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ANALYZING THE DIELECTRIC FUNCTION AND CRITICAL POINTS OF TELLURIUM THIN FILMS OBTAINED BY THE HYDROCHEMICAL METHOD

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Abstract- Spectroellipsometric measurements were employed to investigate the optical properties and determine the critical point energies of tellurium (Te) thin films deposited on glass substrates via a hydrochemical method. The energy-dependent dielectric function, including both real $\varepsilon_1(h\nu)$ an $\varepsilon_2(h\nu)$ imaginary components, was analyzed in detail. In order to accurately identify the critical points, second-order derivatives $d^2\varepsilon/d(h\nu)^2$ of the spectral dependencies were calculated, enhancing visibility of interband transition features.

A fitting procedure was subsequently carried out by matching the experimental data with appropriate analytical models, aiming to achieve the closest possible agreement between theoretical and experimental curves. This analysis was performed using the "Graphical Analysis" program. The fitting results revealed three distinct critical points located at photon energies of E1 = 1.04 eV, E2 = 1.30 eV, and E3 = 1.95 eV.

For all three spectral regions, the best fitting between the experimental data and theoretical model was obtained assuming a two-dimensional (2D) type critical point line shape (k=0), indicating that the dominant electronic transitions in these regions exhibit two-dimensional characteristics. It was found that the experimentally determined critical point energies are in good agreement with previously reported literature values.

EXPERIMENTAL DETAILS

The method is based on the acid decomposition of sodium tellurosulfate (Na_2TeSO_3), resulting in the release of elemental tellurium and its deposition as a thin film on a glass substrate.

Stage 1. Preparation of Precursors

A sodium tellurosulfate precursor solution is prepared through the reaction of tellurium dioxide (TeO_2) with sodium thiosulfate ($Na_2S_2O_3$).

1.1. Preparation of $Na_2S_2O_3$ Solution

Elemental sulfur (3.5 g) was added to a solution of sodium sulfite (15 g Na_2SO_3) in 200 mL of distilled water. The mixture was refluxed at 90 °C for 6 h, yielding a 0.55 M $Na_2S_2O_3$ solution.

1.2. Preparation of TeO_2 Solution

TeO_2 (0.140 g) was dispersed in 10 mL of distilled water and dissolved by gradual addition of NaOH under continuous stirring.

Stage 2. Preparation of Na_2TeSO_3 Working Solution

Twenty milliliters of the 0.55 M $Na_2S_2O_3$ solution were mixed with 10 mL of the TeO_2 solution. The mixture was maintained at 60 °C for 1 h under magnetic stirring to ensure complete reaction, producing a 0.065 M Na_2TeSO_3 solution.

EXPERIMENTAL DETAILS

Stage 3. Deposition of Tellurium Thin Film

Thirty milliliters of the 0.065 M Na_2TeSO_3 solution were transferred to a 60 mL beaker, and 30 drops of concentrated HCl were added, resulting in the formation of a black tellurium precipitate. After stirring, a chemically cleaned glass substrate was immersed vertically in the solution. The deposition process was carried out at room temperature for 16 h, leading to the formation of a tellurium thin film on the substrate surface.

At the end of the process, a homogeneous, highly adhesive, mirror-like thin layer of elemental tellurium is formed on the walls of the beaker and on the glass substrate placed in the solution.

ANALYTICAL FORMULATION

The analytical function describing how the real and imaginary parts of the complex dielectric function (CDF) depend on energy derived from ellipsometric measurements, depends on the value of the parameter k.

In the general case , the analytical expression is given by

$$\varepsilon(h\nu) = C - Ae^{i\theta}\left(h\nu - E + i\Gamma\right)^{k} \qquad (1)$$

here, A represents the amplitude, E signifies the critical point energy, while Γ and θ denote the Spectral broadening and the exciton phase shift, respectively. The parameter k defines the dimensionality of the critical point and assumes the values k= -1, k= -1/2, k= 0 and k=1/2 corresponding to excitonic (0D), one- dimensional (1D), two-dimensional (2D), and three-dimensional (3D) line shapes, respectively.

For the two-dimensional (2D) case (k=0) the expression reduces to the form

$$\varepsilon(h\nu) = C - Ae^{i\theta}\ln\left(h\nu - E + i\Gamma\right) \qquad (2)$$

In order to improve the accuracy of parameter determination and to eliminate the constant term C, the analysis is performed using $d^2\varepsilon/d(h\nu)^2$ -the second derivative of the experimental dielectric function with respect to energy $\varepsilon(h\nu)$.

ANALYTICAL FORMULATION

The Accordingly, the second derivatives of Equations (1) and (2) lead to the expressions presented in Equations (3) and (4) rewritten in trigonometric form, corresponding to $k \neq 0$ and $k = 0$, respectively.

$$\frac{d^2\varepsilon}{d(h\nu)^2} = A^1\left(\Omega\right)^{(k-2)/2}\cos\left[(k-2)\arg\cos\left(\frac{h\nu - E}{\Omega^{\frac{1}{2}}}\right)+\theta\right]+ \\ + A^1\left(\Omega\right)^{(k-2)/2} i\sin\left[(k-2)\arg\cos\left(\frac{h\nu - E}{\Omega^{\frac{1}{2}}}\right)+\theta\right] \quad (3)$$

$$\frac{d^2\varepsilon}{d(h\nu)^2} = \frac{A}{\Omega}\cos\left[-2\arg\cos\left(\frac{h\nu - E}{\Omega^{\frac{1}{2}}}\right)+\theta\right]+ \\ + \frac{A}{\Omega} i\sin\left[-2\arg\cos\left(\frac{h\nu - E}{\Omega^{\frac{1}{2}}}\right)+\theta\right] \quad (4)$$

where $A^1 = -k(k-1)A$ **and** $\Omega = (h\nu - E)^2 + \Gamma^2$

For the fitting procedure, Equations (3) or Equation (4) is employed as the fitting function. The calculated curves are fitted to the corresponding curves obtained from the experimental energy dependence of $d^2\varepsilon_1/d(h\nu)^2$ **And** $d^2\varepsilon_2/d(h\nu)^2$ **. The fitting quality is optimized by adjusting the parameters A, E, Γ, and θ.**

Upon completing the fitting procedure the parameters are automatically extracted using the "Graphical analysis" software.

RESULTS AND DISCUSSION

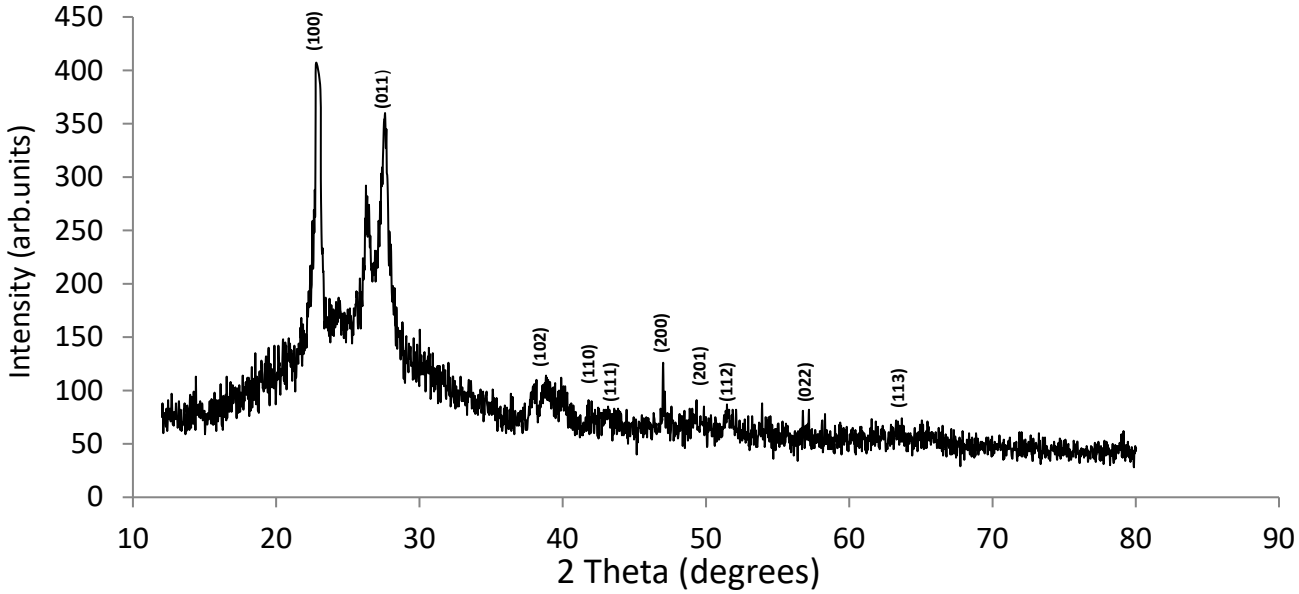


Figure 1. Figure 1. X-ray diffraction analysis tellurium thin film deposited by the hydrochemical method at room temperature

The corresponding XRD pattern, recorded over the 2θ range of 15°–80°. All detected peaks match the standard JCPDS card No. 79–0736 data perfectly. These results confirm the formation of elemental Te with a trigonal crystal structure belonging to the space group $P3_121$ (No. 152).

The experimental real and imaginary CDF curves for the tellurium thin films, generated from a high-resolution dataset of more than 700 coordinates, are illustrated in Figure 2.

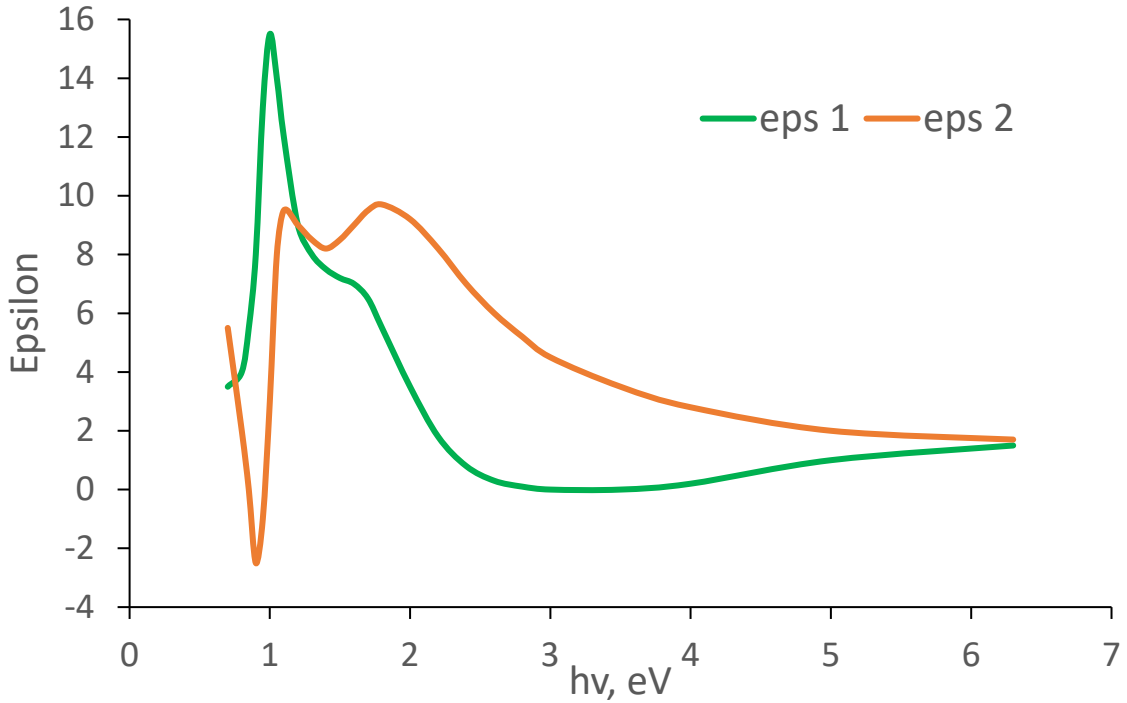


Figure 2. $\varepsilon_1(hv)$ **-real and** $\varepsilon_2(hv)$ **-imaginary parts of the tellurium thin film CDF plotted against photon energy.**

To fit the experimental data to the theoretical expressions and , we calculated the second-order derivatives of the experimental coordinates for the and dependencies (Figure 3).

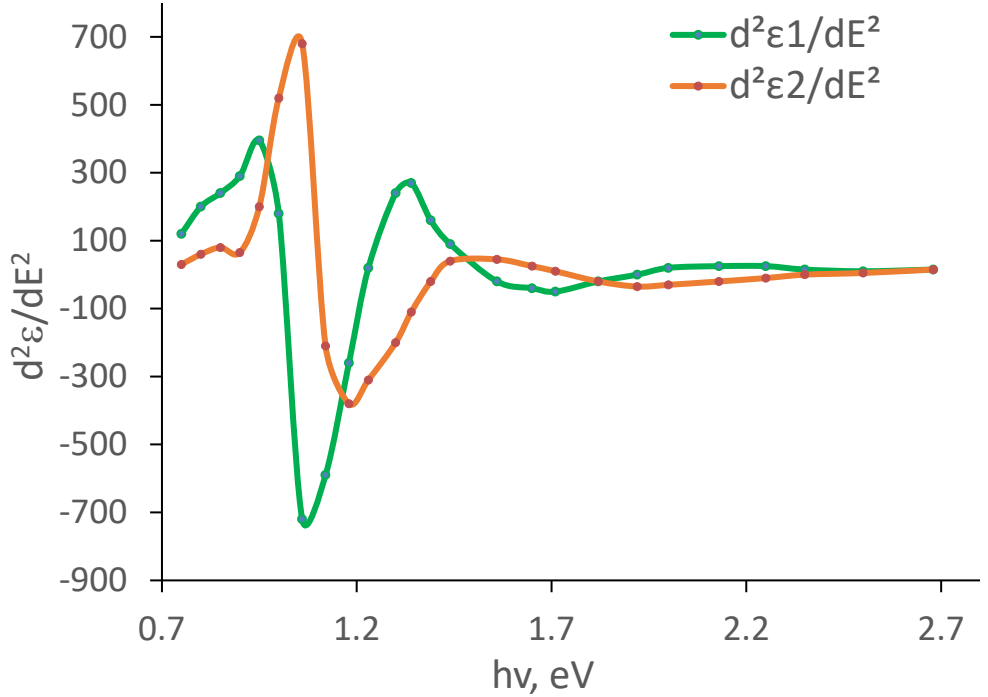


Figure 3. Second-order derivatives of the real and imaginary parts of the tellurium thin film CDF, plotted against photon energy.

Using the "Graphical Analysis" program, we determined that a 2D critical point model ($k=0$) provided the best fit for the area across all three energy regions. Figures 4(a)–(c) illustrate the results of fitting the curves $d^2\varepsilon_1/d(h\nu)^2$ and $d^2\varepsilon_2/d(h\nu)^2$ of the experimental dependences to the real and imaginary parts of expression (6) (k=0) for the energy range E=0.74÷1.22 eV, E=1.16÷1.52 eV and E=1.7÷2.6 eV, respectively.

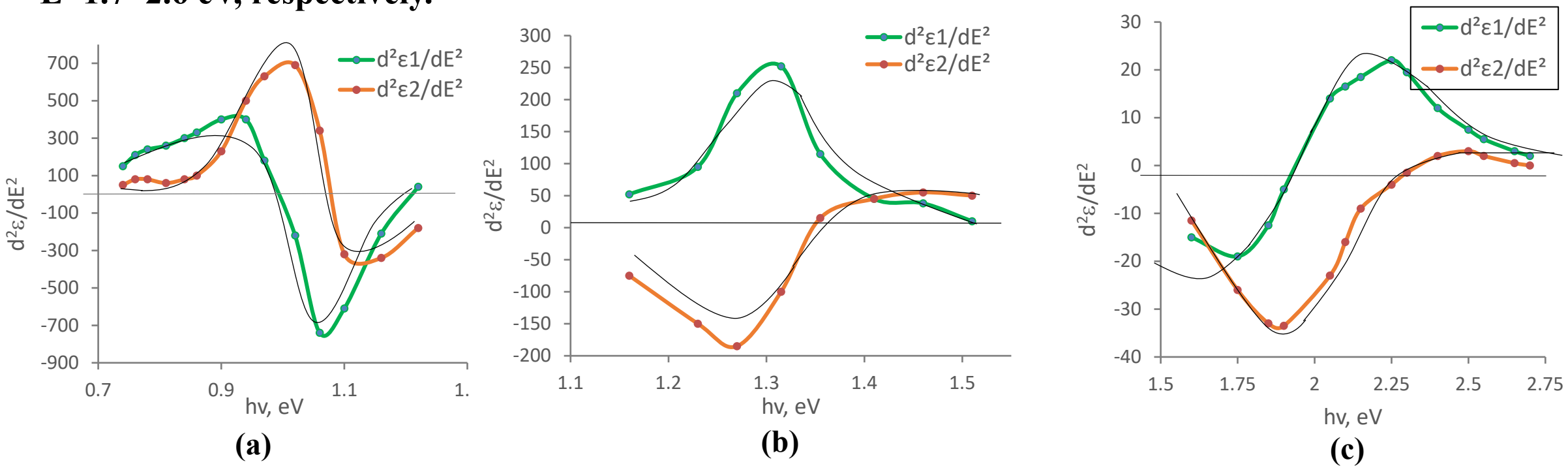


Figure 4. Second-order derivatives for experimental dependences $\varepsilon_1(h\nu)$ (green points) and $\varepsilon_2(h\nu)$ (red points) and their respective best-fit curves for a tellurium thin film. The data spans energy (a) E=0.74÷1.22 eV, (b) E=1.16÷1.52 eV and (c) E=1.7÷2.6 eV, analyzed via the "Graphical Analysis" software.

Using these obtained constants, fitting curves were constructed for the entire spectrum and a general fitting dependence was obtained by summing them.

Figure 5 shows the second-order derivatives $\varepsilon_1(hv)$ and $\varepsilon_2(hv)$ and the general fitting dependence for the entire spectrum (E=0.74÷2.6 eV) and the experimental dependences constructed based on the "Graphical Analysis" program.

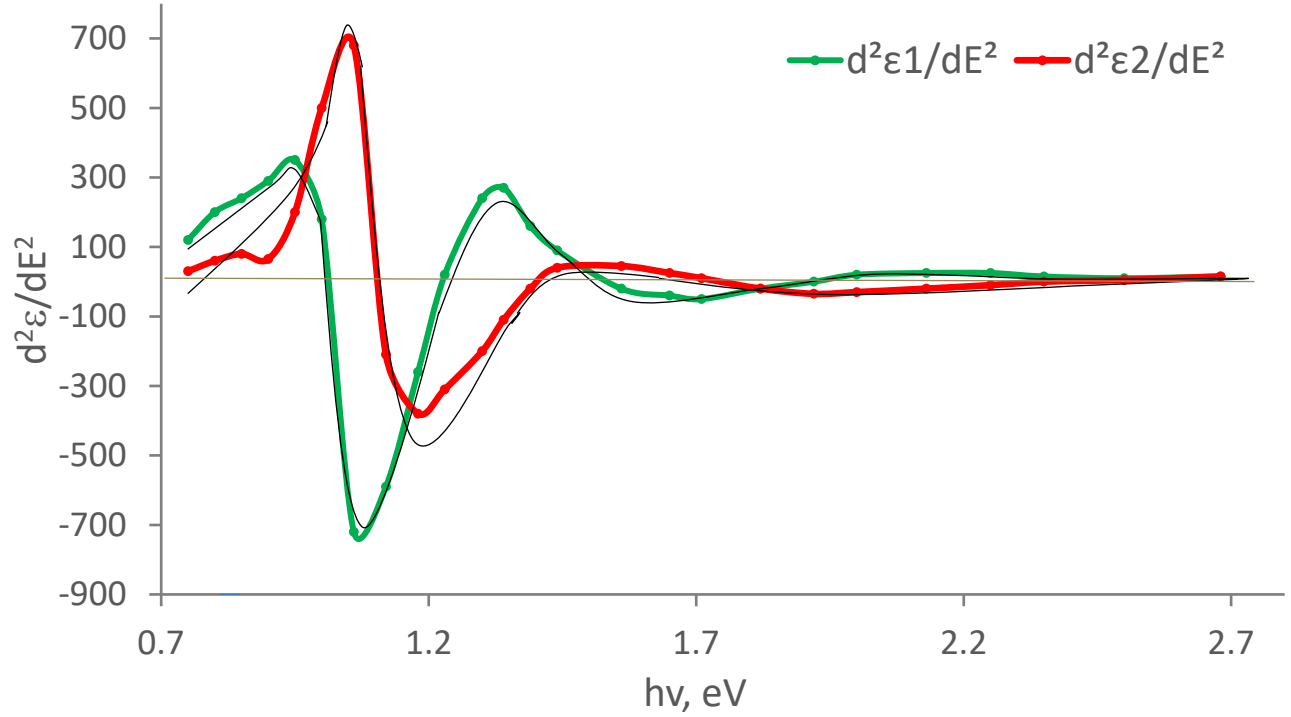


Figure 5. Second-order derivative of the experimental data (curves $\varepsilon_1(hv)$ and $\varepsilon_2(hv)$ alongside the best-fit curve for the entire tellurium thin film spectrum (E=0.74÷2.6 eV).

The existence of electronic transitions corresponding to these energy values (E1=1.04 eV, E2=1.3 eV and E3=1.95 eV) is supported by previously published literature. In [19] the values E1=1.0 eV and E2=1.4 eV - the energy position of critical points appearing in the reflection spectrum of a tellurium crystal at room temperature almost coincide with the values E1=1.04 eV, E2=1.3 eV obtained as a result of fitting. In that work, the next energy position of the critical point was reported to be E = 2.4 eV.

CONCLUSIONS

A tellurium thin film was hydrochemically deposited on a glass substrate, and X-ray diffractometric analysis confirmed that this film was a elemental tellurium crystallized in a trigonal structure. To determine the critical point energies of the tellurium thin films, the experimental data for the real $d^2\varepsilon_1/d(h\nu)^2$ and imaginary $d^2\varepsilon_2/d(h\nu)^2$ components of the CDF were fit to an analytical function. This optimization was performed using the "Graphical Analysis" software package and a detailed examination of these dependences shows that fitting can be performed within the energy ranges of E=0.74÷1.22 eV, E=1.16÷1.52 eV and E=1.7÷2.6 eV. It was determined that, across all three energy regions, the best fit was achieved using a two-dimensional (2D) critical point model ($k = 0$). As a result of the fitting, the values E1=1.04 eV, E2=1.3 eV and E3=1.95 eV were obtained as critical points for the tellurium thin film.

The existence of states corresponding to these energy values obtained from the ellipsometric measurements, has been confirmed by previously published literature data.