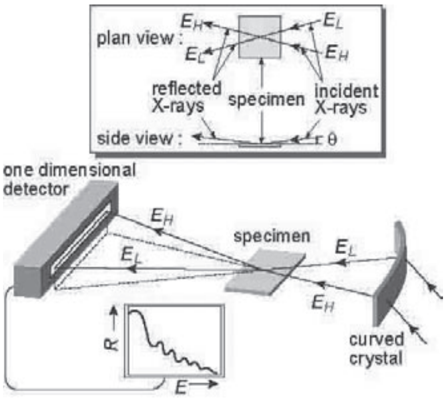
specimen placed at the focus in a geometry that the glancing angle in the vertical direction is the same for all the X-ray components, and they are reflected in the vertical direction by the surface and diverge in the horizontal plane. The perpendicular momentum transfer, given by $q=4\pi\sin\theta/\lambda$, continuously changes as a function of the ray direction even with the fixed glancing angle θ since the wavelength (energy) λ changes. The X-ray intensity distribution across the beam direction measured downstream of the specimen using a one-dimensional detector represents the X-ray reflectivity curve. Some results of static and dynamic measurements will be reported, and the characteristics and potentials of the method will be discussed.



Keywords: specular X-ray reflectivity, time-resolved, simultaneous multiwavelenth dispersive

MS.02.3

Acta Cryst. (2008). A**64**, C17

Structural characterization using the multiple scattering effects in GISAXS

Byeongdu Lee[1], Chieh-Tsung Lo[2], P. Thiyagarajana[3], Dong R. Lee[4], Zhongwei Niu[5], Qian Wang[5]

[1]Argonne National Laboratory, Advanced Photon Source, 9700 S. Cass Ave., Argonne, IL, 63945, USA, [2]Argonne National Laboratory, 9700 S. Cass Ave., Argonne, IL, 60439, USA, [3]Intense Pulse Neutron Source, Argonne National Laboratory, 9700 S. Cass Ave., Argonne, IL, 60439, USA, [4]Pohang Accelerator Laboratory, POSTECH, Pohang 790-784, Republic of Korea, [5]Department of Chemistry and Biochemistry and the Nanocenter, University of South Carolina, 631 Sumter Street, Columbia, SC 29208, USA, E-mail：blee@aps.anl.gov

The multiple scattering effects present in grazing-incidence small-angle X-ray scattering (GISAXS) data and interference between them are addressed theoretically as well as experimentally with measurement of a series of patterns at different incident angles, referred to as `incident-angle-resolved GISAXS' (IAR-GISAXS). X-ray reflectivity (XR), GISAXS and IAR-GISAXS of virus particles on Si-substrate supported-polystyrene films have been measured and compared. It was found that under certain conditions it is possible to extract the correct structural features of the materials from the GISAXS/IAR-GISAXS data using the kinematic SAXS formalisms. Furthermore, the Kiessig fringes in GISAXS enable the measurement of the average distance between the particle and the substrate, similar to the measurement of film thickness using the fringes in the XR data.

Acknowledgements
This work benefited by the use of the APS and other facilities at the Argonne National Laboratory supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

Keywords: GISAXS, reflectivity, virus assembly

MS.02.4

Acta Cryst. (2008). A**64**, C17

Neutron reflectively study of chain conformation in polyelectrolyte brushes at the liquid interface

Atsushi Takahara[1], Motoyasu Kobayashi[1], Yuki Terayama[1], Naoya Torikai[2], Masahiro Hino[3], Kazuhiko Ishihara[4]

[1]Kyushu University, Institute for Materials Chemistry and Engineering, 744 Motooka, Nishi-ku, Fukuoka, Fukuoka, 8190395, Japan, [2]KENS, Tsukuba, Ibaraki 305-0801 Japan, [3]Research Reactor Institute, Kyoto University, Kumatori, Osaka 590-0494, Japan, [4]The University of Tokyo, Bunkyo-ku, Tokyo 110-8536, JAPAN, E-mail：takahara@cstf.kyushu-u.ac.jp

The zwitterionic and cationic polyelectrolyte brushes on the quartz plates were prepared by surface-initiated atom transfer radical polymerization of 2-methacryloyloxyethyl phosphorylcholine (MPC) and N,N-dimethylaminoethyl methacrylate, which was successively converted to methcryloyloxyethyl trimethylammo-nium iodide (METAI) by quarternization with methyl iodide. Neutron reflectivity (NR) was measured by irradiation of neutron beam from the quartz plate to the interface between liquid phase and immobilized polyelectrolyte brush. NR profiles of polyelectrolyte brush/D_2O interface indicated that the polymer chains exhibited stretched conformation and formed concentration gradient of D_2O under swelling states. The effects of ionic strength on the conformation and surface properties of densely grafted polyelectrolyte brush were analyzed by NR. The difference between reflectivity of polyelectrolyte brushes in D_2O and in salt solution was negligible. The authors supposed that quaternary ammonium iodide at the side chain of poly(METAI) chains are bulky and the mobility of iodide ion is limited because of weak hydration. On the other hand, PMPC brush slightly shrunk at the EtOH/Water in cononsolvency region.

Keywords: polymer brush, water Interface, polyelectrolyte

MS.02.5

Acta Cryst. (2008). A**64**, C17-18

Following growth and catalytic reaction of oxide supported metal nanoparticles with GISAXS

Rémi Lazzari[1], Jacques Jupille[1], Frédéric Leroy[2], Gilles Renaud[3], Marie-Claire Saint-Lager[4], Pierre Dolle[4], Odile Robach[3]

[1]Université Pierre et Marie Curie - CNRS, Institut des NanoSciences de Paris, 140 Rue de Lourmel, Paris, Paris, 75015, France, [2]Centre de Recherche en Matière Condensée et NanoSciences, CNRS − Campus de Luminy, Marseille, France, [3]CEA-Grenoble, Département de Recherche Fondamentale sur la Matière Condensée et ESRF BM32, [4]Institut Néel, CNRS, Grenoble, France, E-mail：lazzari@insp.jussieu.fr

X-ray scattering techniques using the grazing incidence geometry offer the opportunity to probe in situ the crystallographic structure and the morphology of metal nanoparticles grown on oxide planar surfaces. Combining wide angle (GIXD) and small angle scattering (GISAXS) can give some insights into connected thermodynamic and kinetic parameters of metal/support interface, namely the role of stress due the lattice mismatch on the epitaxial orientation, the adhesion/wetting properties, the particle equilibrium shape and the peculiarities of the growth modes and the chemical reactivity. One key advantage of X-ray is the capability to perform measurement not only during particle growth under vacuum conditions but also at high pressure during the course of an actual catalytic reaction. This will be illustrated with our recent results on Au/TiO_2(110), a model planar system of gold-based catalyst. Among others, the following points will be discussed:

(i) The theoretical developments made to analyse quantitatively the GISAXS patterns beyond the classical approximations, in particular to account for the profile of refraction index and the particle-particle correlations.
(ii) The self similarity during the dynamic coalescence of Au/TiO2(110) on the size distribution but also on the spatial ordering of the particles and its link with the randomness of the nucleation centers.
(iii) The sintering of nanoparticles during the course of the CO oxidation reaction and the link between particle size and chemical reactivity measured by mass spectrometry.

Keywords: GISAXS, growth, catalysis

MS.03.1

Acta Cryst. (2008). A**64**, C18

Reliable determination of absolute structure using small Bijvoet differences

Rob WW Hooft[1], Leo H Straver[1], Anthony L Spek[2]
[1]Bruker AXS BV, R&D, PO Box 811, Delft, ZH, 2600 AV, The Netherlands, [2]Bijvoet Center for Biomolecular Research, Utrecht University, Padialaan 8, NL 3584 CH Utrecht, The Netherlands, E-mail：rob.hooft@bruker-axs.nl

Hooft et al. 2008 [1] contains a list of 11 data sets with MoKa radiation and 15 data sets with CuKa radiation that have been used to determine the absolute structure of the measured crystals using maximum likelihood and Bayesian statistics. The results compare favorable with the determination of the Flack x parameter [2] in that comparable standard uncertainties have been reduced by a factor of ~2. Since the submission of that paper additional experience was gained with the reliability of the absolute structure determination and the interpretation of associated statistics like the Normal Probability Plot [3] of the Bijvoet differences. We will address this experience and discuss small changes to the method that will further increase the robustness of the results.

[1] J. Appl. Cryst. (2008). 41, 96-103.
[2] Acta Cryst. (1983). A39, 876-881.
[3] Acta Cryst. (1971). A27, 157-165

Keywords: absolute configuration, pharmaceutical compounds, maximum likelihood

MS.03.2

Acta Cryst. (2008). A**64**, C18

Small molecule toolbox

Luc J Bourhis, Oleg Dolomanov, Horst Puschmann
University of Durham, Department of Chemistry, University Science Laboratories, South Road,, Durham, County Durham, DH1 3LE, UK, E-mail：luc_j_bourhis@mac.com

The Computational Crystallography Toolbox (cctbx)[1] provides a solid and comprehensive set of building blocks from which to construct crystallographic programs. Its core crystallographic library, which gave its name to the whole toolbox, is the foundation of the MacroMolecular Toolbox (mmtbx) which is the open source protein-specific component of the PHENIX system [2]. A sister library of the mmtbx, the Small Molecule Toolbox (smtbx), built on the top of the cctbx and addressing the specific need of small molecule single crystal solution and refinement is now under development. Ultimately we aim at writing the code necessary to give the practising crystallographer the tools (s)he is used to. Our focus is mainly on refinement and we will give a synthetic view of our implementation of F^2 refinement, weighting schemes, special position constraints [3], constrained Hydrogen atoms, constrained occupancies and ADP's for disordered atoms. We have also an interest in ab-initio structure determination and so far have coded the charge flipping algorithm. We will also discuss the problems raised by and the advances made in handling anisotropic scattering form factors, which are the key components for charge density refinement.

We gratefully acknowledge the financial support of EPSRC under grant number EP/C536274/1.

[1] CCTBX: http://cctbx.sourceforge.net/
[2] PHENIX: building new software for automated crystallographic structure determination, P.D. Adams, R.W. Grosse-Kunstleve, L.-W. Hung, T.R. Ioerger, A.J. McCoy, N.W. Moriarty, R.J. Read, J.C. Sacchettini, N.K. Sauter and T.C. Terwilliger. Acta Cryst. D58, 1948-1954 (2002) (http://www.phenix-online.org)
[3] cctbx news, in Comp. Comm. Newsletter no. 8, November 2007, Luc J. Bourhis, Ralf W. Grosse-Kunstleve and Paul D. Adams

Keywords: cctbx, small molecule, single crystal

MS.03.3

Acta Cryst. (2008). A**64**, C18

The charge-flipping algorithm and related dual-space structure solution methods

Lukas Palatinus, Gervais Chapuis
EPFL, Laboratory for Crystallography, BSP - Dorigny, Lausanne, Vaud, 1015, Switzerland, E-mail：palat@fzu.cz

The dual-space iterative structure solution methods face an increasing interest among crystallographers, especially after the publication of the charge-flipping algorithm in 2004 [1], and demonstration of its usefulness for realistic crystallographic problems [2,3,4]. However, the history of the applications of the dual-space iterative algorithms for structure solution dates back at least to 1992, when the "low density elimination" method was published [5]. In 2003 a rather general algorithm named Difference Map was published [6]. It can be shown that all these algorithms can be described in a unified way using the language of constraint sets and projections. A constraint set is a set of all images (for example electron density) that fulfill a predefined constraint, for example positivity. A projection is then a mapping that maps any image onto an image in the constraint set. The different algorithms can be described as an iterative application of different combinations of two projections on a starting random image. It turns out, however, that not only the exact choice of the combination of projections is essential for the performance of the algorithm, but also the exact definition of the projections, constraint sets, and image play a crucial role. These settings distinguish the different algorithms that are otherwise conceptually related.

[1] Oszlanyi, G. and Suto, A. (2004). Acta Cryst. A60, 134-141
[2] Wu, J. S., Spence, J. C. H., O'Keeffe, M. & Groy, T. L. (2004). Acta Cryst. A60, 326-330
[3] Palatinus, L. (2004). Acta Cryst. A60, 604-610
[4] Oszlanyi, G., Suto, A., Czugler, M. and Parkanyi, L. (2006). J. Am. Chem. Soc. 128, 8392-8393
[5] Shiono, M. and Woolfson, M. M. (1992). Acta Cryst. A48, 451-456
[6] Elser, V. (2003). Acta Cryst. A59, 201-209

Keywords: *ab-initio* structure determination, small-molecule structure determination, iterative algorithms