Determination of the Point of the Zincblende-to-Wurtzite Structural Phase Transition in Cadmium Selenide Crystals

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Determination of the Point of the Zincblende-to-Wurtzite Structural Phase Transition in Cadmium Selenide Crystals

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Introduction There are quite contradictory data in the literature on the point of the phase transition in cadmium selenide crystals where the zincblende (ZB-3C) crystalline structure transforms into the wurtzite (W-2H) structure. For instance, the authors of /1 to 3/ state that this temperature is between 360 and 480 $^{\circ}$C (357 $^{\circ}$C in the last work /3/), whereas the results of /4, 5/ indicate that it cannot be above 130 and 100 $^{\circ}$C, respectively.

Experimental results The method of determining T (ZB $\rightarrow$ W) we use in this study is based on the exchange process between cations from $A^{II}B^{VI}$ crystals and cations from the melts or solutions of salts, which we have discovered earlier /6 to 8/. In particular, the ion-exchange reaction results in that in the surface region of zinc selenide single crystals there forms a $Cd_xZn_{1-x}Se$ solid solution whose composition depends on the relative concentration of zinc and cadmium ions in the liquid phase and on the temperature of the process /7/. The process takes place under equilibrium conditions, since the composition of the produced solid solution is independent of the process duration. The ion exchange process in the ZnSe powder occurs in a similar way /8/. In contrast to the corresponding process in a single crystal /7/ and to the method used in /1 to 3/, which result in the formation of metastable structures, it is characterized by the absence of introduced mechanical stresses, so that the structure of the $Cd_xZn_{1-x}Se$ crystalline powder is thermodynamically stable at the temperature of the process in which it was formed.

The ion-exchange process of CdSe production was carried out in a solution of cadmium chloride, $CdCl_2$, in glycerine (0.1 mol/l). A fine-dispersed ZnSe powder was used (0.01 mol/l) with the particle size less than 1 μm. The following heterogeneous ion-exchange reaction took place in the solution:

$$CdCl_2(l) + ZnSe(s) = ZnCl_2(l) + CdSe(s) \quad . \tag{1}$$

The processes were carried out at temperatures between 50 and 150 $^{\circ}$C during 6 months. The initial solution contains no zinc ions, and there is much more

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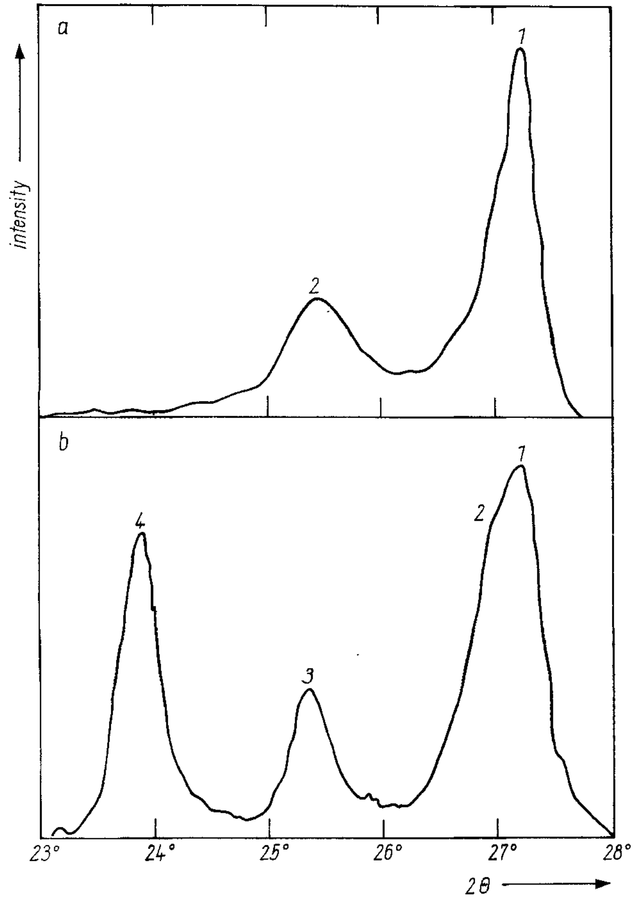

Fig. 1. X-ray diffractograms of powders obtained at different temperatures. a) T = 90 °C: 1: peak with respect to (111) reflection of ZB-ZnSe, 2: ZB-CdSe (111); b) T = 100 °C: 1: ZB-ZnSe (111), 2: W-CdSe (101), 3: W-CdSe (002), 4: W-CdSe (100)

cadmium chloride than zinc selenide. Thus, in accordance with the isotherm of the $Cd^{2+} \leftrightarrows Zn^{2+}$ ion exchange /7, 8/, reaction (1) proceeds to the end, with production of pure cadmium selenide particles on the surface. The structure type and lattice parameters on the CdSe produced were determined by X-ray diffraction (with a D-2 "Rigaku Denki" diffractometer, CuK_{α} radiation). It was found that the CdSe produced at a temperature below 90 °C has zincblende structure (a = 0.607 nm, see Fig. 1a), whereas the one produced at temperatures above 100 °C has wurtzite-type structure (a = 0.430 nm and c = 0.701 nm, see Fig. 1b). The value of the crystalline lattice parameter for zincblende CdSe is close to what has been published in the literature /9/: a = 0.6077 nm. Let us mention that within the time the process took place, the ZnSe powder did not transform into CdSe entirely. This is due to the smallness of ion interdiffusion coefficients at low temperatures of ion exchange /7/. We believe that this fact did not affect the determination of the temperature of the structural phase transition. Indeed, in /8/ we showed that the structure and composition of the solid solution formed at 400 to 600 ^{o}C via exchange reaction did not depend on the exchange time and, therefore, on the degree of powder transformation.

Conclusion It was established that the temperature of the zincblende-to-wurtzite structural phase transition in cadmium selenide crystals is $(95 \pm 5)^{o}C$. Knowing this value, one is able to plot or predict the CdSe-ZnSe, CdSe-HgSe, CdSe-CdTe, and other state diagrams in the low temperature region.

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