

m/sec) and investigated for their hydrogen storage characteristics. The lower cooling rate obtained through low wheel speed (35 m/sec) produces, i- phase grains whose size ranges from 300-350 nm. Whereas higher cooling rates obtained through high wheel speed (45 and 50 m/sec) promote the formation of nano-quasicrystalline grains with size ranges from 50-150 nm in $Ti_{45}Zr_{38}Ni_{17}$ ribbons. It has been found that the ribbons synthesized at 35 m/sec absorbed ~2.0 wt%, whereas ribbons synthesized at 50 m/sec absorbed ~2.84 wt.% of hydrogen. Thus the hydrogen storage capacity of ribbon increases with increasing quenching rate. One of the salient features of the present study is the improvement of hydrogen storage capacity obtained through higher quenching rates (~45 to 50 m/sec wheel speed) lead to the formation of lower grain size.

Keywords: quasicrystals, hydrogen storage, microstructure

MS30.P07

Acta Cryst. (2011) A67, C417

Diffuse scattering and phason modes in the Zn-Sc icosahedral quasicrystal

Tsunetomo Yamada,^{a,b} Holger Euchner,^c Cesar Pay Gómez,^d Ryuji Tamura,^a Marc de Boissieu^b ^a*Department of Materials .Sci. & Tech., Tokyo Univ. of Science, Noda, (Japan).* ^b*SIMaP, Grenoble-INP, CNRS,UJF, Saint Martin d'Hères Cedex, (France).* ^c*ITAP, Universitat Stuttgart, Stuttgart (Germany).* ^d*Ångström Lab., Uppsala University, Uppsala, (Sweden).* E-mail: j8209701@ed.noda.tus.ac.jp

Recently, a new binary icosahedral quasicrystal $Zn_{88}Sc_{12}$ has been obtained by Canfield and co-workers [1]. Because of the chemical order and the x-ray contrast between Zn and Sc, this phase is a nice system for the structure refinement. On the other hand, a large amount of diffuse scattering can be seen on the x-ray diffraction pattern [1]. In this study, we carried out an absolute scale measurement of the x-ray diffuse scattering of the $Zn_{88}Sc_{12}$ to study the possible presence of phason modes (phason diffuse scattering) and estimate phason elastic constants K1 and K2.

Millimeter size single grain of the $Zn_{88}Sc_{12}$ was obtained by slowly cooling from the melt. The sample was polished with a surface perpendicular to 5-fold axis. Systematic Q -scans and diffuse scattering maps have been measured on the D2AM beamline (ESRF) using an incoming x-ray energy equal to 9.3 keV.

Compared with ZnMgSc quasicrystal on an absolute scale [2], we find that the amount of diffuse scattering is larger in the $Zn_{88}Sc_{12}$ sample. Also, the maximal Q_{perp} value necessary for indexing the diffraction pattern was found to be less than 3 (r.l.u.) i.e. much smaller than for ZnMgSc for which it was found to be 7 [2]. In addition, as for other quasicrystals [3] a characteristic diffuse intensity distribution due to phason fluctuations around strong Bragg reflections is clearly visible on the systematic reciprocal space map. The ratio K2/K1 is found to be close to the three-fold instability limit, which results in the strong elongation of the diffuse scattering along directions parallel to a three-fold axis. Finally, the simulation is carried out based on the elastic theory and reproduces well the observed anisotropic shape of the diffuse scattering.

[1] P.C. Canfield, M.L. Caudle, C.-S. Ho, A. Kreyssig, S. Nandi, M.G. Kim, X. Lin, A. Kracher, K.W. Dennis, R.W. McCallum, A.I. Goldman, *Phys. Rev. B*, **2010**, 81, 020201. [2] M. de Boissieu, S. Franoual, Y. Kaneko, T. Ishimasa, *Phys. Rev. Lett.*, **2005**, 95, 105503. [3] T. Janssen, G. Chapuis, M. de Boissieu, *Aperiodic Crystals. From modulated phases to quasicrystals*, Oxford University Press, Oxford, **2007**, 466.

Keywords: quasicrystal, diffuse scattering, phason

MS30.P08

Acta Cryst. (2011) A67, C417

Quantitative modeling of diffuse scattering from a relaxor ferroelectric

Benjamin A. Frandsen,^a Va-yeé Vue,^a Matthew J. Gardner,^b Kevin D. Seppi,^b Branton J. Campbell,^a ^a*Department of Physics & Astronomy, Brigham Young University, Provo, Utah, (USA).* ^b*Department of Computer Science, Brigham Young University, Provo, Utah (USA).*

The lead-based relaxor ferroelectrics like $Pb(Zn_{1/3}Nb_{2/3})O_3$ - $PbTiO_3$ (PZN-PT) are of pressing applied interest due to their exceptional piezoelectric properties [1]. X-ray single-crystal diffuse-scattering techniques have recently yielded insights into the local structures of these compounds, where marked changes have been observed upon the application of a strong electric field [2]. We will present high-resolution reciprocal-space volume reconstructions from PZN-PT from X-ray CCD images, both with and without an in-situ electric field, and also describe quantitative fits of structural models against our diffuse scattering data. The results facilitate a better understanding of the influence of an applied field on the local structure of this material.

[1] H. Fu, R.E. Cohen, *Nature* **2000**, 403, 281. [2] G.Y. Xu, Z. Zhong, Y. Bing, Z.G. Ye, G. Shirane, *Nat Mater* **2006**, 5, 134.

Keywords: relaxor ferroelectric, diffuse scattering, soft phonon

MS30.P09

Acta Cryst. (2011) A67, C417

Framework defects in aluminophosphate ALPO-5

Branton J. Campbell, Nichole Maughan, Daniel G. Robertson, Sumner Norman, *Department of Physics & Astronomy, Brigham Young University, Provo, Utah 84602 (USA).* e-mail: branton_campbell@byu.edu

ALPO-5 is a well-known microporous aluminophosphate framework compound¹ with a one-dimensional channel system consisting of 12-ring tubes formed from 6-ring sheets. Several metal cation-substituted forms of this AF1 framework type are important due to their superior shape-selective catalytic properties. Single-crystal x-ray diffuse scattering data from ALPO-5 reveal oddly-structured rods of diffuse scattering parallel to the hexagonal axis. Diffuse scattering is not expected in this plane due to the constraints of strict Al-O-P linkage ordering. We will present a defect structure model that explains the observed scattering pattern.

[1] J.M. Bennett, J.P. Cohen, E.M. Flanigen, J.J. Pluth, J.V. Smith, *ACS Sym. Series* **1983**, 218, 109-118.

Keywords: aluminophosphate, diffuse scattering, faulting

MS30.P10

Acta Cryst. (2011) A67, C417-C418

Ab-initio lattice dynamics and thermal diffuse scattering in CaTiSiO₅

M. J. Gutmann,^a K. Refson,^b M.V. Zimmermann,^c C.K.D. Stock,^d I. P. Swainson,^e H.A. Dabkowska,^f A. Dabkowski,^f ^a*Rutherford Appleton Laboratory, ISIS Facility, Oxfordshire (United Kingdom).* ^b*Rutherford Appleton Laboratory, Computational Science and Engineering Department, Oxfordshire (United Kingdom).* ^c*HASYLAB-DESY, Hamburg, (Germany).* ^d*NIST center for neutron research,*