Optical gap bowing parameter and spin-orbit splitting in $CdSe_{1-x}S_x$ thin films

Kashuba A.I.[1], Andriyevsky B.[2], Ilchuk H.A.[1], Semkiv I.V.[1], Kashuba N.Yu.[1]

[1]*Department of General Physic, Lviv Polytechnic National University,*
Bandera Str., 12, Lviv-79046, Ukraine
E-mail: andrii.i.kashuba@lpnu.ua

[2]*Faculty of Electronics and Computer Sciences, Koszalin University of Technology, Sniadeckich Str., 2, Koszalin 75-453, Poland*

$CdSe_{1-x}S_x$ thin films are prepared by the method of high-frequency (HF) magnetron sputtering (13.6 MHz) using a VUP-5M vacuum station (Selmi, Ukraine). The target–substrate distance was 60 mm. The start and end of the process were controlled by means of a movable shutter. Before the sputtering process, the chamber was evacuated. The gas pressure inside the chamber was 4×10^{-4} Pa. This pressure is achievable when using a Polifenilovyi Efir 5Φ4E diffusion fluid in the vapor oil vacuum pump, which provides a low partial vapor pressure (9×10^{-7} Pa). The sputtering was carried out at a pressure of argon (Ar) in the range of 1.0–1.3 Pa. The power of the HF magnetron was maintained at the level of 100 W and the temperature of the substrate at 563 K. For heating the substrates, a high-temperature tungsten heater with a power of 300 W was used. The temperature was controlled by means of a proportional–integral–derivative (PID) controller for controlling heating and cooling rates, as well as for ensuring the temperature conditions of deposition.

The phase analysis and crystal structure refinement were examined with using X-ray diffraction data (DRON-2.0M) at the room temperature. The thickness of the films was measured on a Veeco profilometer (model Dektak 8). The mean value of the $CdSe_{1-x}S_x$ film thickness is ~0.5 µm. The X-ray fluorescence spectroscopy (XRF) and energy-dispersive X-ray (EDX) study were used for analyzing the chemical composition of materials. The spectral dependence of the optical transmittance (Shimadzu UV-3600) of the obtained sample in the visible and near-infrared regions is studied at room temperature.

Results of XRF spectra analysis.

Theoretical composition	**Experimental composition (from XRF)**	***x***
$CdSe_{0.75}S_{0.25}$	$CdSe_{0.7}S_{0.3}$	0.3
$CdSe_{0.5}S_{0.5}$	$CdSe_{0.6}S_{0.4}$	0.4
$CdSe_{0.25}S_{0.75}$	$CdSe_{0.4}S_{0.6}$	0.6

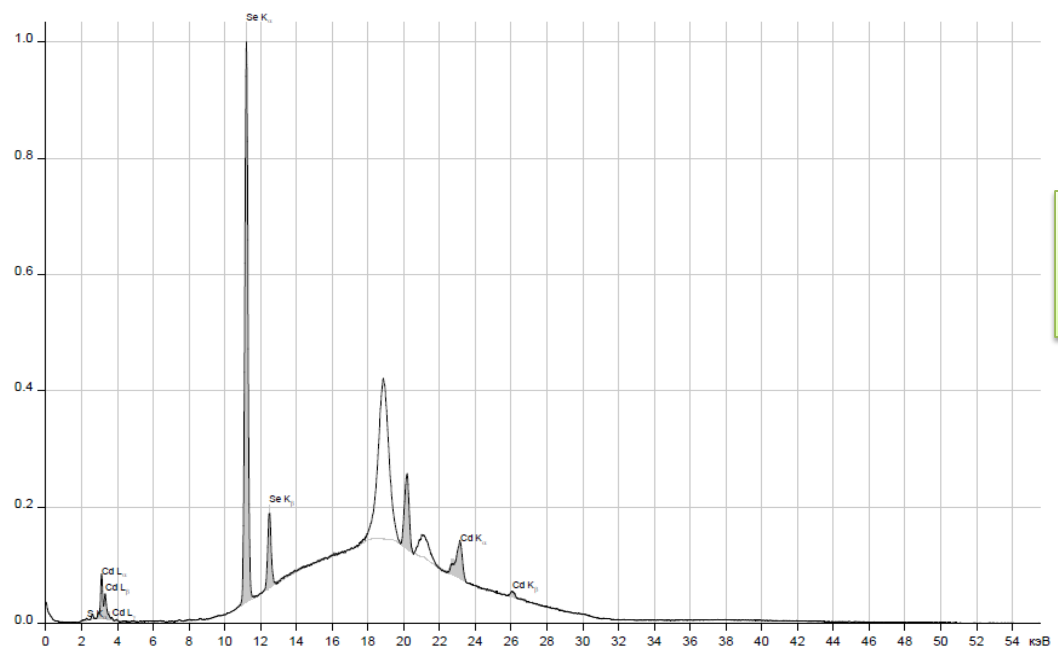

Fig.1. XRF spectra of $CdSe_{0.7}S_{0.3}$ thin film.

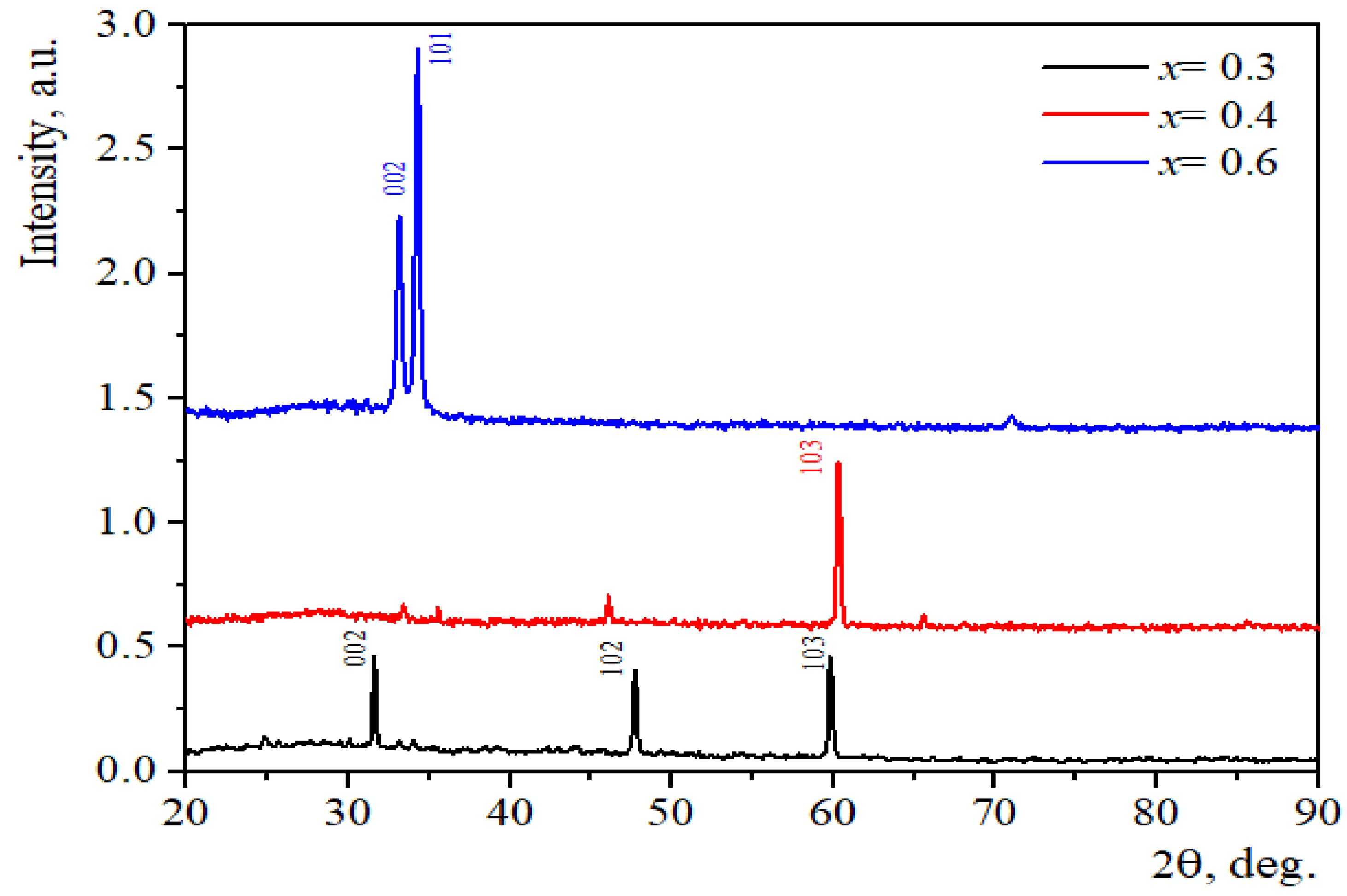

Fig.2. XRD pattern of $CdSe_{1-x}S_x$ thin film.

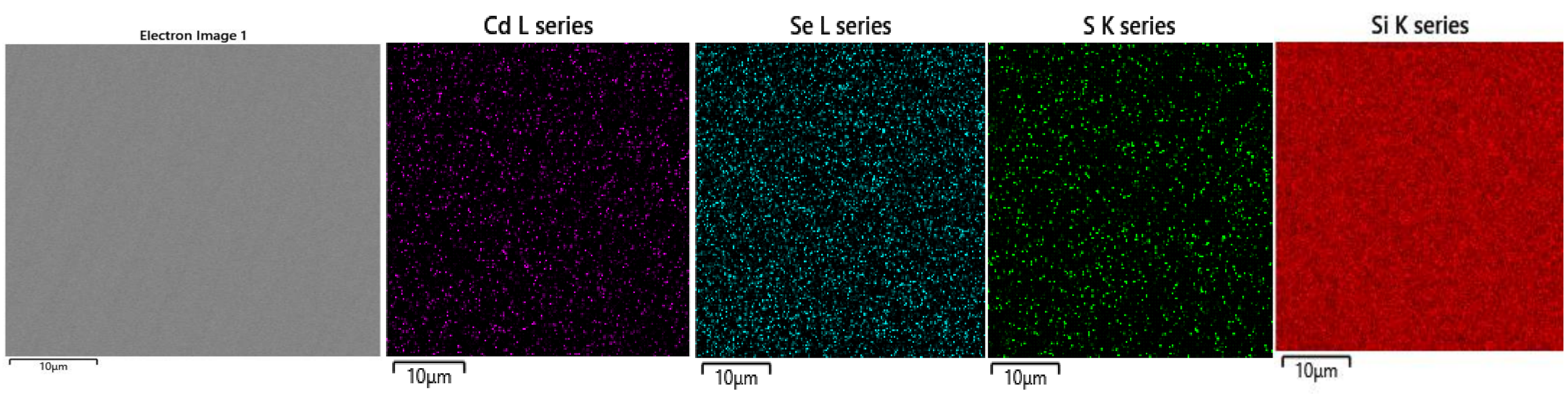

Fig. 3. Morphology of $CdSe_{0.6}S_{0.4}$/Si with the elemental distribution.

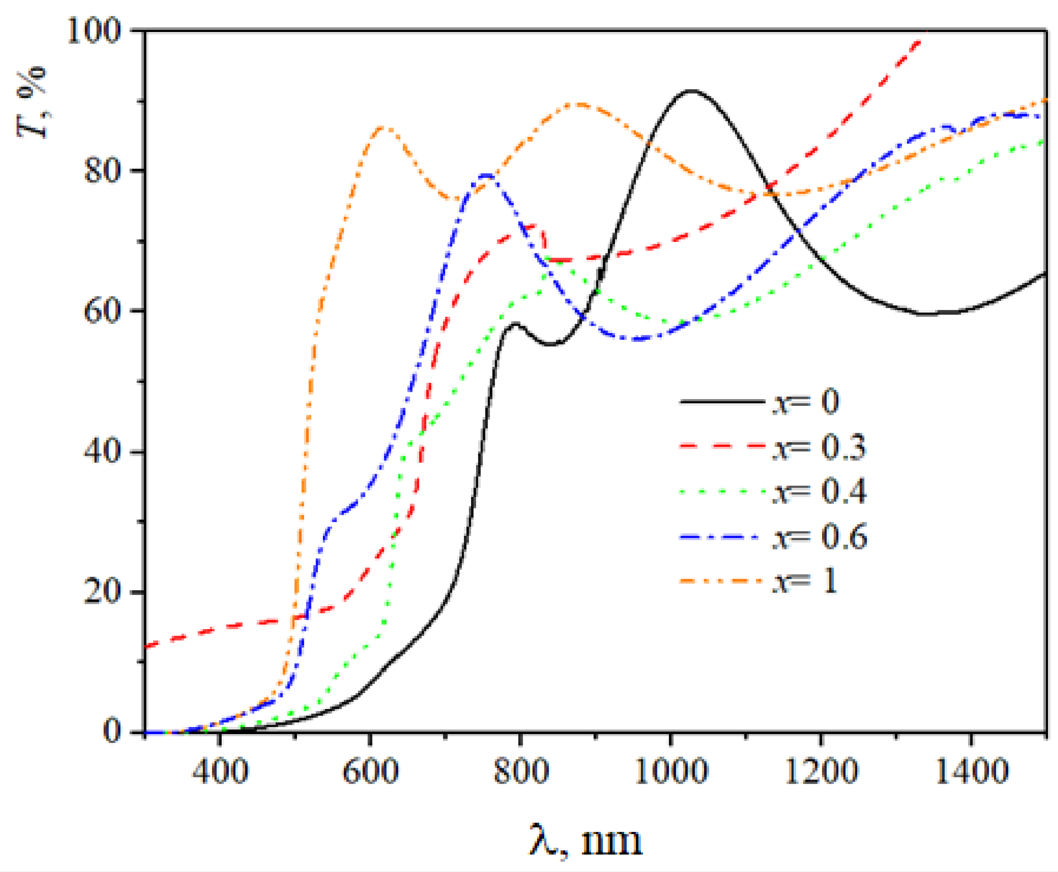

Fig. 4. Optical transmission of the $CdSe_{1-x}S_x$/quartz thin films at room temperature.

$$E(x) = x\cdot E_{CdS} + (1-x)\cdot E_{CdSe} - \delta\cdot x\cdot(1-x)$$
$$\delta = \delta_{VD} + \delta_{CE} + \delta_{SR}$$

Band gap and spin-orbit splitting of $CdSe_{1-x}S_x$ thin films.

Sample	Tauz	d*T*/dλ		
	E_g	E_g	E_{g2}	E_{SO}
CdSe	1.6	1.66	2.04	0.38
$CdSe_{0.7}S_{0.3}$	1.77	1.85	2.14	0.29
$CdSe_{0.6}S_{0.4}$	1.89	1.96	2.28	0.32
$CdSe_{0.4}S_{0.6}$	2.17	2.3	2.46	0.16
CdS	2.34	2.43	2.48	0.05

Optical gap bowing parameter estimated for main optical transitions of $CdSe_{1-x}S_x$ thin films.

Methods/Ref.		GGA+PBEsol	Tauz	d*T*/dλ	[1]	[2]	[3]
Sample		Thin films			Nanoparticle	Thin films	Crystal
Crystal structure		$P6_3mc$				*F*-43*m*	
Optical transitions	$E_g(\Gamma_8^v-\Gamma_6^c)$	0.13	-0.14	-0.24	0.54	0.079	0.53, 0.54
	$E_{g2}(\Gamma_7^v-\Gamma_6^c)$	0.12	–	-0.33	–	0.101	–

References

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