Interaction of the Components in the System Ba-Tb-Cu-O and Related Systems

O. Zaremba, R. Gladyshevskii

Ivan Franko National University of Lviv, 6 Kyryla i Mefodiya Str., UA-79005 Lviv, Ukraine

The interaction of the components in the *A*-*R*-Cu-O systems, where *A* is an alkaline-earth and *R* is a rare-earth metal, has attracted considerable interest for a long time. The compounds of these systems are usually characterized by layered structures and are first of all interesting as high-temperature superconductors. The most prominent among them is undoubtedly $YBa_2Cu_3O_7$ (*YBCO*), the crystal structure and properties of which have been studied meticulously. The interaction of the components in the system Ba-Y-Cu-O and related systems with other alkaline-earth and rare-earth metals has also been widely investigated [1]. In this work we focus on the system Ba-Tb-Cu-O, and some related systems, for which data in the literature are scarce.

Polycrystalline samples of the BaO-Tb_2O_3-CuO system were prepared by solid-state reaction of appropriate amounts of high-purity carbonates and oxides at 1173 K in air in two 24-hour stages. Firstly the reagents were mixed and heated in a corundum crucible to decompose the carbonates. Then, after cooling to room temperature, the mixtures were reground to achieve homogeneity, pressed into pellets and sintered again. Phase and structure analyses were carried out on X-ray powder diffraction data (DRON 2.0M diffractometer, Fe K_α radiation). Samples of nominal composition $A_{0.5}Tb_{0.5}TO_3$, where *A* = Ca, Sr or Ba, *T* = Ni or Zn, were prepared in similar way.

The isothermal section of the phase diagram of the BaO-Tb_2O_3-CuO system at 1173 K was constructed based on the investigation of fifteen samples. The existence of the compounds $BaTbO_3$ ($SrZrO_3$ structure type, *I*4/*mcm*, a = 0.6034(1), c = 0.8576(1) nm, R_B = 0.052) and $Ba_{44}Cu_{45}O_{90}$ (own structure type, *Im*-3*m*, a = 1.8266(3) nm, R_B = 0.237) was confirmed in the pseudo-binary BaO-Tb_2O_3 and BaO-CuO systems, respectively. It was established that the interaction of the components in the ternary region of the BaO-Tb_2O_3-CuO system is characterized by the absence of compounds. The only compound reported in the literature, $TbBa_2Cu_3O_7$ with orthorhombic $YBa_2Cu_3O_7$ structure type [2], was not observed under the conditions of our study. The $BaTbO_3$ phase is in equilibrium with the $Ba_{44}Cu_{45}O_{90}$ and CuO phases. Hence, there are three three-phase and two two-phase regions in the system. It should be noted that, during the synthesis, the initial cubic Tb_2O_3 phase with $(Mn_{0.5}Fe_{0.5})_2O_3$ structure type was oxidized into the rhombohedral Tb_7O_{12} phase with Pr_7O_{12} structure type.

$Ba_{0.5}Tb_{0.5}ZnO_3$ and $Sr_{0.5}Tb_{0.5}ZnO_3$ were found to be two-phase samples, which contained in equilibrium $BaTbO_3$ ($SrZrO_3$ structure type, *I*4/*mcm*, a = 0.6039(1), c = 0.8578(1) nm, R_B = 0.099), or $SrTbO_3$ ($GdFeO_3$ structure type, *Pnma* a = 0.5945(1), b = 0.8347(2), c = 0.5879(1) nm, R_B = 0.160), and ZnO. The investigation of the samples with nominal compositions $Ca_{0.5}Tb_{0.5}ZnO_3$ and $Ca_{0.5}Tb_{0.5}NiO_3$ showed the presence of phases that correspond to the reagents only – CaO, Tb_7O_{12} and ZnO (or NiO), in appropriate ratios.

[1] P. Villars, K. Cenzual (Eds.), Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds, ASM International, Materials Park, OH, USA, Release 2014/15.

[2] H. Ouchi, Preparation and superconducting properties of *Ln*-Ba-Cu-O ceramics, *Ferroelectrics* **95** (1989) 215-220.