

### EFFECT OF IMPURITIES ON POLYTYPISM AND PHASE TRANSFORMATION OF GEL -- GROWN PbI<sub>2</sub> SINGLE CRYSTALS

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Three different kinds of impurities (Ag, Zn, and Br) have been separately incorporated into PbI<sub>2</sub> crystals during their growth from gel and the polytypism of the crystals studied by X-ray diffraction. Subsequently, phase transformation of the as-grown crystals upon heating have also been studied in each case. Higher polytypes have been found to form only in the Ag-doped crystals. The Zn-doped crystals are mostly disordered 2H types, coupled with the presence of polytype 4H in some cases. The Br-doped crystals are all heavily disordered 2H types. The phase transformations resulting from heat treatment of the crystals are also different in the three cases.

An optical microscopic study of the growth features on the basal surfaces of the crystals has been made. Significant differences in the nature of the growth features have also been noticed. The undoped crystals have been found to display single growth spirals, whereas the doped crystals usually display two or more spirals. Besides several different kinds of unusual growth features have been observed on the Zn-doped crystals.

**Keywords: GEL GROWTH-PHASE TRANSFORMATION-POLYTYPISM**

### STUDY OF EPITAXIAL GROWTH OF MIXED CRYSTALS FROM AQUEOUS SOLUTIONS

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Process of heteroepitaxy has been studied for several water soluble binary systems (KAP-RbAP, (Co,Ni)(NH<sub>4</sub>)<sub>2</sub>(SO<sub>4</sub>)<sub>2</sub>\*6H<sub>2</sub>O, KDP-ADP). If the crystal composition is not equilibrium to the saturated mixed solution (the case of heteroepitaxy) it results in some additional ΔG (difference of thermodynamic potentials between the solution and the crystal). This is a reason of dissolution of a "foreign" crystal in the first moment of its interaction with saturated mixed solution. Dissolved crystal substance enriches diffusion solution layer around the crystal making it supersaturated and giving a start to a compositional interchange between the crystal and the solution. Non-regular surface morphology is formed in this case due to simultaneous growth of new crystalline layer and substrate dissolution in the adjacent regions. ΔG can be reduced to zero by some temperature decreasing ΔT. At this supercooling the crystal is in a metastable equilibrium with the solution and crystal dissolution is eliminated that suppresses further interchange reaction. Hence, growth of regular crystalline layer can be realized by temperature decreasing started from initial supercooling ΔT. This ΔT value depends on the solution composition shift relatively equilibrium value for a given crystal and increases as the composition deviation is increased. A type of growing heteroepitaxial layer (continuous layer or island growth) depends on lattice parameter mismatch. A continuous layer can be grown at misfit less than 7%. This limit is lower than that at melt liquid phase epitaxy because generation of misfit dislocations is suppressed under low temperatures typical for solution crystal growth.

**Keywords: SOLUTION CRYSTAL GROWTH, MIXED CRYSTALS, HETEROEPITAXY**

### GROWTH AND CHARACTERIZATION OF NONLINEAR OPTICAL METHYL P-HYDROXY BENZOATE

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Organic systems have become an alternate to the inorganic species because of their fast and large optical nonlinear response over a broad frequency range, and inherent synthetic flexibility. Organic solvents play an important role on the morphology and quality of organic crystals. Hence we have also investigated the effect of various solvents on the growth and morphology

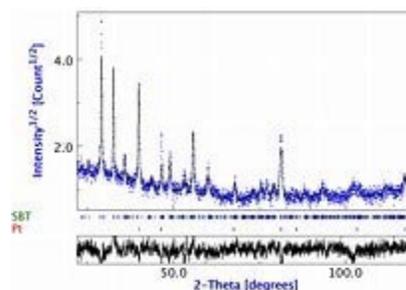
**Keywords: CRYSTAL GROWTH, ORGANIC CRYSTAL, P-MHB**

### COMBINING RIETVELD AND REFLECTIVITY FOR THIN FILM ANALYSIS

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Thin film analysis is still a challenge in the diffraction field when a small thickness is combined with a sharp texture in a multilayer system. The European project (ESQUI, <http://www.ing.unitn.it/maud/esqui>) is under progress to combine diffraction and reflectivity in one instrument and one analysis package based on the Rietveld method. The methodology is completed by a dedicated new instrument equipped with an Eulerian cradle, a very narrow beam for reflectivity and a large position sensitive detector. To test the instrument and methodology some thin films and multilayers have been prepared ranging from very small thickness (lower than 30 nm on a single layer) with extremely sharp textures typical of the electronic industry, to thicker films with not-so-sharp texture prepared by spin coating. The reflectivity and diffraction spectra have been collected according to the characteristics of the films by the custom instrument and the large amount of data has been processed in a global minimization step by fitting all the spectra together (unless the thickness of the layers was too large for reflectivity). The program uses a multilayer arrangement of the sample and all the parameters, from the layer thickness, phase content, crystal structures, microstructure, texture and residual stresses are optimized at the same time in a Rietveld like fashion. The methodology has permitted to analyse all the tests case successfully. The good quantitative results obtained prove the feasibility and potentiality of this technique. In figure a fitting of a SBT film diffraction spectrum is reported.



**Keywords: THIN FILM TEXTURE RIETVELD**