

FA2-MS08-P01

Multi-Energy Anomalous Diffuse Scattering.
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The method of multi-energy anomalous diffuse scattering (MADS) [1] for imaging local atomic structures is presented. MADS solves the phase problem by measuring the anomalous portion of x-ray diffuse scattering by analogy to the x-ray diffuse scattering holography (XDSH) [2]. However, compared to the two-dimensional XDSH experiments [3], MADS profits from the large amount of data recorded in a continuous three-dimensional region of the reciprocal space. Thanks to this approach, MADS solves the fundamental problem of strong artefacts inherent in the images reconstructed from holograms. A three-dimensional anomalous diffuse scattering pattern of a SrTiO₃ single crystal was measured using anomalous scattering from Sr atoms at photon energies near strontium K absorption edge (Figure (left)). The reconstructed real-space image yields the average short-range order atomic arrangement in the vicinity of the anomalous scatterers. Compared to holographic methods, where only the positions of the strontium atoms in the first three coordination shells are resolved [4], MADS gives neat images of all atoms, including the light oxygen atoms, up to a distance of tens of ångströms (Figure (right)).

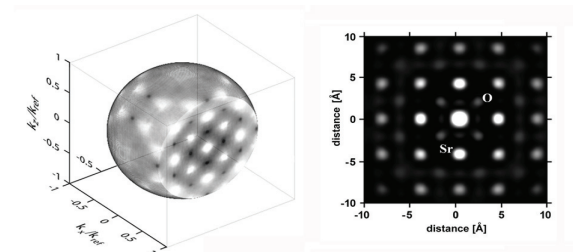


Figure: (Left) The anomalous diffuse scattering pattern of the SrTiO₃ single crystal obtained as a difference between two diffuse scattering patterns recorded at energies of 14 keV and 16.055 keV. (Right) The reconstructed image of the atomic plane parallel to the (001) crystallographic plane at $z = a$, the lattice parameter $a = 3.905 \text{ \AA}$.

[1] M. Kopecký, J. Fábry, J. Kub, A. Lausi, and E. Busetto, Phys. Rev. Lett. 100, 195504, **2008**. [2] M. Kopecký, J. Appl. Cryst. 37, 711, **2004**. [3] M. Kopecký, J. Fábry, J. Kub, E. Busetto, and A. Lausi, Appl. Phys. Lett. 87, 231914, **2005**. [4] M. Tegze and G. Faigel, Nature 380, 49, **1996**.

Keywords: X-ray diffuse scattering; anomalous scattering; atomic structure

FA2-MS08-P02

New Understanding of Anomalous Transmission and Absorption and Additional Unusually Curious Facts[1]. Tetsuo Nakajima. *Saitama Institute of Technology, Fusaiji 1690, Fukaya, Saitama 369-0293, Japan.*

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The recursion formulas of the photon paths in the Borrmann triangle which satisfies a modified Bragg law could be derived from the binomial distribution of t plus d in parentheses to the n th power in the n -multiple X-ray reflections by regarding the permutation of the stochastic variables of the diffracted and transmitted photons [2]. Sub-Borrmann triangle of the diffraction shows perfectly flawless symmetry but that of the transmission shows inevitable asymmetry. Longitudinal and transverse sums of the binomial coefficients in both sub-Borrmann triangles could be depicted by the binomial theorem but the binomial distribution in the latter sub-triangle could not describe it graphically. It means appearance of a new binomial distribution. Novel understanding of both the high intense and very weak photon flows in the binomial distribution, which are popularly known as anomalous transmission and absorption, respectively, are revealed from the standard normal distribution of $N(0, 1)$ through approximation of the binomial distribution. Incident photons into the vertex O of the Borrmann triangle propagate through the bypasses parallel to only the complementary half of the integral whole median with the highest probabilities from the binomial theorem and the reflected high intense photons emanate from a very narrow slit of O'O'' on the base of $\Delta OO'O''$ inscribed in the Borrmann triangle, which could be defined by the standard deviation of $N(0, 1)$. The parallel paths to the whole median of the triangle $\Delta OO'O''$ pass as the very weak photon flows from the terms with the highest exponent of d to the $\approx n$ th power which nearly equals to n in n -degree homogeneous multinomials of d and t . The intensity ratio between the very weak photon flows whose dummy suffix nearly equals to n and the high intense photon flows whose one nearly equals to $n/2$ could be defined by (combination of n things taken near to n at a time) / (combination of n things taken near to n halves at a time) $\div \{(n/2)!\}^2 \div n! \div 0, (1)$ and then the former terms could not be absolutely detectable in experiments. It is for this reason that X-ray photons never emerge from a position on the crystal, which is directly opposite the entrance point on a line segment of the median on the diffraction plane. Similarly, from eq. (1) the nearly parallel paths in both sides of the Borrmann triangle also pass as the very weak photon flows from the terms with the highest exponent of t to the $\approx n$ th power, which is mentioned in the above. In conclusion, both the high intense and very weak photon flows are correctly understood as a natural consequence. An additional unusually curious features pointed out many workers [3-5], for example, single refraction at entrance point O and double refraction at the midpoint of O'O'', could not be understood, since those exceed the realm of the physical possibilities [2]. We prove that the median path does not exist in the above. Much still remains to be done.

[1] T. Nakajima: J. Low Temp. Phys. 153 77, **2008**, [2] T. Nakajima: ibidem 138 1039, **2005**, [3] B. D. Cullity: *Elements of X-ray Diffraction* Addison-Wesley, **1978**, Sec. 8-7, [4] B. E. Warren: *X-ray diffraction* Dover, New York, **1990** Sec. 14.8, [5] L. V. Azaroff: *Elements of X-ray Crystallography* McGraw Hill, New York, **1968** Chap. 9.

Keywords: anomalous transmission and absorption; interference fringe

FA2-MS08-P03

The Phenomenon of Focusing of X-ray in Crystals Under Influence of the Temperature Gradient.

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The phenomenon of diffraction focusing of X-ray radiation in mono crystals under the influence of temperature gradient is analyzed in details. The phenomenon of focusing of X-ray radiation in crystal in simply way is approved.

The parallel plane single crystal samples of quartz (1x10x20mm³) have been experimentally investigated. The topogrammes of diffracted-reflected and diffracted-transmitted beams of Laue geometric have been obtained in the reflecting position of samples after adjustment at the presence of temperature gradient on distance L=3cm from the sample. For the observation of the propagation in the range of diffraction in front of the entrance of the investigated single crystal apart of incident X-ray beam is cut with wedge shaped screen. At the (m,n,n) diffraction scheme on the back side of intersection in the absence of temperature gradient of the reflected beam the wedge has a weak reverse position. The presence and the increasing of the temperature gradient brings to the increase of reflected beam and on the topogramme section the shape of the cut screen is seen more distinctly (in the reverse view). In the scheme (m,n,-n) in the absence of temperature gradient on the reflected beam on the cut height it is observed only the decrease of intensity. However, in the presence and gradually increasing of the temperature gradient, the length of diffracted beam is slowly narrowed and the track of cut at the beginning slowly and then distinctly is appeared on the backside of reflected beam. The above mentioned confirms the well known phenomenon of focusing of incident X-ray radiation inside of single crystal.

[1] Levonyan L.V. // Pis'ma v Zhurnal Tekhnicheskoi Fiziki. № 7. vol. 5 p. 269-272. **1981** (in Russian). [2] Mkrtychyan A.R., Navasardian M.A., Gabrielyan R.G., Kocharian L.A. and Kuzmin R.N. // Solid State Communications, **1986**, v.59, p.147-149.

Keywords: X-ray diffraction; X-ray focusing; X-ray spectrometry

FA2-MS08-P04

Effect of Doping on the Structure of Bi₄Ge₃O₁₂.

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Single crystals of Bi₄Ge₃O₁₂ ($I\bar{4}3d$) doped with V, Co and Mn have been grown by the Czochralski method. Samples with concentration of V= 6.8*10¹⁸ cm⁻³, Co=0.011*10¹⁸ cm⁻³ and Mn = 0.81*10¹⁸ cm⁻³ were studied using single crystal structural analysis and the dependence of the main structural parameters (bond lengths and angles, unit cell parameter) on the doping elements is followed. These data can provide a basis for estimating the incorporation of doping ions in the crystal lattice of such type of materials, which are of importance for their optical properties.

It is found that V, Co and Mn doping affects the BiO₆ octahedrons asymmetry, namely Bi-O(a) bond is shortened while Bi-O(b) bond elongates. The measured relative changes are of the order of 10⁻². On the other hand, the GeO₄ tetrahedron becomes more symmetric. The structural change per a doping atom is strongest for Co, for which the shortening of the Ge-O bond is highest.

Keywords: doped Bi₄Ge₃O₁₂; structure; optical properties