Indian Institute of Science, Bangalore, INDIA, INSTRUMENTATION, Dr T K Mondal, Dept of Instrumentation, IISC Bangalore, INDIA, Pin 560012, BANGALORE, KARNATAKA, 560012, India, E-mail：tushar@isu.iisc.ernet.in

$As_x Te_{100-x}$ 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

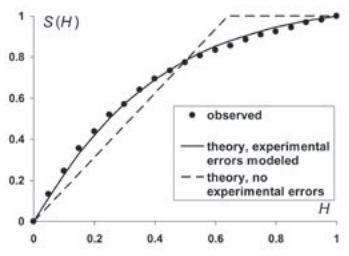
P01.11.90

Acta Cryst. (2008). A**64**, C198

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

Vladimir Y. Lunin[1], Natalia L. Lunina[1], Manfred W. Baumstark[2]
[1]Institute of Mathematical Problems of Biology, Laboratory of Macromolecular Crystallography, 4, Institutskaya str., Pushchino, Moscow Region, 142290, Russia, [2]Medizinische Universitätsklinik Freiburg, Hugstetter Str. 55, 79106 Freiburg, Germany, E-mail：lunin@impb.psn.ru

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.



Yeates, T. O. (1988). Acta Cryst. A44, 142-144.
Lunin V.Y., Lunina N.L., Baumstark M.W. (2007). Acta Cryst.. D63, 1129-1138.

Keywords: merohedral twinning, statistical modelling, likelihood

P01.11.91

Acta Cryst. (2008). A**64**, C198

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

Takashi Ida, Akihisa Oya, Hisashi Hibino
Nagoya Institute of Technology, Ceramics Research Laboratory, Asahigaoka 10-6-29, Tajimi, Gifu, 465-0097, Japan, E-mail：ida.takashi@nitech.ac.jp

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.

[1] T. Ida, J. Appl. Cryst. 40, 964 (2007).
[2] D. R. Chipman, Acta Cryst. A25, 209 (1969).
[3] T. Ida & Y. Iwata, J. Appl. Cryst. 38, 426 (2005).

Keywords: counting loss, statistical error, counting method

P01.15.92

Acta Cryst. (2008). A**64**, C198–199

The XtalFinder imaging system

Erik Brostromer, Jie Nan, Xiao-Dong Su
Peking University, College of Life Sciences, College of Life Sciences R417, Peking University, Beijing, Beijing, 100 871, China, E-mail：brostromer@gmail.com

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.

References:
1. Brostromer E, Nan J, Su XD. "An automated image-collection system for crystallization experiments using SBS standard