

MS.60.3*Acta Cryst.* (2008). A64, C106**High-resolution X-ray diffraction analysis of strain relaxation in epitaxial oxide thin films**Rene Guinebrethiere¹, Florine Conchon¹, Alexandre Bouille¹, Cecile Girardot², Stephane Pignard², Eric Dooryhee³, Jean Louis Hodeau³¹Lab. Science des Procédés Céramique et de Traitements de Surface, ENSCI, 47, Av. A. Thomas, Limoges, Limousin, 87065, France, ²LMGP UMR CNRS 5628, INP Grenoble, MINATEC, 3 parvis Louis Néel BP 257, 38016 Grenoble, France, ³IN CNRS UPR 2940, 25 avenue des Martyrs BP 166, 38042 Grenoble – France, E-mail : rene.guinebrethiere@unilim.fr

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 constraints (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]. RNiO₃ compounds are extremely difficult to stabilize because of the less stable 3+ oxidation state of Ni. We have recently shown [3, 4] that SmNiO₃ (SNO) perovskite can be epitaxially grown on both SrTiO₃ and LaAlO₃ 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.

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[2] A. Bouille 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

MS.60.4*Acta Cryst.* (2008). A64, C106**Paramagnetism and ferromagnetism of TiO₂ and ZnO as seen by XMCD: A way to study defects in oxides**Paolo Imperia¹, A. Barla², N. H. Hong³, J. -P. Kapler⁴, K. R. Whittle¹, G. R. Lumpkin¹¹ANSTO, Institute of Materials Engineering, New Illawarra Road, Lucas Heights, Sydney, NSW, 2234, ²ALBA/CELLS, Barcelona, Spain, ³LEMA, Tours, France, ⁴IPCMS, Strasbourg, France, E-mail : plo@ansto.gov.au

ZnO and TiO₂ have attracted in recent years much attention possessing a large range of potential applications. One field is waste form management. Pyrochlores, A₂Ti₂O₇ 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

TiO₂ 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. TiO₂ is a wide gap diamagnetic semiconductor. If an oxygen vacancy is created, to compensate the charge a Ti⁴⁺ cation must change from the diamagnetic Ti⁴⁺ to a paramagnetic Ti²⁺ or two Ti⁴⁺ cations must change to Ti³⁺. We studied the magnetic properties of doped and undoped TiO₂ 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 through 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

MS.60.5*Acta Cryst.* (2008). A64, C106-107**Mn atoms in GaAs: First evidence for Ga interstitial site occupation**Krystyna Lawniczka-Jablonska¹, Anna Wolska¹, Marcin T Klepka¹, Janusz Sadowski^{1,2}, Elisabeth Holub-Krappe³, Andreas Persson⁴, Dimitri Arvanitis⁴¹Polish Academy of Sciences, Institute of Physics, Al. Lotnikow 32/46, Warsaw, Poland, 02 668, Poland, ²Lund University, Max-Lab, Lund SE-221 00, Sweden, ³Hahn-Meitner Institute, Department of Magnetism, Glienicker Str. 100, D-14109 Berlin, Germany, ⁴Physics Department, Uppsala University, Box 530, 75121 Uppsala, Sweden, E-mail : jablo@ifpan.edu.pl

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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