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Stability and thermal expansion of InN: An X-ray diffraction study

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Thin films built from binary III-V nitrides or from their solid solutions are basic components of modern optoelectronic devices. In particular, indium nitride is a component suitable for high-speed electronics and solar cells. Experimental data on the bulk nitride material behaviour under specific thermal conditions (e.g., on variation of its stability, resistance to oxidation, thermal expansion coefficient with temperature) provide a valuable basic information needed for design and development of such devices. The properties such as decomposition temperature, oxidation rate at elevated temperatures, and thermal expansion are of importance for technologies of growth of low-dimensional structures. The current knowledge of thermal properties [1–3] may require an extension through studies in neutral or oxidizing environment in broad temperature ranges. The aim of the present work is to present selected experimentally determined temperature-dependent properties (thermal decomposition, interaction with air, thermal expansion) and discuss them on the basis of existing literature data.

Polycrystalline indium nitride samples differing by grain size were sealed in capillaries filled with air and in argon, and then studied by X-ray diffraction in a broad temperature range. High-resolution powder diffractometer at the B2 beamline (DORIS-III, Hasylab, DESY) equipped in a position-sensitive detector ensured collection of data with excellent counting statistics. The X-ray diffraction experiments were conducted at increasing temperatures using a step of 50 K or less; the experiments were stopped when the full decomposition of InN was concluded. High-resolution electron microscopy was used for determination of the microstructure and crystallite size. The structures of InN and minority phases as well as those of the oxidation products were refined using the Rietveld method. The obtained results demonstrate that the decomposition is, as expected, much faster for the sample composed of small grains. The oxide formation, observed when heating indium nitride in air, is attributed to oxidation of the nitride (at moderate temperatures) or to interaction of oxygen with indium vapour (at high temperatures). Thermal expansion was determined from the lattice parameters variation between 22 and 900 K. In this range, the unit-cell volume increases from 61.78 to 62.5 Å³, whereas the thermal expansion coefficient, α_v , increases from 0 to $19 \times 10^{-6} \text{ K}^{-1}$.

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A curious case of hexahydroxytriphenylene

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The D_{3h} symmetry molecule 2,3,6,7,10,11-hexahydroxytriphenylene (HHTP) has been an attractive building block for covalent organic frameworks (COFs) [1] and has found use as a mesogen unit in discotic liquid crystals [2]. In the current study the crystal structure of HHTP·4H₂O has been investigated.

Various single crystal x-ray diffraction (SCXRD) measurements performed at different temperatures yielded vital information about the structure and structural changes of the crystals. The as synthesised crystals illustrate the π -stacking motif common to triphenylene systems: the HHTP triphenylene cores assemble in columnar stacks, arranged in a distorted hexagonal array. The solvent water molecules reside in the pores between the stacks and hence an extensive three-dimensional hydrogen bonding network is created. This results in parallel corrugated two-dimensional sheets across the (b,c)-plane.

Our hypothesis is that upon heating and over time the crystals lose the solvate water molecules, resulting in a mixture of phases. Correlating powder x-ray diffraction (PXRD) data with SCXRD data, we can confirm that structural changes do indeed take place over time. It can further be seen that when a sample was left to stand in air for a number of days a phase transition started to occur.

We have taken the first steps to understand this fascinating system and are in the process of finding out more about the structural changes happening upon dehydration.

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Growth, composition, structure and optical properties of ZnO crystals

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Zinc oxide (ZnO) has a great potential in modern opto-, acousto- and microelectronic applications such as semiconductor lighting, piezoelectric transducers and so on. Crystal properties depend on the type and the concentration of the defects, in particular, point defects and their associates. However, the data concerning this topic is almost absent in the literature.

The aim of this work is to establish the relationship between composition, structural peculiarities and perfection, color, optical and electrical characteristics of ZnO crystals.

A series of green (in particular, ZnO1) and light-green (in particular, ZnO2) crystals were grown by the hydrothermal technique combined with a Pt inner container in an aqueous solution of the mineralizers 4M(KOH) + 1M(LiOH) + 0.1M(NH₄OH) by the $t = 330\text{--}350^\circ\text{C}$ and the $P = 30\text{--}50 \text{ MPa}$.

ZnO has the wurtzite structure (sp. gr. P₆mc, Z=2) where each anion is surrounded by four cations at the corners of a trigonal