MULTI-FERROIC MATERIALS (SYMM)

Jointly organized by
Dielectric Materials (DF)
Magnetism (MA)
Metal- and Material Physics (MM)
Dynamics and Statistical Physics (DY)

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OVERVIEW OF INVITED TALKS AND SESSIONS

(lecture room HSZ 04)

Invited Talks

SYMM 1.1	Tue	14:30	(HSZ 04)	**Magnetoelectric Multiferroics from First Principles**, C. Ederer, N. Spaldin
SYMM 1.2	Tue	15:00	(HSZ 04)	**Electrostatic Interface Tuning in Superconducting Oxide Heterostructures**, N. Pavlenko
SYMM 1.3	Tue	15:30	(HSZ 04)	**Modelling realistic ferroic materials - multiscale approaches**, S. Gemming, I. I. Chaplygin, W. Alsheimer, G. Seifert
SYMM 2.1	Tue	16:15	(HSZ 04)	**Multifunctional Complex Oxide Heterostructures**, R. Ramesh
SYMM 2.2	Tue	16:45	(HSZ 04)	**Some Observations about Static Scaling: Domain Widths and Circular and Toroidal Ordering in Ferroelectrics, Ferromagnets, and Magnetoelectrics**, J. Scott
SYMM 2.3	Tue	17:15	(HSZ 04)	**Magnetoelectric Effect and Toroidal Ordering in Multiferroic Manganites**, M. Fiebig, Th. Lottermoser, Th. Lonkai
SYMM 2.4	Tue	17:45	(HSZ 04)	**Magnetoelectric Effects in Multiferroics**, A. Loidl, J. Hemberger, A. Pimenov, P. Lunkenheimer, A. A. Mukhin, V. Tsurkan

Sessions

SYMM 1	**Multiferroic Materials - Theory**	Tue 14:30–16:00	HSZ 04	SYMM 1.1–1.3
SYMM 2	**Multiferroic Materials - Experiment**	Tue 16:15–18:15	HSZ 04	SYMM 2.1–2.4

Sessions

– Invited Talks –

SYMM 1 Multiferroic Materials - Theory

Time: Tuesday 14:30–16:00 Room: HSZ 04

Invited Talk SYMM 1.1 Tue 14:30 HSZ 04

Magnetoelectric Multiferroics from First Principles — •C. Ederer and N. Spaldin — Materials Department, University of California, Santa Barbara

The combination of magnetic and ferroelectric properties in a single material is appealing both because of the interesting coupling effects that emerge as well as due to a variety of technological applications that can be envisaged. Computational methods based on density functional theory have made invaluable contributions to the present understanding of such magnetoelectric multiferroics. In this talk I will present an overview over current research activities in the field of multiferroic materials and illustrate how first principles methods can be used in various ways to investigate these systems. In particular, I will discuss the application of first principles methods to explain the confusing and sometimes contradictory experimental observations for the room-temperature multiferroic $BiFeO_3$, to predict novel effects like electric-field induced switching of magnetic order parameters in $BaNiF_4$, and to design new multiferroic materials with improved properties.

Invited Talk SYMM 1.2 Tue 15:00 HSZ 04

Electrostatic Interface Tuning in Superconducting Oxide Heterostructures — •N. Pavlenko — Institute of Physics, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

In oxide heterostructures consisting of high-temperature superconducting films and ferroelectric/dielectric layers, electric fields can be used to switch between superconducting and insulating states by electrostatically tuning the free carrier density. Analyzing the superconducting pairing in a cuprate film in terms of a developed microscopic model model, we show that a coupling to electric dipoles and phonons at the interface of film and dielectric/ferroelectric gate localizes the injected charge and leads to a superconductor-insulator transition [N. Pavlenko et al., Phys. Rev. B, 72 (2005) 174516]. We find that in the correlated oxide films, the strong interface polaron effect is inherently connected to the stabilization of interface charge orderings and inhomogeneous states. This leads to a dramatic modification of the doping dependent phase diagrams which is expected to shed light on recent electric field-effect experiments with HTSC cuprates. Based on these results, we consider several novel design concepts for superconducting field-effect devices [N. Pavlenko, Phys. Rev. B 70 (2004) 094519; N. Pavlenko et al., Appl. Phys. Lett. 70 (2005) 012507] and discuss the ways to amplify the electric field effect.

Invited Talk SYMM 1.3 Tue 15:30 HSZ 04

Modelling realistic ferroic materials - multiscale approaches — •S. Gemming, I. I. Chaplygin, W. Alsheimer, and G. Seifert — Institut für Physikalische Chemie, TU Dresden, D-01069 Dresden

The complex coupling of electronic and structural degrees of freedom in ferroic materials makes it necessary to treat different physical properties on a different theoretical level. First-principles calculations based on the density-functional theory yield electronic and atomistic structure, potential and field distribution, as well as dielectric properties. Pure bulk or composite compounds, but also nanostructured species and systems including defects such as grain boundaries and vacancies can thus be investigated at the microscopic scale. Beyond this, the calculations provide a database for mesoscopic approaches, for instance for the conductivity mediated by both electronic and ionic contributions. Also the coupling between different spin subsystems in correlated systems is much better described by a modified Heisenberg approach, whose parameters can be based on first-principles data. In this way the phase sequence and transition temperatures in ferroic oxides have been accessed. Examples for bridging the microscopic and macroscopic length scales are provided by finite-element modelling of the elastic properties of realistic compounds, which contain microscopic defects, or by mean-field approaches to derive the long-range potential or field distribution of nanostructured matter.

SYMM 2 Multiferroic Materials - Experiment

Time: Tuesday 16:15–18:15 Room: HSZ 04

Invited Talk SYMM 2.1 Tue 16:15 HSZ 04

Multifunctional Complex Oxide Heterostructures — •R. Ramesh — Department of Materials Science and Engineering, and Department of Physics, University of California, Berkeley, CA 94720

Complex perovskite oxides exhibit a rich spectrum of functional responses, including magnetism, ferroelectricity, highly correlated electron behavior, superconductivity, etc. There exists a small set of materials which exhibit multiple order parameters; these are known as multiferroics. Using our work in the field of ferroelectrics and ferromagnetics as the background, we are now exploring such materials, as epitaxial thin films as well as nanostructures. Specifically, we are studying the role of thin film growth, heteroepitaxy and processing on the basic properties as well as magnitude of the coupling between the order parameters. In single phase multiferroic perovskites, such as $BiFeO_3$, we have found significant enhancements in magnetism and ferroelectricity compared to bulk. Detailed measurements indicate that the enhancement in magnetism is due to a mixed Fe^{2+}/Fe^{3+} state in the films, while the ferroelectric polarization is reasonably commensurate with that predicted from first principles theory. A very exciting new development has been the discovery of the formation of spontaneously assembled nanostructures consisting of a ferromagnetic phase embedded in a ferroelectric matrix that exhibit very strong coupling between the two order parameters. This involves 3-dimensional heteroepitaxy between the substrate, the matrix perovskite phase and spinel phase that is embedded as single crystalline pillars in this matrix. This epitaxial coupling is critical and is responsible for the significantly higher magnetoelectric coupling and magnetic anisotropy in such vertical heterostructures compared to a conventional heterostructure.

This work is supported by the ONR under a MURI program.

Invited Talk SYMM 2.2 Tue 16:45 HSZ 04

Some Observations about Static Scaling: Domain Widths and Circular and Toroidal Ordering in Ferroelectrics, Ferromagnets, and Magnetoelectrics — •J. Scott — Cambridge University, Cambridge, UK

In 1946 Charles Kittel derived a formula for the width w of 180-degree domains, varying as the square root of the sample thickness d, and in the same early paper showed that nano-structures (nano-wires and nano-dots) would have circular ordering of spins. Both ideas were later independently rediscovered, w being proportional to the square root of d by Mitsui and Furuichi (Phys. Rev. 1953), and circular or toroidal ordering in ferroelectrics by Ginzburg in 1981-1984. Very recently the latter idea was put on an atomistic ab initio level by Naumov et al. (Nature 2004). In this talk I combine Kittel's equation with a less well known one of Zhirnov (1959), which shows that the domain wall thicknesses D also varies as the square root of d. The resulting formula is (w-squared)/Dd = G, where G is a dimensionless constant = 32 in barium titanate and 1 in Rochelle Salt. This formula fits barium titanate over six decades of thickness d, from 1.5 nm to 1.5 mm (figure below). Where this formula breaks down depends upon boundary conditions and size, which connects it to circular/toroidal ordering. Moreover, as Ginzburg first showed, the symmetry requirements for toroidal ordering are closely related to those for magnetoelectricity (Schmid, 1994).

Invited Talk SYMM 2.3 Tue 17:15 HSZ 04

Magnetoelectric Effect and Toroidal Ordering in Multiferroic Manganites — •M. Fiebig[1], Th. Lottermoser[1], and Th. Lonkai[2] — [1]Max-Born-Institut, Max-Born-Strasse 2A, 12489 Berlin, Germany — [2]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany; and Hahn-Meitner-Institut, Glienicker Strasse 100, 14109 Berlin, Germany

Recently, an enormous interest in multiferroic compounds which unite two or more different forms of primary ferroic ordering in one phase is observed. Aside from technological aspects the interplay of different forms of (anti-) ferroic ordering is a rich source for exploring the fundamental science of phase control. I will discuss the coexistence of magnetic and electrical ordering in the hexagonal rare-earth manganites $RMnO_3$ (R=Ho,Yb). With ferroelectricity and magnetic Mn^{3+} and R^{3+} ordering the compounds possess 4 ordered sublattices. I will show how microscopic magnetoelectric correlations between sublattices in combination with multiple frustration lead to giant manifestations of macroscopic magnetoelectric behavior. This leads to magnetic phase control by external electric or magnetic fields or temperature. Furthermore, I will argue that in addition to ferromagnetism, ferroelectricity, and ferroelasticity as the three widely known forms of primary ferroic ordering, ferrotoroidicity formation of a spontaneous magnetic vortex must be included as the fourth variety. Toroidic domains can exist and have already been observed in multiferroic $YMnO_3$, but were not recognized as such. However, after introducing toroidic domains as physically independent states the former observation becomes physically sound.

Invited Talk SYMM 2.4 Tue 17:45 HSZ 04

Magnetoelectric Effects in Multiferroics — •A. Loidl, J. Hemberger, A. Pimenov, P. Lunkenheimer, A. A. Mukhin, and V. Tsurkan — Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

Magnetoelectric phenomena were investigated for two different multiferroic systems. The coupling of dielectric and magnetic properties and the simultaneous occurrence of long-range magnetic and polar order are discussed for manganites and spinels. A phase diagram of $Eu_{1-x}Gd_xMnO_3$ as function of temperature and magnetic field is established. It resembles the main features of the well-known magneto-electric phase diagram of $RMnO_3$ (R = rare earth) with a sequence of magnetic and polar phase transitions for varying ionic radii of the rare earth ions. Special attention is paid to the occurrence of electromagnons, i.e. spin waves that can only be excited by an ac electric field. These excitations also allow tuning the index of refraction by moderate magnetic fields. In the second part we discuss the simultaneous appearance of colossal magneto-resistance and colossal magneto-capacitance effects in chromium sulfo spinels. Ferroelectricity appears well above the onset of ferromagnetism in $CdCr_2S_4$ and above a complex antiferromagnetic order in $HgCr_2S_4$. We speculate that the occurrence of ferroelectricity in these multiferroic compounds is rather of electronic than of ionic origin.