Interpretation of infrared spectra of chalcogenide glasses $Se_{95}As_5$ impurited by samarium

Mekhtiyeva S.I, Isayev A.I, Alekberov R.I, Mammadova H.I.

Institute of Physics named after academician G.M. Abdullayev's of the Azerbaijan National Academy of Sciences, AZ1143, Baku, G. Javid Ave131

E-mail: rahim-14@mail.ru

Abstract

In work investigated with method IR of spectroscopy of amorphous selenium andsystem $Se_{95}As_5$ containing impurity samarium. It is certain that, in IR a spectrum of amorphous selenium due to hypervalent defects maxima with different intensity are observed in 230 and 270 cm^{-1}.Increase of the concentration of impurity samarium in spectrum $Se_{95}As_5$, the maximum arises with $400cm^{-1}$ frequency which, are connected with $SmSe_3$ structural elements.

Keywords

Glass-like semiconductor; charged defects; amorphous

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1. INTRODUCTION

Glass-like semiconductor As-Se are more intensive investigatedin comparison with other semiconductors [1,2]. This is connected with their as active layers application in the different optoelectronic and diffraction-devices, planar wave guides, DVD disks, etc. Influence of samarium impurities on the infrared spectrum (IR) of system $Se_{95}As_5$ has been investiqated in this work. In the system As_xSe_{1-x} existing as positive samarium ions influences on the concentration of charged defects, the neutralhipervalence and diamagnit defects which sharply changes optical properties of the system.

II.EXPERIMENTAL METHOD AND DISCUSSION OF THE OBTAINED RESULTS

CGS synthesis of $Se_{95}As_5$ composition with Sm impurity is carried out by melting appropriate qualities of chemical elements of special purity in vacuum guartz ampoules up to 10^{-6} mm Hg at T above 900^0C in rotating furnace with subseguent cooling in regime Off-furnace.The impurity is introduced during the synthesis, its concentration is within 0.01 ÷1 at%.

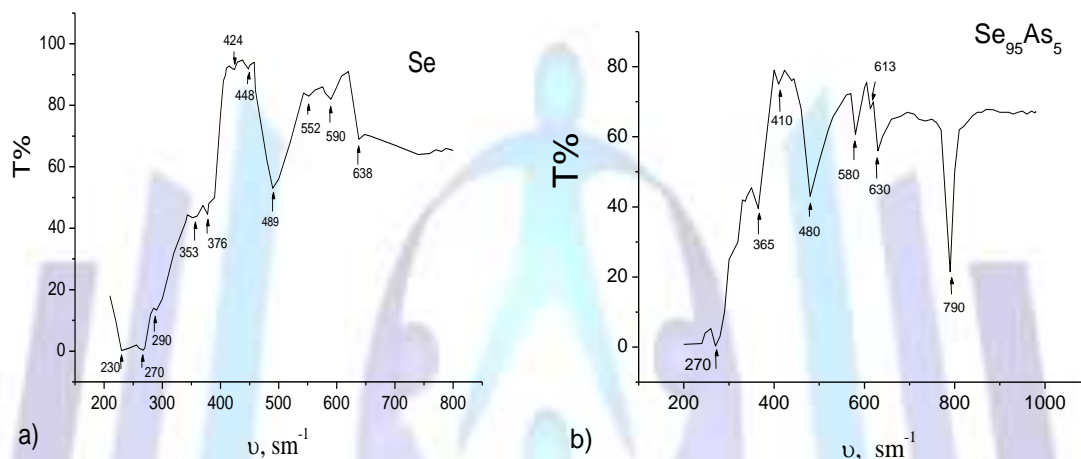In Fig.1 there has been shown spectrums of the IR of the amorphous selenium (a) and of $Se_{95}As_5$ system (b).

Fig.1. Spectrums of the infrared transmission of the amorphous selenium (a) and of $Se_{95}As_5$ system (b).

As it seen from spectrum, the IR transmission of the amorphous selenium consist of different frequency ($230 \div 638$ cm^{-1}) maxima. Addition of the arsenic atoms to selenium leads to slip of the maximums concerning to the selenium to the side of little energies ($\nu=376 \to 365$ cm^{-1}; $424 \to 410$ cm^{-1}; $590 \to 580$ cm^{-1}; $638 \to 630$ cm^{-1}).

In this case maxima ($\nu=353$ cm^{-1}; 448 cm^{-1}; 552 cm^{-1}) of IR spectrum are connected with selenium partial or completely disappear, but diff for frequencies $\nu=613$ cm^{-1}; 790 cm^{-1} maximaarises owing arsenic atoms. In Fig.2 there has been shown spectrums of the infrared transmission of $Se_{95}As_5$ system containing Sm impurities. The influence on the spectra of infrared transmission of $Se_{95}As_5$ system of the samarium impurities are of complex character. In the IR spectra of the amorphous selenium intensity of the maxima with $\nu=230$ cm^{-1}; 270 cm^{-1}; 290 cm^{-1} frequencies sharply decreases with increase in the concentration in of impurity (0,005 to 0,6at% Sm), but in $Se_{95}As_5$ system clean and with Sm impurity less than (0,005 at %) the maximum with $\nu=365$ cm^{-1} frequency does not change energetically. Despite its fact , in the IR spectra of the amorphous selenium observed the weak maximum with $\nu=424$ cm^{-1}; 448 cm^{-1}; 552 cm^{-1} frequencies almost, is not almost observed.

In the IR spectra of the amorphous selenium and the $Se_{95}As_5$ system maxima with $\nu=638$ cm^{-1}; 590 cm^{-1}; 806 cm^{-1} frequencies under influence of the impurity of 0,005 at% Sm slips to side high energies ($590 \to 605$ cm^{-1}; $790 \to 806$ cm^{-1}; $638 \to 640$ cm^{-1}). At rather the large concentration samarium impurity in the spectrum the novel maximum $\nu=400$ sm^{-1} with the intensity is clearly observed.

According to modern ideas [3, 4] the optical, electrical and other properties of the glass-like semiconductors are mainly determined with charged defects existing in them. In these semiconductors of the electron paramagnetic resonancedoes not observing which is connected with existence of neutral and diamagnetic defects [5]. At the present, for the glass-like semiconductors more are a number of models reflecting existence of different defects cases [6,7,8]. Among these the widest is the model with changing valence of charged defects (VAP) [6]. According to this model amorphous selenium has the positive and negative charged coordination defects (C_3^+, C_1^-). These defects in mainly exist in two forms.

1. In the external boundary of the selenium chain and 2 inside of the chain

In the model with hypervalent configuration defects it is assumed that the amorphous semiconductor consists of diamagnetic and neutral defects with high coordination atoms [7,8]. The coordination number of such atoms in semiconductor is the crystal atoms coordination number with the same composition.

As it seen from the IR spectrum of the amorphous selenium the volume of the coefficient optical transmissioncoefficient for low frequencies is very little. In deferent works are explained the nature of the maxima with $\nu=230$ cm^{-1} və 270 cm^{-1} frequencies. During the long period the structure of amorphous selenium is mostly the mixture of, i.e. it consists of eight member rings and spiral chains [5]. These elements of the structures are connected with of the weak Wan-Der-Walsstrengths with each other. But the connection between eight rings (Se$_8$) and chains (Se$_n$) has the covalence feature.
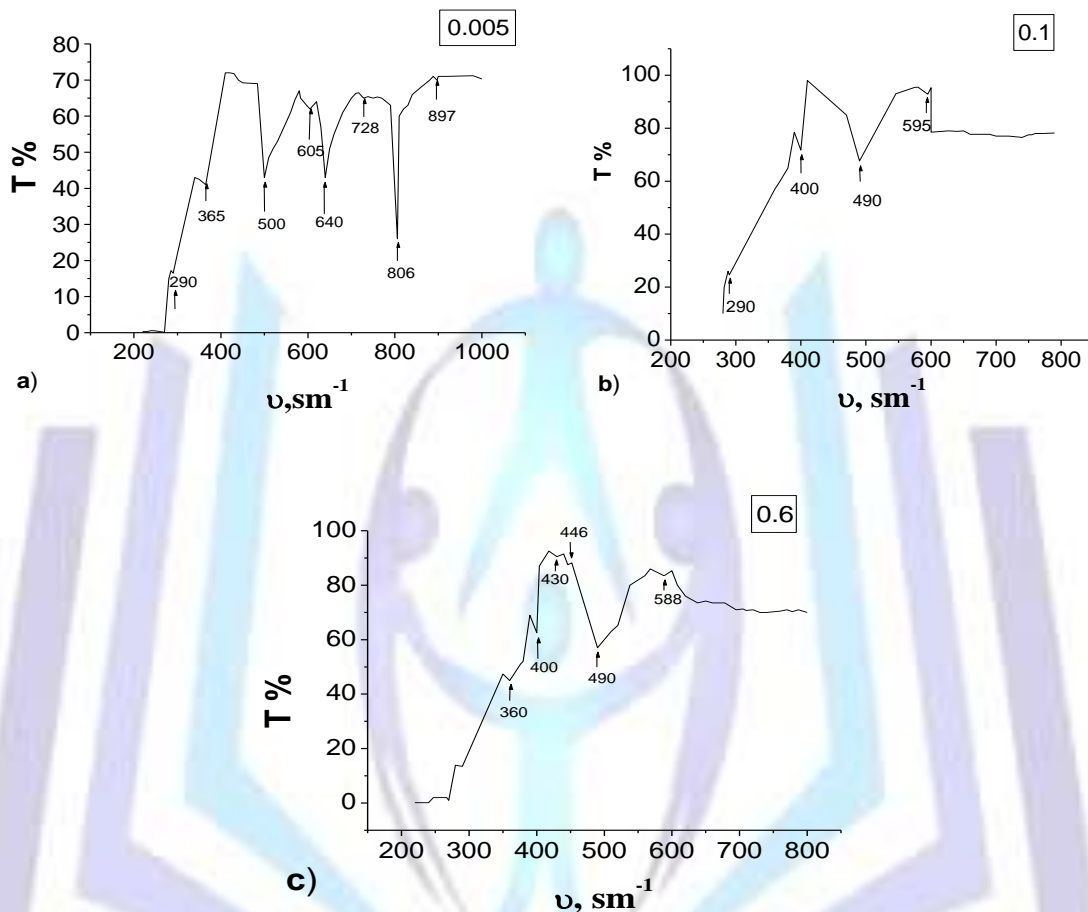

Fig.2 Spectrums of the infrared transmission of Se$_{95}$As$_5$ system with Sm impurity.

a)Se$_{95}$As$_5$:Sm$_{0.005}$; b) Se$_{95}$As$_5$:Sm$_{0.1}$; c) Se$_{95}$As$_5$:Sm$_{0.6}$

The radial distribution function of the amorphous selenium conform of structural models received by different methods which are known from the crystal modifications of the selenium have been guided mostly existence two kind of structural elements. It is known that the trigonal selenium consists of the like spiral chains parallel directed. The atoms inside these chains are situated in the distance 2,32A^0 from each other and the angle of between them is 105^0 A^0. In this case the distance between neighbour chains is 3,46A^0. But the monocline selenium exists in α and βforms. Both of these are formed from eight member rings which are bent. The angle and length of the bond are similar to the trigonal selenium.

But, differently from the trigonal selenium which in the monocline selenium sign of the angle of the bondchanges. Investigations show that the IR and Raman spectra of the amorphous selenium show that consists of not only Se$_8$ rings in [9]. There fore for the structure of the amorphous selenium must be used to the model of chaotic chain. According to this model the atoms of the amorphous selenium is the chain like form. According to investigations observed maxima with $\nu=237$ cm^{-1} and 252 cm^{-1} frequences in the Raman spectrum of the amorphous selenium are connected with Se-Se-Se chains and Se$_8$ rings[10]. The maximum with $\nu=260$ cm^{-1} frequency of the IR spectra are connected with Se$_8$ rings [11]. But, investigations show that the maxima with $\nu=229$ cm^{-1}and 271 cm^{-1} frequences in the IR spectrum of the amorphous selenium are connected with the hypervalent configuration have been eight members rings defects[7]. It is seen from the **fig.1** maxima with 230 cm^{-1} and 270 cm^{-1}frequency confirm the results obtained from the model HVK defects [7].

We noted that the energy of the charges defects is was bigger, than the energy of the HVK defects. On the other hand the energy bond of the charges defects depends on their structure state, too. It is assumed that length of the bond of the

charges defects is less than the length of the bond of the changing valence pairs arising in the outside of the selenium chain but, the energy of the bond is big.

In fig.1 the maxima with $\nu=237$ cm^{-1} and 252 cm^{-1} frequences in IR spectrum of the amorphous selenium and the maxima with $\nu=290$ cm^{-1}; $\nu=353$ cm^{-1} və $\nu=376$ cm^{-1} frequences in the around zone of the base absorption are connected with charge defects (VAP-defects) in outside of the selenium chain. In this case the maxima with the big energies ($\nu=424$ cm^{-1}; 448 cm^{-1}; 490 cm^{-1}; 552 cm^{-1}; 590 cm^{-1}; 638 cm^{-1}) are explained with arising in the chain inside of charge defects. Differing sharply of the maxima concerning with inside charge defects are explained with homogeneous distribute of their concentration in the structure of the amorphous selenium. Adding to the selenium in the x=5 at% amount of the arsenic creates as the $As(Se_{1/2})_3$ structure elements. This structure elements are consist of with less energies homopolar(As-As və Se-Se) and big energies heteropolar(As-Se) bonds. In the IR spectra of $Se_{95}As_5$ system observing the maxima with $\nu_1=613$ cm^{-1} və $\nu_2=790$ cm^{-1} frequenciesare explained with bonds of As-Se and As-Se-Se [12]. Increase of the concentration of impurity samarium in spectrum $Se_{95}As_5$, the maximum arises with 400cm^{-1} frequency which, are connected with $SmSe_3$ structural elements.

III. CONCLUSION

It is established that increase of the concentration of impurity samarium in spectrum $Se_{95}As_5$, the maximum arises with 400cm^{-1} frequency which, are connected with $SmSe_3$ structural elements. Addition to selenium of arsenic (5 at %) leads to occurrence of two additional peaks in high-frequency area (613 and 790 cm^{-1}). These facts are connected with structural units $As(Se_{1/2})_3$ in glass.

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