Modeling the vapor transport of non-stoichiometric zinc oxide

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In many studies on crystal growth and prospect applications of ZnO, it has been shown that a small deviation from the ideal stoichiometry has a significant impact on properties like charge carrier density[1], conductivity, and light absorption[2]. The occurrence of non-stoichiometric ZnO during chemical vapor transport (CVT) applying reducing transport additions such as H_2(g)[3], C(s)[4] or annealing in zinc vapor is frequently mentioned in literature[2,4]. But, a quantitative approach on the relation between predominant experimental conditions such as temperature or ambient gas phase and composition is rarely given. A quantification of the phase width's lower boundary was delivered by TESKE et al.[5] from coulometric measurements.

These experimental data were utilized to perform thermodynamic modeling for chemical vapor transport of non-stoichiometric ZnO. Therefor six representative compositions (see figure 1 left) were defined. Each represents a segment of the homogeneity range between 600 and 1200°C.

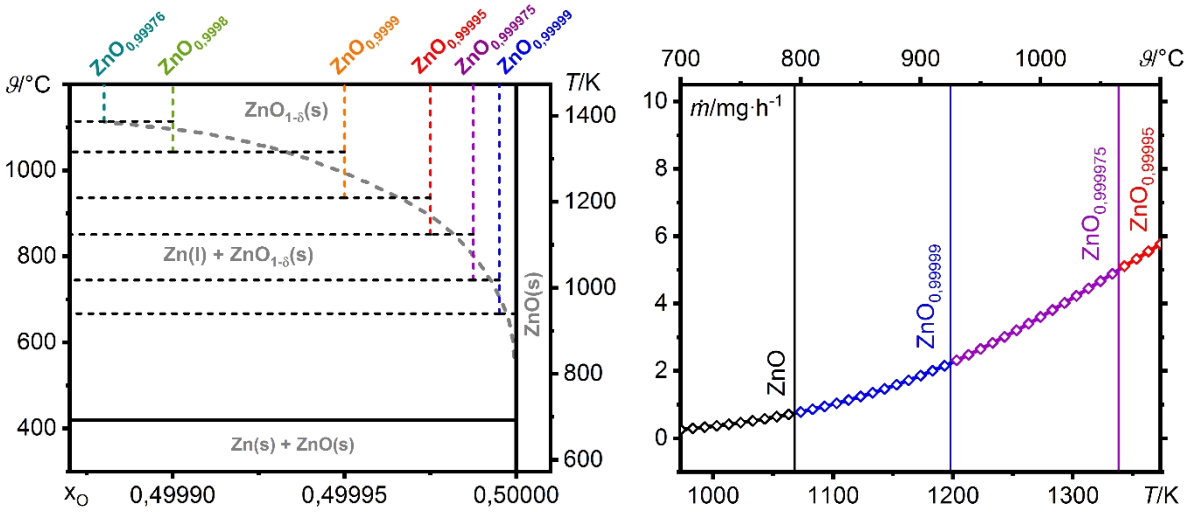

Figure 1: phase width of ZnO according to TESKE et al. (grey dashed line) and defined pseudo components for modelling (left); transport rates calculated for CVT of ZnO phases with hydrogen ($6\ mmol\ ZnO;\ 0{,}8\ mmol\ H_2;\ \Delta T = 50\ K$) (right)

Thermodynamic data for these compounds were assessed by CALPHAD methods using experimental results of TESKE et al[5]. Applying TRAGMIN software package[6] prospects are made on the composition of ZnO phases deposited during chemical vapor transport for different transport additions (e.g. H_2(g), C(s), CO(g)) in a temperature range between 700 and 1100°C (see figure 1 right).

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