

s6.m21.p4 **Elastic and inelastic neutron scattering on hydrogenated austenitic stainless steels.** M. Hoelzel^{a,b}, S.A. Danilkin^c, D.M. Toebbens^c, T.J. Udovic^d, T. Rameriz-Cuesta^e, V. Rajevac^a, H. Wipf^f and H. Fuess^a, ^aTU Darmstadt, *Material- und Geowissenschaften, 64287 Darmstadt, Germany*, ^bFRM-II, *TU München, 85747 Garching, Germany*, ^cHahn-Meitner-Institut Berlin, *14109 Berlin, Germany*, ^dNational Institute of Standards and Technology, *NIST Center for Neutron Research, Gaithersburg, MD 20899-8562, USA*, ^eRutherford Appleton Laboratory, *ISIS Facility, United Kingdom*, ^fTU Darmstadt, *Institut für Festkörperphysik, 64289 Darmstadt, Germany*. E-mail: markus.hoelzel@frm2.tum.de

Keywords: Neutron diffraction; Inelastic neutron Scattering; Metal-hydrogen-system

The effects of hydrogen (and deuterium) on the structure and lattice dynamics of austenitic stainless steels Fe/Cr25/Ni20 and Fe/Cr18/Ni10 have been investigated by elastic and inelastic neutron scattering. Among the postulated mechanisms of hydrogen embrittlement in austenitic stainless steels, the hydrogen-induced formation of brittle hydride and martensite phases is under discussion. High-pressure hydrogenations resulting in various hydrogen contents between H/Me = 0.003 and H/Me = 1 have been performed in order to study the phase transformation behaviour due to hydrogen loading. It was found that hydrogen and deuterium atoms occupy exclusively the octahedral interstitial sites in both steels. In the frame of accuracy, no hydrogen-induced phase transformations have been observed in steel Fe/Cr25/Ni20 for the whole range of hydrogen concentrations up to H/Me = 1. In case of Fe/Cr18/Ni10, the formation of e-martensite occurred due to hydrogenations at 3.0 GPa and 7.0 GPa, corresponding to hydrogen contents of H/Me = 0.56 and H/Me = 1.03, respectively. Additionally, the formation of e-martensite was observed in Fe/Cr18/Ni10 after subjection to 4.0 GPa without the presence of hydrogen. Neither the elastic, nor the inelastic neutron scattering experiments gave indications for hydrides. In the vibrational spectra, a continuous decrease of the vibrational energies of the optical modes has been observed for increasing Me-H interatomic distances. In both steels, the optical modes in the samples with highest hydrogen contents showed a splitting into a two-component profile, which could be explained by longitudinal and transversal optical branches. A description of the modelling of the hydrogen vibrational modes is given by Rajevac et al. in this issue [1]. Even at maximum hydrogen contents, the high-pressure charged samples revealed a lower tendency for the formation of e-martensite compared to results found by electrolytical hydrogenation [2,3]. The results indicate, that the formation of e-martensite might be less determined by the absolute hydrogen concentration rather than the stress states resulting from the particular hydrogen distributions.

- [1] Rajevac et al., this issue.
 [2] Narita et al., *Metal. Trans. A* **13A** (1982) 1355-1365
 [3] Gavriljuk et al., *Metall. et Mater.* **28** (1993) 247-252.

s6.m21.p5 **Origin of the ferroelectricity in YMnO₃.** Gwilherm Nenert, Harold Stokes, Thomas Palstra, *University of Groningen, Solid State Chemistry, Nijenborgh 4, Groningen, The Netherlands*. E-mail: nenert@chem.rug.nl

Keywords: Ferroelectricity; Group theory; Hexagonal manganates

Ferroelectric materials have a spontaneous electric polarization that can be switched by an applied electric field. They are used in a wide range of applications, including data storage and as capacitors, transducers and actuators, as a result of their wide variety of physical and electronic properties. Then a good understanding of the ferroelectricity in magnetic ferroelectric oxides is of both fundamental and technological importance.

Currently two distinctly different chemical mechanisms for stabilizing the distorted structures in ferroelectric oxides have been identified. A recent article on the ferroelectric phase transition in the hexagonal manganite, YMnO₃, using a combination of single-crystal X-ray diffraction, thorough structure analysis and first-principles density-functional calculations claimed the discovery of a new mechanism for ferroelectricity [1]. The ferroelectric phase is characterized by a buckling of the layered MnO₅ polyhedra, accompanied by displacements of the Y ions, which lead to a net electric polarization. They show that the mechanism is driven entirely by electrostatic and size effects, rather than the usual changes in chemical bonding associated with ferroelectric phase transitions in perovskite oxides.

This article does not describe fully the nature of an intermediate phase which is a key element in the derivation of this new mechanism for the ferroelectricity. In the light of some group theoretical elements, we will discuss the possible different scenarios [1], [2] and proposed a new one for explaining the origin of the ferroelectricity in YMnO₃.

- [1] B. van Aken et al. *Nature Materials* **3**, 164 - 170 (2004).
 [2] Lonkai et al. *Physical Review B* (2004) vol. **69** p.134108.