

EFFECT OF SMOOTH FLUCTUATIONS OF THE COMPOSITION OF A SEMICONDUCTING SOLID SOLUTION ON THE SHAPE OF THE INTRINSIC ABSORPTION EDGE

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A quasiclassical approximation is used to calculate the dependence of the effective optical extinction coefficient $\bar{K}(\omega)$ on the frequency near the edge of the fundamental band in semiconducting solid solutions, with allowance for the inevitable fluctuations of the composition and width \mathcal{E}_g of the forbidden band. For the case of a plate made of material in which light is absorbed as a result of allowed direct interband transitions, one measures not the usual function $\bar{K}(\omega) \sim \sqrt{\hbar\omega - \mathcal{E}_g}$ but either $\bar{K}(\omega) \sim (\hbar\omega - \mathcal{E}_g)^{3/2}$ or $(\hbar\omega - \mathcal{E}_g)^1$, depending on the character of the variation of \mathcal{E}_g with the plate thickness.

The dependence of the optical extinction coefficient K on the frequency ω near the intrinsic absorption edge is used to determine the type of interband transitions with which the absorption of light in semiconductors is connected. In the case of semiconducting solid solutions, when the width \mathcal{E}_g of the forbidden band depends strongly on the composition, the unavoidable inhomogeneities in the component distribution give rise to spatial variations of \mathcal{E}_g , and these, as we shall show, can markedly alter the observed shape of the absorption edge. Failure to take this circumstance into account leads to incorrect conclusions concerning the type of the interband transitions.

We consider the long-wave part of the spatial spectrum of the component-concentration fluctuations in a solid solution. This part can be taken into account by introducing the local width $\mathcal{E}_g(\vec{r})$ of the forbidden band and the local complex dielectric constant $\epsilon(\omega, \vec{r}) = \omega_1 + i\epsilon_2$. This description of the optical characteristics of a solid solution should be sufficiently exact when the concentration varies little over the wavelength λ of the light in the substance, and makes it possible to reduce the analysis of the optical properties of the inhomogeneous solid solution to the problem of propagation of an electromagnetic wave in a medium with smoothly varying $\epsilon(\vec{r})$.

The expression for the transmission coefficient $T(\omega)$ of a semiconducting plate whose optical properties vary with thickness can be obtained from two linearly-independent solutions $\vec{E}_+(x)$ and $\vec{E}_-(x)$ of the wave equation for the electric field vector \vec{E} . If we choose the x axis to be the direction of variation of ϵ , then for transverse waves propagating along Ox we have the equation

$$\frac{\partial^2 \vec{E}}{\partial x^2} + \frac{\omega^2}{c^2} \epsilon(x) \vec{E} = 0. \quad (1)$$

In the quasiclassical approximation

$$\vec{E}_+(x) = E_0 [\epsilon(x)/\epsilon(0)]^{-1/4} \exp \left[i \frac{\omega}{c} \int_0^x \sqrt{\epsilon(x')} dx' \right], \quad (2a)$$

$$\vec{E}_-(x) = E_0 [\epsilon(x)/\epsilon(0)]^{-1/4} \exp \left[-i \frac{\omega}{c} \int_0^x \sqrt{\epsilon(x')} dx' \right], \quad (2b)$$

where \vec{E}_+ corresponds to a wave that goes off to $+\infty$, and E_0 to a wave coming from $+\infty$. Since we want to obtain the function $T(\omega)$ in the vicinity of the intrinsic absorption edge, we can put $\epsilon_1 \gg \epsilon_2$, i.e., assume the absorption over one wavelength in the matter to be small. This is true up to $K \approx 10^4 - 10^5 \text{ cm}^{-1}$ [1]. We then have for a plate of thickness d :

$$T(\omega) = \frac{[1 - R(d)][1 - R(0)]e^{-\bar{K}(\omega)d}}{1 + R(d)R(0)e^{-2\bar{K}(\omega)d} - 2\sqrt{R(d)R(0)}e^{-\bar{K}(\omega)d} \cos 2\kappa}, \quad (3)$$

where $R(0)$ and $R(d)$ are the coefficients of reflection from the front and rear faces of the plate, $\kappa = (\omega/c) \int_0^d \sqrt{\epsilon_1(x)} dx$, and

$$\bar{K}(\omega) = \frac{1}{d} \int_0^d K(\omega, x) dx; \quad K(\omega, x) = \frac{\omega}{c} \frac{\epsilon_2(\omega, x)}{2\sqrt{\epsilon_1(\omega, x)}}. \quad (4)$$

We see that in the case of a homogeneous plate $\bar{K}(\omega)$ goes over into the ordinary extinction coefficient. When the variation of ϵ_g inside the plate does not exceed $0.1 \epsilon_g$, then we can determine $\bar{K}(\omega)$ from (3) by putting in first-order approximation $R(d) = R(0)$, since it is easy to show that ($\epsilon_1 \gg 1$)

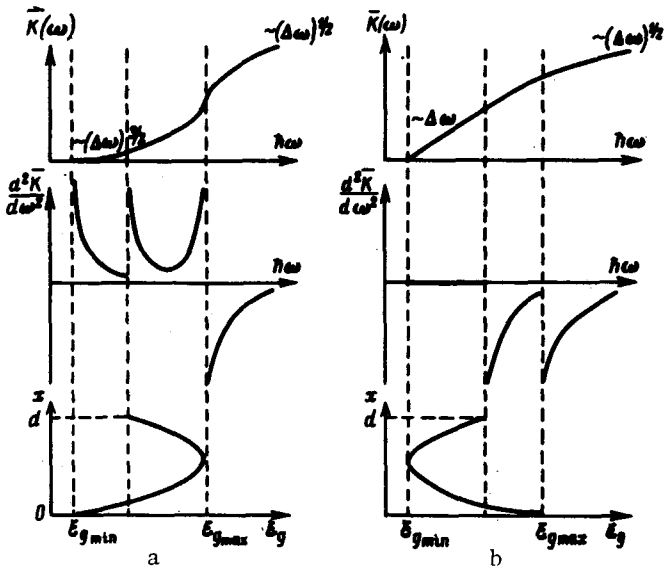
$$\frac{\Delta R}{R} = \frac{\sqrt{\epsilon_1}}{\epsilon_1 - 1} \frac{\Delta \epsilon_1}{\epsilon_1} \text{ and } \frac{\Delta R}{1 - R} = \frac{1}{4} [1 + R] \frac{\Delta \epsilon_1}{\epsilon_1},$$

and it follows quite readily from Moss's empirical formula $1/\epsilon_1^2 \sim \epsilon_g [1]$ that $\Delta \epsilon_1/\epsilon_1 = 2\Delta \epsilon_g/\epsilon_g$. Then formula (3) becomes very similar to the known expression for the transmission of a homogeneous plate, in which the role of the effective extinction coefficient is played by $\bar{K}(\omega)$. We shall show that its frequency dependence differs appreciably from the frequency dependence of the local extinction coefficient $K(\omega, x)$ when $\min \epsilon_g(x) < \hbar\omega < \max \epsilon_g(x)$. We see that in the usual method of determining the plate extinction by using the transmission one measures precisely $\bar{K}(\omega)$.

Assuming that the composition of the solid solution, meaning also ϵ_g , varies little over distances on the order of d , and confining ourselves to terms of second order in the expansion $\epsilon_g(x) = \epsilon_g(0) + \epsilon_g'x + (1/2)\epsilon_g''x^2$, let us investigate the behavior of $\bar{K}(\omega)$ in the case when the light absorption is determined by allowed direct transitions from the valence band to the conduction band. Then¹⁾

$$K(\omega, x) \sim [\hbar\omega - \epsilon_g(x)]^{1/2}.$$

The absorption near the edge then begins to increase in accordance with a law characteristic of forbidden direct transitions



$$\bar{K}(\omega) \sim [\hbar\omega - \epsilon_{g \min}]^{3/2}, \quad (5a)$$

if $\partial \epsilon_g / \partial x > (\partial^2 \epsilon_g / \partial x^2)d$ at the point where the width of the forbidden band is minimal (Fig. a), and

$$\bar{K}(\omega) \sim [\hbar\omega - \epsilon_{g \min}], \quad (5b)$$

if the minimum of $\epsilon_g(x)$ is reached inside the plate ($\partial \epsilon_g \min / \partial x = 0$) (Fig. b)²⁾. At $\hbar\omega > \epsilon_g \max$, the form of $\bar{K}(\omega)$ approaches the usual form for allowed transitions of square-root dependence. At a frequency equal to the maximum value of ϵ_g , where $\bar{K}(\omega)$ is continuous, the function $d^2 \bar{K}(\omega) / d\omega^2$ has a singularity. The character of this singularity is given by

$$(\hbar\omega - \epsilon_{g \max})^{-1}, \quad (6a)$$

if $\max \epsilon_g(x)$ is reached inside the plate (Fig. a), and

$$(\hbar\omega - \epsilon_{g \max})^{-1/2} \quad (6b)$$

if $\partial \epsilon_g / \partial x \neq 0$ at the maximum (Fig. b). Thus, the form and the characteristic values of the

Schematic form of the frequency dependence of the effective extinction coefficient $\bar{K}(\omega)$ at different variations of ϵ_g over the plate thickness, $\Delta\omega = \omega - \epsilon_g \min / \hbar$.

function $\epsilon_g(x)$ can be assessed from the frequency dependence of $\bar{K}(\omega)$.

We note that in the case of direct allowed transitions we have $\partial\epsilon_2/\partial x \sim [\hbar\omega - \epsilon_g(x)]^{-1/2}$, and the usual condition for the validity of the quasiclassical approach is violated near the singular point where $\epsilon_2(\omega, x) = 0$. Nonetheless, the use of the solutions (2) to calculate the absorption coefficient is justified in this case, too, as can be verified by investigating the behavior of the solution of Eq. (1) in the vicinity of the singular point. Analysis shows that the exact solution remains finite, together with its derivative, at the singular point, and is well approximated by the quasiclassical formulas (2) with the distance from the singular point exceeds λ . Owing to the smallness of absorption over one wavelength, the difference between the quasiclassical solution and the exact one is immaterial when it comes to calculation of the absorption of a plate of thickness $d \gg \lambda$. The results concerning the behavior of $d^2\bar{K}/d\omega^2$ also remain in force, except that the growth of this derivative is bounded at the singular points. The order of magnitude of $d^2\bar{K}/d\omega^2$ near the singular points can be estimated by substituting in (6) $\hbar\omega - \epsilon_{g \max} = \max \{(\partial \epsilon_g/\partial x)\lambda, (\partial^2 \epsilon_g/\partial x^2)\lambda^2\}$, where the derivatives are taken at the singular point $\epsilon_2(\epsilon_{g \max}/\hbar, x) = 0$. The influence of the inhomogeneity of the composition in a plane perpendicular to the direction of light propagation, if the fluctuations of ϵ_g are smooth, as before, in comparison with λ , can be determined by using a three-dimensional quasiclassical approximation. It turns out then that the expression for $T(\omega)$ can be obtained by averaging (3) over the area of the plate. In real cases, however, the fluctuations of the composition along the crystal-growth direction can be larger than the fluctuations in the transverse direction. If the plate used to investigate the absorption is cut perpendicular to the growth direction, then its transmission should be adequately described by formula (3).

We note in conclusion that in [2] they reported observation of a relation of type (5a) in the investigation of the shape of the absorption edge in the solid solution $\text{Bi}_x\text{Sb}_{1-x}$, although the optical absorption in this substance should be connected with allowed direct transition. This contradiction, from our point of view, is due to the variation in the concentration of the antimony over the thickness of the plate, and for the $\bar{K}(\omega)$ dependence observed in the interval ~ 2 meV it suffices to have the antimony concentration change by 1%.

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1) We disregard here the change in the local extinction coefficient, which is similar to the Keldysh-Franz effect, and can take place in such an inhomogeneous system. This question will be considered elsewhere.

2) Formulas (5) give the asymptotic values of $\bar{K}(\omega)$ in two limiting and, in our opinion, most probable cases. The exact expressions can be easily obtained by carrying out the integration in (4).

[1] T. S. Moss, Photoconductivity in Solids (Russ. transl.), IIL, 1961.

[2] A. A. Abdullaev, V. G. Alekseeva, et al., ZhETF Pis. Red. 17, 292 (1973) [JETP Lett. 17, 209 (1973)].