Indium complex oxides have tremendously triggered many research efforts due to their exceptional physical properties, such as high electrical conductivity and transparency in the visible range. In our work, subsolidus phase relations of Li$_2$O-In$_2$O$_3$-TiO$_2$ ternary system at 1050 °C and WO$_3$-In$_2$O$_3$-TiO$_2$ ternary system at 1000 °C have been systematically investigated. Samples with different compositions were synthesized by the conventional solid-state reaction method, and their phase assembles were analyzed by means of powder X-ray diffraction method.

The Li$_2$O-In$_2$O$_3$-TiO$_2$ ternary system contains a new compound LiInTi$_2$O$_6$ and is divided into seven three-phase regions. The crystal structure of LiInTi$_2$O$_6$ was solved based on powder X-ray diffraction data by the charge flipping method [1] using Jana2006 program [2], and refined by the Rietveld method [3] using Fullprof-suite program [4]. It crystallizes in a trigonal unit cell of $a = b = 5.1050(5)$ Å, $c = 28.5620(4)$ Å, $V = 644.63(1)$ Å$^3$, and $Z = 6$ in space group $R-3m$ (No. 166). The fundamental building units of this structure are 12-fold coordinated metal-oxygen prisms. It represents a three-dimensional mixed (Li/Ti)O$_{12}$, (In/Li/Ti)O$_{12}$, and TiO$_{12}$ prisms stacking layer by layer along the $c$ axis.

As for WO$_3$-In$_2$O$_3$-TiO$_2$ system, the phase diagram is composed of six three-phase regions. A new compound WIn$_2$TiO$_8$ which was isostructural with InNbO$_4$ was observed in this system. The crystal structure of WIn$_2$TiO$_8$ was also refined by the Rietveld method using Fullprof-suite program. Final agreement factors were converged to $R_B = 4.29\%$, $R_p = 5.00\%$, $R_{wp} = 6.43\%$, and $S = 1.50$. It crystallizes in the space group $P2/c$ (No. 13) with $a = 4.77631(6)$ Å, $b = 5.72598(8)$ Å, $c = 5.08664(7)$ Å, $\beta = 91.9025(6)$ °, $V = 139.038(3)$ Å$^3$, and $Z = 2$. Its crystal structure is alternately layered by InO$_6$ and (W/Ti)O$_6$ octahedra chains in the form of corner- and edge-sharing along the $a$ axis.

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Reference