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

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

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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 constats 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. Francoual, 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

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Quantitative modeling of diffuse scattering from a relaxor ferroelectric

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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

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Framework defects in alumino-phosphate ALPO-5

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ALPO-5 is a well-known microporous alumino-phosphate framework compound[1] with a one-dimensional channel system consisting of 12-ring tubes formed from 6-ring sheets. Several metal cation-substituted forms of this AFI 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

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Ab-initio lattice dynamics and thermal diffuse scattering in $CaTiSiO_5$

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A synthetic specimen of the mineral $CaTiSiO_5$ has been studied using the time-of-flight neutron diffractometer SXD at ISIS and high-energy X-ray diffraction using 100keV X-rays on BW5 at DESY. Diffuse scattering at room-temperature has been recorded using both techniques. The diffuse features appear rather different in the two datasets owing to the relative scattering power of X-rays and neutrons from the various elements.

To model the data, ab-initio phonons have been calculated using density-functional perturpation theory as implemented in CASTEP and reciprocal space maps corresponding to first-order thermal diffuse scattering are compared with the data. Very good visual agreement is obtained with both neutrons and X-rays confirming the thermal nature of the diffuse scattering. The present work provides a basis for studying the diffuse scattering in the high-temperature phase and inelastic spectra away from the zone-centre.

Keywords: diffuse scattering, diffraction, mineral

MS30.P11

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Structural study on zr-based metallic glasses by anomalous X-ray scattering coupled with reverse Monte-Carlo simulation

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Recent discovery of the Zr-based bulk metallic glasses (BMGs) with interesting mechanical properties of high fracture strength, Young's modulus and plasticity have aroused much interests in their practical applications. These findings have also stimulated a variety of advanced structural studies on Zr-based metallic glasses, because their structural information are important for understanding their glass forming ability and thermal stability.

The concept of partial structural functions describing the correlations for individual pairs of chemical constituents in multi-component disordered systems has been emphasized for a long time and the partial structure factors for a binary system can be estimated only by making available at least three independent intensity measurements for which the weighting factors are varied. On the other hand, the anomalous X-ray scattering (hereafter referred to as AXS) method by utilizing the anomalous dispersion effect near the absorption edge provides another answer. Recently, the utility of this AXS method has greatly improved by the intense white X-rays from a synchrotron radiation source. Additionally, the development of the reverse Monte Carlo (RMC) simulation encourages us to reduce the subsequent difficulty by providing partial structural information in a sense of the necessary condition at best [1.2.3]. The main purpose of this paper is to demonstrate the detailed structural information of Zr-based glassy alloys by AXS measurements coupled with RMC modeling (hereafter denoted as AXS-RMC) and to discuss their topological features in the nearest neighbor region.

As an example, the AXS analysis of $Zr_{80}Pt_{20}$ glassy alloy provided the environmental structural information around Zr and Pt, and subsequent reverse Monte Carlo (RMC) simulation allowed us to obtain three partial pair distribution functions together with a three dimensional structural model. The Voronoi polyhedral analysis in the nearest neighbor region, confirmed the structural feature similar to that of the random dense packing hard sphere model together with an icosahedral atomic arrangement as shown in Fig.1. The present analysis also revealed the preference of ideal Pt-icosahedron with covalent Pt-Zr pairs. This particular unit is suggested to introduce the easy formation of the nano-icosahedral phase.

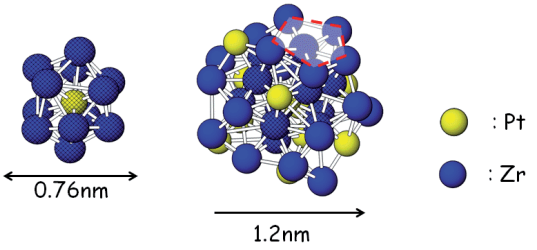

Fig 1. The local atomic arrangement around Pt in $Zr_{80}Pt_{20}$ glassy alloy.

[1] M. Saito, C. Park, K. Omote, K. Sugiyama, Y. Waseda, *J. Phys. Soc. Jpn.* **1997**, *66*, 633-640. [2] M. Saito, C. Park, K. Sugiyama, Y. Waseda, *J. Phys. Soc. Jpn.* **1997**, *66*, 3120-3126. [3] T. Kawamata, Y. Tokoyama, M. Saito , K. Sugiyama, Y. Waseda, *Mater. Tans.* **2010**, *51*, 1796-1801.

Keywords: RDF, glass, synchrotron

MS30.P12

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Kinetics of atomic ordering and diffuse scattering of X-Rays within the nonstoichiometric quasi-binary (W,Ti)B_2 crystal

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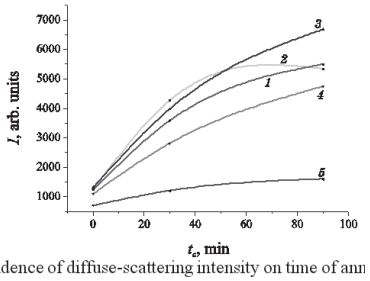
The change of X-ray diffuse-scattering intensity during isothermal annealing of $(Ti_{1-\delta}W_\delta)B_2$ solid solution, in a wide range of concentration, δ, and from various initial states (quenched from various temperatures) is studied. As shown, the intensity of diffuse scattering and, hence, the Cowley's short-range order parameters demonstrate the complicated change during an annealing. The short-range order kinetics in this nonstoichiometric quasi-binary $(Ti_{1-\delta}W_\delta)B_2$ system is nonmonotonous. To reveal the initial stages of concentration decomposition without formation of noncoherent interphase boundaries, the data obtained by the small-angle scattering of X-rays near to zero site of reciprocal (diffraction) lattice [1, 2] are used.



Dependence of diffuse-scattering intensity on time of ann
at different reciprocal-space points, $\mathbf{k} = \frac{2\pi}{c}\zeta[001]$, for
binary $C32$-(W,Ti)B_2 (with hexagonal c axis) [1, 2

[1] A.P. Shpak, O.V. Sobol, V.A. Tatarenko et al., *Metallofiz. Noveishie Tekhnol.* **2008**, *30*, 285–295. [2] A.P. Shpak, O.V. Sobol et al., *Nanosystems, Nanomaterials, Nanotechnologies* **2008**, *6*, 147–152.

Keywords: short-range order, ordering kinetics, diffuse scattering