

**P.12.07.4***Acta Cryst.* (2005). A61, C412**USAXS: A Tool to Probe the Structure and Dynamics of Complex Fluids**Michael Sztucki, T. Narayanan, *European Synchrotron Radiation Facility, BP 220, F-38043, Grenoble, France.* E-mail: sztucki@esrf.fr

For small-angle X-ray scattering (SAXS) experiments requiring high angular resolution and dynamic range, the Bonse-Hart camera [1] is still an attractive technique. The low divergence and high flux of an undulator beam permits to use a crossed-analyser configuration, and obtain the unsmear high resolution scattering data on an absolute scale (without requiring a calibration standard) within an acquisition time of a few minutes. However, Bonse-Hart double-crystal diffractometers with multibounce channel-cut crystals show rocking curves which depart considerably in their wings from dynamical diffraction theory [2]. The aim of this work is to improve and eventually suppress this parasitic scattering background originating from the surface of the crystals. This will make the ultra small-angle X-ray scattering (USAXS) technique suitable for studying weakly scattering biological samples and very dilute systems such as aerosol particles in a flame. This will be demonstrated using bio-colloids exhibiting hierarchical structures on the nanometer to micron scale. Furthermore, an improved USAXS set-up will allow to perform time-resolved experiments in the USAXS region and to exploit the coherence of the beam for scattering and imaging.

[1] Bonse U., Hart M., *Appl. Phys. Lett.*, 1965, 7, 238. [2] Agamalian M., Christen D.K., Drews A.R., Glinka C.J., Matsuoka M., Wignall G.D., *J. Appl. Cryst.*, 1998, 31, 235-240.

**Keywords:** USAXS, complex fluids, microstructure and dynamics**P.12.07.5***Acta Cryst.* (2005). A61, C412**Anomalous SAXS and WAXS for the Structure of Pt/Ru Catalyst Nanoparticles**U-Ser Jeng, Hwo-Shuenn Sheu, Ying-Huang Lai, Ya-Sen Sun, Din-Goa Liu, Jyh-Fu Lee, *National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan.* E-mail: usjeng@nsrc.org.tw

With the high flux ( $3 \times 10^{11}$  photons/s) and wide photon spectrum (5-35 keV) provided by the newly constructed superconducting wavelength shifter at the National Synchrotron Radiation Research Center, Taiwan, we study the structure of Pt and Pt/Ru nanoparticles embedded in carbon grains for fuel cell applications, using anomalous small angle X-ray scattering (ASAXS) and wide angle X-ray scattering. Using photon energies near 11.5 and 22.1 keV for the L and K absorption edges of Pt and Ru, respectively, in ASAXS, we have extracted the structural information for the Pt nanoparticles, including a mean dia. of 2.3 nm and a polydispersity of 25%. Whereas the ASAXS result for the Pt/Ru nanoparticles indicates clearly a core-shell structure with Pt taking the core position. On the other hand, at a temperature above 450 °C WAXS reveals a sign of core-shell structural inversion for the Pt/Ru nanoparticles of an average dia of 3.3 nm. The structural inversion results in a significant growth in particle size, from a diameter of 3.3 nm to 5.0 nm, due to the reorganization and fusion of the nanoparticles. The coordinating numbers of Pt and Ru extracted from EXAFS data for the nanoparticles support the core-shell structure revealed by ASAXS and WAXS.

**Keywords:** anomalous scattering, small-angle X-ray scattering, nanoparticles**P.12.07.6***Acta Cryst.* (2005). A61, C412**Interface Structure in Solid Oxide Fuel Cells by Anomalous/High-Energy SAXS/WAXS**Andrew Allen<sup>a</sup>, Jan Ilavsky<sup>b</sup>, Jon Almer<sup>b</sup>, Pete Jemian<sup>c</sup>, <sup>a</sup>*NIST, Gaithersburg, MD, USA.* <sup>b</sup>*APS, Argonne National Lab. Argonne, IL, USA.* <sup>c</sup>*University of Illinois, Urban-Champaign, IL.* E-mail: andrew.allen@nist.gov

Control of solid oxide fuel cell (SOFC) microstructure and

chemistry is needed to optimize SOFC performance and cost. Within the composite electrodes, the variation in the triple-phase-boundary (TPB) morphology (where the gas-, electron- and ion-conducting phases all meet), as a function of distance from the electrolyte layer, is particularly significant in defining electrochemical performance. Thus, characterization of the void and phase microstructures within the anode and cathode, at sufficient resolution to infer a quantitative characterization of the TPB interface, is highly desirable. This has become possible by utilizing the high brilliance and high x-ray energies available at a 3rd generation hard x-ray synchrotron source.

Anomalous ultrasmall-angle x-ray scattering (USAXS), close to the Zr absorption edge, has been combined with high-energy small-angle and wide-angle scattering (HE-SAXS and HE-WAXS). For the first time this has provided correlated variations in void size distribution, interface surface area, and solid phase, to below 10 micrometers spatial resolution, and has enabled the ion-conducting YSZ phase to be distinguished from the voids and electron-conducting phase (LSM or Ni). From these data, TPB properties can be inferred.

[1] Allen A.J., Dobbins T.A., Ilavsky J., Zhao F., Virkar A., Almer J., DeCarlo F., *Ceramic Engineering and Science Proc.*, 2004, 25, 275.

**Keywords:** small-angle X-ray scattering, interface structure, solid oxide fuel cells**P.12.07.7***Acta Cryst.* (2005). A61, C412**Structural SAXS Studies of the Human Amyloid Precursor Protein**Iris L. Torriani<sup>a,b</sup>, Cristiano L.P. Oliveira<sup>a,b</sup>, Matthias Gralle<sup>c</sup>, Carlos H.I. Ramos<sup>b</sup>, Sergio T. Ferreira<sup>b,c</sup>, <sup>a</sup>*IFGW Universidade Estadual de Campinas, Campinas, Brazil.* <sup>b</sup>*Laboratorio Nacional de Luz Sincrotron, Campinas, Brazil.* <sup>c</sup>*Instituto de Bioquímica Médica, UFRJ, Rio de Janeiro, Brazil.* E-mail: torriani@ifw.unicamp.br

The amyloid precursor protein (APP) gives rise to the  $\beta$ -amyloid peptide, considered to be a causal factor for Alzheimer's disease. The soluble extracellular domain of APP released by  $\alpha$ -secretase cleavage (sAPP $\alpha$ ) has several important physiological functions. Several APP fragments have been structurally characterized at atomic resolution, but the structures of APP and full-length sAPP $\alpha$  have not been determined. In this work, *ab initio* reconstruction of molecular models from solution X-ray scattering (SAXS) data for the two main isoforms of sAPP $\alpha$  (sAPP $\alpha_{695}$  and sAPP $\alpha_{770}$ ) provided models with enough resolution to identify distinct domains. Using the *ab initio* models and molecular docking tools, the fragments whose structures are known at the atomic level were optimally fit within the models of full-length sAPP $\alpha$ , allowing localization of important functional sites (glycosylation, protease inhibition and heparin-binding sites). Furthermore, SAXS and analytical ultracentrifugation (AUC) results indicate that both sAPP $\alpha$  isoforms are monomeric in solution. AUC measurements further show that sAPP $\alpha_{695}$  forms a 2:1 complex with heparin, in agreement with SAXS results. Possible implications of such complex formation for the dimerization of sAPP $\alpha$  and biological signalling are discussed in terms of the structural models proposed. Sponsors: FAPESP, LNLS, CNPq

**Keywords:** SAXS, human amyloid precursor protein, molecular model reconstruction**P.12.08.1***Acta Cryst.* (2005). A61, C412-C413**Diffuse Scattering of Pt-Rh in Grazing Incidence**Christian Steiner<sup>a</sup>, B. Schönfeld<sup>a</sup>, M.M.I.P. van der Klis<sup>a</sup>, G. Kostorz<sup>a</sup>, P.R. Willmott<sup>b</sup>, B. Patterson<sup>b</sup>, <sup>a</sup>*ETH Zürich, Institute of Applied Physics, 8093 Zürich, Switzerland.* <sup>b</sup>*Paul Scherrer Institut, 5232 Villigen PSI, Switzerland.* E-mail: steiner@iap.phys.ethz.ch

The near-surface microstructure of Pt-47 at.% Rh was investigated by diffuse scattering under grazing incidence at 730°C and UHV condition. The (110) and (111) surfaces investigated had a crystallographic misorientation of less than 0.05°. The samples were polished, then sputtered and aged prior to the diffraction experiments done at the Materials Science Beamline 4S of the SLS. The incident