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$As_x Te_{100-x}$ glasses with $x \leq 40$ show single stage crystallization and those with $x \geq 40$ exhibit a double stage crystallization and at $x = 40$, this is associated with "rigidity percolation" and "chemical stoichiometric ordering". In the present study the effect of pressure on the thermal crystallization of $As_x Te_{100-x}$, $As_x Te_{100-x-y} Se_y$ glasses has been investigated by differential thermal analyzer at high pressure (HP-DTA). For As = 40 and 50 system, in $As_x Te_{100-x}$ and $As_x Te_{100-x-y} Se_y$, the first exothermic peaks are converted to endothermic under pressure and this is considered as rigidity percolation. The second exothermic peak do not converted to endothermic or no structural transformation takes place. This is considered as electron localization to delocalization. In As = 30, 40 and 50 system, as the Se content increases, the volume decreases from the initial value and the shifting of the temperature of the peaks reduces than the basic system because of less structural transformation. Thus it is concluded that the second peak is generated because of the electron localization.

Keywords: glasses, crystallization, coordination

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The modelling of experimental errors improves statistical description of merohedrally twinned data

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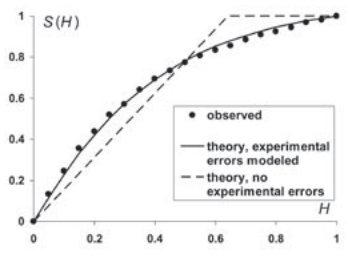
An advanced statistical model is suggested, designed to estimate the twinning fraction in merohedrally twinned macromolecular crystals. The model takes into account experimental errors of the measured intensities and is adapted to the accuracy of a particular X-ray experiment through the standard deviations of the reflection intensities. The theoretical probability distributions for the improved model are calculated using a Monte Carlo-type simulation procedure. The use of different statistical criteria (the method of moments, likelihood, chi-square, Kolmogorov-Smirnov criterion) to choose the optimal statistical model is discussed. The improved model enables obtaining better qualitative agreement of theoretical and observed cumulative distribution functions and produces twinning fraction estimates closer to the refined ones in comparison to the conventional model, which disregards experimental errors. Cumulative distributions for Yeates's statistic H are shown below for Low Density Lipoprotein data. The work was supported by RFBR and DFG grants.



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Lunin V.Y., Lunina N.L., Baumstark M.W. (2007). Acta Cryst.. D63, 1129-1138.

Keywords: merohedral twinning, statistical modelling, likelihood

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Statistical properties of measured X-ray intensities affected by counting loss of detection system

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Counting methods are widely used to measure the intensity of X-rays. Statistical errors of measured intensities are usually assumed to be equal to the square root of the observed number of counts, because independently generated signal pulses obey the Poisson distribution, where the statistical variance is exactly identical to the average number of pulses. However, the intensity measured with a realistic counting system does not strictly obey the Poisson distribution because of finite response time of the detection system. Statistical properties of two conventional theoretical models for counting loss, non-extended and extended deadtime models, examined by Monte Carlo simulations, have shown that statistical variances as well as means deviated from those predicted by the Poissson model are well approximated by simple mathematical formulae [1]. In this study, experimental evaluation of statistical variance of counted pulses based on a repeated Chipman's method [2] has been conducted for a laboratory powder x-ray diffractometer (Rigaku RAD-2C) and a synchrotron powder diffractometer (KEK-PF BL-4B2 MDS system). The dependence of the observed average count on the expected count rate has been rather well fitted by an intermediately extended deadtime model [3] than the conventional models. It has been suggested that the statistical errors of the observed counts can also be predicted by applying the intermediate model, assuming hypothetical series of detection components with non-extended and extended deadtime characters.

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Keywords: counting loss, statistical error, counting method

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The XtalFinder imaging system

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The XtalFinder is an automated imaging system for collecting crystallization results from SBS format (48-, 96-, 192-, 384-wells) microplates. The system has previously been described [1]. Our recent updates include: A mono microscope for straight viewing angle of the sample; An LED cold light source with center and radial intensity control, to improve the contrast and sample illumination for multiple sample types; A new software version with a more user-friendly graphical interface and simpler, straight forward, functions; Use of a third party software for Z-batching of multiple images (slices) of the same drop, with different focus levels, to generate one focused image per collected drop. For future developments, algorithms and software to automatically recognize crystals or potential crystalline states are underway.

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Keywords: automation, crystallization, imaging

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Possibilities and limitations of X-ray diffraction using high energy X-rays on a laboratory system

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Recent interest in nanomaterials has increased the need to analyze structures on a local (nano) scale. However, the atomic structures of nanoparticles and nanostructured materials are not accessible by conventional methods used to study crystalline materials, because of the short ordering range in these materials. One of the most promising techniques to study nanostructures using X-ray diffraction is total scattering pair distribution function (PDF) analysis. This technique is successfully applied in a number of application areas in materials science and technology. The PDF analysis technique makes use of high quality, high energy X-ray scattering data, usually obtained at synchrotron facilities, available in several national and international research centers around the world. Despite the advantages and data quality that measurements at synchrotron beam lines offer to the researcher, in practice it can be difficult and time-consuming to get access to the facilities required. In order to be prepared as good as possible and to make optimal use of the valuable experiment time offered, it is highly desirable to perform selective measurements on candidate samples in the own research laboratory. New developments in XRD technology have been directed towards the possibility of performing nanocrystallography experiments on a standard laboratory X-ray diffraction system. In this presentation we will report on the possibilities and limitations of the use of high-energy X-rays on a homelab system.

Keywords: nanocrystalline materials, pair distribution function, X-ray diffraction

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Super high resolution powder diffractometer at J-PARC

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Neutron Science Division of High Energy Accelerator Research Organization (KEK) is constructing a Super High Resolution Powder Diffractometer (SuperHRPD) at Materials and Life Science Experimental Facility (MLF) of Japan Proton Accelerator Research Complex (J-PARC). SuperHRPD is designed to have the world best resolution $\delta d/d$ = 0.03%, which changes quite slowly in its covered d-range. SuperHRPD is located at about 100 m from a thin side of a decoupled poisoned moderator, which has been developed to produce a high-resolution & good S/N data to achieve the 0.03 % resolution within 100 m flight path. It has a 32 m curved guide and 50 m straight guide section between the instrument and the moderator. To prevent frame overlap caused for a long flight path, the disk choppers were installed in two places of the beam line. The measurement in various wavelength ranges is possible by using these disk choppers, and the adjustment of the choppers are scheduled. To install the beam line of long flight path, we constructed beam line building (MLF SuperHRPD BL building) and annex experimental hall (MLF SuperHRPD building) on the east side of MLF experimental hall. As soon as these buildings were completed in the end of 2007, a guide tube, various shielding blocks, etc. were set up. The *Sirius* diffractometer chamber, which had been used in the previous neutron facility, KENS, at KEK was installed at the SuperHRPD beam line (BL08). At the end of May in 2008, the first neutron was produced successfully at a spallation neutron source in MLF, and the high resolution Bragg reflections were obtained using the *Sirius* diffractometer chamber. The obtained data will be used in designing a new diffractometer chamber for BL08, which will be installed in the summer of 2009.

Keywords: neutron instrumentation, neutron powder diffraction, time-of-flight powder diffraction

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4SEASONS: A high-intensity chopper spectrometer for inelastic neutron scattering at J-PARC/MLF

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4SEASONS is one of the chopper spectrometers for the spallation neutron source in Materials and Life Science Facility (MLF), Japan Proton Accelerator Research Complex (J-PARC). It is intended to provide very high counting rate up to 300 meV neutron energy with medium resolution ($\Delta E/E_i$~6% at E=0) to efficiently collect weak inelastic signals from novel spin and lattice dynamics especially in high-T_c superconductors and related materials. To achieve this goal, the spectrometer equips advanced instrumental design such as an elliptic-shaped converging neutron guide coated with high-Q_c (m=3-4) supermirror, long-length (2.5m) ^{3}He position sensitive detectors arranged cylindrically inside the vacuum scattering chamber. Furthermore, the spectrometer is ready for multi-incident-energy measurements by the repetition rate multiplication method with a special Fermi chopper (the MAGIC chopper), and polarization analysis with ^{3}He spin filters. 4SEASONS is now under construction and will be ready to use in December 2008. In this paper, we show the design of 4SEASONS and current status of its construction. 4SEASONS is supported by Grant-in-Aid for Specially Promoted Research (No. 17001001) from MEXT of Japan.