Structural Study of Sn-doped In_2O_3

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Tin doped In_2O_3 (ITO) is widely used in phototronic, opto-electronic and microelectronic devices. There are numerous studies on ITO, but the understanding of its defect structure is rather incomplete. In_2O_3 possesses a cubic structure, the space group Ia^3[1]. The structure contains two different six-fold-coordinated cation sites referred as sites B and D, respectively. This paper focuses on X-ray diffraction and ^{119}Sn Moessbauer studies of the polycrystalline ITO samples containing 2-14 at% Sn. Nanocrystalline ITO powders were prepared by a sol-gel technique using $InCl_3$ and $SnCl_4$ reagent grade chemicals and annealed at 300°C for 5 h. Lattice parameter *a* of doped In_2O_3 increased with Sn-doping level up to 8 at% and decreased above. Such behavior of lattice parameter suggests that tin substitution for In^{3+} on sites B and D is non-uniform and depends on tin content. ^{119}Sn Moessbauer spectra indicated that only the Sn^{4+} state is present in ITO samples. The least square fitting of spectra was performed by assuming presence of two doublets. In accordance with [2], doublets with isomer shifts (IS) in the range 0.09–0.17 and 0.36–0.464 mms^{-1}, respectively, correspond to the D and B sites in the cation sublattice of the In_2O_3 structure. The area ratio of the two doublets depended on tin content.

[1] Marezio M., *Acta Cryst*., 1966, **20**, 723. [2] Binczycka H., et al., *Phys. Stat. Sol. (B),* 2005, *in press*.

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