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Surface-active and electrophysical semiconductors properties of the CdTe-CdSe system

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Abstract. Surface properties (acid-base, adsorptive, electrophysical) of binary and multicomponent semiconductors of the CdTe-CdSe system have been holistically studied. Changing patterns of the studied surface properties correlated among themselves and with changing patterns of the bulk physical and chemical properties have been revealed. The nature of active centers, acid-base, adsorptive and electronic interactions mechanisms have been determined with due account for local and collective factors. The most active discovered adsorbents are recommended as primary transducers of CO trace impurities measuring cells.

Keywords – binary and multicomponent semiconductors, surfaces acidity, adsorption, electrical conductivity, measuring cells.

1. Introduction

The research question here is the surface properties of the binary (CdTe, CdSe) and multicomponent ((CdTe)_x(CdSe)_{1-x}) semiconductors of the CdTe-CdSe. Possessing unique properties (electrical, optoelectrical, optical, etc.), binary semiconductors (A^{II}B^{VI} type) they are widely used in engineering: heterojunctions, laser radiating elements, luminescent and electrical luminescence display, diverse photo- and piezoelectric converters, ionizing-radiation detector, etc are based on them.

The subject of special concern is multicomponent semiconductors – substitution solid solutions, implicating even greater possibilities. Preserving many unique properties of the initial binary compounds, they can detect unexpected, specific effects related to the peculiarities of internal processes accompanying solid-solution formation: ordering, structure hardening, combined effect of constituent components as macro- and micro effects and possible high concentrations of impurity centers [1]. Such unexpected, specific effects are useful both for science and sophisticated technology.

At the same time, the potential for use the designated objects in sophisticated technology, in particular in nano- and sensor technology, are considerably determined by awareness of their bulk and surface physico-chemical properties in particular. The determining role of the latter grows with the growing trend to miniaturization of semiconductor devices and facilities.

The issue is acid-base, adsorptive and electrophysical surface properties of the CdTe-CdSe system semiconductors.

2. Problem statement



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To study in an integrated manner acid-base, adsorptive (in relation to CO), electrophysical properties of binary and multicomponent semiconductors of the CdTe-CdSe system. To determine the nature of active centers, mechanisms and patterns of surface interactions, their connection with bulk and physico-chemical changing patterns.

To identify the most active adsorbents – possible primary transducers of CO (carbon monoxide) trace impurities measuring cells with subsequent practical guidelines.

3. Experimental part

The research subjects were powders ($S_{sp} = 0.405 \dots 0.91 \text{ m}^2/\text{g}$) and nanosized films ($d = 20 \dots 100 \text{ nm}$) of CdTe, CdSe, and solid solutions $(\text{CdTe})_x(\text{CdSe})_{1-x}$ ($x = 15; 25; 50; 75; 85 \text{ mol. \%}$). Solid solutions powders were obtained by isothermal diffusion of binary compounds (CdTe, CdSe) in vacuum-sealed quartz vessel at temperature close to the melting point of more easily melted binary compound (CdTe), followed by homogenizing annealing, according to the created program [1]; binary compounds and solid solutions films – by discrete thermal spraying in vacuum ($T_{\text{cond}} = 298 \text{ K}$, $P = 1.33 \cdot 10^{-3} \text{ Pa}$) on electrodes of AT – cut piezoquartz resonators [2, 3]. Simultaneously, on the same film samples the resistance change according to electrical conductivity (σ_s) and the surface charging under adsorption conditions were investigated (using the probe compensation method [3]). The film thickness was determined from frequency deviation of the piezoquartz resonator [3].

To identify solid solutions, the results of X-ray research were mainly used, indirectly supported by the results of IR and UV spectroscopic studies [4].

X-ray studies were carried out on diffractometers DRON-3, in $\text{CuK}_{\alpha,\beta}$ – radiation ($\lambda = 0.154178$ and 0.139217 nm), and D8 Advance from «Bruker»(Germany), in CuK_{α} – radiation ($\lambda = 0.154056 \text{ nm}$), by method of high-angle scattering [5, 6], using the position-sensitive detector Lynxeye, as well as data base ICDIPDF-2 and software ICDIPD 3.0 (Bruker).

Surface properties were judged by the results of acid-base and adsorption properties studies. Acid-base properties were examined by methods of hydrolytic adsorption, mechanochemistry and non-aqueous conductometric titration [1, 7, 8], adsorption properties were examined by methods of piezoquartz crystal microbalance (sensitivity $10^{-11} \text{ g/cm}^2 \cdot \text{Hz}$) and by volumetric method [3] at temperature $258 \dots 477 \text{ K}$ and pressure $6 \dots 18 \text{ Pa}$ intervals.

Adsorbate gas (CO) was obtained according to a well-known method [8].

Reproducibility and accuracy of the experimental data were checked based on the results of parallel measurements using mathematical statistics, quantitative analysis results processing methods and computer programs.

4. Results and discussion

According to X-ray study findings [9], in the system CdTe – CdSe solid substitutional solutions are formed with sphalerite structure (excessive CdTe) and wurtzite (excessive CdSe). This is evidenced by the relative position and distribution by intensity of the basic lines on binary compounds and solid solutions radiographs, dependence on crystalline grids parameter values composition (a , c), interplanar spacing (d_{hkl}), density (ρ_r) (for example, see Fig. 1, [9]).

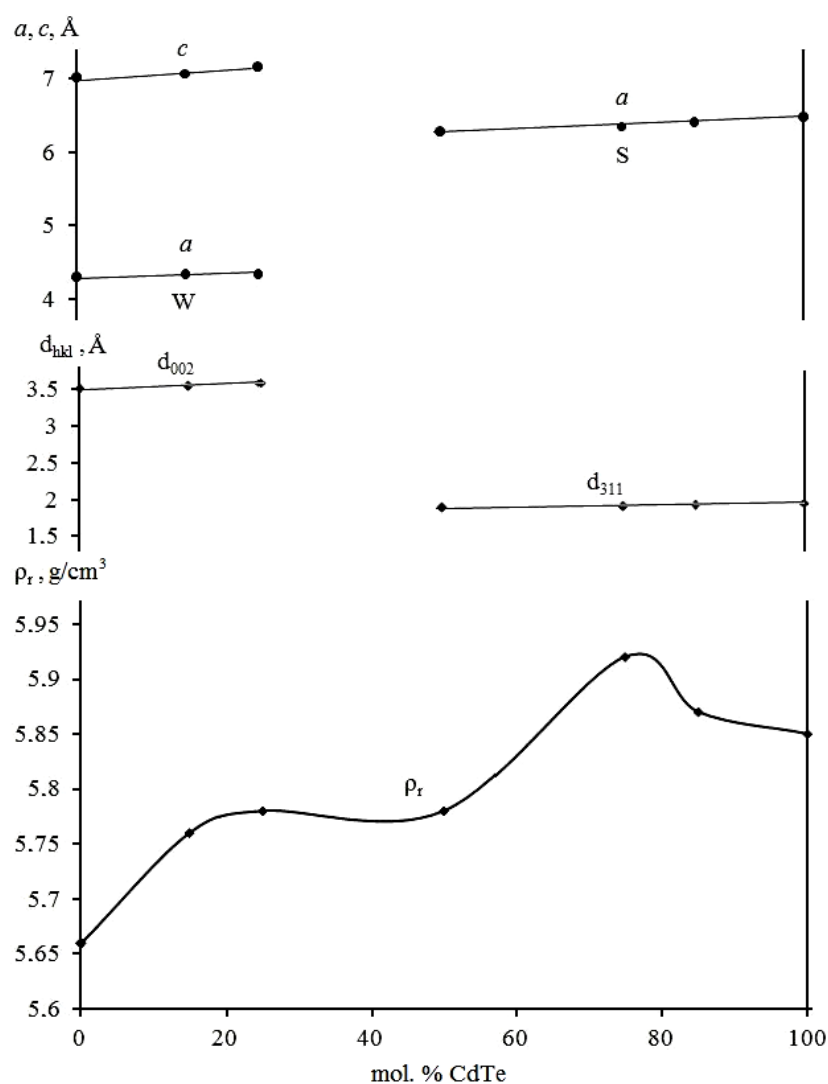


Figure 1. Dependence on crystalline grids parameter values composition (a , c), interplanar spacing (d_{hkl}) and theoretical calculated crystal density (ρ_r) of the system CdSe-CdTe components; W – wurtzite, S – sphalerite.

Study of the surfaces acid-base properties made it possible to determine the strength (isoelectric state $\text{pH} - \text{pH}_{\text{iso}}$), overall concentration (C_{overall}) (Table 1), acid sites nature.

Table 1. Acid-basic surface characteristics of the system CdTe – CdSe components.

System component	pH_{iso}	C_{overall}
CdTe	6.29	2.0
$\text{CdTe}_{0.85}\text{CdSe}_{0.15}$	6.13	2.6
$\text{CdTe}_{0.75}\text{CdSe}_{0.25}$	5.88	2.8
$\text{CdTe}_{0.5}\text{CdSe}_{0.5}$	5.99	4.3
$\text{CdTe}_{0.25}\text{CdSe}_{0.75}$	5.84	4.4
$\text{CdTe}_{0.15}\text{CdSe}_{0.85}$	5.86	3.9
CdSe	6.81	3.4

According to the strength of acid sites (pH_{iso}), CdTe – CdSe system components are arranged on the initial surfaces in the following sequence:

$\text{CdTe} \rightarrow (\text{CdTe})_x(\text{CdSe})_{1-x} \rightarrow \text{CdSe}$, with changes in pH_{iso} values from 6.29 to 6.81.

The latter indicates the faintly-acid nature of such surfaces and respectively the prevailing contribution of Lewis acid sites charged by coordination unsaturated atoms [1, 7].

The impact of the increased acidity of the CdTe surface (compared to CdSe) on the acidity of the solid solutions surfaces (Table 1) comes under notice. The basis is a regular change in the bulk physical and chemical properties of binary compounds (at transition from CdTe to CdSe). Here it is logical to talk about the melting point (T_m), band gap (ΔE), electronegativity differences (Δx) (Table 2), which determine the A-B bonds strength; possibility of electrons transitions from the valence band to the conduction band and their localization on coordinatively unsaturated atoms (Lewis sires), responsible for the acidity of the surfaces, and ionicity, and the surfaces hydration.

Table 2. Values of bulk (T_m , ΔE , Δx) and surface (pH_{iso}) initial binary compounds properties of the CdTe–CdSe system.

Composition	Melting point (T_m), °C	Band gap (ΔE), eV	Electronegativity differences (Δx)	pH_{iso}
CdTe	1092	1.51	0.4	6.29
CdSe	1258	1.88	0.8	6.81

As the Table 2 shows, growth of the indicated bulk physical and chemical properties provides growth of pH_{iso} . Such parallels in bulk and surface properties changes additionally confirm the defining role of coordinatively unsaturated atoms as the acid Lewis sites in this case. They are also responsible for the adsorption of molecules of CO, CO₂, H₂O [1, 7] type.

The results of the adsorption properties of the CdTe–CdSe system components (relative to CO) studies make it possible to claim of chemical activated adsorption leak at room temperature [10]. The reason for such statement is the appearance of adsorption isobars (see, for example, Fig. 2) the results of the analysis of equilibrium ($\alpha_T = f(p)$) and kinetic ($\alpha_T = f(t)$) adsorption isotherms, performed activation energy calculations (E_a) and adsorption heat (q_a) as well as the results of electrical conductivity measurements (σ_s) under adsorption conditions (Fig. 2, 3).

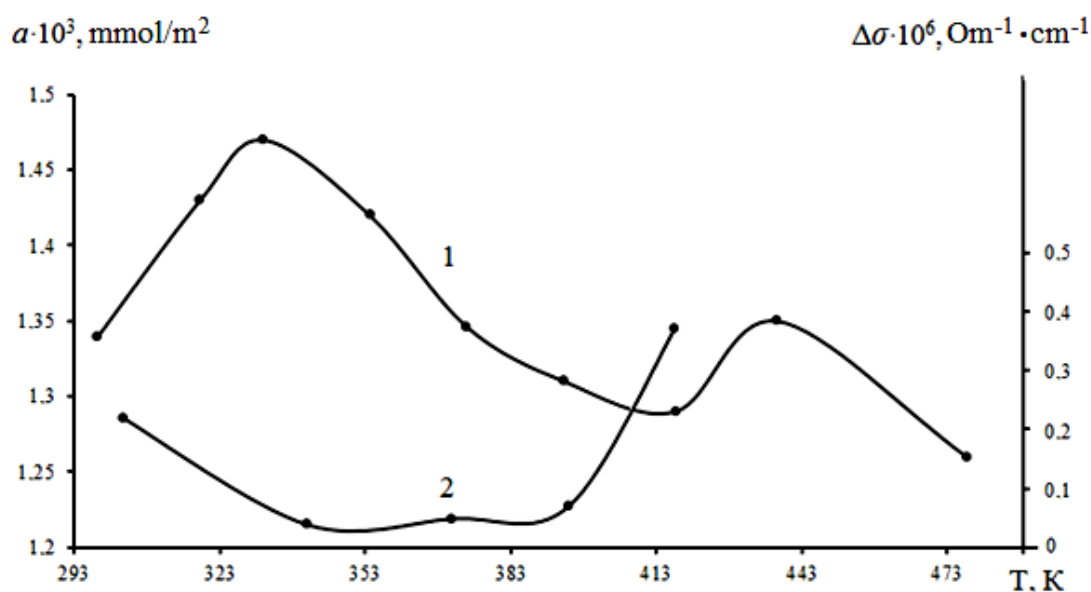


Figure 2. Temperature dependence of CO adsorption amount on the solid solution $(\text{CdTe})_{0.85}(\text{CdSe})_{0.15}$ (1) and the change in its electrical conductivity during CO adsorption at $P_0 = 16 \dots 18$ Pa.

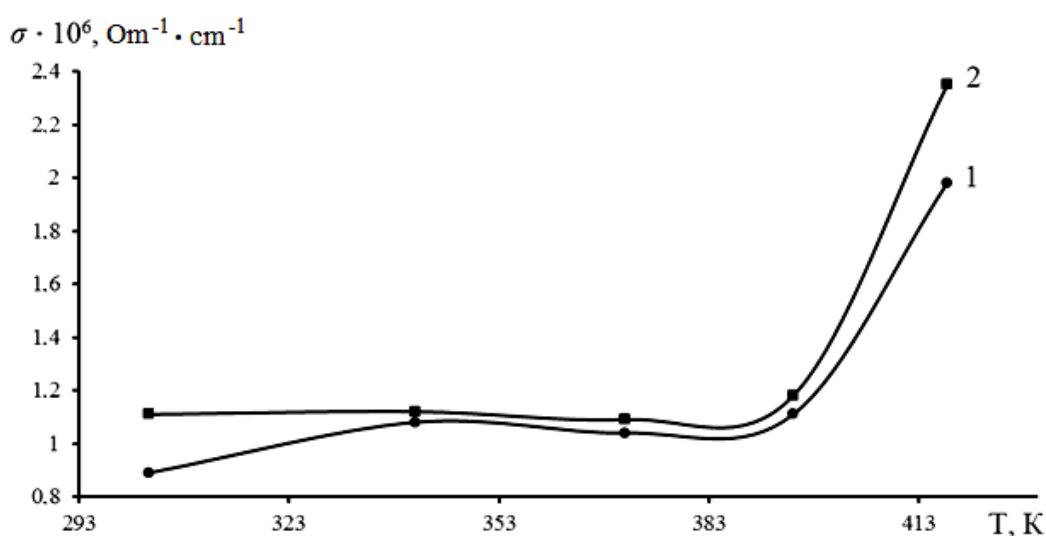
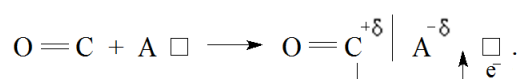


Figure 3. Temperature dependence of the solid solution electrical conductivity $(\text{CdTe})_{0.85}(\text{CdSe})_{0.15}$ in vacuum (1) and during CO adsorption (2) at $P_b = 16 \dots 18$ Pa.

When thoroughly considering the said results, taking into account the acid-base properties of adsorbent surfaces, electronic structure of adsorbate (CO) molecules and their “behavior” on other diamond-like semiconductors [1, 7] it is apparent that CO adsorption proceeds by the donor-acceptor mechanism with predominantly surface A atoms (with free d- and p- orbitals and more evident metallic properties) as acceptors, and adsorbate molecules as donors:



Formation of donor-acceptor bonds is indicated by the presence of the corresponding bands in the IR spectra after CO adsorption [10], and the possible role of CO molecules as electron donors – by the increase in electrical conductivity (σ_s) under CO adsorption conditions (Fig. 2, 3).

Noting the preferential formation of donor-acceptor bonds in the adsorption systems under study one can not exclude due to the peculiarities of the electronic nature of CO molecules the possible definite contribution of back donation and hydrogen bonds [1, 7].

The results of the electrical conductivity measurements under adsorption conditions (Fig. 2, 3), indicating its change and respectively, charging of adsorbent surfaces indicate the dependence of the adsorption capacity of CO molecules not only on the local factor (chemical properties of molecules and active sites) but also on the collective (electronic) factor, which is determined by the position of the Fermi level and the character of the surfaces energy spectrum [1, 7]. That is, with such features of the donor-acceptor bonds $\text{CO}^{\delta+} - \text{A}^{\delta-}$, the participation of free carriers in the elementary adsorption act is inevitable, although the selectivity of gas adsorption is determined by the local properties of the surface [3, 11].

It is appropriate to recall that the free carriers concentration (electrons - n and holes - p) in crystalline bodies is related to the width of the forbidden band and the position of the Fermi level in it. It is the reason for the statement in the framework of the electron theory of adsorption and catalysis by F.F. Wolkenstein on the role of the Fermi level as a regulator of adsorption and catalytic activity [11].

5. Summary and conclusions

Complex studies of acid-base, adsorption (in relation to CO), electrophysical properties of binary and multicomponent semiconductors of the CdTe-CdSe system have been performed.

Taking into account their physical and chemical properties, the following has been established:

- the nature of active sites and mechanisms of acid-base, adsorption and electronic interactions;
- the role of local and collective factors;
- changing patterns of the studied surface properties correlated among themselves and with changing patterns of the bulk physical and chemical properties.

The most active adsorbents, cadmium telluride and solid solution with its excess have been discovered, proposed as primary transducers of CO trace impurities measuring cells (carbon monoxide). Footnotes should

be avoided whenever possible. If required they should be used only for brief notes that do not fit conveniently into the text.

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