

Poster Sessions

of Oxford, South Parks Road, Oxford (UK). ^bISIS Facility, STFC Rutherford Appleton Laboratory, Didcot (UK). ^cThe School of Physics, Queen Mary, University of London, London (UK). E-mail: callum.young@chem.ox.ac.uk

Fe₃O₄ (magnetite) is a ferrimagnetic material that has been known to man for thousands of years, and was used to make the first magnetic compasses as early as the 8th century AD. In more recent times it has been greatly studied by the scientific community, with much effort going into investigation of the Verwey transition [1] and the associated structural changes [2]. Despite this, a definitive model for the low temperature structure has remained elusive.

In this study neutron total scattering data from a highly stoichiometric powder sample collected at 10K have been used to perform reverse Monte Carlo (RMC) refinements using the program RMCProfile [3]. These refinements produce large box atomic configurations consistent with experimental data on both local and average length scales. Atoms may be translated and magnetic moments swapped and rotated during the refinement, allowing both the atomic and magnetic structures to be refined.

The results and their implications are discussed within the context of charge ordering models and space group assignments produced by previous studies.

[1] E.F.W. Verwey, *Nature* (London) 1939, 144, 327 [2] F. Walz, *J. Phys.: Condens. Matter* 2002, 14, R285-R340 [3] M.G. Tucker, D.A. Keen, M.T. Dove, A.L. Goodwin, Q. Hui, *J. Phys.: Condens. Matter* 2007, 19, 335218.

Keywords: diffraction, magnetite, RMC

MS26.P07

Acta Cryst. (2011) A67, C402

Studying the 3-dimensional structure of proteins in solution by small-angle X-ray scattering

Heiner Santner, Christian Moitzi, Petra Kotnik, Anton Paar GmbH, Graz (Austria) E-mail: heiner.santner@anton-paar.com

Small-angle X-ray Scattering (SAXS) is an important method for the characterization of biological macromolecules. Usually, the structure of proteins is characterized by protein crystallography and NMR. However, the results obtained with these methods do often not reflect the protein structure and its behavior in the native state. With SAXS, the 3-dimensional structure of proteins in solution, i.e. under biological conditions can be determined. The method determines the size and shape of proteins and protein complexes. Furthermore, SAXS is very sensitive to any structural or size changes caused e.g. by external effects (changed temperature or pH, ligand binding, etc.).

The main challenge for measuring proteins in solution with laboratory SAXS systems is the low contrast of these samples (contrast in SAXS is the difference in electron density between the nanoparticle and the matrix). Therefore, the design, collimation concept [1] and quality of the SAXS system is crucial for achieving excellent data quality at reasonable measurement times.

In this contribution we will show some examples of structural characterization of proteins in solution with the SAXSess mc² laboratory system. These examples include the determination of the overall protein size, of the folding state and of the 3-dimensional envelope describing the structure of the protein in solution. The determined solution structures can be well compared with structural data from protein crystallography.

SAXSess mc² is ideally suited for the analysis of e.g. low-concentrated protein solutions or drug delivery systems within minutes. Therefore, it can be used for time-resolved monitoring of

structural changes. Furthermore, many samples can be screened by use of a fully integrated autosampler.

[1] O. Glatter and O. Kratky, Small Angle X-ray Scattering, Academic, London, 2006

Keywords: SAXS, Proteins, 3D-envelope

MS26.P08

Acta Cryst. (2011) A67, C402

New GI-SAXS capabilities for the home-lab

Petra Kotnik, Heiner Santner, Heimo Schnablegger, Anton Paar GmbH, Graz (Austria) E-mail: petra.kotnik@anton-paar.com

Grazing-incidence small angle X-ray scattering (GI-SAXS) is an established technique for the characterization and analysis of nanostructured surfaces and thin films. Typical applications include thin organic films, quantum dot arrays or nanomaterials deposited and arranged on surfaces. However, GI-SAXS is mainly performed on dedicated synchrotron (GI-)SAXS beamlines due to the requirement of high primary beam intensity and parallel-beam requirements.

In this contribution we will present the new GI-SAXS stage for the SAXSess mc² laboratory small- and wide-angle X-ray scattering system. The precise GI-SAXS stage in conjunction with the SAXSess mc² system enables to perform GI-SAXS experiments even in the home laboratory. Samples with a nano-structured surface can be precisely tilted in order to perfectly obtain grazing incidence conditions. In addition, samples can be rotated in-plane in order to study the arrangement of the nanostructured surface. We will discuss technical aspects of the GI-SAXS stage and will present selected results of nanostructured thin film samples.

Keywords: GI-SAXS, grazing incidence, surface

MS26.P09

Acta Cryst. (2011) A67, C402-C403

Non-crosslinking aggregation of DNA-functionalized nanoparticles

Masahiro Fujita, Mizuo Maeda, Bioengineering Laboratory, RIKEN, Saitama (Japan). E-mail: mfujita@riken.jp

Recently, it was discovered that DNA-functionalized nanoparticles assemble by hybridization in a non-crosslinking configuration. When single-stranded (ssDNA) molecules grafted on the nanoparticles hybridize to the complementary ones, the resulting nanoparticles, which are covered with double-stranded DNA (dsDNA), assemble immediately at high salt concentrations without molecular crosslinking, while the nanoparticles with ssDNA molecules remain stable. The colloidal stability is very sensitive to the terminal base-pair of DNA duplex. When the tethered ssDNA hybridizes with a single-base mismatched DNA, the nanoparticles still disperse stably at the high salt concentrations. However, the mechanism of the non-crosslinking aggregation has not been understood yet. In this study, the non-crosslinking aggregation was explored from the structural point of view, using mainly small-angle X-ray scattering (SAXS). The structural characterization of the gold nanoparticles with ss- or dsDNA was performed, and the effects of DNA length, core size, and temperature on the non-crosslinking aggregation were also investigated.

Gold nanoparticles (ca. 5, 15 and 40 nm) were functionalized with ssDNA. Here, the DNAs with various bases were used. The functionalized gold nanoparticles were suspended in 10 mM phosphate