Structural Changes of Sol-Gel derived Sn-doped In_2O_3 due to Annealing at 1000 ºC

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Sn doped In_2O_3 (ITO) is an n-type, highly degenerate, wide-gap semiconductor. Its electrical and optical properties are associated with microstructure as well as with the preparation methods and conditions [1]. Although it is widely used in optoelectronic devices, its structure is not well understood yet. A set of ITO samples containing 0-14 at% Sn was prepared by a sol-gel technique from $InCl_3$ and $SnCl_4$ [2]. The samples were additionally annealed at 1000 ºC for 1 h, slowly cooled to RT and examined by XRD and ^{119}Sn Moessbauer spectroscopy. XRD revealed that the samples were isostructural with In_2O_3 [3]. Lattice parameter *a* increased almost linearly with Sn-content from the value of 10.1215(5) Å for pure In_2O_3 to 10.1319(4) Å for 14 at% Sn. While ^{119}Sn Moessbauer spectra of the as-prepared samples are characterized with two doublets corresponding to two different cation sites (B and D, respectively), the spectra of annealed samples contained extremely broad subspectrum in addition. Decrease of temperature from 300K to 10K caused disappearance of the broad component. This unusual broad Moessbauer subspectrum could be explained by a diffusional motion of Sn^{4+} ions.

[1] Shigesato Y., Paine D. C., *Thin Solid Films*, 1994, **238**, 44. [2] Tkalcec E., et al., *XX Congress IUCr*, 2005. [3] Marezio M., *Acta Cryst*., 1966, **20**, 723.

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