

# SKM-Symposium Diffusionless Transformations in Magnetic and Ferroelectric Bulk and Thin Films (SKM-SYDT)

jointly organized by  
 the Metal and Material Physics Division (MM),  
 the Thin Films Division (DS),  
 the Dielectric Solids Division (DF), and  
 the Magnetism Division (MA)

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Diffusionless phase transformations are the decisive mechanism for multifunctional properties like the magnetic shape memory effect, ferroelectricity, magnetocaloric and multiferroic properties. These phase transformations can be controlled by external electric or magnetic fields as well as stress and pressure. Hence these complex materials exhibit multiple new physical effects, which are currently examined with dedicated theoretical and experimental methods.

By highlighting the close connections between the different classes of functional materials this symposium brings together different communities. As external constraints significantly affect these transformations, in particular thin films and nanostructures helped to understand the underlying coupling mechanism. Hence a particular focus will be on scale effects in functional materials exhibiting diffusionless transformations.

## Overview of Invited Talks and Sessions

(lecture room TRE Ma)

### Invited Talks

SKM-SYDT 1.1	Thu	10:30–11:00	TRE Ma	<b>Domain boundaries as active elements in multiferroics and martensites: steps towards Domain Boundary Engineering</b> — ●EKHARD K.H. SALJE
SKM-SYDT 1.2	Thu	11:00–11:30	TRE Ma	<b>Intermediate Phases in Perovskite Solid Solutions</b> — ●IAN REANEY, CLIVE RANDALL, DAVID WOODWARD
SKM-SYDT 1.3	Thu	11:30–12:00	TRE Ma	<b>Adaptive martensite and giant strain effects in multiferroics</b> — ●ULRICH K. RÖSSLER
SKM-SYDT 1.4	Thu	12:00–12:30	TRE Ma	<b>Nature of magnetic coupling in Ni-Mn-based martensitic Heusler alloys</b> — ●MEHMET ACET, SEDA AKSOY, EBERHARD F. WASSERMANN, LLUIS MANOSA, ANTONI PLANES
SKM-SYDT 1.5	Thu	12:30–13:00	TRE Ma	<b>Orthorhombic to tetragonal transition of SrRuO<sub>3</sub> layers in Pr<sub>0.7</sub>Ca<sub>0.3</sub>MnO<sub>3</sub>/SrRuO<sub>3</sub> superlattices</b> — ●MICHAEL ZIESE, FRANCIS BERN, IONELA VREJOIU, ECKHARD PIPPEL, ELIZAVETA NIKULINA

### Sessions

SKM-SYDT 1.1–1.5	Thu	10:30–13:00	TRE Ma	<b>Diffusionless Transformations in Magnetic and Ferroelectric Bulk and Thin Films</b>
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## SKM-SYDT 1: Diffusionless Transformations in Magnetic and Ferroelectric Bulk and Thin Films

Time: Thursday 10:30–13:00

Location: TRE Ma

**Invited Talk** SKM-SYDT 1.1 Thu 10:30 TRE Ma  
**Domain boundaries as active elements in multiferroics and martensites: steps towards Domain Boundary Engineering** — ●EKHARD K.H. SALJE — University of Cambridge, Cambridge CB2 3EQ, UK

Domain boundaries can contain properties, which are absent in the bulk of the material. Typical examples which can be used for applications in Domain Boundary Engineering are ferroelectric boundaries in ferroelastic matrices. A similar example is piezoelectricity in boundaries where the matrix remains non-piezoelectric and materials with reversed contrast. In addition, electronic and ionic transport are often greatly enhanced in boundaries. An extreme case are superconducting twin walls in a ferroelectric matrix. Increased ionic transport is common in twin boundaries of most materials with perovskite-type structures. While much progress has been made in ceramics, we also find indications for specific domain boundary effects in shape memory metals. The mobility of martensitic twins depends greatly on their internal structure, e.g. their ability to anchor dislocations. All materials have in common that strain interactions are strong and hence long correlations prevail. This makes the system amenable to Landau theory including appropriate coupling terms which modify the bulk and the domain walls differently. The general concept and some examples will be discussed.

Ref.: E.K.H. Salje (2010) Multiferroic domain boundaries as active memory devices: trajectories towards domain boundary engineering, *Chemphyschem* 11, 940.

**Invited Talk** SKM-SYDT 1.2 Thu 11:00 TRE Ma  
**Intermediate Phases in Perovskite Solid Solutions** — ●IAN REANEY<sup>1</sup>, CLIVE RANDALL<sup>2</sup>, and DAVID WOODWARD<sup>3</sup> — <sup>1</sup>Department of Materials Science and Engineering, University of Sheffield, Sheffield, S1 3JD, UK — <sup>2</sup>Department of Physics, University of Warwick, Gibbet Hill Road, Coventry CV4 7AL, UK — <sup>3</sup>144 MRL Bldg., Penn State University, University Park, PA 16802, USA

The intermediate monoclinic (M) phase in  $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$  (PZT) in-between rhombohedral (R) and tetragonal (T) displacive variants is considered as a high profile example of a more general phenomenon in which low symmetry intermediate phases are stabilised between higher symmetry displacive variants. In the case of the M phase, the order parameter is dominated by polarisation but similar situations are reported where the order parameter is dominated by strain, amplitude of octahedral rotation or combinations thereof. This article presents examples of intermediate phases and discusses their structures and functional properties.

**Invited Talk** SKM-SYDT 1.3 Thu 11:30 TRE Ma  
**Adaptive martensite and giant strain effects in multiferroics** — ●ULRICH K. RÖSSLER — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Ferroelastic behavior in martensitic microstructures relies on the orientation of twin variants under applied external fields. Giant strains driven by multiferroic couplings, as in ferromagnetic shape-memory alloys (FSMA) and in ferroelectric perovskites, have been achieved in modulated lattice structures only. The concept of adaptive martensite introduced by Khachatryan and co-workers explains these lattice structures by twinning at the unit cell level. The formation of such nanoscale microstructures is determined by lattice geometry and the compatibility at the habit plane. The martensite transformation creates metastable states with a maximum density of twin boundaries. For FSMA as  $\text{Ni}_2\text{MnGa}$  or  $\text{Co}_2\text{NbSn}$  the modulated low symmetry phases can be identified as nanotwinned structures of a tetragonal

lattice in accordance with results on the ground state from ab initio calculations. The adaptive nature of modulated structures and microstructure in the Heusler  $\text{Ni}_2\text{MnGa}$  alloys has been demonstrated in experiments. In epitaxial films the modulated structure at the habit plane is found to be rigidly connected to the coexisting tetragonal martensite by branching. In these constrained films, the habit plane acquires a fractal geometry which fixes the lengths in the microstructure from the lattice cells up to the coarsened twins. Metastability and hierarchical organization of adaptive martensites are suggested as essentials for the easy variant re-arrangement in mesoscale twinned microstructures.

**Invited Talk** SKM-SYDT 1.4 Thu 12:00 TRE Ma  
**Nature of magnetic coupling in Ni-Mn-based martensitic Heusler alloys** — ●MEHMET ACET<sup>1</sup>, SEDA AKSOY<sup>1</sup>, EBERHARD F. WASSERMANN<sup>1</sup>, LLUIS MANOSA<sup>2</sup>, and ANTONI PLANES<sup>2</sup> — <sup>1</sup>Experimentalfysik, Universität Duisburg-Essen, 47048 Duisburg — <sup>2</sup>Departament d'Estructura i Constituents de la Matèria, Facultat de Física, Universitat de Barcelona, Diagonal 647, E-08028 Barcelona, Catalonia, Spain

To understand the cause of magnetic field induced effects in shape memory alloys, it is necessary to understand the nature of the magnetic coupling in the temperature-neighborhood of the martensitic transition. Neutron diffraction, and neutron polarization analysis experiments on Ni-Mn-based martensitic Heusler systems show that at temperatures just below the martensitic transformation, the magnetic short-range correlations are antiferromagnetic in a spin-liquid type state. The correlations are mixed ferromagnetic and antiferromagnetic at temperatures above the martensitic transition; and well beyond the Curie temperature of the austenite state. The results of further ferromagnetic resonance studies show that antiferromagnetic exchange in the martensite state persists down to the lowest temperatures and coexists with the long-range ferromagnetism below the austenite Curie temperature. These results are also in line with the presence of a spin liquid state just below the martensitic transition.

**Invited Talk** SKM-SYDT 1.5 Thu 12:30 TRE Ma  
**Orthorhombic to tetragonal transition of  $\text{SrRuO}_3$  layers in  $\text{Pr}_{0.7}\text{Ca}_{0.3}\text{MnO}_3/\text{SrRuO}_3$  superlattices** — ●MICHAEL ZIESE<sup>1</sup>, FRANCIS BERN<sup>1</sup>, IONELA VREJOIU<sup>2</sup>, ECKHARD PIPPEL<sup>2</sup>, and ELIZAVETA NIKULINA<sup>2</sup> — <sup>1</sup>Div. of Superconductivity and Magnetism, University of Leipzig, D-04103 Leipzig, Germany — <sup>2</sup>Max Planck Institute of Microstructure Physics, D-06120 Halle, Germany

In perovskite superlattices (SLs) the intimate interplay between structural, magnetic and electronic properties can be modified by geometrical constraints. This is explored in this work by the study of the crystallographic, magnetic and magnetotransport properties of ultrathin  $\text{SrRuO}_3$  (SRO) layers embedded in SLs.  $\text{Pr}_{0.7}\text{Ca}_{0.3}\text{MnO}_3/\text{SrRuO}_3$  (PCMO/SRO) SLs were grown by pulsed laser deposition on vicinal  $\text{SrTiO}_3$  substrates with a miscut angle of about  $0.1^\circ$ , uniform  $\text{TiO}_2$ -termination and an atomically flat terrace morphology. The SRO layer thickness was kept constant at 4 nm, whereas the PCMO layer thickness was varied between 1.5 and 4 nm. High resolution TEM investigations of the PCMO/SRO SLs showed that the PCMO layers were orthorhombic throughout, whereas the SRO layers were orthorhombic when adjacent to 1.5 nm thick PCMO layers and transformed to tetragonal when adjacent to 4 nm thick PCMO layers. This structural transformation profoundly changed the form of the angular dependent magnetoresistance (MR) as well as the direction of the magnetic easy axes. Further the antiferromagnetic interlayer exchange coupling between PCMO and SRO layers was stronger in the orthorhombic than in the tetragonal phase.