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The spectrums of fundamental optics functions of thin films p-CuAgTe

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The paper presents a new data on reflection and absorption and fundamental optics functions of thin films p-CuAgTe. The treatment of data by Kramers-Kronigs relations allowed to estimate the complete of fundamental optical constants: ε_1; ε_2; $-\mathrm{Im}\varepsilon^{-1}$, n, k in the energy range 0.05÷0.50 and 1.0÷6.2 eV and make suppositions about the electrons transmissions from low-lying level to conduction zone. Also the effective mass of charge carriers, the lifetime of the plasma oscillations, the plasma energy and direct transition energy in between the zones was estimated.

Keywords: reflection, absorption, optics functions, thin films.

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There are very few papers on narrow-band triple chalkogenides of I group in the literature. The optical spectra of CuSSe, CuSeTe with anion substitution of components were investigation in energy range 0.5 ÷ 5.0 eV [1].

By differential-thermal and electro-physical methods it is shown, that similarity of structural types and the nature of bond-strength in copper and silver chalkogenides allowes obtaining of the triple chalkogenides CuAgS (Se, Te) by equimolar cation substitution in Ag_2X-Cu_2X systems. The formation of the triple compounds takes a peritectic reaction course at 903 K (p-CuAgS), 1033 K (n-CuAgSe) and 1123 K (p-CuAgTe) [2].

The edge absorption and the absorption by free carriers in n-CuAgSe are investigated in [3,4].

In paper with the object to investigation of energy band structure of p-CuAgTe in the range of own absorption the fundamental optical functions: refractive index – n(ω), absorption index-k(ω), dielectric constants-$\varepsilon_1(\omega)$, $\varepsilon_1(\omega)$, ε_∞, the function of the characteristic volume energy losses-$\mathrm{Im}\varepsilon^{-1}(\omega)$, the effective mass of charge carriers are estimated.

p-CuAgTe is undergoes polymorphism at 473 ÷ 478 K. The law-temperature α-modification crystallizes into rhombic lattice with parameters

$$a = 4.19\,\overset{0}{A};\ b = 20.02\,\overset{0}{A};\ c = 6.38\,\overset{0}{A}.$$

The thin films of p-CuAgTe (0.25 ÷ 0.35) mkm were obtained by vacuum deposition (10^{-3} Pa) on newly made spall surface NaCl and optical glass heated up to 350 ÷ 370 K. By X-ray and electronographic analyses determined the identity of thin films p-CuAgTe with parent compound.

The transmission and reflection spectra (at perpendicular incidence of beam) in non-polarized light, in range 0.05 ÷ 0.50 and 1.0 ÷ 6.0eV are measured on two-beam and double-wave spectrometer Hitachi (model 556-557) and two-beam spectrometer

"Specord-75-JR" and dublicated on IKS-29. The treatment of experimental spectra on known Kramer-Kronig's relations are produced.

In fig. 1 have been presented reflection spectra in the range (1.0 ÷ 6.2) eV (a) and (0.05 ÷ 0.50) eV (b). There are two minima on reflection spectra in the IR range: at 0.05 and 0.141 eV. By higher steep of low-energy slope and the peak frequency of $-\mathrm{Im}\varepsilon^{-1}(\omega)$ it is established that plasma minimum corresponds to 0.056 eV. From $\omega_{min.} = \omega_\rho(\varepsilon_0/\varepsilon_0-1)^{1/2}$ and $\omega_\rho^2 = 4\pi e^2 n / m^* \varepsilon_0$ giver the carrier concentration $n = 6.2\cdot10^{18}\,cm^{-3}$ has been determined the plasma resonance frequency $\omega_\rho = 0.85\cdot10^{14}\,c^{-1}$ and the effective mass of charge carriers $m_\rho^x = 0.3m_e$. From relation $\chi = ne^2/\omega_{min}^2 \cdot \omega_\rho^2$ dielectric susceptibility of p-CuAgTe X = 0.6 is determined. In energy range (1.0 ÷ 6.2) eV on reflection spectra have been developed two distinct maxima without any particular peaks and steps. With rise of energy a reflection increases monotonically from 0.32 (at 1.3 eV) up to 0.55 (1.7 eV), then

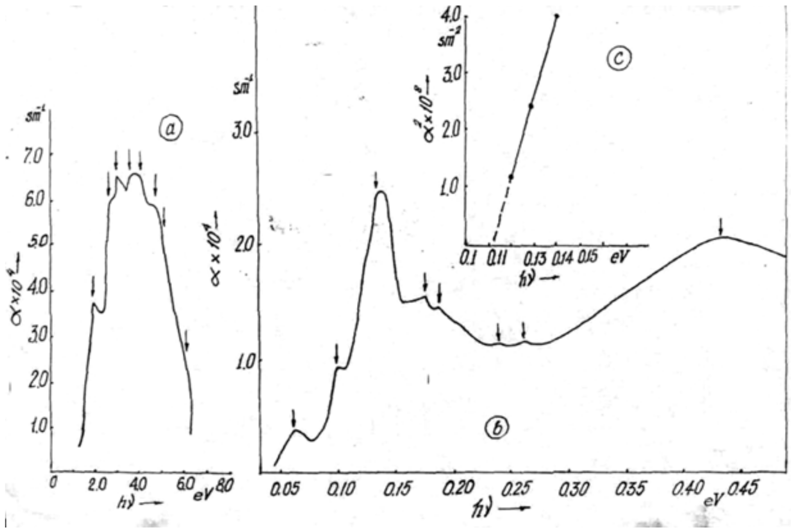

Fig. 2. The absorption spectrums of p-CuAgTe a - in range 1.0 ÷ 6.2 eV b - in range 0.05 ÷ 0.50 eV c - $\alpha^2 \sim h\gamma$

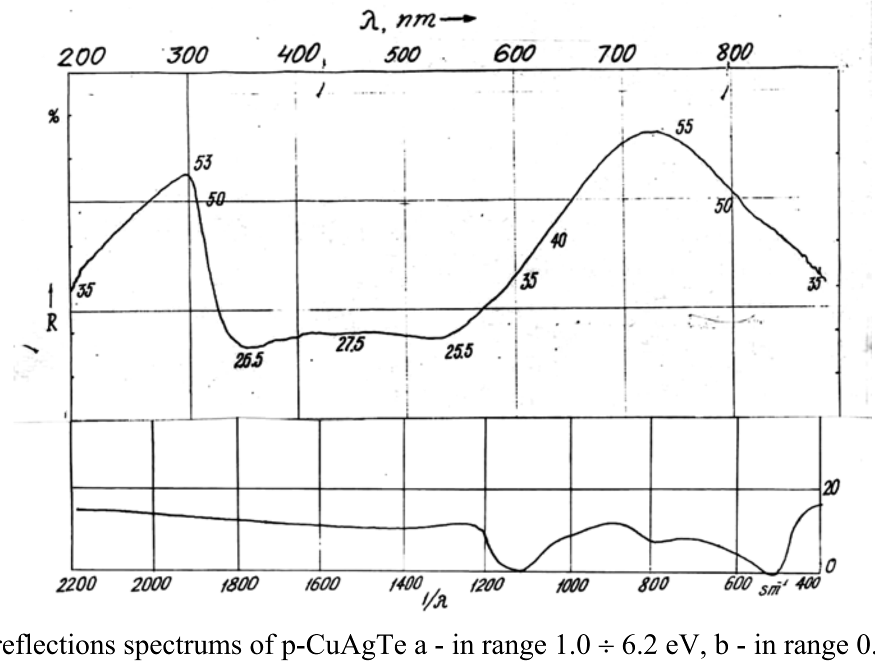

Fig. 1. The reflections spectrums of p-CuAgTe a - in range 1.0 ÷ 6.2 eV, b - in range 0.05 ÷ 0.50 eV

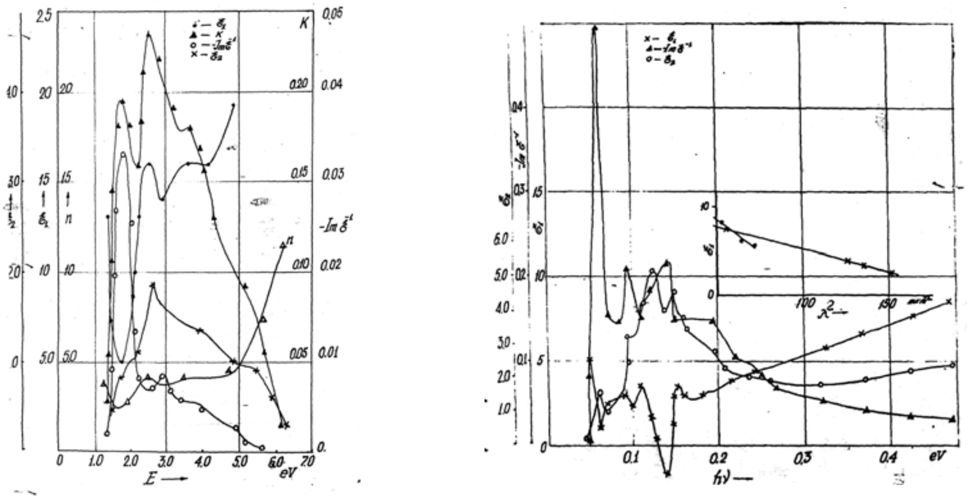

Fig. 3. Spectrum of characteristic electronic losses ($-Im\varepsilon^{-1}$) and fundamental optics constants (ε_1; ε_2; n, k) a - in range 1.0÷6.2 eV, b - in range 0.05÷0.50 eV

decreases down to 0.26 and keep one's in the range (2.30 ÷ 3.65) eV, and then suddenly increases up to 0.54 (4.10 eV). The ultraviolet reflection allows locate the electrons states, distant from edges of forbidden band. These two maxima 1.7 eV and 4.1 eV are taken as symptom of direct interband transitions from lower valent bands into conduction band.

In fig. 2 (a, b) have been presented the absorption spectra in IR (0.05 ÷ 0.50) eV, visible and close UV (1.0 ÷ 6.2) eV regions. In absorption spectrum occurs a number of intensive peaks at 1.4; 1.9; 2.6; 2.9 eV.

The property of silver and copper chalkogenides is the presence of high cation conductivity [5]. These structures arise from ionic skeleton. In energy scale they underlies well below of valent band. A few lines of oscillation type are observed in close UV region (4.0 ÷ 6.2) eV. They can to correspond to transitions from the top of 3d-band of copper into conduction band near Fermi energy. The transition's strips from d-band into conduction band are wide, as they take place in different points of Brillouin zone and lifetime $-\tau$ is short, respectively. Duplex in the interval 3.0 ÷ 3.5eV is due to spin-orbit splitting of copper's 3d level, i.e. splitting like that is not observed on Ag_2Te spectrum [6]. The frequency ranges near $\omega \geq \omega_g$ is the most important section of spectrum to yield the quantitative data about energy band structure near absolute extremum of Brillouin zone. In fig.1b the absorption spectrum covers just this region. By extrapolation of straight line $\alpha^2 \sim (h\nu)$ have been determined optical band gap $E_{opt} = 0.12$eV. Has been exceeded forbidden band (0.10 eV) by 0.02 eV. In general, in ionic crystals the cutoff of direct transitions can be a few higher than band gap due to polarization of crystal lattice, do not manage to change for short time of interaction of photon with electron [7]. The difference is equal to polaron energy for p-CuAgTe – 0.02 eV beyond of absorption edge have been observed peaks at 0.17; 0.26; 0.37; 0.43; 0.5 eV. There are special points in zone structure p-CuAgTe, of pointing to energy of vertical transitions between the extremum points of Brillouin zones. The structures at 0.07 and 0.10 eV are due to selective absorption by free carriers and acceptor impurity level, respectively.

In fig. 3 (a, b) have been presented the spectral dependencies ε_1; ε_2; $-Im\varepsilon^{-1}$, n, k in the energy range 1.0 ÷ 6.2 and 0.05 ÷ 0.50 eV. On spectrum $-Im\varepsilon^{-1}$(3b) expect main peak at 0.056 eV (pointing to plasma frequency) there have been found features as extra peaks at 0.096; 0.14; 0.18; 0.28 eV. Extra peak energies correlate with direct interband transitions in corresponding points CuAgTe, pointing to energy of vertical transitions between the extremum points of Brillouin zone. In fig. 3 a have been derived the dependence $\varepsilon_1 = f(\lambda^2)$. By extrapolation this straight line to $\lambda = 0$, the high-frequency dielectric constant-$\varepsilon_\infty = 7.8 \div 8.2$ is found. The

Table 1

ω_{min} c^{-1}	ω_ρ c^{-1}	$\hbar\omega_\rho$ eV	τ_{opt} c	χ	ε_1	ε_2	ε_∞
$0.88\cdot10^{14}$	$0.85\cdot10^{14}$	0.05	$4.7\cdot10^{-13}$	0.6	1.0	3.0	7.8÷8.2

Magnitudes of direct interband transitions

Table 2

Energy range eV	E_8 eV	E_7 eV	E_7^1 eV	E_6 eV	E_5 eV	E_4 eV	E_3 eV	E_2 eV
1.0÷6.2	6.0	5.0	4.7	4.0	3.5	3.0	2.6	1.9
0.05÷0.50	0.43	0.26	0.24	0.17	0.14	0.132	0.097	0.06

real part of dielectric constant ε_1 reaches the biggest values 3.5 (0.11 eV); 8.8 (0.50 eV) and it is negative in the range (0.13 ÷ 0.46) eV. Consequently, in this range n<K.

Spectra ε_2, λ, K are similar in all energy ranges. Their biggest values are equal to $\varepsilon_2 = 5.1$ (0.132 Ev0, K = 1.77 (0.136 eV), $\lambda = 2.46\cdot10^4$ cm^{-1} (0.136 eV) and closely resembles on energy.

The time of life of the plasma oscillations is calculated from peak -Im$\varepsilon^{-1}(\omega)$ on the half-width level by relation $\Delta\omega/\omega = 2/\omega_\rho\tau$ [5]. It is equal to $\tau = 4.7\cdot10^{-13}$c. The plasma resonance energy $\hbar\omega_\rho = 0.05$ eV. Maximal of main volume plasmons: 0.21 (0.10 eV) and 0.22 (0.144eV) indicates that in excitation of volume plasmons besides valent electrons also deeper level's electrons are taken place. The shift of main peak - Jm$\varepsilon^{-1}(\omega)$ about maximum ε_2 on 0.07 eV (fig. 3 b) and in visible region on 0.75 eV determines energy of longitudinal-cross splitting of transitions.

In conclusion in Table 1 have been given set of fundamental optic functions of p-CuAgTe close to plasma resonance.

So by investigation of fundamental optic functions in infrared, visible and close UV regions have been determined peculiarities of interband transitions in p-CuAgTe and obtained the first data about structure of energy zones near absolute extremum of Brillouin zone.

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Спектри основних оптичних функцій тонких плівок p-CuAgTe

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Дослідженням фундаментальних оптичних функцій тонких плівок p=CuAgTl в інтервалі енергій (0,05÷0,50) та (1,0÷6,2) eВ вперше отримано дані про структуру енергетичних зон біля абсолютних екстремумів зони Бріллюена. Розраховано комплекс фундаментальних оптичних функцій: ε_1; ε_2; ε_∞ ; $-\mathrm{Im}\,\varepsilon^{-1}$; n, k в околі плазмового резонансу, час релаксації плазмових коливань $\tau=4,7\cdot10^{-13}$c, енергія плазмового резонансу $h\ \omega_p=0,05$ eВ, ефективна маса носіїв струму $m^*=0,3\ m_e$, енергії прямих міжзонних переходів та спін-орбітального розщеплення.