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Examination of Absorption Spectra of Amorphous Silicon in the Infrared Range

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The paper discusses the amorphous materials in terms of absorption of electromagnetic infrared radiation (IR) as the integral characteristic of a photoelectric converter. The spectrum obtained experimentally was shown with the consideration of the main absorption peak. The interaction physics was described and the basic characteristics of the main defect levels was defined which strongly influence the absorption of optical radiation.

Keywords: Polycrystalline and amorphous materials, Quantum structure, Stoichiometric and structural parameters, Band gap, Defect centres, IR spectrum, Hydrogenated silicon, Absorption.

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1. THEORETICAL FOUNDATIONS

The integral parts of modern optoelectronics are thin-film converters whose efficiency is already close to the efficiency of single-crystal devices. They are based on polycrystalline and amorphous materials, which are used as receivers and transform matrices of photoelectric elements. However, the obtaining of strictly disordered semiconductors with optimal optical properties is technologically challenging task. Nevertheless, the implementation of this task is the importance of application of these materials in the semiconductor industry. It is necessary to solve a number of problems related to the understanding of the processes taking place in the matrix material for further producing of structures with optimal parameters [1-3].

The purpose of our work is to describe the quantum structure of the active layers of optoelectronic devices by the determinacy of the energy spectrum in the tails of the band gap and determination of the absorption coefficient of the atomic structure [4]. To fully understand the process it is necessary the theoretical justification based on micro- and macroparameters, and the agreement with the experimental results. To explain the optical and the electrical processes in amorphous structures we proposed a model for describing the optoelectronic characteristics of disordered matrix, based on the stoichiometric and structural parameters.

2. DETERMINACY OF DEFECT LEVELS IN AMORPHOUS SILICON

Currently, there are several models of the interaction of optical radiation with amorphous semiconductors. Nonetheless, the complexity and diversity of amorphous and polycrystalline materials require additional recesses in the theory of interaction. At the same time, despite the complexity of the theoretical representation of the absorption coefficient of amorphous material the sequential approximation can decrypt the passing spectrum of amorphous silicon and determine the defective spectrum in band tails. The attractiveness of a-Si as promising material optoelectronics is its bandwidth, which is provided not only by increasing the optical band gap, but the presence of a large number of defect centres, giving numerous quantum transitions. Therefore, we considered the IR spectrum of amorphous silicon in long wavelengths (Fig. 1).

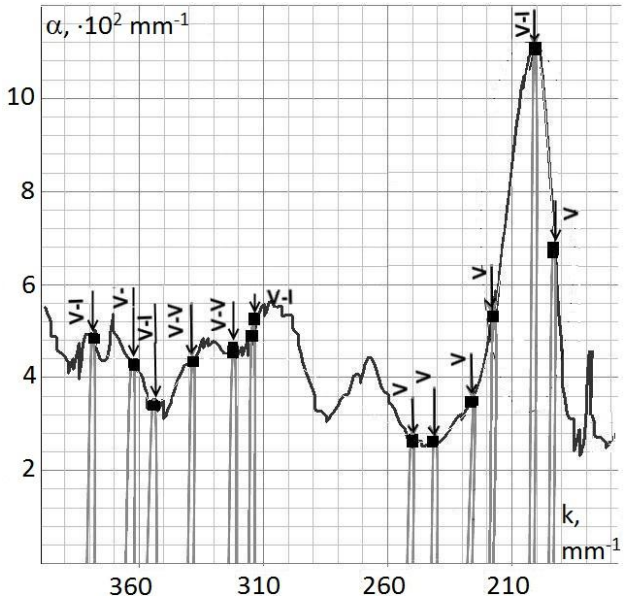

Fig. 1 – Infrared absorption spectrum of amorphous silicon films in the range of wave numbers of 160-390 mm^{-1}. The insert is the detailed examination of the peak in the range of 190-220 mm^{-1}

The experimental film samples were hydrogenated silicon (a-Si and a-Si: H) and were obtained on a magnetron type URM3.279.014 installation at a pressure in the working chamber 10^{-2}-10^{-3} Pa, a voltage and a current of the target – 500-650 V and 1.5-2 A respectively. The growth rate of the films was 0.1-0.4 m/min [5].

As the basis of substrates used in the deposition of films based on the structure of the glass-ceramic (SCHEO 781,001 0y, SchU 7. 002-15 817, St-50-1-1-0.6) and high-quality glass. The glass substrate having the optical transparency serves as a protective screen against external influences for the thin films, in particular from the interaction with oxygen, and mechanical damage.

The main structure of noncrystalline silicon is warp of its tetrahedral symmetry and can have many irregularities. Basic from them we can consider as the vacancy atoms in the nodes (V), interstitial (I) lattice (Fig. 1), as well as charged and neutral divacancy ($V\text{-}V^{-}$, $V\text{-}V^{+}$, $V\text{-}V^{0}$) and the complex with donor and acceptor impurities [6, 7].

The experimental absorption spectrum is a complex curve having mixed picture noise (Fig. 1). For understanding the physics of the interaction, we have analyzed all possible defective components taking place in defect formation in amorphous silicon.

According to the experimental data, selected continuous spectrum was represented by the sum of the absorption coefficients at fixed wavelengths:

$$\alpha_a(\lambda) = \alpha_1(2.64) + \alpha_2(2.76) + \alpha_3(2.82) + \alpha_4(2.95) + \alpha_5(3.1) + \alpha_6(3.18) + \alpha_7(4.0) + \alpha_8(4.13) + \alpha_9(4.43) + \alpha_{10}(4.59) + \alpha_{11}(4.96) + \alpha_{12}(4.17),$$

where in brackets there is the wavelength in micrometres.

To determine the nature of each absorption coefficients, we compared the set of resonators formed by defect centres in the forbidden zone. So α(2.64), from our point of view, belongs to a proper interstitial atom located on level $E = (E_c - 0.47)$ eV ± 0.04 eV.

Absorption coefficient at 2.95 microns is due to the interaction of a vacancy with the impurity atom of phosphorus. As the acceptor level, it forms the energy centre on $E = (E_c - 0.44)$ eV ± 0.04 eV. More complicated is the energy centre at 0.4 eV. The physics of its formation is very ambiguous and depending on the nature of forming the semiconductor structure may be different. On the one hand, it can be represented by the self-interstitial atom located in the split dumbbell state of the electron, which can be interpreted as a double interstitial. On the other hand, the same energy level takes a complex vacancy with a hydrogen atom having acceptor properties, or the vacancy combining with itself similarly forms divacancy. Almost merging with the energy centre at 0.39 eV, the vacancy combining with interstitial centred on 314.5 mm^{-1}, forms the following absorption peak.

The next group of defect centres lies in the region of 190-220 mm^{-1}. A vacancy in this spectral region forms the energy centre: $E = (E_c - 0.27)$ eV ± 0.03 eV, whereas an interstitial defective silicon atom is located on the 0.25 eV below the conduction band. Resonant absorption at the centre wavelength of 5.17 microns is either a vacancy or a divacancy.

The contact of centres with microscopic parameters of silicon structure is performed by the selection of coefficients b_j and ξ_j, characterizing completely amorphous materials. The first parameter indicates the frequency of this type of considered defect in the material, in turn ξ_j, allows us to estimate the energy level relative to the mid-energy band gap. Description of the whole spectrum requires a long calculation and is the subject of our further research. As the efficiency of the approach we have attempted to describe the peak at the interval of 190-220 mm^{-1}, which is shown in more detail in the inset in Figure 1. This monopeak of absorption, from our point of view, is formed by the three defect levels: the vacancies occurring at the level of 0.27 eV from the conduction pseudozone, interstitial silicon atoms lying at 0.25 eV, double divacancy on 0.24 eV.

Qualitative and quantitative model calculation gave the following values b_j and ξ_j. For the first level of the defect located at a wavenumber of 217.7 mm^{-1}, the calculated values of b_j totalled about $3.8 \cdot 10^6$ at approximately 0.63 eV for ξ_j. With regard to the second level with the wave number 201.6, it is characterized by the value $b_j = 7.7 \cdot 10^6$ and $\xi_j = 0.65$ eV. Double divacancy with wavenumber of 193.6 cm^{-1} has $b_j = 1.5 \cdot 10^6$ and $\xi_j = 0.66$ eV.

3. CONCLUSIONS

Technologists need to solve the problem of obtaining materials with certain distribution of defects necessary for absorption of optical radiation. The resulting absorption spectrum can provide the important information about the internal structure of amorphous silicon, namely, about the number and location of impurity centres.

Based on these results, the oscillation modes were identified, allowing to determine the energy distribution in the tails of the band gap (ξ_j) and determine the frequency of each of the types of defects (b_j), which reveal the internal structure of the material.

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