its Q-resolution is about 0.3 % at back scattering detectors. By utilizing the broadband width of neutron wavelength, it can observe a wide Q range of 0.01 < Q < 100 Å^{-1} in one experiment. These features provide diffraction pattern with reasonable resolution for PDF analysis as well as Rietveld refinement. Also, with the low Q data, larger scale structure and/or fluctuation will be observed. The expecting neutron flux at the sample position of NOVA is 5 x 10^8 neutron / sec at 1 MW operation of the proton accelerator. Typical measurement time is expected to be several minutes for full Q-range measurement. By introducing state-of-art data acquisition technique, each neutron detection event at detectors will be recorded separately and it is possible to relate values of outer fields of the sample with the time of the neutron scattered. In some cases such as structural changes in reversible phenomena, msec order measurements of the full Q-range can be realized with the technique. In-situ measurements of hydrogen absorbing/desorbing process are planning to understand local structural changes in hydrogen storage materials. Despite it is still open question how we can analyze the full Q-range data consistently, it is promising that NOVA will provide new opportunities for non-crystalline structure of materials. This research is supported by NEDO (New Energy and Industrial Technology Department Organization) under "Advanced Fundamental Research Project on Hydrogen Storage Materials"

Keywords: neutron diffraction techniques, noncrystalline materials, hydrogen storage

MS.39.3

Negative thermal expansion and local crystal structure

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The structures of a significant group of materials which contract on heating consist of flexibly-linked polyhedra. This group is typified by ZrW_2O_8, with a maximum negative thermal expansion (NTE) of -9.1MK^{-1} and isotropic NTE over ~1000K. The WO_4 and ZrO_6 polyhedra are joined together at their corners by oxygen atoms and this flexibility, enhanced by the presence of a non-bonded oxygen atom on each WO_4 tetrahedron, gives rise to the NTE in ZrW_2O_8 [1,2]. Bonding via a molecular bridge---even one as simple as CN---can give rise to more extreme behaviour. For example, $Ag_3[Co(CN)_6]$, whose CoC_6 octahedra are joined via a pentanuclear --CN--Ag--NC-- linkage, displays colossal NTE and positive thermal expansion of more than +/-100MK^{-1} along orthogonal directions throughout its ~500K stability range [3]. This presentation will describe how analysis of the local structure of ZrW_2O_8 and $Ag_3[Co(CN)_6]$ from reverse Monte Carlo modelling of total scattering data has been used to understand the local structural changes associated with unusual thermal expansion behaviour. Furthermore we will show how pressure-induced amorphisation might be explained in ZrW_2O_8 [4] and how weak argentophilic interactions govern the thermal expansion in $Ag_3[Co(CN)_6]$ [5].

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Keywords: thermal expansion, pair distribution function, cyanides

MS.39.4

High-resolution structure of disordered materials by high-energy X-ray diffraction

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Atoms in countless materials, both nature and man made, are not arranged in a perfectly periodic pattern over long-range distances as they are in crystals. The x-ray diffraction (XRD) patterns of such materials show only a few, Bragg-like peaks, if any, and a very pronounced diffuse component rendering traditional crystallographic techniques very difficult to apply. An alternative and very successful approach is that of the atomic pair distribution function (PDF) analysis (1,2). In the talk we will show results from recent high-energy (~ 100 keV) XRD and atomic PDF studies on materials of various degrees of structural disorder including water, ultra small (~1nm) metallic clusters grown inside polymeric hosts, semiconductor QDs, fast Li-ion conducting glasses and nanosized ferroelectric ceramics. The experimental and data reduction procedures needed to obtain good quality PDF data with x-rays will be discussed as well.
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Keywords: synchrotron X-ray scattering, atomic pair distribution functions, disordered materials

MS.39.5

Atomic pair distribution function analysis on nanomaterials

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Atomic pair distribution function (PDF) analysis is very powerful tool for the structural analysis of a nanomaterial [1], because the crystal structure cannot be well reproduced by a unit cell with periodic boundary condition due to the limited size. Recently, there are active researches about the structure determination of nanomaterials [2-7]. Here, we will discuss three finite size effects on PDF. The fast one is the particle form factor effect. The second one is the small angle scattering effect. The last one is the particle-particle correlation effect. So far, we have studied the former two cases [6]. Here, in addition, we would like to discuss the last effect for a