

The Quantization of the Absorption Spectrum for Aamorphous Semiconductor Films

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Approach to the description of the photoelectric converter built on the basis of nanosized semiconductor film was presented. The absorption coefficient of the incident quantum flux was presented as the sum of the vibration modes, determined by their own energies have been picked up from the Schrödinger equation, which describes the disordered atomic matrix.

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1. AMORPHOUS SEMICONDUCTORS

Amorphous materials are integral structure modern optoelectronics, are used as receptors and matrix of photoelectric converting elements. However, the production of amorphous semiconductors with optimum optical properties is a difficult task. Modern quantum physics does not give a clear description of nanostructured materials, as well as isn't standard approach to the description of such microscopic aperiodic. Therefore it is necessary to solve a number of problems associated with understanding the construction of this matrices.

2. REPRESENTATION OF THE STRUCTURE

2.1 Specific of Structure

The specificity of the optical absorption spectrum of active layers of optoelectronic devices is the unique energy spectrum in the tails of the band gap. Videlicet, a large number of energy conversions create a wide range of absorption. Therefore, for a description of the optical absorption spectrum of the amorphous matrix is necessary to know the distribution of energy levels in the band gap, i.e., the density of states depending on the type of construction of the base lattice [1].

2.2 Quantum Formalism for Amorphous Matrix

Since at disordered materials is not have long-range order, directly, we can not directly use the quantum formalism for amorphous materials. Quantitative evaluation of each type of defect can be set from the proposal even distribution of its components by volume material. This in turn makes it possible to input a certain periodicity of defects and taking into account the localization allows to describe the energy distribution in the band tails as [2]:

$$\begin{cases} E_c = E_a + C_{\sim} + 2A_{\sim} \cos\left(\vec{\mathbf{k}} \quad \vec{a}\right) \\ E_{d_j} = \left(\left(E_a + E_{a-1}\right)/2 + C_{d_j} + \xi_j\right) \left(1 + \sqrt{\ln\left(\cos\left(2\pi \cdot \vec{\mathbf{k}} \cdot \overrightarrow{\mathbf{b}_j}\right)\right)}\right) \end{cases}$$

A feature of this representation is the existence of two energy distributions embedded in each other. The solution for the E_c is similar to the solution for the crystal structure in the space of the wave vector \boldsymbol{k} [1] (Fig. 1), but with constants C_{\sim} and A_{\sim} which consider the irregular lattice. The second equation for E_{dj} is a builtenergy state in the band gap. In its energy E_a and E_{a-1} are determined by the energy levels in an isolated atom. The constant C_d order to C_{\sim} and is also respon-sible for the shift of the energy level in the structure, which is connected with the interaction of a periodic lattice and defect [3]. This relation must be considered in a more rigorous description of the inhomogeneous structure, for the condition of the weak interaction, they can be considered as constants. The shift in energy ξ is responsible for the details of the selected localized in the center of the mobility gap. Quantitative parameter is specified intervals defective component and is described below.

This distribution allows, in primary approximation, determine the energy structure of the ordered nano material. The first equation describes the position of the conduction band and gives the optical band gap of the semiconductor the defective. The second equation introduces both quantitative and qualitative assessment of disordered centers, i.e. it sets the offset in the E_g for *j*-type of defect $E_{dj} = ((E_a - E_{a-1}) / 2 + C_{dj} + \xi_j)$ and it describes the real spectrum.

Quantitative evaluation of the defective component for nanoscale matrix is concretized by entering the periodicity, that is inputting |bj| = bj in the second equation. This ratio is defined as the ratio of the defect centers N_{dj} to number of atoms in the base lattice N_c :

$$b_j = a \frac{N_{d_j}}{N_c},$$

with the coefficient of proportionality a, which is determined by the structure of a periodic lattice. Generally, this ratio is also a vector quantity, but in the simplest case it can be assumed as constant. Therefore, by setting the qualitative and quantitative parameters, we can be modeled the disordered structure.

The first equation forms the conduction band and virtually defines direct and indirect optical jumps. Subsequent *j* equations are giving a quantitative and qualitative assessment of built-in defect subsymmetry and provide a spectrum of localized centers by sequential displacement of energy $E_{dj} = ((E_a - E_{a-1}) / 2 + C_{dj} + j)$ for *j*-type imperfection.



 ${\bf Fig.}\,1-{\rm The}$ three-dimensional energy centers in the amorphous material

It is generally accepted that at the initial formation of the atomic packing the density of matrix from layer to layer is not homogeneous. This the ambiguity persists to a certain thickness and depends on the roughness of the substrate and on its structure. In addition, the palpable influence is impacting operating conditions precipitating the installation and applied techniques [2, 4].

Therefore, this leads to different distances between the atoms in the different layers. For this state of affairs the distance between atoms is modified, consequently it is forms a different size of band gap. Therefore, the energy distribution, which describes a periodic structure [5],

$$\begin{split} E\left(\vec{k}\right) &= E\left(k_{0}\right) + \frac{\hbar^{2} \left[\left(k_{x} - k_{0x}\right)^{2} + \left(k_{y} - k_{0y}\right)^{2}\right]}{2m_{1}} + \\ &+ \frac{\hbar^{2} \left(k_{z} - k_{0z}\right)^{2}}{2m_{2}} \end{split}$$

must be entered by averaging by E_c (dash dotted line in Fig. 1). Here the mass of the electrons in the atomic plane of m_1 and of the film growth direction m_2 , and $E(k_0)$ – the energy of an electron at the point k_0 .

3. THE ABSORPTION COEFFICIENT OF THE TRANSITION

Based on the assumptions introduced in the previous section, and considering the defect as a separate periodicity we can use the well-developed theory of the absorption of crystals. In this case, the allowed transitions cause the absorption coefficient [6]:

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$$\alpha = \frac{1}{\pi} \frac{e^2}{m^2 c n \omega} \int d^3k \left| \vec{\mathrm{ep}}_{cv} \right|^2 \delta \left[\varepsilon_c \left(\vec{\mathrm{k}} \right) - \varepsilon_v \left(\vec{\mathrm{k}} \right) - \hbar \omega \right]$$

where \vec{e} – the unit vector, \vec{p}_{cv} – the transition matrix for the momentum, e – electron charge, c – the speed of light, n – refractive index of the material, ε_c – the energy of the conduction band, ε_v – the energy of the conduction band, $\hbar\omega$ - the energy of the transition.

Therefore we obtain the absorption coefficient for direct transitions:

$$\alpha_{per} = \frac{2e^2}{m^2 cn\omega} \left(\frac{2\mu}{\hbar^2}\right)^{3/2} \sum_{j=1}^{R} \left|\vec{\mathrm{ep}}_{cvj}(0)\right|^2 \left(\hbar\omega - \varepsilon_{0j}\right)^{1/2}.$$

For indirect transition zone-zone:

$$\alpha_{for} = \frac{2e^2}{3m^2 cn\omega} \left(\frac{2\mu}{\hbar^2}\right)^{5/2} \sum_{j=1}^{R'} \left|\frac{\partial}{\partial \vec{\mathbf{k}}} \left[\vec{\mathrm{ep}}_{cvj}(0)\right]\right|^2 \left(\hbar\omega - \varepsilon_{0j}\right)^{3/2} \,. \label{eq:aformula}$$

Accounting for the defective portion of the amorphous semiconductor gives account of the absorption coefficient of the defect parameters:

$$\alpha_{a}(\lambda) = \sum_{j=1}^{K} \frac{4\pi e^{2} s_{j} b_{j} \omega^{2} \gamma_{j}}{cm \left[\left(\left(\xi_{j} + \frac{E_{g}}{2} \right)^{2} - \omega^{2} \right)^{2} + \omega^{2} \gamma_{j}^{2} \right]}$$

CONCLUSION

Based on the above mentioned model representations of active photovoltaic layers of semiconductor devices, it is possible to draw the following conclusions.

The absorption coefficient of amorphous semiconductors which are used as active layers in optoelectronic devices may describe as the sum of the pseudo crystalline and amorphous components.

Effective management of the absorption spectrum of the optical receiver is possible by using the energy spectrum in the tails of the band gap of the amorphous semiconductor.

Quantifying the value of the absorption coefficient is achieved by increasing the parameter b_j , scilicet, we are setting the periodicity and regularity of defects.

The frequency absorption spectrum is determined by the coefficient ξ_j , which are characterizes the existence of a specific vibration mode.

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