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Physicochemical and optical properties of glasses from the Cu-S-Se system

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Based on the results of the micro-hardness, HV, density, d, and the glass-transition temperature, T_g measurements, the thermo-mechanical characteristics (micro-voids volume, V_h, and the energy for micro-void formation, E_h), the compactness, C, and the elasticity modulus, E, of glasses from the Cu-S-Se system are calculated. The mean values of the overall bond energy, <E>, coordination number, <Z>, bond energy of the average cross-linking/atom, $\bar{E}_c$, and that of the "remaining matrix", $\bar{E}_{rm}$, are determined using the known formalism. The average heteropolar bond energy, E_{hb}, and the degree of "cross-linking/atom", P, are also calculated employing the same experimental finding. The dependence between T_g and <E> is linear: $T_g = 314(0.004\langle E\rangle+0.88)$. The optical band gap, $E_{g,o}$, of as-deposited thin films with composition $Cu_5Se_{95-y}S_y$ ($0 \le y \le 30$) is determined using the Tauc's power law. The $E_{g.o}(y)$ dependence is linear: $E_g^{opt} = 0.0057y + 1.797$. Correlations between the investigated properties and the glass composition are established.

Keywords: chalcogenide glasses; physicochemical properties, bond energy, optical band gap.

INTRODUCTION

During the last years the chalcogenide glassy semiconductors are widely investigated due to their various properties (switching and memory effects, photosensitivity and transparency in the IR spectral region, chemical and radiation stability, ionic conductivity, etc.), which determine multiple possibilities for their application [1–4].

On the one hand, the investigations referred are focused on already familiar chalcogenide glasses, and on the other hand, on the development of new ones. The experimental investigations include the outlining of glass-forming regions in new systems, and complex investigation on the structure, properties and application areas of the chalcogenide glasses.

When the component number in a given system is increased, the glass-forming ability grows due to the increased probability of formation of new structural units which impede crystal nucleation [5]. Most often two-component systems are used, one of them usually being the glass-forming elements, and the other being the modifier. The S-Se system is very suitable as a base binary system due to the presence of large glass-forming area and it spreads from 50 to 100 at.% Se [6]. Liquid selenium and sulphur form equilibrium melts, built by linear polymer molecules and 8-ring monomers.

The unarranged interweaking of Se and S chains with rings is stimulated by structure amorphization and by the fact that both S and Se are glass-formers. For example, about 60 at.% As [7] and 30 at.% Ge [8] can be introduced in the S-Se system.

The region of glass-formation in the Cu-S-Se system is outlined by V. Vassilev *et al.* [9] on the basis of the results from visual, X-ray diffraction and electron-microscopic analyses (see Figure 1 below).

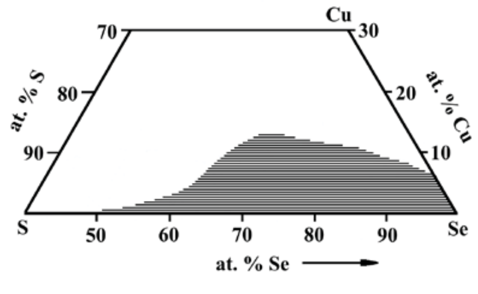

Fig. 1. Region of glass-formation in the Cu-S-Se system [9].

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The aim of the present paper is the investigation of the main physicochemical and optical properties of glasses with composition $Cu_xS_ySe_z$ (x+y+z=1), and the analysis of the respective composition-property diagrams.

EXPERIMENTAL

The glassy samples, used for the investigations, were synthesized applying the method, described in [9]: direct monotemperature synthesis in evacuated and vacuum sealed quartz ampoules; maximum synthesis temperature of 1100 ± 5 ºC; synthesis duration – 24 h, and subsequent quenching of the smelter in water+ice+NaCl mixture.

The microhardness, HV, was measured by the Vickers' method using a metallographic MIM-7 microscope with built in microhardness meter, PMT-3, at loading of 10 g (accuracy ± 4 %). The density, d, is measured by hydrostatic method in toluene as immersion fluid (accuracy ± 4 %). The glass-transition temperature, T_g, is determined by differential-thermal analysis (accuracy ± 5 ºC) at heating rate of 16 ℃ min^{-1} and with α-Al_2O_3 as reference substance.

Using the results of these measurements, the thermomechanical characteristics (micro-voids volume, V_h, and energy for micro-voids formation, E_h), the elasticity modulus, E, and the compactness, C, are calculated.

Based on a free volume approach in calculating cohesion glasses, Sanditov [10] proposed to determine microhardness as HV = E_h/V_h. Using this concept we derived in [11] the following expressions for the quantities E, V_h, and E_h:

$$V_h = 5.04\cdot10^{-3}.\frac{T_g}{HV}\ [nm^3];\ E_h = 29.75.T_g\ [J\ mol^{-1}];$$

$$E = 0.147.HV\ [GPa], \qquad (1)$$

where HV – micro-hardness [kgf mm^{-2}]; T_g – glass-transition temperature [K].

The compactness, C, expresses, in arbitrary units, the deviation in the glass density from that of a corresponding crystal with the same composition ($C=\Delta/d_i$; $\Delta=d_i-d$). It is calculated using the equation [13]:

$$C = d\left\{\sum_i^n \frac{M_i x_i}{d_i} - \sum_i^n \frac{M_i x_i}{d}\right\}\left[\sum_i^n M_i x_i\right]^{-1}, \qquad (2)$$

where d – density of the sample; d_i, M_i and x_i are the density, the molar (atomic) mass and molar (atomic) part of the i^{th} component, respectively. The compactness can acquire both positive and negative values. The negative ones respond to looser structure, and the positive to a denser structure, compared to a crystal with the same composition.

The properties of the chalcogenide glasses are directly related to the overall mean bond energy, which is a function of the mean coordination number and the type and the energy of the chemical bonds between the atoms, building the glasses.

The mean coordination number <Z> of the glasses is calculated by an equation (3), proposed by Tanaka [13]. The following values of the atom coordination numbers are used for the investigated system: $Z_{Se}=Z_S=2$ [14] and $Z_{Cu}=2$ [15].

$$< Z >= x.Z_{Cu} + y.Z_S + z.Z_{Se} \qquad (3)$$

where x, y and z are the atomic parts of Cu, S and Se, respectively.

The overall mean bond energy <E> is calculated using Tichy's equation [16] for complex chalcogenide systems:

$$< E >= \overline{E}_c + \overline{E}_{rm}, \qquad (4)$$

where $\overline{E}_c$ is the average bond energy of cross-linking/atom and $\overline{E}_{rm}$ is the average bond energy per atom of the "remaining matrix".

The value of $\overline{E}_c$ is calculated by the equation:

$$\overline{E}_c = P.E_{hb}, \qquad (5)$$

where P is the degree of cross-linking/atom; E_{hb} – average heteropolar bond energy. For glasses with composition $Cu_xS_ySe_z$, the E_{hb} is calculated by the equation (6):

$$E_{hb} = \left(x.Z_{Cu}.E_{Cu-S} + x.Z_{Cu}.E_{Cu-Se}\right)/\left(x.Z_{Cu}\right), \qquad (6)$$

where: E_{Cu-S} and E_{Cu-Se} are the heteropolar bond energies of Cu-S and Cu-Se – Table 1.

Table 1. Energy of chemical bonding in the Cu-S-Se system.

Bond	Se-Se	S-S	Cu-Cu	Se-S	Se-Cu	S-Cu
Bond energy, eV	1.90	2.20	1.83	3.85	2.60	2.86
Reference	[16]	[16]	[17]	[18]	[19]	[19]

The coefficient R is used for determination of the chalcogen content in the glasses:

$$R = \left(y.Z_S + z.Z_{Se}\right)/\left(x.Z_{Cu}\right). \qquad (7)$$

At R>1 the system is chalcogen rich and heteropolar chalcogen-chalcogen bonds are present. In this case P = P_r, and

$$P_r = x.Z_{Cu}/(x+y+z) \quad (8)$$

At R=1 the system is with stoichiometric composition thus there are only heteropolar bonds to be expected.

At R<1 the system is chalcogen poor and heteropolar metal-metal bonds are present. In this case $P=P_p$.

$$P_p = z.Z_{Se}/(x+y+z) \quad (9)$$

The average bond energy per atom of the "remaining matrix" is defined by:

$$\overline{E}_{rm} = 2(0.5.<Z>-P_r).E_{<>}/<Z>, \; R>1 \quad (10)$$

$$\overline{E}_{rm} = 2(0.5<Z>-P_p)E_{A-A}/<Z>, \; R<1, \quad (11)$$

where $E_{<>}$ - average bond energy between the S and Se atoms:

$$E_{<>} = \frac{1}{3}.(E_{S-S}+E_{Se-Se}+E_{S-Se}) \cdot \quad (12)$$

The measurement of the optical absorption (at $\alpha<10^4$ cm^{-1}) gives information about the density of the states in the tail area. Since in amorphous semiconductors the doubled value of the electrical conductivity activation energy corresponding to a frequency, equivalent to = 10^4 cm^{-1}, Stuke [20] suggested the optical band gap, E_g^{opt} to be defined at this α value. According to Tauc [21] in the $\alpha \geq 10^4$ cm^{-1} area the optical absorption is due to transitions of electrons from the delocalized states in the valence band ($E<E_v$) to the delocalized states in the conductivity band ($E>E_c$), as the value of α increases with the photon energy (hν) according the equation:

$$\alpha h\nu = A[h\nu-(E_c-E_v)]^n, \quad (13)$$

A is a constant, characteristic for the material, and n is another constant, characterizing the transition type (for direct transitions n=1/2 and for indirect – n = 2).

The absorption coefficient is calculated from the transmission spectra using the equation

$$\alpha = -\frac{1}{d}\ln T, \quad (14)$$

where T=I/I$_o$ (I and I$_o$ are the intensities of the transmitted and incident light, respectively).

RESULTS AND DISCUSSION

1. Physical and thermo-mechanical characteristics

The T_g,, d, and HV values, needed for calculation of the thermo-mechanical characteristics of glasses from the Cu-S-Se system, are shown in Table 2, as well as the obtained results for E, E_h, V_h, and C, derived using equations (1) and (2).

Table 2. Physical and thermo-mechanical properties of glassy phases with composition $Cu_xS_ySe_z$ ((x+y+z)=1; m=z/(y+z)).

№	Composition, at. parts			m	T_g, K	d, g cm^{-3}	HV, kgf mm^{-2}	E, GPa	E_h., kJ mol^{-1}	V_h 10^{-3}, nm^3	C
1	0.00	0.00	1.00	1.000	315	4.25	40	5.88	9.37	39.69	-0.1127
2	0.00	0.05	0.95	0.950	310	4.15	35	5.15	9.22	44.64	-0.1124
3	0.00	0.15	0.85	0.850	305	3.92	31	4.56	9.07	49.59	-0.1335
4	0.00	0.25	0.75	0.750	300	3.67	28	4.12	8.93	54.00	-0.1272
5	0.05	0.00	0.95	1.000	330	4,18	36	5.29	9.82	46.20	-0.1438
6	0.05	0.05	0.90	0.947	325	4.03	32	4.70	9.67	51.19	-0.1542
7	0.05	0.10	0.85	0.895	318	3.88	30	4.41	9.46	53.42	-0.1649
8	0.05	0.15	0.80	0.842	312	3.81	28	4.12	9.28	56.16	-0.1848
9	0.05	0.20	0.75	0.789	307	3.61	27	3.97	9.13	57.31	-0.1804
10	0.05	0.30	0.65	0.684	305	3.40	25	3.68	9.07	61.49	-0.2006
11	0.10	0.10	0.80	0.889	325	3.80	27	3.97	9.67	60.67	-0.1515
12	0.10	0.15	0.75	0.833	317	3.69	25	3.68	9.43	63.91	-0.2047
13	0.10	0.20	0.70	0.778	310	3.58	24	3.53	9.22	65.10	-0.2027
14	0.10	0.25	0.65	0.722	305	3.43	23	3.38	9.07	66.83	-0.2047

The increase of the glass-transition temperature, T_g, at raising the Se content at constant copper concentration (x=const) is expected since in this case the concentration of the glass-former increases as seen from Table 2. The influence of copper on the T_g-value of the glasses seems "unusual". It rises with the increase of the Cu-content (at m=const) (Table 2). It has to be noticed that up to a certain concentration copper breaks the (–S–S–), (-Se–Se-), and (–S–Se–) bonds and participates equally in the linear chains formed by the S and Se atoms in the chalcogenide glass. At Cu-content higher than a critical value, defined by the glass-forming boundaries in the Cu-S-Se system, a crystalline phase of composition Cu, Cu_2S and/or Cu_2Se is formed. The T_g-value decreases quickly in this case.

The density, d, increases noticeably with the raise of the Se-content (i.e. m increases) at a constant value of Cu (x=const) which is related to the great difference between the densities of the elements S and Se ($d_{Se}=4.25 \gg d_S=2.09$ g cm^{-3}) – Table 2. In spite of the great difference between the density values ($d_{Cu}=8.93$ g cm^{-3}), the density of the chalcogenide glasses lightly increases with the raise of the Cu content at m=const (Table 2) which is connected to the circumstance that with the inclusion of Cu the total micro-pore volume increases $V_{\mu p}$. This increase compensates the glass mass increase m_g ($d=m_g/(V_g+V_{\mu p})$, where V_g is the glass volume without the pores. This assumption is confirmed by the HV(x) dependencies at m=const (Table 2). HV decreases with the x raise since the glass structure becomes looser, i.e. the $V_{\mu p}$ increases.

The elasticity modulus, E, follows the path of the microhardness.

The minimum micro-void volume, V_h, decreases with the increase of the Se-content (at x=const), and increases with the addition of Cu (at m=const) since both dependencies are almost linear. This change of the V_h of the chalcogenide glass composition is caused, on the one hand, by the fact that the atomic radius of Se is larger than this of the S and with the gradual substitution of S- with Se-atoms (at x=const) the structure becomes denser. On the other hand, the Cu-atoms are built into the structure, formed by (–S–Se–)-chains (at m=const), as a result of which it becomes looser.

The E_h(x;m) dependencies go over the path of the T_g(x;m) dependencies. In the cases when m increases (the Se replaces the S) at x=const, as it was shown above, the structure of the glasses is denser. This process opposes the further substitution of S with Se, which by its side requires higher E_h values. The introduction of Cu in the glasses at m=const does not lead to substitution of S and/or Se but breaks their chains at different places (–S–S–; –Se–Se– и –S–Se–), builds into them, and forms fragments form the type: –S–Cu–S–; –Se–Cu–Se– и –S–Cu–Se–. Additional amount of energy is needed for these processes to take place and this is why E_h increases with the increase of the Cu content (at m=const).

The compactness of the investigated glasses has negative values and depending on the composition changes in very narrow limits (the experimental values of C are from – 0.21 to – 0.10).

2. Energy of the Chemical Bond

Based on the model shown in the Experimental Part, the average parameters (<Z>, R, P, E_{hb}, $\bar{E}_c$, $E_{<>}$, $\bar{E}_{rm}$, and <E>) of the chemical bond are calculated. Their values are shown in Table 3.

Table 3. Physicochemical properties of the samples with composition $Cu_xS_ySe_z$.

№	Composition, at. parts			m	T_g, K	Z	R	P_r	E_{hb}	$\bar{E}_c$, eV	$E_{<>}$, eV	$\bar{E}_{rm}$, eV	<E>, eV
1	0.00	0.00	1.00	1.000	315	2	∞	0	0	0	2.65	2.650	2.650
2	0.00	0.05	0.95	0.950	310	2	∞	0	0	0	2.65	2.650	2.650
3	0.00	0.15	0.85	0.850	305	2	∞	0	0	0	2.65	2.650	2.650
4	0.00	0.25	0.75	0.750	300	2	∞	0	0	0	2.65	2.650	2.650
5	0.05	0.00	0.95	1.000	330	2	19	0.1	5.46	0.546	2.65	2.385	2.931
6	0.05	0.05	0.90	0.947	325	2	19	0.1	5.46	0.546	2.65	2.385	2.931
7	0.05	0.10	0.85	0.895	318	2	19	0.1	5.46	0.546	2.65	2.385	2.931
8	0.05	0.15	0.80	0.842	312	2	19	0.1	5.46	0.546	2.65	2.385	2.931
9	0.05	0.20	0.75	0.789	307	2	19	0.1	5.46	0.546	2.65	2.385	2.931
10	0.05	0.30	0.65	0.684	305	2	19	0.1	5.46	0.546	2.65	2.385	2.931
11	0.10	0.10	0.80	0.889	325	2	9	0.2	5.46	1.092	2.65	2.120	3.212
12	0.10	0.15	0.75	0.833	317	2	9	0.2	5.46	1.092	2.65	2.120	3.212
13	0.10	0.20	0.70	0.778	310	2	9	0.2	5.46	1.092	2.65	2.120	3.212
14	0.10	0.25	0.65	0.722	305	2	9	0.2	5.46	1.092	2.65	2.120	3.212

The investigated system is rich of chalcogen, since R>1 [R=(0.05.2+0.9.2)/(0.05.2)=19>1] - Table 3.

For description of the temperature dependence on the viscosity, equation (15) is used:

$$\mu(T) = \mu_o \exp(E_\mu / kT). \tag{15}$$

It is known that at T_g the value of $\mu = 10^{13}$ dPa.s [22]. Tanaka [13] assumes that $\mu_o = 10^0 – 10^{-5}$ dPa.s. If one puts $\mu_o = 10^{-3}$ dPa.s the following dependence will be obtained: $T_g = 314E_\mu$

Taking into consideration the above dependence, we determined that between T_g and <E> exists a linear dependence of the type: T_g = 314 (0.004<E>+0.88). It guarantees accuracy not worse than ± 0.1.T_g which is fully acceptable. The obtained value of the straight line slope (314 K/eV) is in full conformance with the theoretically expected one.

3. Optical Characteristics

For determination of the optical band gap the compositions lying on the $Cu_5Se_{95-y}S_y$ section (0≤y≤30) are used, since in this section the S/Se proportion varies in wide limits for the tri-component system. The thin films are deposited using vacuum-thermal evaporation (P≈0.01 Pa) on Na-Ca substrates. The film thickness varies from 0.2 to 0.4 μm. The optical transmittance spectra are recorded in the range of 200–900 nm. The dependence between the absorption edge on the film composition is shown in Fig. 2a where it can be seen that with the increase of the sulphur content, the optical edge shifts towards shorter wave lengths, i.e. the material band gap value increases – Fig. 2b.

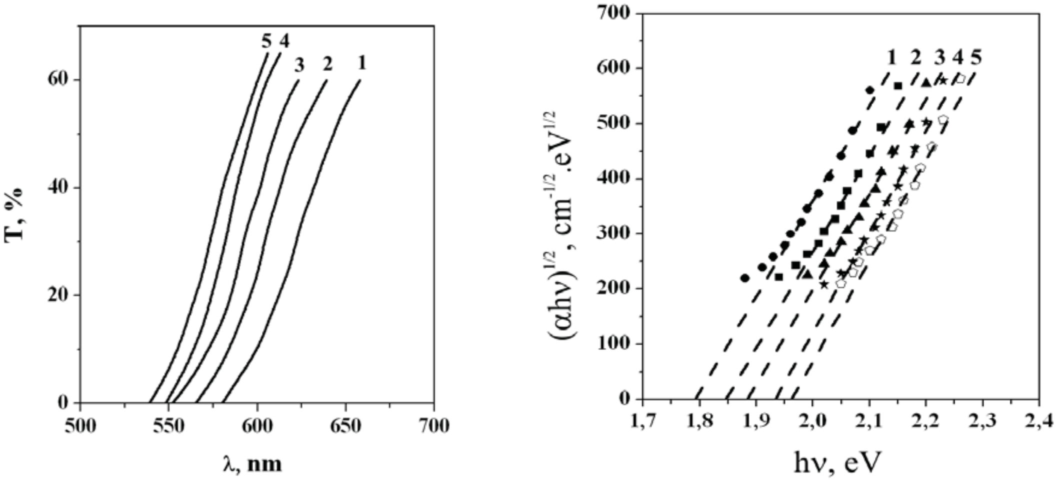

Fig. 2. Optical characteristics of thin films from the Se-S-Cu system (1 - x = 0 %; 2 - x = 10 %; 3 - x = 15 %; 4 - x = 20 %; 5 - x = 30 %):
a – transmission spectra; b – dependence $(\alpha h\nu)^{1/2} = f(h\nu)$

Since the obtained values for α are higher than 10^4 cm^{-1}, Tauc's power law is applicable. E_g^{opt} is determined by extrapolation of the linear part of the $(\alpha h\nu)^{1/2} = f(h\nu)$ dependence at α=0 - Fig. 2b.

A linear dependence between the optical band gap and the S-content in the $Cu_5Se_{95-y}S_y$ glasses is observed: E_g^{opt}=0.0057x + 1.797 – Fig. 3.

With the increase of the sulphur at constant Cu content, the E_g^{opt} increases, since

$$E_g^{opt}(Se) < E_g^{opt}(S)\ (E_g^{opt}(Se) = 1.7 \div 1.9 \text{ eV } [23]$$
$$E_g^{opt}(S) = 2.4 \text{ eV } [24]).$$

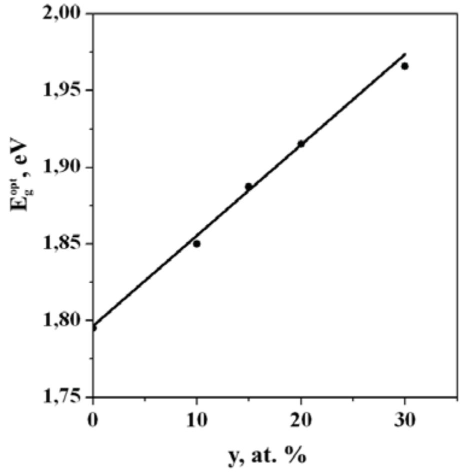

Fig. 3. Dependence of the optical band gap $\Delta E_{g,0}$ from the sulphur content in the film.

CONCLUSIONS

1. The glass-transition temperatures, density and microhardness of glasses from the Cu-S-Se system are determined. Based on the obtained results, the compactness, elasticity modulus, and the main thermo-mechanical properties of the investigated systems are calculated. A correlation between the composition and these properties is found.

2. Linear dependence between the glass-transition temperature and the overall mean bond energy is found ($T_g = 314\ (0.004\langle E\rangle+0.88)$).

3. Transmittance spectra of the synthesized glasses are recorded in the wave length range of 200-900 nm, and are used to calculate the optical band gap $\Delta E_{g,0}$. A linear dependence between $\Delta E_{g,0}$ and the sulphur content in the film is observed ($\Delta E_{g,0}$=0.0057x+1.797).

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ФИЗИКО-ХИМИЧНИ И ОПТИЧНИ СВОЙСТВА НА СТЪКЛА ОТ СИСТЕМАТА Cu-S-Se

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(Резюме)

На базата на резултатите от измерването на микротвърдостта (HV), плътността (d) и температурата на размекване (T_g) са изчислени термомеханичните характеристики обем (V_h) и енергия за образуване на микропразнина (E_h); компактността (C) и модула на еластичност (E) на стъкла от системата Cu-S-Se. По позната методика са изчислени още средните стойности на пълната енергия на връзките (<E>), координационното число (<Z>), енергията на средно омрежване за атом ($\bar{E}_c$) и тази на „останалата матрица" $\bar{E}$ ($_{rm}$), средната енергия на хетерополярната връзка (E_{hb}) и степента на омрежване за атом (P). Зависимостта между T_g и <E> е линейна: $T_g = 314(0.004\langle E\rangle + 0.88)$. Оптичната ширина на забранената зона (E_g^{opt}) на свежо отложени тънки слоеве със състав $Cu_5Se_{95-y}S_y$ ($0 \leq y \leq 30$) е определена от закона на Тауц. Зависимостта E_g^{opt} (y) е линейна: $E_g^{opt} = 0.0057y + 1.797$. Установени са закономерности между изследваните свойства и състава на стъклата.