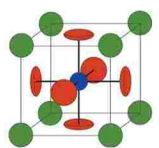


 *IUCrJ* (2016). **3**, 20–31
<http://dx.doi.org/10.1107/S2052252515018722> 

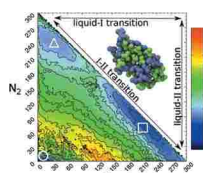


Total scattering and PDF analysis in modelling disorder in PZN

R. E. Whitfield, D. J. Goossens and T. R. Welberry

The ability of the pair distribution function analysis of total scattering from a powder to determine the local ordering in ferroelectric PZN ($\text{PbZn}_{1/3}\text{Nb}_{2/3}\text{O}_3$) is explored by comparing it with a model established using single-crystal diffuse scattering.

 *IUCrJ* (2015). **2**, 256–266
<http://dx.doi.org/10.1107/S2052252514027626> 



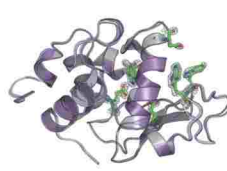
Metadynamics studies of crystal nucleation

F. Giberti, M. Salvalaglio and M. Parrinello

Crystallization processes are characterized by activated events, thus the application of enhanced sampling techniques such as metadynamics in order to study phenomena occurring at the molecular scale through molecular modelling. This paper provides an introduction to metadynamics and an overview of its applications in the context of crystal nucleation.

Neutron and synchrotron science and technology

 *IUCrJ* (2016). **3**, 43–50
<http://dx.doi.org/10.1107/S2052252515018795> 

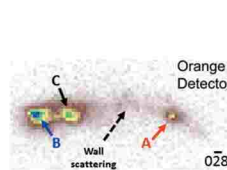


Protein crystal structure from non-oriented, single-axis sparse X-ray data

J. L. Wierman, T.-Y. Lan, M. W. Tate, H. T. Philipp, V. Elser and S. M. Gruner

Using the *EMC* algorithm, the three-dimensional intensity was successfully reconstructed from millions of non-oriented, sparse data frames collected from a hen egg-white lysozyme crystal rotating about a single axis. The protein structure was solved from the reconstructed intensity. This result is encouraging for the development of synchrotron-based serial microcrystallography.

 *IUCrJ* (2015). **2**, 635–642
<http://dx.doi.org/10.1107/S2052252515015031> 

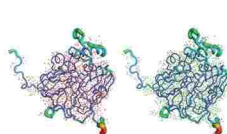


Full elastic strain and stress tensor measurements from individual dislocation cells in copper through-Si vias

L. E. Levine, C. Okoro and R. Xu

A ground breaking new capability for measuring complete strain and stress tensors nondestructively from deeply buried, sub-micrometre sample volumes within microstructurally complex and multicomponent specimens is presented. The method is demonstrated on technologically important copper through-Si vias that are used in advanced three-dimensional microelectronics.

 *IUCrJ* (2015). **2**, 464–474
<http://dx.doi.org/10.1107/S2052252515011239> 

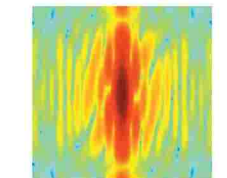


Sub-atomic resolution X-ray crystallography and neutron crystallography: promise, challenges and potential

M. P. Blakeley, S. S. Hasnain and S. V. Antonyuk

Neutron crystallography and sub-atomic X-ray crystallography complement each other in defining hydrogen positions in macromolecules. Significant advances have been made but much effort is still required if neutron crystallography is to become a mainstream activity.

 *IUCrJ* (2015). **2**, 106–125
<http://dx.doi.org/10.1107/S2052252514024178> 

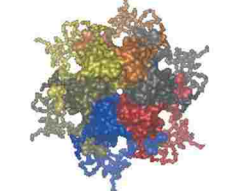


Advanced GI techniques for modern soft-matter materials analysis

A. Hexemer and P. Müller-Buschbaum

Advanced grazing-incidence (GI) techniques have developed significantly during recent years. With the on-going progress in instrumentation, novel methods have emerged which allow for an in-depth morphology characterization of modern soft-matter materials. Examples are *in situ* and *in operando* GISAXS, micro- and nanofocused GISAXS, time-of-flight GI SANS and surface-sensitive resonant soft X-ray scattering techniques.

 *IUCrJ* (2015). **2**, 207–217
<http://dx.doi.org/10.1107/S205225251500202X> 



Advanced ensemble modelling of flexible macromolecules using X-ray solution scattering

G. Tria, H. D. T. Mertens, M. Kachala and D. I. Svergun

New developments in the modelling of flexible biological macromolecules from SAXS data offer extended possibilities of using high-resolution models and provide metrics for quantitative characterization of the reconstructed ensembles.

 *IUCrJ* (2015). **2**, 230–245
<http://dx.doi.org/10.1107/S2052252514024269> 





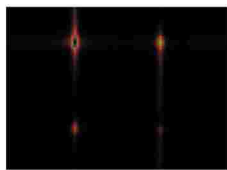
The potential of future light sources to explore the structure and function of matter

E. Weckert

The new generation of SR light sources will drive analytical methods for the determination of the structure and function of molecules and crystals towards new limits in sample size and temporal resolution.

Physics and free electron laser science and technology

 *IUCrJ* (2016). **3**, 127–138
<http://dx.doi.org/10.1107/S2052252516001238> 

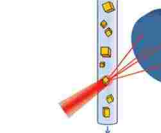


Whole-pattern fitting technique in serial femtosecond nanocrystallography

R. A. Dilanian, S. R. Williams, A. V. Martin, V. A. Streltsov and H. M. Quiney

The whole-pattern fitting technique, originally designed for one-dimensional powder diffraction crystallography, is reconsidered and applied to the analysis of higher-dimensional serial femtosecond X-ray crystallography data. For nanocrystals with a small number of unit cells, the whole-pattern fitting approach is shown to be more accurate than integration-based Monte Carlo methods.

 *IUCrJ* (2015). **2**, 246–255
<http://dx.doi.org/10.1107/S205225251402702X> 

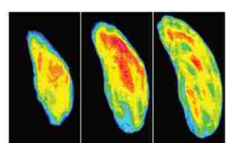


Serial femtosecond crystallography: the first five years

I. Schlichting

The advent of hard X-ray free-electron lasers has opened a new chapter in macromolecular crystallography. Recent results, developments and prospects of serial femtosecond crystallography are described.

 *IUCrJ* (2015). **2**, 575–583
<http://dx.doi.org/10.1107/S205225251501235X>  

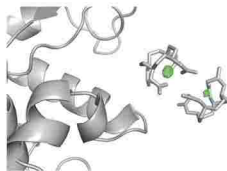


3D coherent X-ray diffractive imaging of whole frozen-hydrated cells

J. A. Rodriguez *et al.*

The first experimental demonstration of cryogenic coherent diffractive imaging for quantitative 3D imaging of whole frozen-hydrated cells is reported. As a proof of principle, the 3D mass density of the sub-cellular organization of a *Neospora caninum* cell is determined based on its natural contrast.

 *IUCrJ* (2015). **2**, 627–634
<http://dx.doi.org/10.1107/S2052252515014049> 

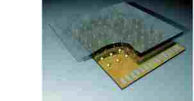


Towards phasing using high X-ray intensity

L. Galli *et al.*

Analysis of serial femtosecond crystallography data collected at the Linac Coherent Light Source using two distinct photon fluxes shows different degrees of ionization of Gd atoms bound to a lysozyme protein, due to electronic damage processes. The charge contrast on the heavy atoms is quantified using difference Fourier maps, and the way in which this could be applied to phasing is discussed.

 *IUCrJ* (2015). **2**, 371–383
<http://dx.doi.org/10.1107/S205225251500010X> 

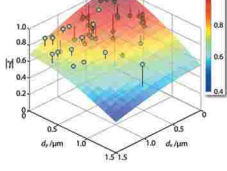


X-ray imaging detectors for synchrotron and XFEL sources

T. Hatsui and H. Graafsma

Hybrid and monolithic detectors for X-ray imaging are reviewed.


 *IUCrJ* (2015). **2**, 620–626
<http://dx.doi.org/10.1107/S2052252515015523> 

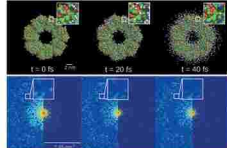


Characterizing transverse coherence of an ultra-intense focused X-ray free-electron laser by an extended Young's experiment

I. Inoue, K. Tono, Y. Joti, T. Kameshima, K. Ogawa, Y. Shinohara, Y. Amemiya and M. Yabashi

A new interference technique to measure the transverse coherence of XFELs is proposed and applied to the characterization of the coherence properties of ultra-intense focused X-ray pulses from SACLA.

 *IUCrJ* (2015). **2**, 661–674
<http://dx.doi.org/10.1107/S2052252515016887> 



Single-molecule imaging with longer X-ray laser pulses

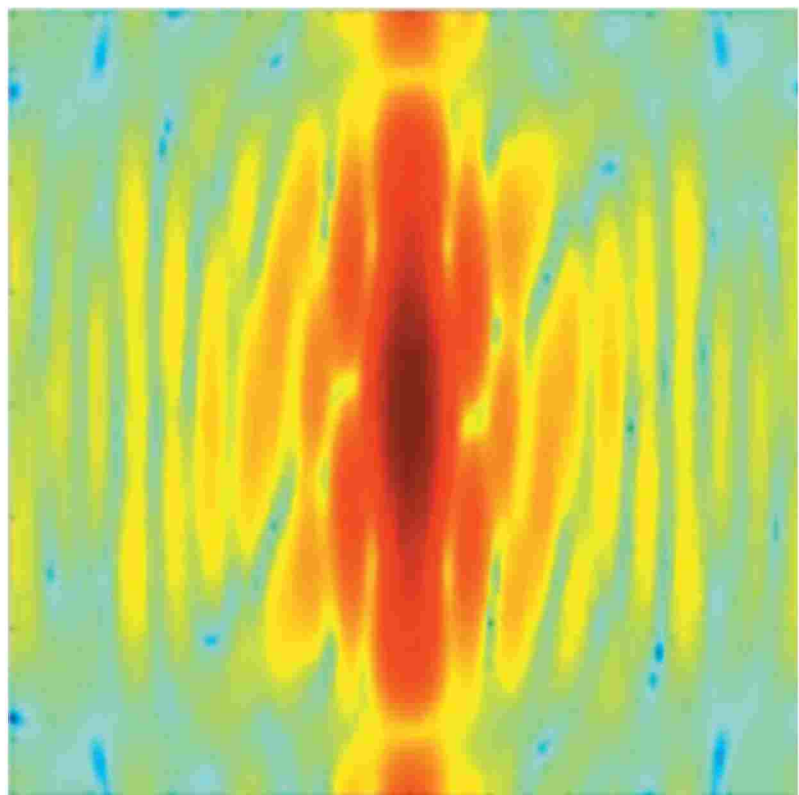
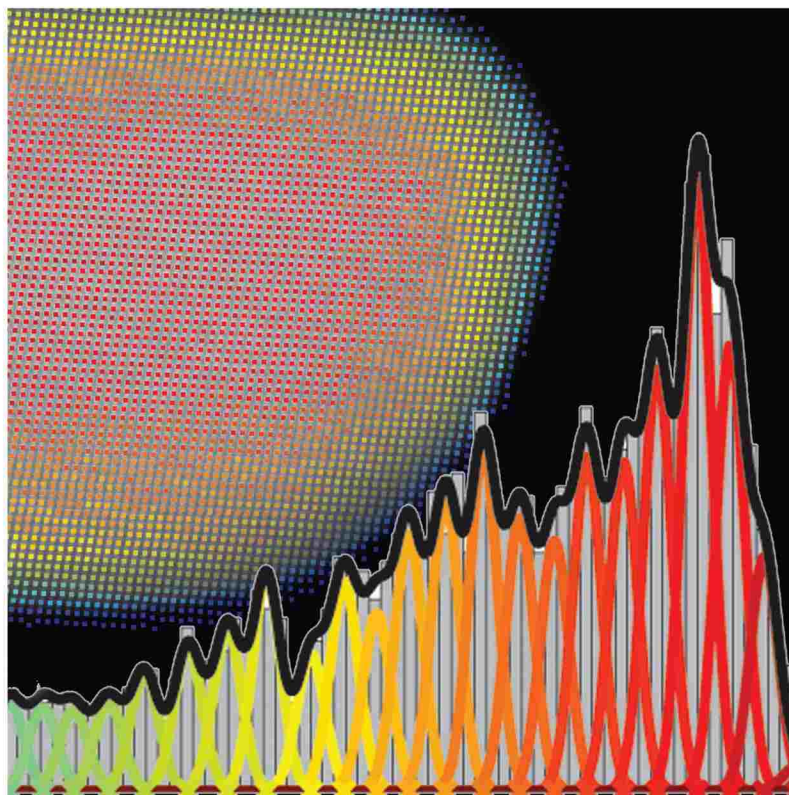
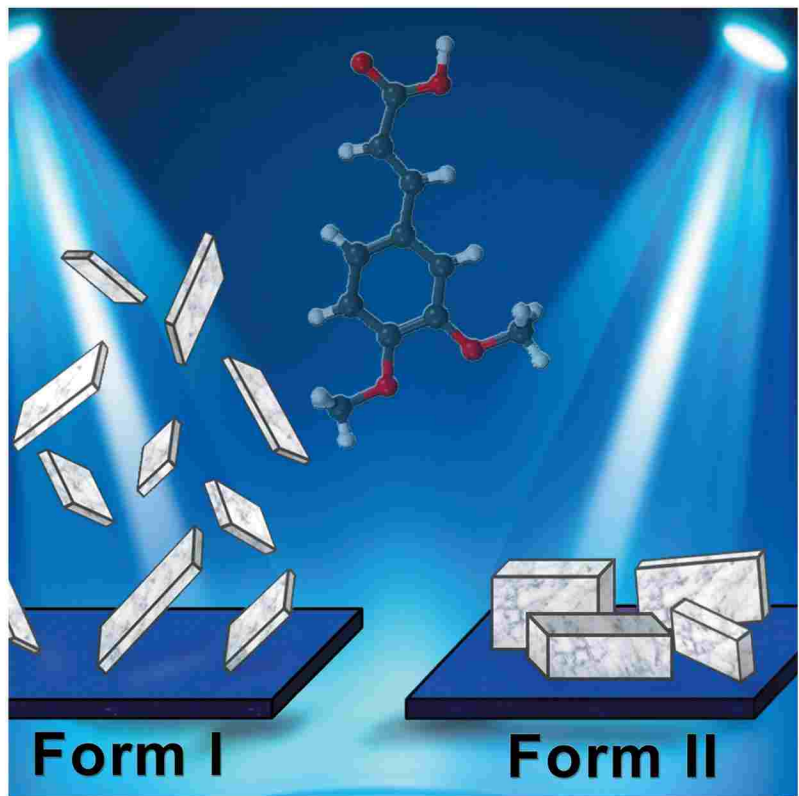
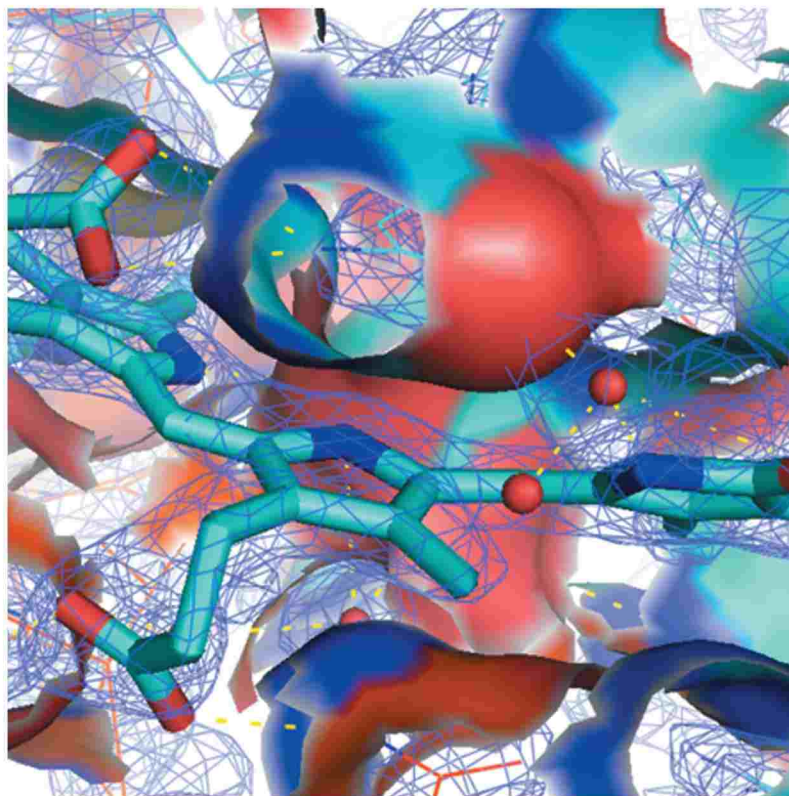
A. V. Martin, J. K. Corso, C. Caleman, N. Timneanu and H. M. Quiney

A theoretical investigation is presented of how radiation damage gates X-ray laser diffraction from single isolated protein molecules. The impact of this effect on the feasibility of X-ray laser single-molecule imaging with pulse durations of the order of 10 fs is discussed.

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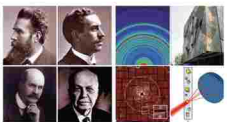


journals.iucr.org

 *IUCrJ* (2015). 2, 602–604
<http://dx.doi.org/10.1107/S2052252515017509> 

Crystallography in the 21st century

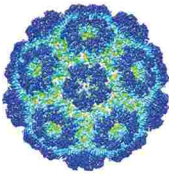
S. S. Hasnain



The field of crystallography, which has had a major impact on the sciences in the last 100 years, is continuing to expand scientific horizons as technical and conceptual boundaries are overcome. Structure–function–dynamics will become an integrated theme for many studies as will obtaining structures without the ‘benevolent tyranny’ of crystals.

Biology and medicine

 *IUCrJ* (2016). 3, 3–7
<http://dx.doi.org/10.1107/S2052252515023738> 

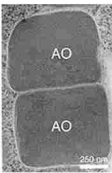


CryoEM at IUCrJ: a new era

S. Subramaniam, W. Kühlbrandt and R. Henderson

In this overview, the authors briefly outline recent advances in electron cryomicroscopy (cryoEM) and explain why the journal **IUCrJ** can provide a natural home for publications covering many present and future developments in the cryoEM field.

 *IUCrJ* (2016). 3, 88–95
<http://dx.doi.org/10.1107/S2052252515022927> 

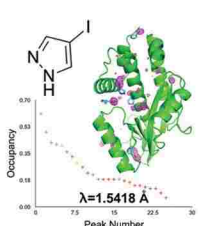


In cellulo serial crystallography of alcohol oxidase crystals inside yeast cells

A. J. Jakobi *et al.*

The application of serial femtosecond crystallography to naturally occurring peroxisomal protein crystals within yeast cells is described. The concept of utilizing peroxisomes for the production of protein nanocrystals is outlined.

 *IUCrJ* (2016). 3, 51–60
<http://dx.doi.org/10.1107/S2052252515021259> 

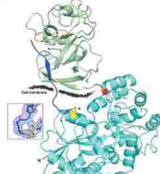


Rapid experimental SAD phasing and hot-spot identification with halogenated fragments

J. D. Bauman, J. J. E. K. Harrison and E. Arnold

4-Bromopyrazole and 4-iodopyrazole bind to many small molecule binding hot spots in target proteins. This promiscuous binding enables the use of these compounds for experimental phase determination by single-wavelength anomalous dispersion (SAD). The low cost and safety of the compounds make them excellent choices for addition to the protein crystallographer’s toolkit.

 *IUCrJ* (2016). 3, 10–19
<http://dx.doi.org/10.1107/S2052252515019971> 

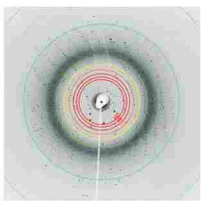


Peptide binding to a bacterial signal peptidase visualized by peptide tethering and carrier-driven crystallization

Y. T. Ting, P. W. R. Harris, G. Batot, M. A. Brimble, E. N. Baker and P. G. Young

Utilizing a peptide-anchoring strategy, transient signal-peptide complexes of a Gram-positive bacterial signal peptidase were trapped, revealing the atomic details of their interaction.

 *IUCrJ* (2015). 2, 168–176
<http://dx.doi.org/10.1107/S2052252514026487> 

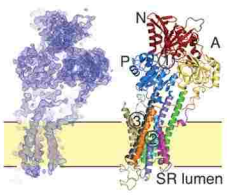


Lipidic cubic phase serial millisecond crystallography using synchrotron radiation

P. Nogly *et al.*

This article describes the structure determination of a membrane protein by serial injection of microcrystals in lipidic cubic phases into a synchrotron microfocus beam. The method is discussed with respect to serial femtosecond crystallography at free-electron lasers.

 *IUCrJ* (2015). 2, 409–420
<http://dx.doi.org/10.1107/S2052252515008969> 

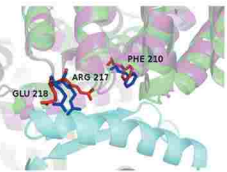


Structural studies of P-type ATPase-ligand complexes using an X-ray free-electron laser

M. Bublitz *et al.*

The structure determination of P-type ATPase-ligand complexes from microcrystals by serial femtosecond crystallography using a free-electron laser is described. The feasibility of the method for ligand screening is demonstrated, and SFX data quality metrics as well as suitable refinement procedures are discussed.

 *IUCrJ* (2015). 2, 643–652
<http://dx.doi.org/10.1107/S2052252515015250> 

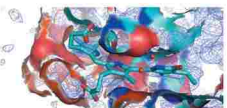


Changes in protein structure at the interface accompanying complex formation

D. Chakravarty, J. Janin, C. H. Robert and P. Chakrabarti

To understand molecular recognition, one needs to characterize the conformational changes that take place when a free (unbound) molecule forms a complex with another protein. An analysis of 281 protein components is presented, delineating such changes in terms of accessible surface area, secondary structure, crystallographic *B* factors and disorder-to-order transitions.

 *IUCrJ* (2015). 2, 545–551
<http://dx.doi.org/10.1107/S2052252515013160> 



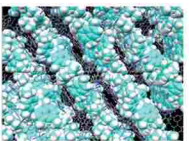
Serial femtosecond crystallography of soluble proteins in lipidic cubic phase

R. Fromme *et al.*

A new approach of using lipidic cubic phase as a carrier matrix for delivering soluble protein microcrystals for serial crystallography helps to dramatically reduce protein consumption. The structures of two soluble test proteins have been determined by this method using less than 0.1 mg of each protein.

Chemistry and crystal engineering

 *IUCrJ* (2016). 3, 139–151
<http://dx.doi.org/10.1107/S2052252515024379> 

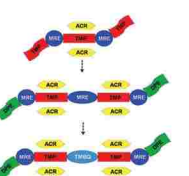


The crystalline sponge method updated

M. Hoshino, A. Khutia, H. Xing, Y. Inokuma and M. Fujita

The protocols of the crystalline sponge method, particularly those in the soaking, data collection and refinement processes, are considerably improved to give reliable structural information.

 *IUCrJ* (2016). 3, 96–101
<http://dx.doi.org/10.1107/S2052252515023945> 

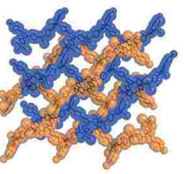


Four- and five-component molecular solids: crystal engineering strategies based on structural inequivalence

N. A. Mir, R. Dubey and G. R. Desiraju

A logic driven synthetic approach is used in this first report of the isolation of stoichiometric four-component molecular solids. A possible extension to a five-component solid is also described.

 *IUCrJ* (2015). 2, 675–690
<http://dx.doi.org/10.1107/S2052252515014608> 

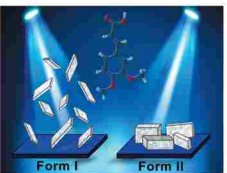


Supramolecular interactions in the solid state

G. Resnati, E. Boldyreva, P. Bombicz and M. Kawano

Supramolecular interactions in the solid state are discussed in the context of crystal engineering. Specific topics include halogen bonding, ambient and non-ambient conditions, isostructurality and polymorphism, and kinetic assembly of coordination polymers.

 *IUCrJ* (2015). 2, 653–660
<http://dx.doi.org/10.1107/S2052252515017297>  

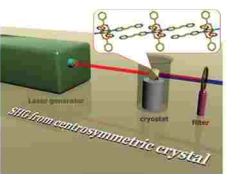


Crystal chemistry and photomechanical behavior of 3,4-dimethoxy-cinnamic acid: correlation between maximum yield in the solid-state topochemical reaction and cooperative molecular motion

M. K. Mishra, A. Mukherjee, U. Ramamurty and G. R. Desiraju

A new monoclinic polymorph, form II, of 3,4-dimethoxycinnamic acid has been isolated and shows a different photochemical and photomechanical property from the previously reported triclinic form I. The solid-state 2 + 2 photodimerization of these polymorphs is rationalized on the basis of minimum and maximum molecular movement during the reaction.

 *IUCrJ* (2015). 2, 317–321
<http://dx.doi.org/10.1107/S2052252515002183> 

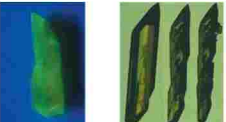


Second harmonic generation from the ‘centrosymmetric’ crystals

V. Nalla, R. Medishetty, Y. Wang, Z. Bai, H. Sun, J. Wei and J. J. Vittal

Based on the observation of second harmonic generation (SHG), the solid state structure of a Zn(II) complex has been reinterpreted in terms of the non-centrosymmetric space group *Cc*, with residual polarity arising from unequal antiparallel packing. Temperature-dependent measurements showed that the highest SHG has been observed at 50 K and the lowest at 170 K.

 *IUCrJ* (2015). 2, 611–619
<http://dx.doi.org/10.1107/S2052252515015134> 

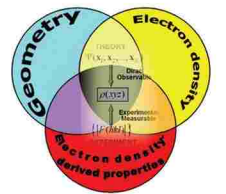


Structure–mechanical property correlations in mechanochromic luminescent crystals of boron difluoride dibenzoylmethane derivatives

G. R. Krishna, R. Devarapalli, R. Prusty, T. Liu, C. L. Fraser, U. Ramamurty and C. M. Reddy

Structure–mechanical property studies confirm that the extent of mechanochromic luminescence in crystalline organic fluorophores positively correlates with the extent of plasticity.

 *IUCrJ* (2015). 2, 161–163
<http://dx.doi.org/10.1107/S2052252515002067> 



On atom–atom ‘short contact’ bonding interactions in crystals

C. Lecomte, E. Espinosa and C. F. Matta

The electron density distribution $\rho(\mathbf{r})$ contains the information needed to quantitatively analyze bonding interactions between atoms, exhibiting short, medium or long inter-nuclear distances. Atom–atom bonding interactions, the orientation of molecules in the space and crystal structure are all inter-determined.

 *IUCrJ* (2015). 2, 157–158
<http://dx.doi.org/10.1107/S2052252515002006> 



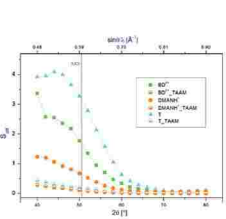
Intermolecular atom–atom bonds in crystals?

J. D. Dunitz

Some questions are raised concerning the interpretation of distances between atoms of neighbouring molecules in crystals.

Materials and computation

 *IUCrJ* (2016). 3, 61–70
<http://dx.doi.org/10.1107/S2052252515020941> 

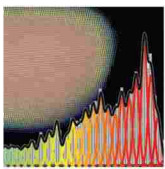


Yes, one can obtain better quality structures from routine X-ray data collection

W. F. Sanjuan-Szklarz, A. A. Hoser, M. Gutmann, A. Ø. Madsen and K. Wozniak

Single-crystal X-ray diffraction data should be collected to the highest resolution as this allows for refinement of more reliable structural, thermal and dependent parameters. The results of refinements using a Transferable Aspherical Atomic Model of electron density (TAAM) appear to be in far better agreement with neutron results than the corresponding Independent Atom Model (IAM) results for all parameters, all resolutions and all compounds, and we advocate the use of this approach instead of IAM.

 *IUCrJ* (2016). 3, 71–83
<http://dx.doi.org/10.1107/S2052252515019727> 

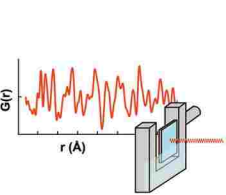


Advanced electron crystallography through model-based imaging

S. Van Aert, A. De Backer, G. T. Martinez, A. J. den Dekker, D. Van Dyck, S. Bals and G. Van Tendeloo

An overview of statistical parameter estimation methods is presented and applied to analyse transmission electron microscopy images in a quantitative manner.

 *IUCrJ* (2015). 2, 481–489
<http://dx.doi.org/10.1107/S2052252515012221> 

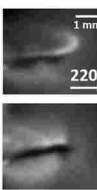
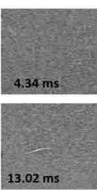


Demonstration of thin film pair distribution function analysis (tfPDF) for the study of local structure in amorphous and crystalline thin films

K. M. Ø. Jensen, A. B. Blichfeld, S. R. Bauers, S. R. Wood, E. Dooryh e, D. C. Johnson, B. B. Iversen and S. J. L. Billinge

It is shown how normal-incidence X-ray total scattering can be used to obtain high-quality pair distribution functions from amorphous and crystalline thin films on much thicker substrates, allowing a range of studies of the local structure in film materials.

 *IUCrJ* (2016). 3, 108–114
<http://dx.doi.org/10.1107/S205225251502271X>  



Real-time direct and diffraction X-ray imaging of irregular silicon wafer breakage

A. Rack, M. Scheel and A. N. Danilewsky

Crack propagation in an Si wafer under thermal stress is depicted by combining diffraction and transmission X-ray imaging. The use of synchrotron radiation allows for the high imaging frame rates required to follow the crack dynamics in real time.