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A synthetic specimen of the mineral  $\text{CaTiSiO}_5$  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 perturbation 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

*Acta Cryst.* (2011) A67, C418

#### 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  $\text{Zr}_{80}\text{Pt}_{20}$  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.

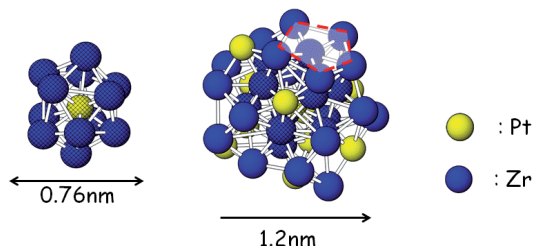


Fig 1. The local atomic arrangement around Pt in  $\text{Zr}_{80}\text{Pt}_{20}$  glassy alloy.

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**Keywords:** RDF, glass, synchrotron

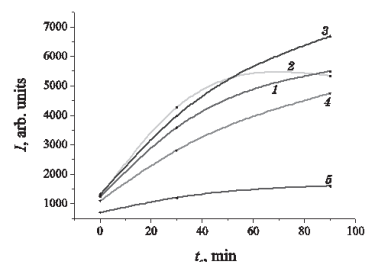
### MS30.P12

*Acta Cryst.* (2011) A67, C418

#### Kinetics of atomic ordering and diffuse scattering of X-Rays within the nonstoichiometric quasi-binary $(\text{W,Ti})\text{B}_2$ crystal

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The change of X-ray diffuse-scattering intensity during isothermal annealing of  $(\text{Ti}_{1-\delta}\text{W}_\delta)\text{B}_2$  solid solution, in a wide range of concentration,  $\delta$ , 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  $(\text{Ti}_{1-\delta}\text{W}_\delta)\text{B}_2$  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 annealing at different reciprocal-space points,  $\mathbf{k} = \frac{2\pi}{c} z[001]$ , for binary  $\text{C32}-(\text{W,Ti})\text{B}_2$  (with hexagonal  $c$  axis) [1, 2].

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