

PS10.07.18 THE POPULATION AND STRUCTURAL CHANGES OF THE METASTABLE STATE II IN SODIUMNITRO-PRUSSIDE ($\text{Na}_2[\text{Fe}(\text{CN})_5\text{NO}] \cdot 2\text{H}_2\text{O}$) AT 60 K. J. Schefer(*), T. Woike(**), S. Hauss hl(**), T. Fernandez(***) and G. McIntyre (***) (*) Laboratory for Neutron Scattering ETHZ+PSI, Paul Scherrer Institute, CH 5232 Villigen PSI, Switzerland (** Institute for Kristallographie,) University at K In, D 50764 K In, Germany (** Institute Laue Langevin ILL, Rue des *) Martyres, F-38042 Grenoble Cedex, France

Long-living metastable states are of fundamental interest for information storage and for the investigation of the correlation between electron density, chemical bond and structural behavior. This is of special interest as such systems can be used for holographic data storage yielding storage densities of up to 10 GByte/cm³.

We present population dynamic and structural properties of the metastable electronic excited state MS_{II} in nitroprusside $[\text{Fe}(\text{CN})_5\text{NO}]_2$. The population of MS_{II} was performed in a two step process: Firstly by irradiation with light of $\lambda=476.5\text{nm}$ in order to excite MS_I by about 50% and secondly by irradiation with light of $\lambda=1064\text{nm}$ to transfer 30% of the anions from MS_I to MS_{II}. The population is determined by Mössbauer spectroscopy in dependence on light exposure. Structure analysis of a single crystal with 30% of the anions in MS_{II} and 70% in the ground state has been done using neutron single crystal diffraction.

PS10.07.19 CALCULATION OF THE LINEAR AND NON-LINEAR OPTICAL SUSCEPTIBILITIES IN KTP AND MXO₄ CRYSTALS (M=Ga, Al; X=P, As) Ch. Schetelich and P.A.Thomas Physics Department, University of Warwick, UK.

Bond polarisability calculations were carried out using Levine's model of the linear and nonlinear susceptibilities, which is based on the Phillips - Van Vechten dielectric theory. Bond properties, such as homopolar and heteropolar energy gaps, the ionicities and susceptibilities have been computed for the different bonds in KTP (KTiOPO_4) and MXO₄ crystals (M=Ga, Al; X=P, As). We found a satisfactory agreement between the theoretical and experimental values of the averaged macroscopic linear susceptibilities. The simple extension to the anisotropic linear case using a sum over the products of the direction cosines and the isotropic bond polarisability has been proved as inappropriate. A different approach using anisotropic bond polarisabilities suggested by Levine is under investigation. A comparison of the values of the nonlinear optical susceptibility obtained by both calculations and experiments is given for KTP.

PS10.07.20 AGGREGATION OF DIVALENT IMPURITIES IN CODOPED NaCl AND KCl SINGLE CRYSTALS. Jacques Soullard, Instituto de Fisica, UNAM, 01000 Mexico D.F., Mexico

The formation energy of small clusters in NaCl and KCl single crystals codoped with Mn²⁺ and Pb²⁺ impurities has been calculated by means of a static simulation of ionic crystals. The results are used to study quantitatively the structure of the equilibrium state of crystals as a function of temperature.

At high temperature, in both systems, the equilibrium state is characterized by isolated defects: doubly charged substitutional impurities, cation vacancies and dipoles. The manganese dipoles are found in the n.n. and n.n.n. configurations, the ratio of their concentration being dependent on the host matrix. For the lead dipoles the n.n. configuration is dominant in both systems.

In the system NaCl : Mn,Pb dimers and trimers form when the temperature is less than 450K. The nucleation planes of dimers are {110} and {111}, at 300K the trimer concentration is much greater than the dimer concentration and about 50% of trimers have a mixed character. In the system KCl : Mn,Pb, the formation of dimers and trimers becomes significant for temperature less than 500K. The nucleation planes of dimers

are {110} and {100}, at 300K the equilibrium state is characterized by a high concentration of dimers, only 10% of dimers are of mixed type.

These results agree qualitatively well with the experimental results. The host matrix where the concentration of closed Mn-Pb pairs is the highest (NaCl) is the most efficient to transfer energy from Pb to Mn; as a consequence, it presents the most intense fluorescence. The differences between the aggregation processes of the two systems can be understood considering the relative solubility of impurities and the binding energy per dipole of clusters.

PS10.07.21 ANTIMONY - DOPED TIN OXIDE THIN FILMS (SnO_x) MADE BY EVAPORATION METHOD. Vo Vong, Laboratory of Electron Microscopy, Vietnam National Center for Natural Science & Technology, Nghiado - Tuliem-Hanoi - Vietnam

Tin and Antimony, which have mass-rate 10:1; pure 99,99%, were evaporated simultaneously at the two differential sources in high vacuum of 10⁻⁵ Torr. The substrate temperature is changed as following 100°C, 120°C, 150°C and 200°C.

Thin films Sn(In)_xO_x were annealed in air and in oxygen for 120 min. at the temperatures 150, 180, 210, 230, 250, 300, 350, 400 and 450°C. Changes of the films in process of the heat treatment were studied by transmission electron microscopy, scanning electron microscopy, electron and X-ray diffraction and measurements of transmittances as the function of wavelength.

High-quality Sn(In)_xO_x thin films are found to be strongly dependent on parameters such as the antimony content, a deposition temperature, a temperature of the annealing

Under optimum conditions we received thin films with a electrical resistivity of 15 Ω□. Thickness of the films above 0,3 - 0,5 μm, λ = 0,4 - 0,7 μm transmittance is reachable 92%.

Based on our experimental results the changes of mechanical, chemical and physical properties of films can be explained by the changes of the x-value.

PS10.07.22 Ba₂ErCl₇: A NEW TERNARY RARE EARTH CHLORIDE WITH BARIUM. M. S. Wickleder, Ph. Egger and J. Hulliger, Institute for Inorganic Analytical and Physical Chemistry, University of Berne, Freiestr. 3, 3012 Berne, Switzerland

Our search for new erbium based upconversion materials has lead to the new compound Ba₂ErCl₇ with isolated sevenfold coordinate Er³⁺ ions within a network of edge and corner sharing [BaCl₉] polyhedra. The [ErCl₇] polyhedron can be described as a monocapped trigonal prism which, due to the site symmetry C₁ of the Er³⁺ ions in the space group P2₁/c, is slightly distorted (for the crystallographic data see table 1). The structure contains two crystallographically different Ba²⁺ ions (Ba1 and Ba2). Each of them is ninefold coordinated by Cl⁻ ions and the [BaCl₉] polyhedra are linked to form chains running along the c-axis (Ba1) and the a-axis (Ba2), respectively. The chains are connected to form a three dimensional network that contains the Er³⁺ ions.

Tab.1 Crystallographic Data for Ba₂ErCl₇

Crystal System	monoclinic	Atomic Coordinates			
		x/a	y/b	z/c	
Space group	P2 ₁ /c	Er	0.2170	0.6269	0.2180
Lattice Parameters	a = 679.4 pm b = 1552.5 pm c = 1049.6 pm β = 90.54°	Ba1	0.7365	0.7798	0.4508
		Ba2	0.2644	0.5610	0.6765
		Cl1	0.9991	0.6044	0.4294
		Cl2	0.4892	0.7573	0.1980
		Cl3	0.0007	0.7725	0.2053
		Cl4	0.4875	0.6049	0.4145
		Cl5	0.2932	0.4595	0.2133
Z	4	Cl6	0.8693	0.5705	0.1236
		Cl7	0.2896	0.6399	0.9710