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CALCULATION OF THE EINSTEIN COEFFICIENTS FOR CO DOPED (80 − x)Sb_2O_3−20Na_2O−xWO_3 (x% mol of WO_3) GLASSES

P. Petkova, P. Vasilev

SHUMEN UNIVERSITY "KONSTANTIN PRESLAVSKY", 115
UNIVERSITETSKASTREET, 9712 SHUMEN, BULGARIA

Abstract: *We have measured the absorption of the glasses (80−x)Sb_2O_3−20Na_2O−xWO_3 (x% mol of WO_3) in the spectral regions 10 500 – 24 500 cm^{-1}. The samples are doped with 0.05% mol of Co_3O_4 from x = 10% until x = 50%. The observed absorption band is due to the Co-impurity in the visible spectral region. This absorption band of glasses contains information about the exactly values of the Einstein coefficients which will be useful for their application in laser technologies.*

Key words: *Co doped glasses, absorption coefficient, Einstein coefficients*

1. Introduction

The antimony oxide as part of the heavy metal oxide (HMO) glasses is attractive to researchers in recent years. These glasses have low energy of photons, high refractive indexes and they are conductive to study in IR region [1, 2]. They are used as nonlinear optical amplifiers and lasers. The cobalt doped glasses were synthesized in silicate crucibles. The content of 0.05%mol Co_3O_4 is added to the combination Sb_2O_3–WO_3–Na_2O [3]. The glasses are synthesized after mixing and melting of the starting materials at room temperature. The cobalt is used as a colouring agent [4]. The undoped glasses have yellow colour. The blue colour of 10% mol WO_3 transforms in green (40% mol WO_3), when the speed of appending increases. Spectroscopic studies on transition metal doped glasses have been implemented in the scope of active applications while the ability of tungsten, to have several oxidation states open possibilities for their application in the laser technologies. These materials are suitable for the study of the macromolecular segments arranged in the crystalline phase with the various X-ray methods [5]. This is the reason of the investigation of Co doped (80−x)Sb_2O_3−20Na_2O−xWO_3 in our work.

2. Experiment and results

The experimental set up for the measurement of the absorption spectra consists of: a halogen lamp with a stabilized rectifier 3H-7, a monochromator

SPM-2, a system of quartz lenses, a polarizer, a crystal holder with a sample and a detector of Hamamatsu S2281-01.

The investigated glasses are two series: undoped (80 − x)Sb_2O_3−20Na_2O−xWO_3 and doped with 0.05% mol Co_3O_4. The values of x changes are from 10% mol WO_3 to 50% mol WO_3. The concentration of the cobalt ions in the glass structures is N = 3,01x10^{18} cm^{-3}.

The thickness of the glasses varies between 2.15 mm and 2.75 mm. The absorption spectra of the Co doped glasses are presented in the spectral region 10 500 – 24 500 cm^{-1}, where the Co structure is observed (Fig. 1). It is seen that the cobalt structure is complicated and its shape does not give information about the number of the electron transitions in Co^{2+} ion. Therefore, the calculation of the first derivative of the absorption coefficient gives information about the number of the electron transitions in the investigated Co complexes (Fig. 2). The exact energetic position of the electron transitions in the Co ion is determined by calculation of the second derivative of the absorption coefficient (Fig. 2).

3. Disscusion

Several parameters are commonly used to describe the strength of atomic and molecular optical transitions. The Einstein A and B coefficients, oscillator strengths f and transition dipole moments are all atomic and molecular parameters related to the "strength" of the transition. In many practical situations, on the other hand, it is useful to define an absorption coefficient to describe the absorption of a beam of light passing through a medium consisting of the atoms or molecules of interest. From a "kinetics" point of view, the absorption or scattering of radiation is described as a reaction or scattering process and the probability of absorption or scattering is given in terms of a cross section.

In this connection, the frequency-integrated absorption coefficient is equals to:

$$\alpha_0 = \int_{\omega_1}^{\omega_2} \alpha(\omega) d\omega \qquad (1).$$

The line shape function is given by the equation:

$$g(\omega) = \frac{\alpha(\omega)}{\alpha_0} \qquad (2).$$

The next important parameter is the frequency-integrated cross section:

$$\sigma_0 = \frac{\sigma_a(\omega)}{g(\omega)}, \qquad (3)$$

where $\sigma_a(\omega)$ is the absorption cross section. The cross-section of the impurity absorption is of great significance for the application of doped materials

in practice [6]. It is used to estimate how radiation is absorbed by the impurity ions in the crystals. The total cross-section $\sigma_a(\omega)$ of the impurity absorption is determined by the integration of the impurity ions within the absorption band

$$\sigma_a(\omega) = \frac{1}{N}\int_{\omega_1}^{\omega_2} \alpha(\omega)\, d\omega \qquad (4)$$

Where:

N is the number of the impurity ions in the unit volume;

$\alpha(\omega)$ is the impurity absorption coefficient, typical for the energy interval from ω_1 to ω_2.

The values of the oscillator strength are determined by the formula:

$$f = \frac{\sigma_0 \omega g(\omega)}{\sigma_a(\omega) 2\pi} \qquad (5).$$

The Einstein coefficient which characterized the induced absorption is:

$$B_{12}^{\omega} = \frac{\sigma_a(\omega)c}{\hbar\omega g(\omega)} \qquad (6).$$

The number n_1 of atoms in level 1 (per unit volume) that the beam intercepts is:

$$n_1 = \alpha(\omega)/\sigma_a(\omega) \qquad (7).$$

The next parameter R_{12} denotes the number of absorption events per unit time and per photon of frequency ω:

$$R_{12} = c\alpha(\omega) \qquad (8).$$

The atomic frequency response is expressed by the next equation:

$$b_{12}(\omega) = \frac{\sigma_a(\omega)c}{\hbar\omega} \qquad (9).$$

The Einstein coefficient A_{12} describes spontaneous emission:

$$A_{21} = \frac{\sigma_0^3 \omega^2\, g^2(\omega)}{\sigma_a^2(\omega)\pi^2 c^2} \qquad (10).$$

The resonance frequency of the transition is determined as follow:

$$\omega_{21} = 2\pi f \qquad (11).$$

The ratio of the degeneracy factors g_1 and g_2 of the two levels is:

$$\frac{g_2}{g_1} = \frac{4\sigma_0}{\omega_{21}^2 A_{21}} \qquad (12).$$

The Einstein coefficient which characterized the stimulated emission is equal to:

$$B_{21}^{\omega} = \frac{B_{12}^{\omega}}{\left(\frac{g_2}{g_1}\right)} \qquad (13).$$

Our next step is connected with the determination of the absorption oscillator strength to the A value:

$$f_{12} = (g_2/g_1)\, 2\pi\varepsilon_0 mc^3/(\omega_{21}^2 e^2) \qquad (14).$$

The square of the transition dipole moment is given by:

$$\mu_{21}^2 = A_{21} \frac{3hc^3\varepsilon_0}{2\omega_{21}^3} \qquad (15).$$

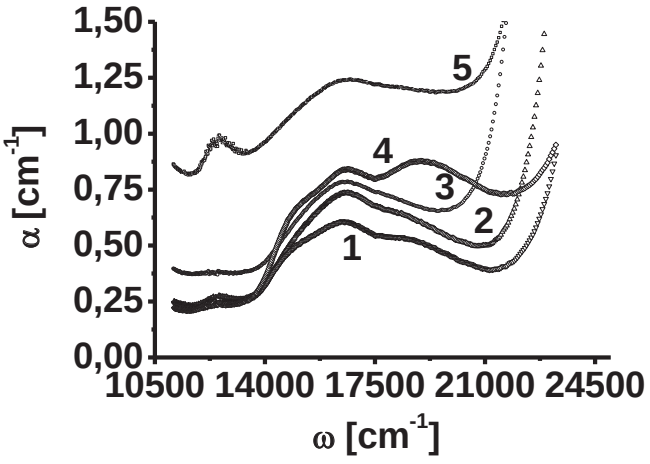

Fig. 1 The absorption spectra of the cobalt doped glasses $(80-x)Sb_2O_3-20Na_2O-xWO_3$ (x% mol of WO_3) in the spectral region 10 500 – 24 500 cm^{-1} as follow: 1 – 10 mol% WO_3; 2 – 20 mol% WO_3; 3 – 30 mol% WO_3; 4 – 40 mol% WO_3; 5 – 50 mol% WO_3.

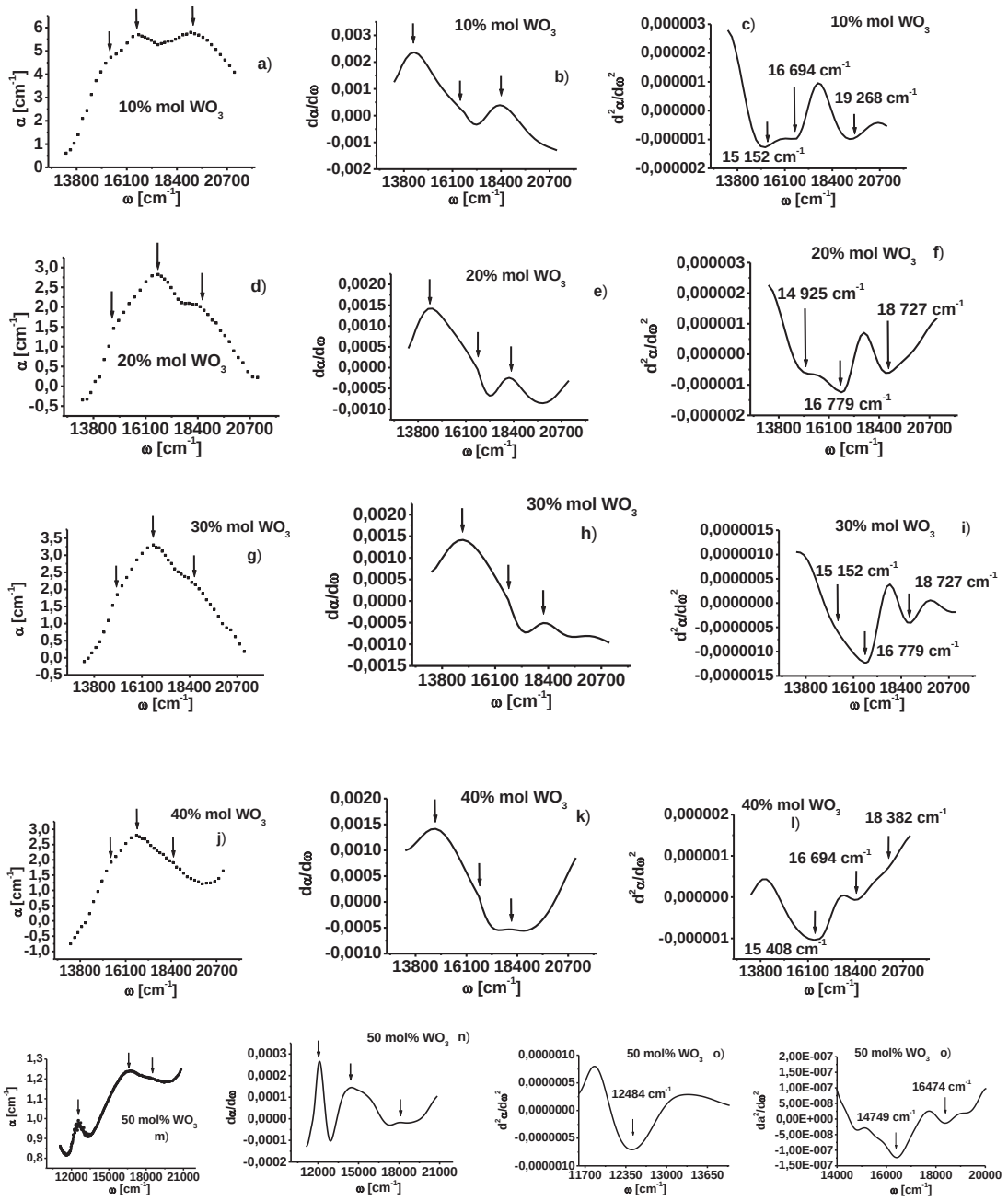

Fig. 2 The second derivative of the absorption coefficient of the cobalt doped glasses $(80-x)Sb_2O_3-20Na_2O-xWO_3$ (x% mol of WO_3) in the spectral region 10 500 – 21 000 cm^{-1}.

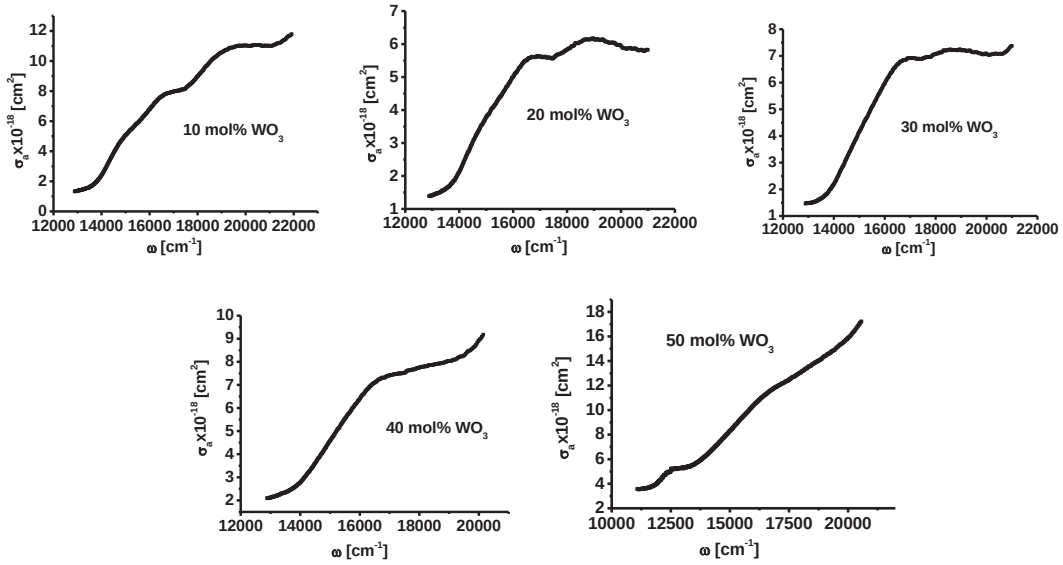

Fig. 3 The impurity cross section as function of the frequency of the cobalt doped glasses $(80-x)Sb_2O_3-20Na_2O-xWO_3$ (x% mol of WO_3) in the spectral region 10 800 – 22 250 cm^{-1}.

Table 1 Parameters which describe the strength of atomic and molecular optical transitions when x = 10% mol of WO_3.

e- tran-sition	B_{12}^{ω}	$b_{12}(\omega)$	A_{21}	B_{21}^{ω}	μ_{21}^2
ω_1	0,0921x10^{24}	0,0987x10^{20}	1,993x10^{-27}	0,0215x10^{15}	1,3615x10^{40}
ω_2	0,1007x10^{24}	0,1326x10^{20}	2,9154x10^{-27}	0,0346x10^{15}	1,4898x10^{40}
ω_3	0,1163x10^{24}	0,1586x10^{20}	5,176x10^{-27}	0,0709x10^{15}	1,7203x10^{40}

Table 2 Parameters which describe the strength of atomic and molecular optical transitions when x = 20% mol of WO_3.

e- tran-sition	B_{12}^{ω}	$b_{12}(\omega)$	A_{21}	B_{21}^{ω}	μ_{21}^2
ω_1	0,0531x10^{24}	0,0693x10^{20}	1,098x10^{-27}	0,0117x10^{15}	0,7841x10^{40}
ω_2	0,0594x10^{24}	0,0949x10^{20}	1,7452x10^{-27}	0,0208x10^{15}	0,8768x10^{40}
ω_3	0,0663x10^{24}	0,0931x10^{20}	4,0759x10^{-27}	0,0543x10^{15}	1,4756x10^{40}

Table 3 Parameters which describe the strength of atomic and molecular optical transitions when x = 30% mol of WO_3.

e- transition	B_{12}^{ω}	$b_{12}(\omega)$	A_{21}	B_{21}^{ω}	μ_{21}^2
ω_1	0,0653x10^{24}	0,0912x10^{20}	1,4138x10^{-27}	0,0152x10^{15}	0,9647x10^{40}
ω_2	0,069x10^{4}	0,1151x10^{20}	2,029x10^{-27}	0,0242x10^{15}	1,0217x10^{40}
ω_3	0,0748x10^{24}	0,1091x10^{20}	3,0571x10^{-27}	0,0407x10^{15}	1,1049x10^{40}

Table 4 Parameters which describe the strength of atomic and molecular optical transitions when x = 40% mol of WO_3.

e- transition	B_{12}^{ω}	$b_{12}(\omega)$	A_{21}	B_{21}^{ω}	μ_{21}^2
ω_1	0,0745x10^{24}	0,0982x10^{20}	1,6953x10^{-27}	0,0186x10^{15}	1,1001x10^{40}
ω_2	0,0805x10^{24}	0,1233x10^{20}	2,3306x10^{-27}	0,0277x10^{15}	1,1904x10^{40}
ω_3	0,0885x10^{24}	0,1214x10^{20}	3,4193x10^{-27}	0,0447x10^{15}	1,3092x10^{40}

Table 5 Parameters which describe the strength of atomic and molecular optical transitions when x = 50% mol of WO_3.

e- transition	B_{12}^{ω}	$b_{12}(\omega)$	A_{21}	B_{21}^{ω}	μ_{21}^2
ω_1	0,2816x10^{24}	0,2544x10^{20}	3,4095x10^{-27}	0,0303x10^{15}	4,1629x10^{40}
ω_2	0,1485x10^{24}	0,1485x10^{20}	2,9646x10^{-27}	0,0311x10^{15}	2,1955x10^{40}
ω_3	0,0736x10^{24}	0,0856x10^{20}	2,0473x10^{-27}	0,024x10^{15}	1,0882x10^{40}

Conclusions:

The cross-sections of cobalt absorption are similar in the cases of x = 20 mol% WO_3 and x = 30 mol% WO_3 and in the cases of x = 10, 40 and 50 mol% WO_3.

There have been calculated and compared Einstein A and B coefficients and transition dipole moments for all Co doped glasses (x = 10-50 mol% WO_3). The spontaneous emission of glasses increases when the concentration of WO_3 increases. The same situation is observed with values of transition dipole moment. These two conclusions are not valid in the case of x = 50 mol% WO_3

Acknowledgments

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References

[1] T. Abritta, F. H. Black, J. Lumin., 48 558 (1991).
[2] M. B. Camargo, R. D. Stultz, M. Birnbaum, M. Kokta, Opt. Lett., 20 339 (1995).
[3] V. Sudarsan, S. K. Kulshreshtha, J. Non-cryst. Solids, 286 99 (2001).
[4] B. Ancora, M. Magini, A. F. Sedda, J. Chem. Phys., 88 2015 (1988).
[5] V.Velev, A. Popov, P. Kyurkchiev, L. Veleva, R. Mateva, Journal Scientific and Applied Research, Vol. 4 235 (2013).
[6] Optical Properties of Condensed Matter and Applications, Edited by Jai Singh, John Wiley & Sons (2006).