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Chemical transport of restricted solid solutions of In_2O_3 and SnO_2: experiments and thermodynamic process analysis [1]

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Abstract

The preparation of mutual dissoluted In_2O_3/SnO_2 single crystals by the chemical transport method has been investigated. The transport reactions were performed using either iodine and sulphur simultaneously or chlorine as transporting agents and a mixture of pure oxides (4N) as source material. The highest concentration values of dissolved oxide were obtained after a sequential transport starting from a two phase region from 1250 to 1200 K. In this case, the maximum solubilities have been determined, indium oxide crystals with 8.2 mol% tin oxide and tin oxide crystals with 2.4 mol% indium oxide were grown. The experiments were explained with thermodynamical process calculations introducing the description of the solid phases as regular solid solutions consisting of nonstoichiometric binary oxides.

1. Introduction

In-Sn-O compounds have been widely used in thin films, thick films and ceramics as transparent electrodes, heat reflectors, resistors, gas sensors and in solar cells. The physical properties are determined by both, bulk and surface behaviour. Well-defined single crystals are necessary to divide the influence of bulk properties.

Due to the small mutual solubility, two types of solid solutions (ss) occur in the In-Sn-O system the structure of which is determined by the host lattice. The CaF_2-type ss1 is stable only in the $InO_{1.5}$ (In_2O_3) rich region and the rutile-type ss2 is stable only in the SnO_2-rich region. Single crystals of SnO_2 and In_2O_3 were obtained in Refs. [1-5].

Chemical transport is a convenient tool for preparing single crystalline materials with defined composition in multicomponent and multiphase systems. Typically, a sequential transport of the coexisting phases as well as composition shifts between source and sink materials have to be expected in such multiphase systems with restricted solubilities [6-8]. This behaviour can be applied to determine phase boundary compositions where the crystals are saturated by the minor component.

The present experiments will be supported by a thermodynamical analysis in which the solid phases are described by a model based on a regular solution of binary oxides [7].

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[1] Dedicated to Professor Erich Wolf on the occasion of his 65th birthday.

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