

Journal of Applied Crystallography

research papers

- 633** **A method for the non-destructive analysis of gradients of mechanical stresses by X-ray diffraction measurements at fixed penetration/information depths**
A. Kumar, U. Welzel and E. J. Mittemeijer
A rigorous measurement strategy for (X-ray) diffraction stress measurements at fixed penetration/information depths has been developed. Thereby errors caused by lack of penetration-depth control in traditional (X-ray) diffraction ($\sin^2\psi$) measurements have been annulled.
- 647** **Small-angle X-ray scattering measurements of helium-bubble formation in borosilicate glass**
A. Y. Terekhov, B. J. Heuser, M. A. Okuniewski, R. S. Averback, S. Seifert and P. R. Jemian
He⁺ implantation at doses from 9×10^{13} to 2.8×10^{16} ions cm⁻², corresponding to a local concentration range of 40 to 11200 atomic parts per million (a.p.p.m.) averaged over the implantation depth of $\sim 1 \mu\text{m}$, was used to study helium-bubble formation in borosilicate glass. The fitting of the scattering data yielded helium-bubble radii and helium-bubble volume fractions that vary from 5 to 15 Å and from 10^{-3} to 10^{-1} , respectively, as the dose increased.
- 652** **A new approach to wide-angle dynamical X-ray diffraction by deformed crystals**
S. G. Podorov, N. N. Faleev, K. M. Pavlov, D. M. Paganin, S. A. Stepanov and E. Förster
A new approach is proposed for X-ray dynamical diffraction theory in distorted crystals. The theory allows one to perform dynamical diffraction simulations between Bragg peaks for non-ideal crystals, using a simple approach of two distorted waves.
- 656** **Tailoring the structure of hybrid organic inorganic nanomaterials built on tetra- and polyfunctional alko-oxo-titanium clusters in polystyrene**
S. Trabelsi, G. Fornasieri, L. Rozes, A. Janke, A. Mensch, C. Sanchez and M. Stamm
Functional titanium oxo-clusters $\text{Ti}_{16}\text{O}_{16}(\text{OEt})_{32-4}(\text{OPh}-\text{CH}=\text{CH}_2)_x$ with different numbers of styrenic groups, where $x = 4$ (tetra) and $x = 16$ (poly), have been synthesized and copolymerized with styrene. The influence of the number of functional groups borne by the oxo clusters on the structure of the resulting hybrid nanomaterials has been investigated by a combination of small-angle X-ray scattering, transmission electron microscopy and energy-filtering transmission electron microscopy.
- 661** **Inferring orientation distributions in anisotropic powders of nano-layered crystallites from a single two-dimensional WAXS image**
Y. Méheust, K. D. Knudsen and J. O. Fossum
A method to determine the orientation distribution probability function of a population of nano-stacks from the dependence of a given diffraction peak's amplitude on the azimuthal angle is proposed. It is applied to two different types of orientational order observed in systems of sodium fluorohectorite clay particles.
- 671** **ELLSTAT: shape modeling for solution small-angle scattering of proteins and protein complexes with automated statistical characterization**
W. T. Heller
A method for producing models from related sets of small-angle scattering data is presented that uses statistical methods to characterize the structural variability and interdependence between structural parameters.
- 676** **Analysis of polydisperse bubbles in the aluminium-hydrogen system using a size-dependent contrast**
M. Paskevicius and C. E. Buckley
A volume-fraction size distribution of hydrogen bubbles in aluminium was obtained from small-angle scattering data. The distribution was then adjusted using a size-dependent contrast to provide a more accurate description of the physical system.
- 683** **Compositional depth profiling of polycrystalline thin films by grazing-incidence X-ray diffraction**
I. M. Kötschau and H. W. Schock
A novel pattern-matching method for compositional depth profiling of polycrystalline thin films using grazing-incidence X-ray diffraction is proposed. As an example, the Cu and S gradients in a $\text{Cu}(\text{In,Ga})(\text{S,Se})_2$ thin film are accurately refined.

- 697** **A novel optimization-based pole-figure inversion method: comparison with WIMV and maximum entropy methods**
 J. V. Bernier, M. P. Miller and D. E. Boyce
 An optimization-based pole-figure inversion method is presented that utilizes the orientation distribution function gradient for conditional control of the solution. The novel pole-figure inversion method, coined the hybrid \mathcal{H}^1 -seminorm minimization, is empirically shown to be versatile, general and robust in the presence of simulated experimental errors.
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- 714** **SXD – the single-crystal diffractometer at the ISIS spallation neutron source**
 D. A. Keen, M. J. Gutmann and C. C. Wilson
 SXD, the single-crystal diffractometer at the ISIS spallation neutron source, CCLRC Rutherford Appleton Laboratory, is described.
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- 723** **Determination of microstructure and twinning relationship between martensitic variants in 53 at.%Ni–25 at.%Mn–22 at.%Ga ferromagnetic shape memory alloy**
 D. Y. Cong, Y. D. Zhang, Y. D. Wang, C. Esling, X. Zhao and L. Zuo
 The microstructure and twinning relationship between the martensitic variants in a newly developed Ni–Mn–Ga ferromagnetic shape memory alloy with non-modulated structure were experimentally investigated by high-resolution electron backscatter diffraction with a field emission scanning electron microscope.
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- 728** **Use of Patterson-based methods automatically to determine the structures of heavy-atom-containing proteins with up to 6000 non-hydrogen atoms in the asymmetric unit**
 M. C. Burla, R. Caliendo, B. Carrozzini, G. L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori and D. Siliqi
 The range of complexity for protein *ab initio* phasing is extended to more than 6000 non-hydrogen atoms in the asymmetric unit.
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- 735** **Location of Mn sites in ferromagnetic Ga_{1-x}Mn_xAs studied by means of X-ray diffuse scattering holography**
 M. Kopecký, J. Kub, E. Busetto, A. Lausi, M. Cukr, V. Novák, K. Olejník, J. P. Wright and J. Fábry
 A three-dimensional image of the local neighbourhood of Mn atoms in a Ga_{1-x}Mn_xAs ($x = 0.02$) layer has been obtained by using X-ray diffuse scattering holography.
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- 739** **Chlorartinite, a volcanic exhalation product also found in industrial magnesia screed**
 K. Sugimoto, R. E. Dinnebier and T. Schlecht
 The building units of the volcanic exhalation product chlorartinite consist of MgO₆ octahedra forming 15-membered puckered rings which are interconnected by CO₃ triangular moieties. The rings are stacked to form a honeycomb-like three-dimensional framework structure with large isolated channels, in which free chlorine atoms and disordered water molecules are located.

short communications

- 745** **Folding a two-dimensional powder diffraction image into a one-dimensional scan: a new procedure**
 A. Cervellino, C. Giannini, A. Guagliardi and M. Ladisa
 The robustness of a method to fold a two-dimensional powder diffraction pattern into a one-dimensional scan is demonstrated, along with its capability of efficiently tagging the pixels in a two-dimensional readout system by matching the ideal geometry of the detector to the real beam-sample-detector frame.
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- 749** **Silver behenate as a calibration standard of grazing-incidence small-angle X-ray scattering**
 B. Lee, C.-T. Lo, S. Seifert and R. E. Winans
 Grazing-incidence small-angle X-ray scattering patterns of a silver behenate composite film, which has a typical layered structure, are described.

computer programs

- 752** **WCEN: a computer program for initial processing of fiber diffraction patterns**
 W. Bian, H. Wang, I. McCullough and G. Stubbs
 A computer program for initial analysis of fiber diffraction patterns is described.

757	SHADE web server for estimation of hydrogen anisotropic displacement parameters A. Ø. Madsen	The <i>SHADE</i> web server accepts an input structural model in CIF format. By combining a rigid-body analysis with estimates of internal atomic displacements, it returns an estimate of anisotropic displacement parameters of H atoms in the structure.
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759	XtalBase – a comprehensive data management system for macromolecular crystallography W. Meining	The crystallography data management system <i>XtalBase</i> is described. <i>XtalBase</i> helps designing, preparing, documenting and evaluating crystallization experiments and is a versatile tool for storing data associated with a macromolecular structure analysis.
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laboratory notes

767	Energy spectrometer on a diffractometer using a charge-coupled device X-ray detector H. Abe, H. Saitoh, H. Nakao, K. Ito and K. Ohshima	By the combination of energy spectroscopy and diffraction, using a wavelength-dispersive X-ray spectrometer mounted on a six-circle diffractometer and a CCD detector, simultaneous real-time data acquisition of both the momentum and the energy transfer was performed.
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771	The use of an acoustic levitator to follow crystallization in small droplets by energy-dispersive X-ray diffraction J. Leiterer, W. Leitenberger, F. Emmerling, A. F. Thünemann and U. Panne	Crystallization from aqueous solution in a levitated droplet was observed by energy-dispersive X-ray diffraction using synchrotron radiation. It was found that crystallization during evaporation of the solvent can be easily followed <i>in situ</i> .
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774	books received
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775	forthcoming meetings
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776	calendar of events
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