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In this contribution recent results by neutron diffraction on technological important functional materials are reported. Hydrogen storage materials, shape memory alloys and ferroelectrics were investigated under special environmental conditions: hydrogen pressure, mechanical load or electrical fields, respectively. All experiments were carried out at the high-resolution neutron powder diffractometer SPODI (FRM-II, Garching). This instrument offers possibilities for the in-situ analysis of functional materials under special environmental conditions.

A rotatable load frame available at SPODI allows materials characterisation at different orientations of the load axis with respect to the scattering vector. Besides tensile stress, also pressure and torsion can be applied. Monoclinic nickel titanium shape memory alloys were measured at different strain levels to determine load-induced elastic strains, changes in twinning texture and resulting microstrains. In addition, diffraction studies under different sample orientations (i.e. different orientations of load axis) were carried out to analyse the anisotropy of the elastic response.

Hydrogen storage materials of the system LiD/Mg(ND)₂ were investigated at 220 °C and different deuterium pressures (up to 70 bars) to study the phase transformation behaviour during desorption and re-deuteration. It has been shown that the deuteration occurs via intermediate reaction steps. The appearing phases could be structurally analysed by Rietveld refinement.

An apparatus for high electric fields was developed to analyse the poling mechanisms in ferroelectrics at fields up to 7 kV/mm. The studies were carried out on samples of technological relevant systems like PbZr_xTi_{1-x}O₃ with compositions close to the morphotropic phase boundary as well as lead-free ferroelectrics of system NBT-BT-KNN. Here, the electrical field induced strain could be correlated with a field-induced phase transformation. The phase transition is accompanied by a change of the oxygen octahedral tilt system correlated with superlattice reflections in the neutron diffraction patterns.

Keywords: hydrogen storage, ferroelectrics, shape memory alloys

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Effect of high pressure treatments on the structure of R₂(MoO₄)₃ (R=Eu, Gd, Sm) single crystals. Elena Kudrenko, Salavat Khasanov, Semen Shmurak, Boris Redkin, Vitaly Sinitsyn. *Institute of Solid State Physics RAS, Chernogolovka, Russia.*

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Early was established [1] that powder samples of some rare earth molybdates undergo phase transformation from initial metastable crystalline β'-phase to the amorphous state at relatively moderate pressures ~7-9 GPa. However treatments of Eu₂(MoO₄)₃ single crystal samples in the same pressure range displayed more complex X-ray pattern [2]. To clarify the structural peculiarities of the transformation the number of R₂(MoO₄)₃ (where R = Eu, Gd, Sm) single crystal samples

were investigated by X-ray method after their high pressure treatment at P=9 GPa.

It was found that X-ray diffraction patterns of the "treated" single-crystal samples can be represented as diffuse-like scattering rings and strong sharp peaks within the first diffuse ring ($\leq 0.3 \text{ \AA}^{-1}$). The observed diffraction peaks were indexed in the framework of the orthorhombic lattice with a parameters $a = 9.69 \text{ \AA}$, $b = 10.61 \text{ \AA}$, $c = 19.25 \text{ \AA}$ and $V = 1977 \text{ \AA}^3$ (for R = Eu) which corresponds to the decrease of the cell volume on ~15% in compare with initial β'-phase ($V=1166 \text{ \AA}^3$). Integration and reduction of the diffraction patterns to Debye patterns show that the diffuse scattering is considerably higher than the Bragg diffraction. This means that the most part of the crystal sample is composed of amorphous-like structure and contain crystalline inclusions. These nanocrystalline domains are highly correlated over the sample, due to what high pressure phase produces single-crystal diffraction patterns. Luminescence spectra measured at different wavelengths revealed that such unusual structural state is the characteristic of whole sample. It was found that "treated" single-crystal samples returned to the initial β'-structure at heating to 550°C.

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[1] V. Dmitriev et al., *Journal of Physics and Chemistry of Solids*, vol. 64, pp.307-312, 2003. [2] A.P.Kiselev, S.Z.Shmurak, V.V.Sinitsyn, S.S. Khasanov, B.S.Redkin, A.V. Alekseev, Ponyatovsky E.G. *Bulletin of RAS:Physics*, vol.72, No9, pp.1297-1302, 2008.

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XIPHOS: Expanding the experimental envelope to extreme sample environments. M.R. Probert, J.A.

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The details of a newly installed and configured high intensity single crystal X-ray diffractometer, XIPHOS, will be presented. This machine has been designed for structural investigations under combined extremes of sample environments, i.e. high pressure, very low temperature and light irradiation. XIPHOS provides a unique facility giving unparalleled access to 'in house' diffraction data, as for example a minimum temperature of 1.9 K. The major components of the system and their complementary aspects will be outlined, highlighting the potential experimental conditions that can be achieved. Methodologies for the operation and monitoring of the system will also be demonstrated together with examples of its research capabilities. Additionally, the development of a new dispex vacuum chamber, to allow irradiation of samples by a laser beam without thermal contact to the outer vacuum sleeves, will be discussed. Irradiation of crystalline samples at reduced temperatures allows the study of different electronic states under the same thermal conditions. Finally, we will highlight some of the unlocked potential in manufacturers programs and also the need for novel solutions to allow operation under extreme environmental conditions.