the reflectance within the small angles of the incidence area (in and near the complete external reflection area). NaCl monocrystals have been used as investigated objects. Crystal faces quality after splitting, short and long time processes of solution and growth have been estimated.

[1] Bushuev V.A., Petrakov A.P., *Crystallography*, 2001, **46**, N 2, 209-214.
Keywords: X-ray crystal analysis methods, X-ray reflectometry, X-ray crystallography

P.12.06.1
Acta Cryst. (2005). A**61**, C411
Hydrogen-Bonded Structure of Alcohols Adsorbed on Silica Surface in Cyclohexane
Kazue Kurihara[a], Masashi Mizukami[a], Satoshi Endo[b], [a]*IMRAM, Tohoku University.* [b]*CREST-JST, Sendai 980-8577, Japan.* E-mail: kurihara@tagen.tohoku.ac.jp

Liquid molecules at the solid-liquid interface often exhibit quite different properties from those in the bulk, which is attributed to the surface-induced structuring of liquids. We recently found a hydrogen-bonded ordered structure, which we call a "molecular macrocluster", of alcohols when we investigated the adsorption of them on silica (glass and oxidized silicon) surfaces from cyclohexane.

Alcohols studied were monohydric alcohol such as methanol and ethanol [1], and dihydric alcohol (ethylene glycol)[2]. A combination of colloidal probe atomic force microscopy, FTIR-ATR spectroscopy, and adsorption excess isotherm measurement was employed. The force measurement revealed the long ranged attraction (e.g. ca. 35 nm for ethanol) between silica (glass) surfaces, which was ascribed to the attraction due to the contact of the opposed adsorption layers bearing the high interfacial energy. FTIR-ATR spectroscopy demonstrated that alcohol molecules adsorbed on the silica (silicon oxide) surfaces formed hydrogen-bonded clusters (polymers), which extended 15~20 nm (for monohydric alcohol) from the surface silanol groups. Practically no cluster was formed on the hydrogen-terminated silicon surfaces. Interesting differences were observed in the mode of adsorption depending on the chemical structures. Dynamic properties of adsorbed alcohols were studied by NMR spectroscopy.

[1] Mizukami M., Moteki M., Kurihara K., *J. Am. Chem. Soc*., 2002, **124**, 12889. [2] Kurihara K., Nakagawa Y., Mizukami M., *Chem. Lett*., 2003, 84.
Keywords: solid-liquid interaction, interfacial liquid structure, hydrogen bonding

P.12.07.1
Acta Cryst. (2005). A**61**, C411
ATSAS 2.1 - A Program Suite for Small-angle Scattering Data Analysis
Petr V. Konarev[a,b], Maxim V. Petoukhov[a,b], Vladimir V. Volkov[b], Dmitri I. Svergun[a,b], [a]*EMBL, Hamburg Outstation, Germany.* [b]*Institute of Crystallography RAS, Moscow, Russia.* E-mail: konarev@embl-hamburg.de

A new release 2.1 of the program package ATSAS for small-angle scattering data analysis is presented. The package allows one to perform a complete analysis of the scattering data covering major steps from data reduction to automated 3D modelling. ATSAS is primarily oriented towards macromolecular solutions but can also be used for other types of systems. Its main components are:

1) Primary data processing and reduction package PRIMUS [1], which also computes overall structural parameters and characteristic functions and permits to invoke major data analysis programs from a single graphical user interface.

2) An *ab initio* three-dimensional modelling suite including e.g. programs DAMMIN and GASBOR bead and dummy residues modelling [2,3].

3) A rigid body modelling suite (programs MASSHA [4], GLOBSYMM, SASREF etc) to characterize macromolecular complexes in terms of the structure of sugbunits.

4) A suite for quantitative analysis of interacting systems and mixtures (programs PEAK, SVDPLOT, MIXTURE etc [1]).

[1] Konarev P.V., et.al., *J. Appl. Cryst*., 2003, **36**, 1277. [2] Svergun D.I., *Biophys. J*., 1999, **76**, 2879. [3] Svergun D.I., et.al., *Biophys. J.*, 2001, **80**, 2946. [4] Konarev P.V., et.al., *J.Appl. Cryst.*, 2001, **34**, 527.
Keywords: small-angle scattering, data processing software, macromolecules

P.12.07.2
Acta Cryst. (2005). A**61**, C411
Probing Intermediate Filament Structure and Assembly with Small-angle X-ray Scattering
Anna V. Sokolova[a,b], L. Kreplak[c], H. Herrmann[d], U. Aebi[c], D. I. Svergun[a,e], S. V. Strelkov[b,c], [a]*Institute of crystallography, Moscow, Russia.* [b]*Institute of bioorganic chemistry, Moscow, Russia.* [c]*Biozentrum, University of Basel, Switzerland.* [d]*German Cancer Research Centre, Heidelberg, Germany.* [e]*EMBL c/o DESY, Hamburg, Germany.* E-mail: sokolova@crys.ras.ru

Intermediate filaments (IFs) together with microtubules and actin filaments, form the cytoskeleton of most living cells. IFs are long macromolecular aggregates, with about 10 nm cross-section. While crystallographic data on the dimer representing the elementary IF 'building block' have recently become available, little structural detail is known on both the mature IF architecture and their assembly pathway.

We have applied small angle X-ray scattering (SAXS) to investigate the *in vitro* assembly of human IF protein vimentin in varying pH and ionic strength conditions. SAXS is a method allowing one to analyze protein structure in solutions at different external conditions and also to quantitatively characterize of mixtures of different oligomeric states. We demonstrate that formation of tetramers, octamers and IFs represent the principal steps along the vimentin assembly pathway. By combining the SAXS data with the atomic structures and additional structural restraints, three-dimensional models of these assembly intermediates are constructed and refined. These results are further confirmed by electron microscopy observations.
Keywords: intermediate filaments, filament assembly, small angle X-ray scattering

P.12.07.3
Acta Cryst. (2005). A**61**, C411
Grazing Incidence Small Angle X-ray Scattering from Nanoparticles : beyond Classical Analysis Approximations
Rémi Lazzari[a], Gilles Renaud[b], Frédéric Leroy[b], [a]*Institut des NanoSciences de Paris, Paris, France.* [b]*CEA-DRFMC, Grenoble France.* E-mail: Lazzari@gps.jussieu.fr

GISAXS (Grazing incidence small angle X-ray scattering) has emerged in the past years as a powerful technique for probing the morphology of nanostructures elaborated on surfaces by recording the diffuse scattering around the specular reflected beam. A recent experimental breakthrough [1] allowed using this synchrotron technique to record background free scattering patterns during the undisturbed growth of islands in ultra-high vacuum environment.

Contrary to real space techniques, extracting morphological parameters as the shape, sizes and size distributions for a classical Volmer-Weber growth implies a complete data analysis that is hampered by the multiple reflection effects induced by the grazing geometry and by the correlations between the size of the scatterers and their separation. It will be shown that suitable models can improve the analysis by (i) including the gradient of index of refraction seen by the incoming and scattered beams contrary to classical Distorded Wave Born Approximation for substrate only [2] and (ii) by calculating the parallel diffuse scattering within the framework of the paracrystal model, thus going beyond the classical Local Monodsiperse Approximation [2,3].

[1] Renaud G., Lazzari R., Revenant C., et al., *Science*, 2003, **300**, 1416. [2] a) Revenant C., Leroy L., Lazzari R., Renaud G., *Phys. Rev. B*, 2004, **69**, 035411-1; b) Lazzari R., *J. Appl. Cryst*., 2002, **35**, 406. [3] Leroy L., Lazzari R., Renaud G., *Acta. Cryst*., 2004, **60**, 565.
Keywords: grazing incidence, SAXS, nanoparticles