

PS14.02.19 TIME-RESOLVED SOLUTION SCATTERING STUDIES ON A MUTANT VERSION OF *E. coli* ASPARTATE TRANSCARBAMOYLASE. H. Tsuruta, D.P. Baker,* T.T. Tibbitts,* S.C. Pastra-Landis,**† P. Vachette,‡ E. R. Kantrowitz*, SSRL, Stanford Univ.; Dept. Chemistry, Boston College*; Dept. Chem. Wheaton College†; LURE, Université Paris-sud‡.

E. coli aspartate transcarbamoylase (ATCase) undergoes a large quaternary structure change in the allosteric transition upon binding of various combinations of substrate analogues and natural substrates. Glu-50 near the carbamoyl phosphate binding site is involved in the interdomain interaction that is essential in transforming the enzyme from T state to R state. The Glu-50 → Ala (E50A) mutation results in an enzyme with low activity, low aspartate affinity and little cooperativity. Enzyme kinetics studies have shown that E50A ATCase may be in an intermediary structure during the enzyme catalysis and that the allosteric effector ATP or the bisubstrate analog N-phosphonacetyl-L-aspartate (PALA) can activate the mutant fully to R state. Indeed the three-dimensional structure of the E50A ATCase co-crystallized with PALA is found to be in fully R state. We have carried out time-resolved solution x-ray scattering studies of E50A ATCase during the enzyme reaction with the natural substrates carbamoyl phosphate and aspartate, aimed at characterizing the possible intermediate structure which is short-lived and difficult to study by x-ray crystallography.

A concentrated enzyme solution was mixed with a substrate solution within a stopped-flow rapid mixer, and collection of time-resolved solution scattering curves in the range of 18-130 Å in Bragg spacing immediately followed, using a synchrotron radiation beam. The subsidiary scattering peak recorded during the enzyme reaction was intermediary between the curves recorded for the complete T and R states. The additional presence of ATP converts the curve all the way to that of R structure while at low PALA concentrations there is a lag phase in which the peak stays intermediary for a while then evolves to the curve of the full R structure. Along with the biochemical results, these observations demonstrate the existence of a quaternary structure intermediary between T and R, rather than the coexistence of T and R structures.

Other

PS14.03.01 DESCRIBING ORIENTATION TEXTURE IN SMALL ANGLE SCATTERING. John D. Barnes, NIST Polymer Structure and Mechanics Group, NIST, Gaithersburg, MD 20899

This presentation attempts to demonstrate how crystallite orientation distribution functions of the kind used in texture analysis for wide-angle x ray diffraction can be extended to provide tools for simulating small-angle scattering from anisotropic materials.

In WAXD the crystallite orientation distribution causes a single point of the reciprocal lattice to be distributed over the surface of a sphere (pole figure). In many materials SAS arises from microdomains that possess an orientation distribution. The scattering from the contents of these microdomains is, however, finite over extended regions of reciprocal space. This contrasts with the situation in WAXD where the scattering is confined to the discrete points of the reciprocal lattice for the domains. One must also account for the fact that microdomains in SAS are not all identical. This means that the distribution functions must account for variations in such parameters as element size, shape, and degree of perfection as well as orientation. These considerations are illustrated by SAS results from highly anisotropic scatters including block copolymers, semicrystalline polymers, and track etched membranes.

PS14.03.02 2-D SMALL ANGLE X-RAY SCATTERING PATTERNS OF COLLOIDS AND PHOTONIC COLLOIDAL CRYSTALS M. Megens¹, W. L. Vos¹, C. M. van Kats¹, and P. Bösecke², ¹van der Waals-Zeeman Instituut, Universiteit van Amsterdam, 1018 XE Amsterdam, The Netherlands, ²European Synchrotron Radiation Facility, 38000 Grenoble, France.

We have started small angle x-ray scattering (SAXS) experiments on BL4/ID2 of the ESRF to study photonic colloidal crystals. These crystals have an as large as possible refractive index contrast in the optical regime, and are thus multiply scattering (photonic), which impedes optical diffraction experiments [1].

Monochromatic radiation (~0.1 nm) was focused on the samples. Scattered radiation was collected with a 2 dimensional gas detector at the maximum distance of ~10 m [2].

The diffraction patterns clearly reveal several features. 1) Sharp diffraction peaks are observed that originate from the colloidal crystals. The 2D nature of the information combined with rotation of the samples reveals a wealth of information on the structure and order of the samples that cannot be obtained from 1D diffraction patterns. Yet, we have observed lattice spacings on the order of several hundred nm. 2) The concentric ring pattern caused by the formfactor of the colloidal spheres is seen. It extends far into reciprocal space due to the high degree of monodispersity (single size). The possibility to measure the size distribution of the spheres for the first time *in-situ* will be discussed.

The information from the SAXS studies already proves to be essential for the interpretation of optical studies of the samples.

[1] W.L. Vos *et al*, in *Photonic Band Gap Materials*, ed. C. Soukoulis (Kluwer, Dordrecht, in press); Phys. Rev. B (submitted).

[2] P. Bsecke *et al*, Rev. Sci. Instr. **66**, 1636 (1995).