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SPECTROSCOPIC ELLIPSOMETRY STUDY OF PbSSe THIN FILMS OBTAINED BY CBD METHOD

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Abstract- **The spectroscopic ellipsometry method was applied to investigate the optical properties of PbSSe thin films obtained by chemical bath deposition. For a better resolution of the structure of interband transitions and for determination of critical points the function $\frac{d^2\varepsilon}{d\omega^2}$, obtained by numerical differentiation of the experimental data of the dielectric function $\varepsilon(\omega)$ is used. Fitting, i.e., the process of determining the theoretical dependences that can overlap with the experimental curve as much as possible, was performed with the "Graphical Analysis" program.**

Two critical points corresponding to the values of E1=1.6 eV and E2=3.2 eV are determined. For the first energy area the best fitting corresponded to the 2D critical point shape case ($m = 0$), and for the second energy area the best fitting corresponded to the 1D ($m = -\frac{1}{2}$) critical point shape case.

EXPERIMENTAL DETAILS

The solution used for the deposition of nanostructured PbSe thin films by CBD method is prepared by mixing of equal (13 ml) volumetric amounts of each of the following solutions: 0,07 M lead acetate ($Pb(CH_3COO)_2$); 0,3 M sodium hydroxide (NaOH); 0,06 M triethanolamine ($C_6H_{15}NO_3$) and 1:1 mixture of 0.17 M of sodium selenosulfate Na_2SSeO_3 with 0.17 M of thiourea $(NH_2)_2CS$. Sodium selenosulphate was prepared by refluxing 0,425 q. of selenium powder with 1,245 gm of anhydrous sodium sulphite (Na_2SO_3) in a three round bottom flask containing 100 ml of distilled water for 7 hours at 90^0C. Undissolved selenium particles were filtered out after the solution was cooled to room temperature. The resultant product yielded clear sodium selenosulphate solution [20].

The PbSSe thin films obtained in a 60 ml beaker on the cleaned in acidic media microscope glass substrate. Glass substrate was dipped into beaker vertically. The mixed solutions were stirred well magnetically. The bath temperature was kept at 50^0C. After a deposition period of 20 min. substrates were removed from the beaker, washed with distilled water and dried.

After these processes a deep brown, homogeneous, with good adhesion PbSSe ($PbS_{0.5}Se_{0.5}$) thin film was obtained on the glass substrate. X-ray diffractometric analyzes of PbSSe thin films were investigated by "D-8 ADVANCE" diffractometer for values of 2θ ranging from 20° to 70° for CuKα (λ= 1,54 A) radiation.

Optical measurements was carried out by "J. A. WOOLLAM COMPANY - M 2000 ELLIPSOMETER".

The measurements were performed at angles from 60 to 75 ° with a step of 5 ° in the spectral range of 0.74–6.45 eV. The angle of 60° was used for modeling; the thin film – semi-infinite substrate system was chosen as the model.

MAIN EXPRESSIONS

The method consists of fitting the second derivative of the complex dielectric function to standard analytic functions.

(1)

$$\varepsilon(\omega) = C - Ae^{i\theta}\ln(\omega - E + i\Gamma) \qquad m \neq 0 \qquad \textbf{(2)}$$

$$\varepsilon(\omega) = C - Ae^{i\theta}\ln(\omega - E + i\Gamma) \qquad m = 0$$

if we write in trigonometric form

$$\frac{d^2\varepsilon}{d\omega^2} = A^1(\Omega)^{(m-2)/2}\cos\left[(m-2)\arg\cos\left(\frac{\omega - E}{\Omega^{\frac{1}{2}}}\right) + \theta\right] + A^1(\Omega)^{(m-2)/2}\, i\sin\left[(m-2)\arg\cos\left(\frac{\omega - E}{\Omega^{\frac{1}{2}}}\right) + \theta\right] \qquad m \neq 0 \qquad \textbf{(3)}$$

$$\frac{d^2\varepsilon}{d\omega^2} = \frac{A}{\Omega}\cos\left[-2\arg\cos\left(\frac{\omega - E}{\Omega^{\frac{1}{2}}}\right) + \theta\right] + \frac{A}{\Omega}i\sin\left[-2\arg\cos\left(\frac{\omega - E}{\Omega^{\frac{1}{2}}}\right) + \theta\right] \qquad m = 0 \qquad \textbf{(4)}$$

ANALYSIS METHODOLOGY

To perform the fitting process, the real $d^2\varepsilon_1/d\omega^2$ and imaginary $d^2\varepsilon_2/d\omega^2$ components of the function (4) (for $m \neq 0$) or (6) (for $m = 0$) written in trigonometric form are used.

In other words, the curves $d^2\varepsilon_1/d\omega^2$ and $d^2\varepsilon_2/d\omega^2$ calculated from the experimental dependence of $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ participate to fitting with the curves $d^2\varepsilon_1/d\omega^2$ and $d^2\varepsilon_2/d\omega^2$ obtained from functions (4) or (6) and A, E, Γ and θ -parameters are determined for a better fitting condition.

It should be noted that the "Graphical analisys" proqram gives these constants as a result.

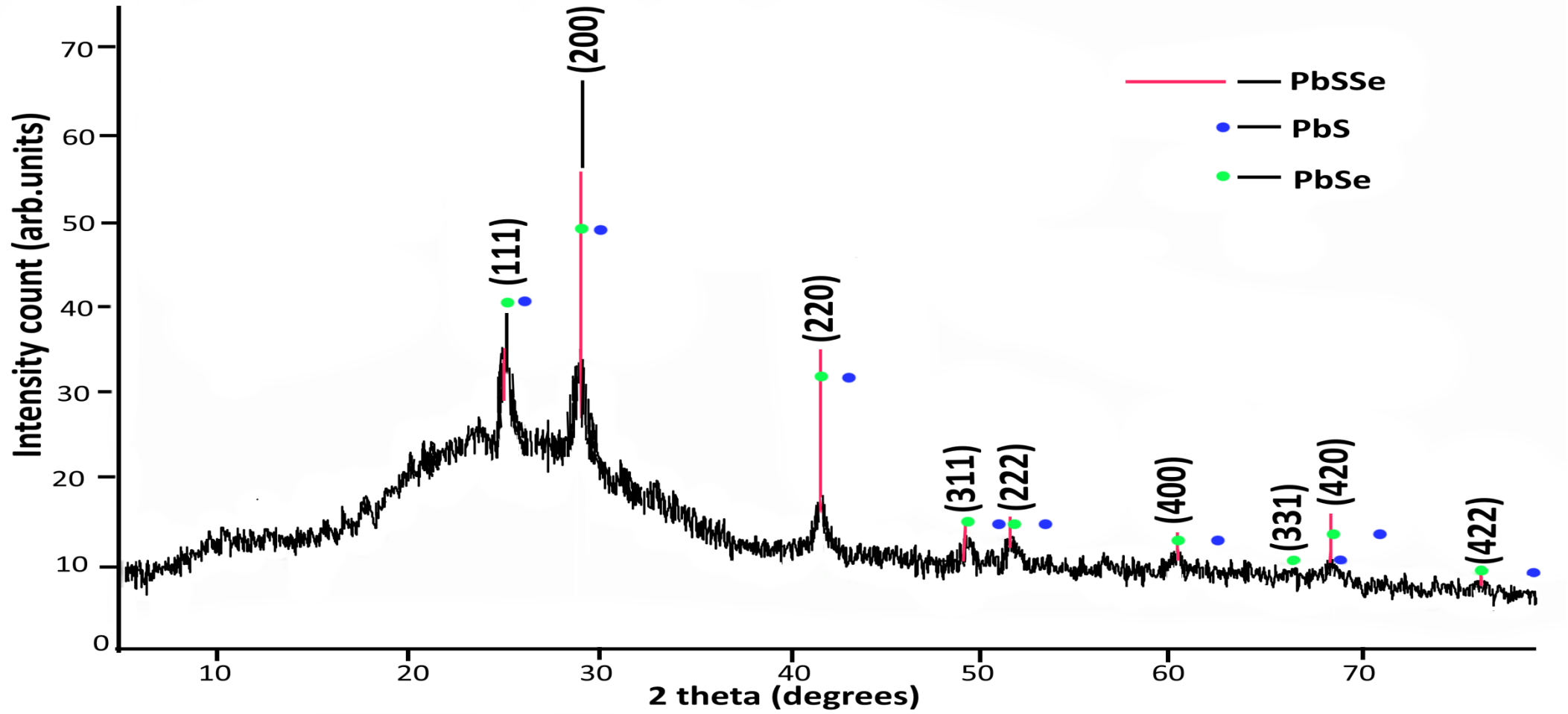

Figure 1. X-ray diffraction spectrum of PbSSe thin film obtained by chemical bath deposition (green and blue dots are peaks corresponding to PbSe and PbS compounds, respectively).

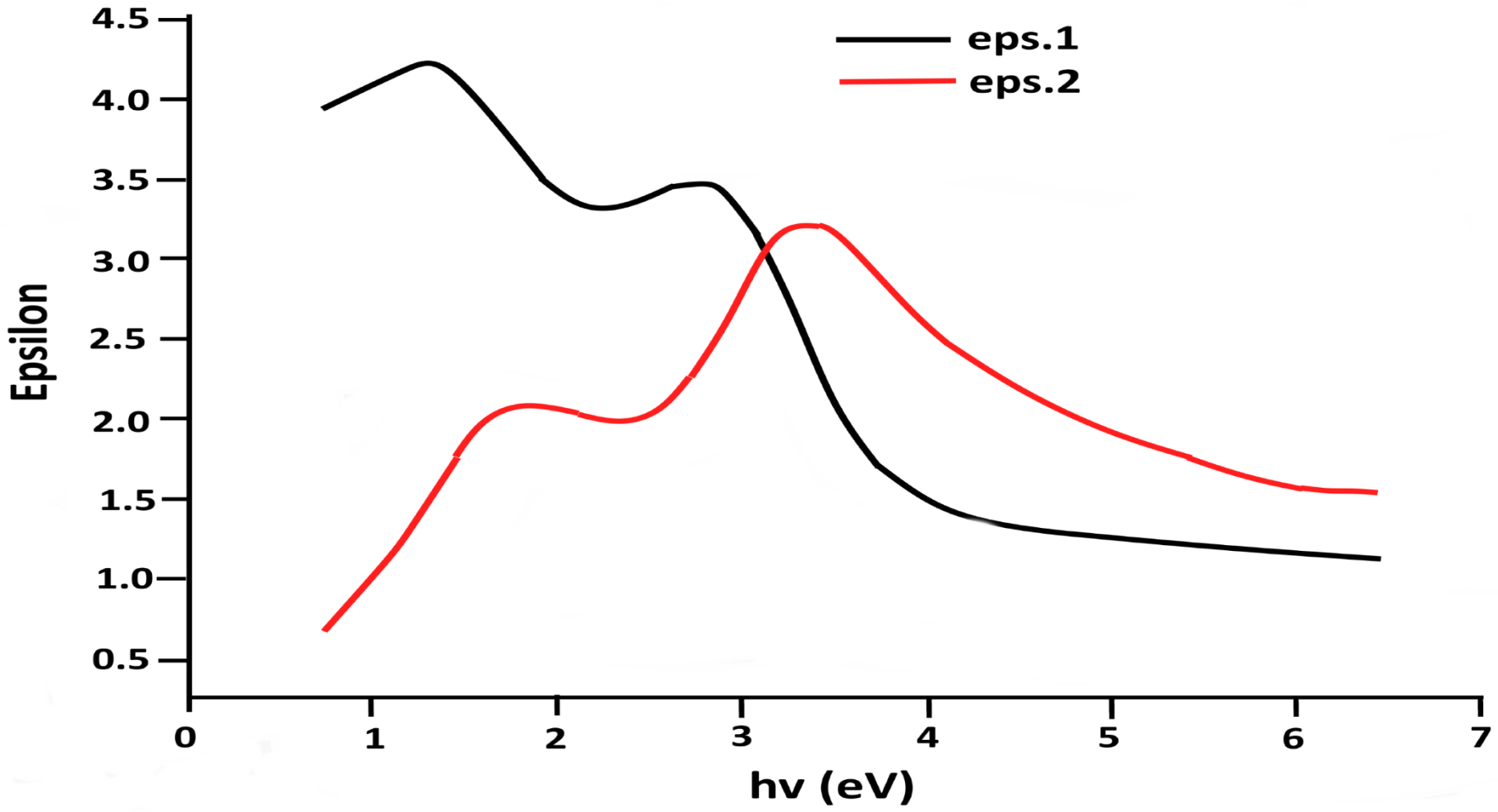

Figure 2. Spectral dependencies of the $\varepsilon_1(\omega)$ -real and $\varepsilon_2(\omega)$ -imaginary components of the complex dielectric function of PbSSe thin film

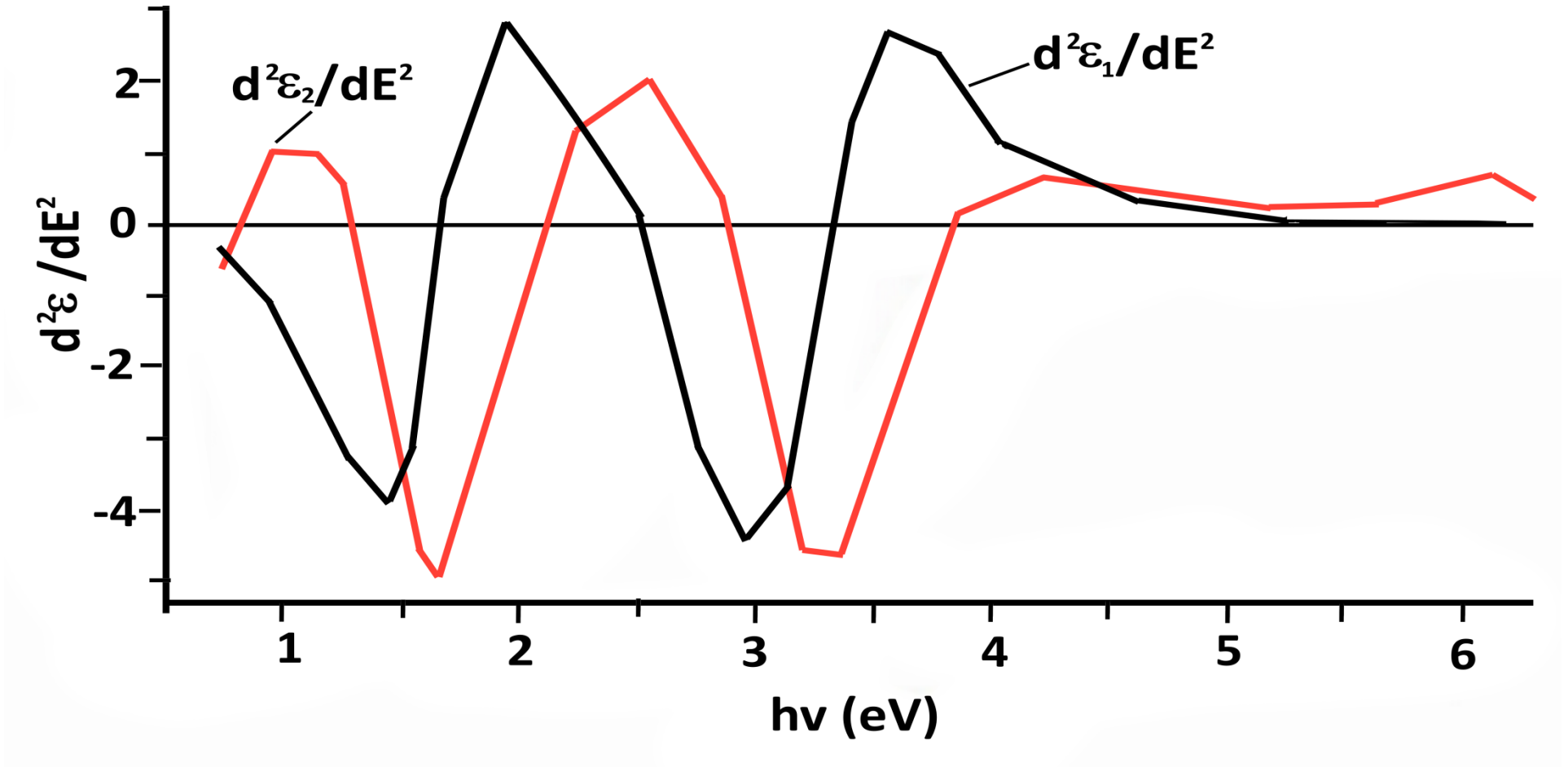

Figure 3. Spectral dependencies of the second derivatives of the $\varepsilon_1(\omega)$ and $\varepsilon_1(\omega)$ components of the complex dielectric function of PbSSe thin film

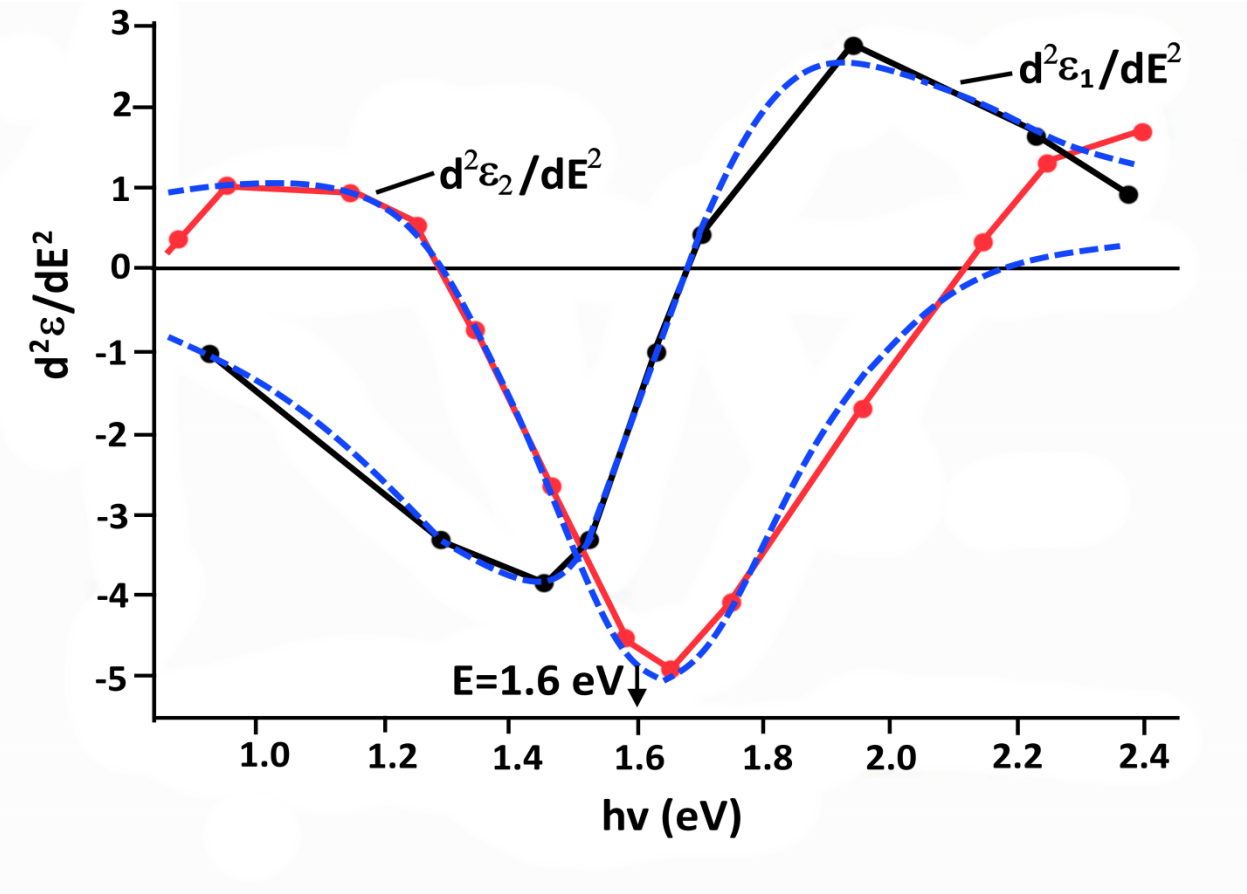

Figure 4. Second derivatives of the experimental dependences $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ (points) and curves of the best fit (dashed lines) for the energy range E=0.9 ÷ 2.4 eV of PbSSe thin film using the "Graphical Analysis" program.
A=0,89; E=1,6 eV; Γ=0,42; θ =1,22.

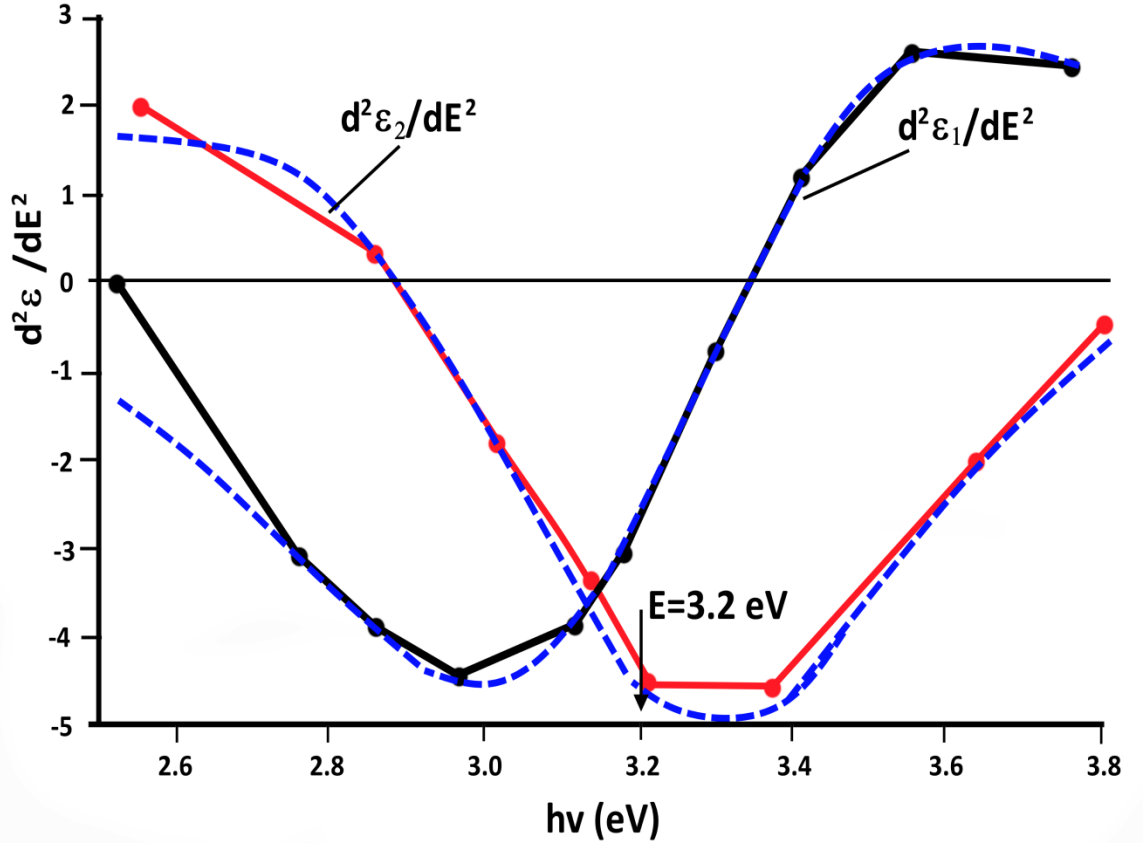

Figure 5. Second derivatives of the experimental dependences $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ (points) and curves the best fit (dashed lines) for the energy range E=2.5 ÷ 3.8 eV of PbSSe thin film using the "Graphical Analysis" program.
A=2,5; E=3,2 eV; Γ =0,66; θ =5.

CONCLUSIONS

To perform the fitting process, the real and imaginary components of the experimental dates of PbSSe thin films to analitical function, "Graphical Analysis" proqram was used.

The value of the critical point equal to the energy pozition E=1.6 eV in the band structure of PbSSe thin films, completely coincides with the theoretically calculated values for both PbS compounds and PbSe compounds and this value of the critical point in these compounds was characterized as $L5 \rightarrow L7$ transition. Therefore, we can assume that the value of the critical point E=1.6 eV in PbSSe thin films also arises due to the $L5 \rightarrow L7$ transition.

The second value of critical point E = 3.2 eV, which we obtained as a result of fitting for PbSSe thin film, is between E = 3.5 eV and E = 2.9 eV, which corresponds to the $\Delta 5 \rightarrow \Delta 6$ transition for PbS and PbSe, respectively, this value can also be attributed to the transition $\Delta 5 \rightarrow \Delta 6$.