilities to create the given dislocation structures and to develop the new methods of revealing the dislocation electronic states.

The deepest bound electronic states related to a dislocation core may have a radius of order of the lattice constant. However, there are always numerous shallow-level bound states. Their radius significantly exceeds the lattice constant. These shallow states can be considered in the framework of the effective mass method. The role of deep and shallow dislocation states varies in the different physical processes. In optical spectra, the manifestations of deep and shallow states are spectrally

separated. The spectrum of shallow states is determined by the interaction of carriers with the long-range field of dislocations, which is well described in the quasiclassical approximation, whereas the influence of the structure of a dislocation core is insignificant.

To interpret the experimental spectra in semiconductors with dislocations near the fundamental absorption edge, the coefficient of light absorption is to be calculated taking into account that the deformation field affecting the carrier motion is formed by many dislocations, in general. In this paper, we investigate the deformational classical absorption [1], i.e. the absorption related to a local change of the gap width caused by the deformation field which is assumed to be a field of randomly distributed parallel dislocations. This absorption is found to be polarized and has different spectral dependences for different polarizations. The results are compared to the corresponding ones obtained in the framework of the same approximations concerning the edge dislocations [1].

1. Influence of Dislocations on Interband Absorption

The calculation for edge dislocations [1] has shown that the spectrum of interband light absorption in a crystal with randomly distributed dislocations in the quasiclassical region is characterized by a certain broadening Γ and consists of three substantially different regions: (a) $\hbar\omega - \varepsilon_g \gg \Gamma$ — the fundamental absorption region, (b) $|\hbar\omega - \varepsilon_g| \leq \Gamma$ — the broadened fundamental absorption edge, and (c) $\varepsilon_g - \hbar\omega \gg \Gamma$ —

the dislocational wing of absorption. The broadening Γ depends on the basic mechanism of the interaction of carriers with dislocations and is expressed in terms of a certain characteristic energy ε_d , an exponent ν , and the dislocation density σ ($\Gamma \sim \sigma^\nu \varepsilon_d$).

The characteristic feature of the long-wave wing of the dislocational absorption is a linear dependence of the absorption coefficient on the dislocation density. In this frequency region, the absorption occurs in the field of every individual dislocation independently. Therefore, the shape of the dislocational wing does not depend on the structure of the dislocation ensemble and is determined by the characteristics of an individual dislocation and the mechanism of absorption. The wing of the dislocational absorption is characterized by the power-law frequency dependence

$$K(\omega) \sim (\varepsilon_g - \hbar\omega)^{-\delta},$$

where the positive exponent δ is determined by the mechanism of absorption. The polarization-related peculiarities of the absorption wing in a semiconductor with dislocations are discussed by us in [2–4].

The broadened fundamental absorption edge is the region where the dislocational absorption continuously transforms into the fundamental absorption (where the influence of dislocations is insignificant). In the region of the broadened edge, the influence of dislocations on the absorption is maximal. In this case, the absorption depends nonlinearly on their density σ being determined by the overlapping fields of many dislocations.

As shown below, the general picture of a dislocation spectrum described above is also valid for screw dislocations but with other characteristic parameters.

2. Changes in Electron Spectrum Caused by Screw Dislocations

For simplicity, consider a cubic direct-gap semiconductor. The cubic approximation may be also applied to some extent to hexagonal crystals [5]. The effect of the strain field is considered within the framework of the deformation potential method [5] using the effective mass approximation for the particle motion. The deformation potential of a screw dislocation for a simple isotropic band is equal to zero. Therefore, the threefold degeneracy of the valence band maximum in the absence of deformations is taken into account. The valence band in the ideal crystal consists of three subbands that are generated at the Γ -point ($\mathbf{k}=0$). The Wannier functions of the subbands are analogous to the wave functions of atomic p -electrons of the x -, y -,

and z -types with respect to the cubic crystal symmetry transformations. Therefore, the subbands will be labeled by the indices x , y , and z . In the ideal crystal, the x -, y -, and z -directions are equivalent, but, for a given subband, the direction of the corresponding cubic axis is selected, i.e. each separate subband is anisotropic.

We suppose that the effective mass is isotropic. In the approximation of an elastically isotropic medium, the orientation of the x -, y -, and z -axes may be arbitrary. The components of the envelope wave function within the effective mass method form a vector $\vec{\Psi} = \{\psi_x, \psi_y, \psi_z\}$. Let Oz be the direction of dislocation lines.

Now we will investigate how the deformation field of an ensemble of randomly distributed parallel screw dislocations affects the spectrum of electron states.

According to the isotropic theory of elasticity, the strain components of an ideal straight screw dislocation are [6]

$$u_{xz} = u_{zx} = -b \sin \varphi / 4\pi r, \quad u_{yz} = u_{zy} = b \cos \varphi / 4\pi r,$$

Here, b is the Burgers vector, r , φ are cylindrical coordinates. All other strain components are zero. In the presence of the ensemble of parallel screw dislocations, the electron spectrum is determined with the Schrödinger equation

$$\left(\frac{\hat{p}^2}{2m} + \hat{V} \right) \vec{\Psi} = E \vec{\Psi}, \quad (1)$$

where the potential energy \hat{V} is the operator of interaction of holes with the strain deformation field [5]:

$$\hat{V} = \begin{pmatrix} 0 & 0 & a \\ 0 & 0 & b \\ a & b & 0 \end{pmatrix},$$

$$a = \sum_{n=1}^N u_{zx}^{(n)} D_3, \quad b = \sum_{n=1}^N u_{zy}^{(n)} D_3, \quad (2)$$

Here, $u_{\alpha\beta}^{(n)}$ are the strain tensor components of the n -th individual screw dislocation, N is the number of dislocations in a crystal, D_3 is the deformation potential constant related to the shear deformation [5]. As the further calculation shows, the strain fields of screw dislocations in the model of a crystal considered lead to local changes of the gap width. It has been shown in [1] that, in such a case, one may neglect the tunneling effects when calculating the absorption coefficient and consider the motion of carriers in the approximation that the crystal is locally homogeneous and the wave function of a carrier is a plane wave. The absorption caused by this

mechanism is called “deformational classical” according to the classification proposed in [1]. The equality of the determinant to zero,

$$\begin{vmatrix} -\lambda & 0 & a \\ 0 & -\lambda & b \\ a & b & -\lambda \end{vmatrix} = 0,$$

where $\lambda = E - \hbar^2 k^2 / 2m$, yields that the anisotropic field of dislocations removes the degeneracy at the Γ -point and three branches are formed: $\lambda_1 = 0$, $\lambda_2 = |u|$, $\lambda_3 = -|u|$, where $|u| = \sqrt{a^2 + b^2}$. They correspond to zero, repulsive, and attractive potentials of dislocations. The corresponding wave functions are $\tilde{\Psi}^j = \tilde{\Psi}_0^j e^{i\vec{k}\cdot\vec{r}}$, where

$$\begin{aligned} \Psi_0^1 &= \begin{pmatrix} \beta \\ -\alpha \\ 0 \end{pmatrix}, & \Psi_0^2 &= \frac{1}{\sqrt{2}} \begin{pmatrix} \alpha \\ \beta \\ 1 \end{pmatrix}, \\ \Psi_0^3 &= \frac{1}{\sqrt{2}} \begin{pmatrix} \alpha \\ \beta \\ -1 \end{pmatrix}, & \alpha &= \frac{a}{|u|}, & \beta &= \frac{b}{|u|}. \end{aligned} \quad (3)$$

It should be noted that the vector of the dipole momentum \vec{p}^j of the transition from the state described by the function $\tilde{\Psi}_0^j$ in the effective mass method to a state of the conductive band is parallel to the vector $\tilde{\Psi}_0^j$.

3. Local Value of the Absorption Coefficient

The local value of the absorption coefficient is determined by the expression

$$K = \frac{2\pi\omega}{\varepsilon_0 n c V} \sum_{\vec{k}} \sum_{j=1}^3 (\vec{p}^j \cdot \vec{e})^2 \delta \left(\hbar\omega - \varepsilon_g - \frac{\hbar^2 k^2}{2m} - \lambda_j \right),$$

where ε_0 is the dielectric susceptibility of a vacuum, n is the refractive index, c is the light velocity, V is the volume of a crystal, \vec{e} is the unit vector of light polarization, and ε_g is the gap width. The local value of the absorption coefficient K is to be averaged over the random arrangement of parallel dislocations. After this averaging, the crystal becomes a uniaxial medium. Therefore, it is enough to calculate the averaged values of the absorption coefficient for $\vec{e} \parallel Oz$ and for $\vec{e} \perp Oz$ only, which we denote K_{\parallel} and K_{\perp} , respectively. After calculating the sum over all of \vec{k} , the local value of the absorption coefficient can be expressed through the light absorption coefficient in this crystal in the absence of dislocations $K_0(\varepsilon) = R_0 \theta(\varepsilon) \sqrt{\varepsilon}$, where $\varepsilon = \hbar\omega - \varepsilon_g$.

Taking into account the form of vectors (3), we obtain the local value of K_{\parallel} as

$$K_{\parallel} = \frac{1}{2} [K_0(\varepsilon - |u|) + K_0(\varepsilon + |u|)]. \quad (4)$$

To obtain K_{\perp} , the local value of the absorption coefficient for $\vec{e} \perp Oz$ may be at first averaged over orientations of the vector \vec{e} in the plane perpendicular to Oz . Then, taking into account (3), the local value of K_{\perp} is expressed via the local value of K_{\parallel} and K_0 :

$$K_{\perp} = \frac{1}{2} (K_0 + K_{\parallel}). \quad (5)$$

Obviously, this universal relation preserves the validity after averaging over the arrangement of parallel dislocations.

4. Probability Distribution Function

After averaging over a random arrangement of parallel dislocations, the value of a local change of the gap width (for the states $j = 2, 3$) $u = \pm\sqrt{a^2 + b^2}$ runs in total from $-\infty$ to $+\infty$. Introducing the corresponding probability distribution function $P(u)$, we obtain, as a result of averaging (4),

$$K_{\parallel}(\varepsilon) = \int_{-\infty}^{\infty} K_0(\varepsilon - u) P(u) du. \quad (6)$$

In order to find the even function $P(u)$, it is convenient to consider the distribution function $P(u^2)$ of $u^2 = a^2 + b^2$ determined in the interval $[0, \infty)$ by the following formula:

$$P(u) = |u| P(u^2). \quad (7)$$

The function $P(u^2)$ can be found by calculating some characteristic function

$$\overline{e^{-pu^2}} = \int_0^{\infty} e^{-pu^2} P(u^2) du^2$$

at first and then performing the inverse Laplace transformation

$$P(u^2) = \frac{1}{2\pi i} \int_{s-i\infty}^{s+i\infty} e^{pu^2} \overline{e^{-pu^2}} dp, \quad (8)$$

where the overline means the average over the random arrangement of parallel dislocations. The average value of the exponent $\overline{\exp(-pu^2)}$ can be calculated directly by

factorizing the contributions of individual dislocations. For this purpose, we use the integral representation

$$e^{-pu^2} = \frac{p}{\pi} \int e^{-pq^2} e^{-2ip\vec{q}\cdot\vec{u}} d^2\vec{q},$$

where \vec{q} is a two-dimensional vector in the plane perpendicular to the dislocation lines, and $\vec{u} = \{a, b\}$ is the vector with the components defined in (2).

Let's introduce the dimensionless variables

$$p' = p\Gamma^2, \quad \vec{q}' = \vec{q}/\Gamma,$$

where Γ is an energy parameter defined below. The strokes will be further omitted. Then

$$\overline{e^{-pu^2}} = \frac{p}{\pi} \int e^{-pq^2} \overline{e^{-pU}} d^2\vec{q}, \tag{9}$$

where $U = 2i\vec{q}\cdot\vec{u}/\Gamma$. The average value of the exponent under the integral can be calculated as in [7]:

$$\begin{aligned} \overline{e^{-pU}} &= e^{-p \overline{\sum_{n=1}^N U_n}} = \prod_{n=1}^N \overline{e^{-pU_n}} = \left(\overline{e^{-pU_n}}\right)^N = \\ &= \left(1 - \overline{(1 - e^{-pU_n})}\right)^N = \\ &= \left(1 - \frac{\sigma}{N} \int (1 - e^{-pU_n}) dS\right)^N \rightarrow e^{-T}, \end{aligned} \tag{10}$$

where $T = \sigma \int (1 - e^{-pU_n}) dS$, σ is the dislocation density, $N = \sigma S \rightarrow \infty$ is the number of dislocations in a crystal, S is the cross section of a cylindrical crystal with an axis parallel to dislocation lines, and U_n is defined by the field of an individual dislocation. In a local coordinate system $U_n = 2i\vec{q}\cdot\vec{u}_n/\Gamma$, $\vec{u}_n = \Delta\{-\sin\varphi, \cos\varphi\}/\rho$, $\Delta = bD_3/4\pi$. Let's choose the direction of the Ox -axis to be parallel to \vec{q} . Then

$$\begin{aligned} T &= \sigma \int_0^\infty \rho d\rho \int_0^{2\pi} \left(1 - e^{2ipq \frac{\Delta}{\Gamma\rho} \sin\varphi}\right) d\varphi = \\ &= 2\pi\sigma \int_0^\infty \rho \left(1 - J_0\left(2pq \frac{\Delta}{\Gamma\rho}\right)\right) d\rho. \end{aligned}$$

In the last integral, there is a logarithmic divergence. This divergence is eliminated by replacing the upper limit of integration by the characteristic dimension L (radius) of the crystal [7]:

$$T = \sigma \int_0^L \rho d\rho \int_0^{2\pi} \left(1 - e^{2ipq \frac{\Delta}{\Gamma\rho} \sin\varphi}\right) d\varphi =$$

$$= 2\pi\sigma A^2 \int_0^{L/A} z \left(1 - J_0\left(\frac{1}{z}\right)\right) dz, \tag{11}$$

where $A = 2pq\Delta/\Gamma$. Assuming $l_N = \ln\sqrt{N} \gg 1$, where N is of the order of the total number of dislocations in a crystal, we retain the main term of the expansion which is proportional to l_N for the energy region $|u| \leq \Gamma$ (i.e. for the spectral region of the broadened dislocational edge) in (11). Then, defining the energy parameter Γ in the form

$$\Gamma = \Delta\sqrt{2\pi\sigma l_N}, \tag{12}$$

we obtain

$$T = p^2 q^2. \tag{13}$$

Consequently using (13), (10), (9), (8), (7), for $|u| \leq \Gamma$, it is found that

$$P(u) = \frac{|u|}{\Gamma^2} \exp\left(-\frac{u^2}{\Gamma^2}\right). \tag{14}$$

Thus, the parameter Γ (12) determines the dispersion of the local values of the gap width related to dislocations.

Finally, for the broadened edge region, the light absorption coefficient K_{\parallel} (4) becomes

$$\begin{aligned} K_{\parallel}(\hbar\omega - \varepsilon_g) &= R_0 \int_{-\infty}^{\hbar\omega - \varepsilon_g} \sqrt{\hbar\omega - \varepsilon_g - u} P(u) du = \\ &= R_0 \sqrt{\Gamma} \alpha(\Omega), \end{aligned} \tag{15}$$

where $\alpha(\Omega)$ is the universal function of the dimensionless frequency:

$$\begin{aligned} \alpha(\Omega) &= \int_{-\infty}^{\Omega} |\nu| \sqrt{\Omega - \nu} \exp(-\nu^2) d\nu, \\ \Omega &= \frac{\hbar\omega - \varepsilon_g}{\Gamma}. \end{aligned} \tag{16}$$

The absorption coefficient under the light polarization $\vec{e}_{\perp} \perp Oz$ is determined from (5).

In the energy region $|u| \gg \Gamma$, the approximation $e^{-T} \approx 1 - T$ can be used. Then we obtain

$$P(u) = \Gamma^2 / (2|u|^3). \tag{17}$$

As a result, in the region of the dislocational wing $\varepsilon_g - \hbar\omega \gg \Gamma$, the dependence (15) is transformed to the power-law asymptote

$$K_{\parallel}(\varepsilon_g - \hbar\omega) = R_0 \frac{\pi}{16} \frac{\Gamma^2}{(\varepsilon_g - \hbar\omega)^{3/2}}. \tag{18}$$

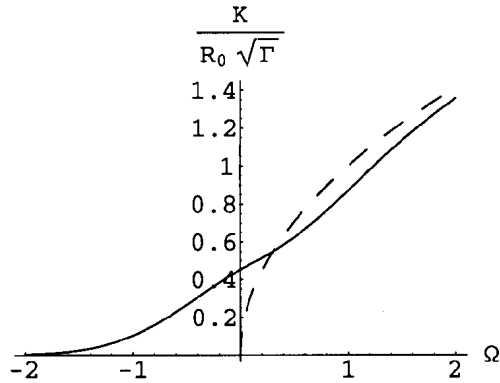


Fig. 1. Dependence of the light absorption coefficient in a crystal with dislocations K_{\parallel} in the broadened edge region in units of $R_0\sqrt{\Gamma}$ on the dimensionless frequency $\Omega = (\hbar\omega - \varepsilon_g)/\Gamma$ (solid curve) in comparison to the absorption coefficient dependence on frequency in the ideal crystal (dashed curve) in the same units

5. Discussion

Fig. 1 presents the dependence of the light absorption coefficient in a crystal with dislocations K_{\parallel} in the broadened edge region in units of $R_0\sqrt{\Gamma}$ on the dimensionless frequency $\Omega = (\hbar\omega - \varepsilon_g)/\Gamma$ calculated from (15) and (16) (solid curve) in comparison to the absorption coefficient dependence on frequency in the ideal crystal (dashed curve) in the same units.

One can see that, in the case of screw dislocations, the redistribution of the absorption from the region $\hbar\omega > \varepsilon_g$ to the region $\hbar\omega < \varepsilon_g$ is observed. A similar behavior takes place for edge dislocations [1]. However, for screw dislocations, the shape of the broadened edge is different since the distribution function $P(u)$ for edge dislocations is strictly Gaussian, while function (14) is not.

In the region of the dislocational wing, the expression for the absorption coefficient for edge dislocations [1] and that for the absorption coefficient K_{\parallel} (18) coincide when taken for equal values of the parameter Γ , while $K_{\perp} = K_{\parallel}/2$. At the same time, the analysis shows that the dislocational absorption coefficient for screw dislocations in the broadened edge region exceeds the corresponding absorption coefficient for edge dislocations when taken for equal values of the parameter Γ .

What distinguishes the dislocational absorption in the case of screw dislocations is its characteristic dependence on light polarization in respect to the direction of dislocation lines, i.e. to the direction of the

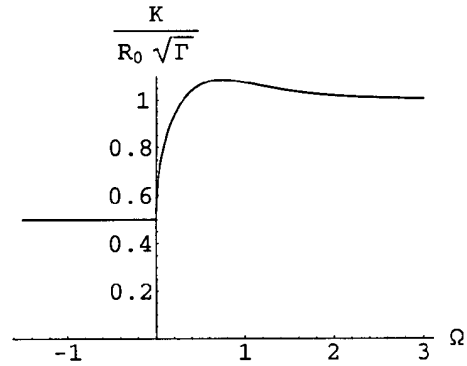


Fig. 2. Dependence of K_{\perp}/K_{\parallel} on the dimensionless frequency

Burgers vector \vec{b} . The absorption coefficients K_{\parallel} and K_{\perp} are not only different but also have different frequency dependences as illustrated by Fig. 2. This creates additional possibilities to investigate the dislocational absorption experimentally and to compare the effects of screw and edge dislocations.

It should be noted that, deeper in the gap, the discreteness of the spectrum of the transverse (in respect to a dislocation line) motion of electrons reveals itself, and therefore the quasiclassical approximation ceases to be valid. In this case, it is necessary to carry out a consistent quantum-mechanical calculation of the localized states in the field of dislocation and of the contributions of the corresponding one-dimensional bands to the absorption coefficient. As was shown in [4], in this region of the absorption spectrum, the dislocational absorption at the light polarization \vec{e} parallel to the Burgers vector \vec{b} dominates both for edge and screw dislocations.

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ПОЛЯРИЗАЦІЙНІ ОСОБЛИВОСТІ СПЕКТРІВ
ПОГЛИНАННЯ СВІТЛА В ПРЯМОЗОННИХ
НАПІВПРОВІДНИКАХ З ГВИНТОВИМИ
ДИСЛОКАЦІЯМИ ПОВЛИЗУ КРАЮ
МІЖЗОННОГО ПОГЛИНАННЯ

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Резюме

Розраховано спектр міжзонного поглинання світла в прямозонному напівпровіднику з хаотично розташова-

ними гвинтовими дислокаціями поблизу краю фундаментального поглинання в області квазінеперервного спектра дислокаційних станів. Показано, що поглинання, зумовлене дислокаціями, пов'язане з локальною зміною ширини забороненої зони, спричиненою далекодійними деформаційними полями дислокацій. Порівняння з відповідними результатами для крайових дислокацій виявляє ряд спільних рис поряд з істотними відмінностями. Встановлено, що спектр поглинання дислокацій є різним для різних поляризацій світла, що створює додаткові можливості для експерименту.