

implying that YCrO_3 became more distorted with increasing pressure. The polyhedral bulk moduli for YO_{12} and CrO_6 polyhedra led to: $V_{0,\text{poly}}, K_{p0}$: 46.09(2) \AA^3 , 254(2) GPa for YO_{12} , and 10.40(1) \AA^3 , 251(5) GPa for CrO_6 . The volume compressibilities of the YO_{12} and CrO_6 sites are therefore equivalent. That results are different to those previously reported for the orthorhombic YAIO_3 perovskite in which the b -axis is significantly more compressible than both c and a [4]. Considering the elastic moduli of both YCrO_3 and YAIO_3 , the two structures under pressure show a different anisotropic behavior along [101] (both YCrO_3 and YAIO_3 structures). Furthermore, for the YAIO_3 perovskite the compressibility of the A site is ~15% less than that of the AlO_6 octahedron [4]. Such contrasting trends can be explained by the stronger confinement of Y ions in YAIO_3 due to the smaller size of octahedral network in the orthoaluminate compared to the orthochromate. As known from previous work [3], the decrease of mean octahedral bond distance, $\langle\text{B-O}\rangle$, from YCrO_3 to YAIO_3 is accompanied by shortening of the average $\langle\text{A-O}\rangle$ distance and decreasing of interpolyhedral tilting. The associated strong confinement of Y cation in YAIO_3 does not occur in YCrO_3 . Here the A site is easier to compress and does not hamper the enhance of octahedral tilting and rotation expected at high pressure conditions.

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Keywords: perovskites, synchrotron powder diffraction, high pressure.

FA2-MS19-T04

Pressure-induced Phase Transformations in Lead-based Relaxor Ferroelectrics. B. J. Maier^a, R. J. Angel^b, B. Mihailova^a, W. G. Marshall^c, C. Paulmann^a, J. M. Engel^d, M. Gospodinov^e, U. Bismayer^a.

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The structural peculiarities of relaxor ferroelectrics, exhibiting very high dielectric and elastoelectric response, remain a challenging problem. Pressure is a strong driving force that can trigger incipient atomic clusters existing at ambient conditions to develop into long-range ordered domains detectable by conventional diffraction methods. Thus, the analysis of pressure-induced transformation processes can help to elucidate the structural complexity of relaxors. Our high-pressure X-ray diffraction data on lead scandium tantalate (PST) and lead scandium niobate (PSN) as well as doped variants reveal a thermodynamically second-order phase transition for all compounds [1,2]. An increase in the intensities of $h,k,l = \text{all odd reflections}$ is observed while the intensity of h,h,h peaks, $h = 2n+1$, does not change with pressure. This indicates a glide-plane pseudo-symmetry of the

structural distortion along the $\langle 111 \rangle$ cubic directions and unambiguously reveals anti-phase octahedral tilting as the cause for the increased reflection intensities.

Rietveld refinements to neutron powder diffraction data on PST and PSN reveal anti-phase octahedral tilts already below the critical pressure that continuously evolve with pressure [3]. The high-pressure phase has either or symmetry, depending on whether the presence of 1:1 cation ordering is neglected or taken into account.

The influence of Ba^{2+} , Bi^{3+} , and La^{3+} substitution for Pb^{2+} on the phase transition will be discussed. Ba^{2+} smears out the phase transition and enhances the local ferroic distortion, while Bi^{3+} lowers the critical pressure and enhances the structural distortions associated with the phase transition. La^{3+} substitution for Pb^{2+} yields a smaller tolerance factor, thus octahedral tilting occurs already at room pressure, although the average structure remains metrically cubic.

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Keywords: Ferroelectrics and Related Materials, High-pressure Phase Transitions, X-ray and Neutron Diffraction

FA2-MS19-T05

Correlations between microstructures evolution and elastic properties of LEK 94. Giovanni Mazzolai^a,

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It is well known that high-cycle fatigue (HCF) is the main source of failures in the components made from single crystal Ni-base superalloys of today's aircraft and spacecraft propulsion systems. Under fatigue loading cyclic stress produces alternating slip reversals on the critical slip systems which eventually results in fatigue crack initiation along "critical" octahedral $\langle 111 \rangle$ planes. It is important to determine the stresses and strains along these planes and corresponding slip systems in order to use them to calculate several multiaxial critical plane parameters to determine the amount of fatigue damage and also the "critical planes" along which HCF failures would initiate [1]. The intensity of the stress levels and the stress states are related to the geometry of the component, to the orientation of the crystal lattice with respect to the component geometry, and to the micromechanics of the deformation and slip mechanisms observed in corresponding single crystal materials and to the temperature histories during cyclic operation and most important to the elastic constants and thermal expansion coefficients of the material.

In the course of our project we investigate the elastic anisotropy of the quasi single crystal Ni-base superalloy LEK94 between room temperature and 1200°C with the aid of resonant ultrasound spectroscopy. This method yields sets of elastic constants of high internal consistency because all independent constants are determined on one single sample in one run.

The influence of microstructure evolution on fatigue crack initiation has been shown to play a dominant role, especially on cracks which are of a size comparable to the scale of characteristic microstructural features. Microstructures

variations at high temperature are mainly induced by the rafting process which is basically due to stress assisted diffusion controlled process. Rafting/directional coarsening in single crystal superalloys is strongly controlled by the sign of applied stress, lattice misfits between and elastic constants of γ/γ' phases and varies with service temperature due to the different thermal expansion coefficients of these phases. The elastic anisotropy of LEK94 can be interpreted by a quasi-single crystal composite consisting of a single crystalline γ matrix with coherently distributed precipitates of well oriented γ' crystallites.

The microstructure of superalloys can be manipulated to obtain different microstructures by altering heat treatments and creep deformation conditions allowing variation in the amount and size distribution of γ' precipitates in order to improve the overall fatigue lifetimes. The main aim of our work is therefore to investigate the correlation between the anisotropic elastic behavior of LEK94 and the evolution of its microstructure in order to optimize modeling and characterization of the thermal fatigue response of this material.

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Keywords: elastic properties, microstructure evolution, fatigue