

Nanocomposites and nanomaterials

Physico-chemical interaction in CuSbSe_2 -“ P_2Se_4 ” system

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Modern device engineering needs the devices with different semiconductor materials. Among them quaternary compounds $\text{Me}^{\text{I}}\text{Me}^{\text{III}}\text{P}_2\text{X}_6$ (Me^{I} -Cu, Ag; Me^{III} -In, Sb, Bi, Cr, V; X-S, Se) which were intensively studied recent years can be interesting as ferroelectrics and thermoelectrics.

$\text{CuSbP}_2\text{Se}_6$ is one of such compounds. This report describes physico-chemical interaction in CuSbSe_2 -“ P_2Se_4 ” system where this compound is formed.

Samples of CuSbSe_2 -“ P_2Se_4 ” system were obtained from elementary components in evacuated silica ampoules. Weight of the sample was 5 g. Temperature of synthesis was controlled by Chromel-Alumel thermocouple. During the synthesis of the alloys firstly we stopped the heating for 24 hours at 450-500 K. Next stop was at 670 K also for 24 hours. At the maximum temperature of synthesis which was 950-1000 K the samples were endured for 1 week. In order to homogenize the alloys they were annealed at 550 K during 2 weeks.

Obtained compounds were investigated by differential thermal analysis. On the base of DTA phase diagram of CuSbSe_2 -“ P_2Se_4 ” system has been built till 50 mol. % “ P_2Se_4 ”. We established that quaternary compound $\text{CuSbP}_2\text{Se}_6$ is forming by peritectic reaction at 713 ± 5 K. Composition of the peritectic point is 91 mol. % CuSbSe_2 – 9 mol. % “ P_2Se_4 ”. Eutectic point in this system (683 ± 5 K) has a composition 94 mol. % CuSbSe_2 – 6 mol. % “ P_2Se_4 ”.

X-ray diffraction pattern of $\text{CuSbP}_2\text{Se}_6$ was obtained by DRON-3 diffractometer. It was established that $\text{CuSbP}_2\text{Se}_6$ crystallizes in trigonal lattice (P-31c) with unit cell parameters: $a=6,507(1) \text{ \AA}$; $c=13,272(5) \text{ \AA}$; $Z=4$; $\rho_{\text{calc.}}=4,92 \text{ g/cm}^3$, unit cell volume $V=486,578 \text{ \AA}^3$.

The density of $\text{CuSbP}_2\text{Se}_6$ determined by picnometry is $\rho_{\text{exp.}}=4,74 \text{ g/cm}^3$.

Enthalpy of melting of $\text{CuSbP}_2\text{Se}_6$ was calculated using quantitative thermography method ($\Delta H=41,18 \text{ kJ/mol}$).

Obtained data of this compound may be added to a database of new quaternary compounds. Its crystallochemical characteristics can be used for identification of related compounds.