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High-resolution X-ray diffraction analysis of strain relaxation in epitaxial oxide thin films

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It is now well accepted that epitaxial strains can be used to stabilize out of equilibrium phases [1]. This approach is especially interesting in the case of functional oxide thin films usually subject to many solid-state phase transitions as a function of external constrains (i.e temperature or pressure variations). The precise evaluation of strains and strain gradients is thus one of the main issues in the development of devices based on functional oxides. High-resolution x-ray diffraction (HR-XRD) is one of the most efficient non-destructive methods to extract such information [2]. $RNiO_3$ compounds are extremely difficult to stabilize because of the less stable 3+ oxidation state of Ni. We have recently shown [3, 4] that $SmNiO_3$ (SNO) perovskite can be epitaxially grown on both $SrTiO_3$ and $LaAlO_3$ single crystalline substrates. Those two different cases are corresponding to different lattice mismatch between the film and the substrate. In this communication we present a detailed study of the microstructure of SNO films. This analysis is mainly based on HR-XRD and more specifically on Reciprocal Space Mapping. The contribution of chemical and mechanical effects to the lattice parameters can be rigorously separated using both laboratory and synchrotron HR-XRD. The effect of relaxation-induced misfit dislocations has been investigated and the dislocation densities were derived from the reciprocal space maps. The presence of misfit dislocations induces asymmetrical longitudinal profiles recorded at synchrotron source, those profiles were quantitatively analysed.

[1] N.A.Pertsev et al., PRL, 80 (1998) 1988-1991.
[2] A. Boulle et al., JAC, 36 (2003) 1424-1431
[3] F. Conchon et al., APL, 91 (2007) 192110, 1-3.
[4] F. Conchon et al., JPCM, 20 (2008) 145216, 1-7.

Keywords: strain, high-resolution X-ray diffraction, epitaxial thin films

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Paramagnetism and ferromagnetism of TiO_2 and ZnO as seen by XMCD: A way to study defects in oxides

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ZnO and TiO_2 have attracted in recent years much attention possessing a large range of potential applications. One field is waste form management. Pyrochlores, $A_2Ti_2O_7$ fluorite based materials have been considered for long-term stabilization of high and medium level nuclear waste, including future generation-IV nuclear technologies. Understanding the basic physics of radiation damage is undeniable and the quest should clearly start from simple systems like TiO_2 and ZnO. The magnetic properties in both compounds can be related to the presence of oxygen vacancies. X-ray magnetic circular dichroism (XMCD) gives a direct proof of it conjugating the atomic specificity and sensitivity of a synchrotron based spectroscopic technique to the magnetic properties. TiO_2 is a wide gap diamagnetic semiconductor. If an oxygen vacancy is created, to compensate the charge a Ti^{4+} cation must change from the diamagnetic Ti^{4+} to a paramagnetic Ti^{2+} or two Ti^{4+} cations must change to Ti^{3+}. We studied the magnetic properties of doped and undoped TiO_2 and ZnO measuring the dichroic signal at the Ti $L_{2,3}$ edges and O and Zn K edges. Evidence of ferromagnetism at the K edge of O and at the $L_{2,3}$ edges of Ti associated with oxygen vacancies, has been found, while no ferromagnetic behavior has been observed at the K edge of Zr. From the magnetic properties information could be obtained about the defects. A further step is the study of irradiated samples with opportunely induced defects. This will highlight trough the evolution of the magnetic properties the irradiation induced defect formation. Here we set forth a conceptually different approach; instead to evaluate the crystalline to amorphous fraction we propose to analyze magnetic defects created by irradiation in otherwise diamagnetic crystals.

Keywords: thin-film properties, defects, magnetic properties

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Mn atoms in GaAs: First evidence for Ga interstitial site occupation

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$Ga_{1-x}Mn_xAs$ is commonly considered as a promising material for microelectronic applications utilizing the electron spin. The location of the Mn atoms in the by MBE grown layers is correlated with all important physical properties of the final material, therefore it is the subject of many studies. A powerful tool for this kind of study is x-ray absorption spectroscopy (XAS) as it probes the local atomic order and the electronic structure. We calculate the influence of the Mn atom location within the GaAs matrix on the shape of the XANES spectra by means of the ab initio calculations using FEFF 8.4. Different Mn positions within the GaAs matrix were considered: (a) substitutional MnGa, (b) interstitial (As); with As atoms as the first neighbours, (c) interstitial (Ga) ; with Ga atoms as the first neighbours. The theoretical predictions were compared with the experimental K and L edge XANES of Mn measured on the samples without any thermal treatment and after annealing to different temperatures. It is shown that in the considered samples the Mn atoms may occupy more than one position in the crystal lattice, therefore a superposition of possible locations was considered. This allows to determine the possible distribution of Mn between all possible lattice locations. We find for the first time that Mn atoms clearly prefer the Ga interstitial positions.

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Keywords: X-ray absorption spectroscopy, magnetic semiconductor, occupancy

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Application of representation theory and SARAh to magnetic structure determination

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The determination of complex magnetic orderings and the study of coupling between different types of order, such as magnetic and electric dipole in multiferroics, requires the application of advanced symmetry arguments. These provide frameworks within which symmetry rules can be developed and expressed. They also enable an understanding to be developed of exactly what a particular order is and why it occurs. SARAh was initially developed in order to allow the calculation of the different types of symmetry modes using representational theory, and refinement of neutron diffraction spectra in terms of the results. In the new release tools have been added to improve the generality of these calculations and aid the visualisation of the different types of magnetic structures. An engine has also been developed to allow the determination of commensurate and incommensurate ordering wavevectors, based on a new procedure whereby the different points, lines and planes in the Brillouin zone are explored sequentially. This procedure, termed 'Brillouin zone indexing', follows from the physical nature of the magnetic ordering transition and enables the translational symmetry of the magnetic order to be explored thoroughly. In SARAh its application is based on the application of reverse-Monte Carlo algorithms to the complete powder diffraction pattern, and it allows even structures with several unrelated wavevectors to be studied through automatic cycling.

Keywords: magnetic ordering, magnetic neutron scattering, symmetry theory generalization and applications

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The determination of magnetic structures by simulated annealing using the FullProf Suite

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The propagation vector formalism for describing magnetic structures is the best way to treat the neutron diffraction (ND) data in order to determine experimental magnetic structures. The magnetic structure in the infinite crystal can generally be described as a finite Fourier series. The Fourier coefficients, labeled by the propagation vector and the index of the particular atom in the cell, are complex vectors to be determined experimentally. These vectors define the magnetic structure and they correspond to the unknowns of the magnetic structure. This kind of formalism is implemented within the program *FullProf* [1]. The steps for solving magnetic structures from ND are the following [2]: (a) Search for the propagation vector(s). (b) A symmetry analysis is needed to find the smallest set of free parameters. In general the Fourier coefficients are linear combinations of the basis functions of the irreducible representations of the propagation vector group. (c) Use an appropriate method for determining the coefficients of the above linear combinations. This implies an evaluation of the observed versus calculated intensity of the magnetic reflections. A trial and error method using least squares is only possible for simple magnetic structures. In general a starting model should be obtained. The simulated annealing technique is extremely efficient, for whatever kind of magnetic structure, in getting an initial model and eventually for determining hidden symmetries. In this communication we will present all the steps in solving magnetic structures by using the programs of the FullProf Suite[3].

[1] J. Rodriguez-Carvajal, Physica B 192, 55 (1993)
[2] J. Rodriguez-Carvajal, Materials Science Forum 378-381, 268 (2001)
[3] See the web site: http://www.ill.eu/sites/fullprof/

Keywords: magnetic structures, neutron diffraction, simulated annealing

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International-like tables for magnetic crystallography

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We discuss the structure, symbols, and properties of magnetic groups. While the focus is on three-dimensional magnetic space groups, analogous information on one- and two-dimensional space groups and two- and three-dimensional subperiodic magnetic groups is available. Properties of the magnetic space groups have been tabulated and are available in a format and content similar to that of the International Tables of Crystallography. For each group we have tabulated diagrams of symmetry elements, diagrams of general positions, symmetry operations, generators selected, origin, general and special positions, and symmetry of special projections. The magnetic moments allowed by magnetic symmetry are given in the diagrams of general positions and in the listing of general and special positions. The present availability of tabulations of subgroups of magnetic groups, 3D rotateable general position diagrams, and a brief review of the history of magnetic group tabulations will also be given.

Keywords: symmetry, magnetic crystal structure, magnetic ordering

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Ab initio magnetic structure refinement: Total scattering and RMCProfile

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