

**FA2-MS19-T01**

**Isostructural phase transitions and crossovers under non-ambient conditions.** Vladimir Dmitriev, Dmitry Chernyshov. *Swiss-Norwegian Beamlines at ESRF, Grenoble, France.*

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It is convenient to consider a change in the structure of crystalline material as a reason for remarkable modifications in its physical properties: a structural phase transition often results in the anomalous behaviour of macroscopic parameters in condensed matter. However, is it always true that a detected change in properties, discontinuous or smooth, manifests itself as a change in the crystal structure? Isostructural transformations exemplify a violation of such a rule. They connect phases with identical structures but with different properties; a volume collapse, giant magneto-elastic coupling, or negative thermal expansion may serve as examples of corresponding macroscopic responses.

Isostructural phase transformations have two possible regimes: the transition can be discontinuous (first-order) or transformation can be smooth (crossover regime). One finds a limited number of examples of discontinuous isostructural phase transitions. At the same time, many examples of anomalous but continuous variation of material parameters within the stability range of the same phase have been reported. Normally structural information collected for non-ambient conditions are limited and therefore an isostructural transformation occurring in the crossover regime may be easily mixed with a second order phase transition. In our talk, we show typical anomaly types for isostructural phase transformations. Generic model-free phase diagrams, with their specific features as critical lines and points, will be presented and analyzed. Phase transformations observed in rare-earth metals and their compounds provide an experimental illustration of different transformation regimes.

**Keywords:** phase transition, isostructural, crossover

**FA2-MS19-T02**

**Elastic and non-elastic response of shape memory alloys to stress fields.** W. W. Schmahl<sup>a</sup>, S.

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Pseudoplastic or pseudoelastic shape memory is based on recoverable ferroelastic twin domain accommodation in stress fields. The twins are associated to a martensitic phase transition. Pseudoelasticity (superelasticity) occurs when the high-symmetry phase (paraelastic “austenite”) is thermodynamically stable in the stress-free state, and the phase transition to the distorted phase (ferroelastic “martensite”) is induced by the application of stress. Those ferroelastic twin variants which are suitably oriented in the stress field become stable and the spontaneous strain of the

martensitic transition leads to a large shape change during the process. When stress is released, the system falls back to the (stable) austenite state and the original shape is “pseudoelastically” recovered. Pseudoplastic shape memory occurs when ferroelastic “martensite” is thermodynamically stable, and the effect is due to ferroelastic domain switching in the stress field. In this case a release of stress does not recover the original domain configuration. The original shape (and domain configuration) is then restored via a thermal transition to the paraelastic austenite and stress-free cooling to martensite.

Microdiffraction experiments using 100keV x-rays at beamline BW5@HASYLAB reveal the formation of stress-induced martensite in the stress field concentrated at the tips of cracks progressing through austenitic NiTi [1] and in localized shear transformation bands in uniaxially stressed NiTi [2]. Careful examination of neutron diffraction 2.54 Å neutron diffraction data on SPODI@FRM-II show that the macroscopic strain of the material is dominated by twin re-accommodation, while the observable crystallographic distortions on unit-cell level reflect residual stresses arising in the twin-microstructure (rather than elastic distortions).

[1] Gollerthan, S., M.L. Young, A. Baruj, J. Frenzel, W.W. Schmahl, G. Eggeler (2009) *Acta Materialia*, 2009, 57, 1015. [2] Hasan, M., W.W. Schmahl, K. Hackl, R. Heinen, J. Frenzel, S. Gollerthan, G. Eggeler, M. Wagner, J. Khalil-Allafi and A. Baruj, *Mater. Sci. and Eng. A*, 2008, 481/82, 414.

**FA2-MS19-T03**

**Elastic properties of YCrO<sub>3</sub> perovskite up to 60 GPa.**

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Perovskite compounds are largely applied in several technological fields due to their peculiar electric, magnetic, piezoelectric and optical properties. YCrO<sub>3</sub>, a GdFeO<sub>3</sub>-type perovskite, has become an attracting material due to its multifunctional biferroic behavior [1], and to its recent use as interconnection for the SOFC's [2]. A recent work revealed that the YAlO<sub>3</sub>-YCrO<sub>3</sub> system exhibits the lowest relaxation coefficient, if compared with other structures hosting Cr<sup>3+</sup> in octahedral coordination [3]. In the last decade, many studies have been devoted to assess the high pressure behavior of orthorhombic perovskites. However, data on YCrO<sub>3</sub> under high-pressure conditions are lacking. For these reasons, we investigated the high pressure evolution of the YCrO<sub>3</sub> perovskite (s.g. *Pbnm*) using synchrotron powder diffraction, up to 60 GPa. The P-V data, fitted with a third-order Birch-Murnaghan equation of state gave a  $V_0 = 218.23(4) \text{ \AA}^3$ , and to a volumetric bulk modulus  $K_{T0} = 208.4(5) \text{ GPa}$ , with a  $K'_0 = 3.7(1)$ , with a volume reduction of ~17.5% in the studied pressure range. The elastic moduli of the individual crystallographic axes showed that the *b*-axis is appreciably less compressible than both *a*- and *c*-axis ( $K_{a0} = 195(5) \text{ GPa}$ ,  $K_{b0} = 223(7) \text{ GPa}$ , and  $K_{c0} = 200(6) \text{ GPa}$ , respectively),