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Studies of material structure and process with coherent diffraction and time-resolved X-ray imaging

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The success of structural science today is largely based on the use of X-ray diffraction on crystalline specimens. However, not all materials can be crystallized. This is especially true for membrane proteins and for larger multi-protein macromolecular assemblies. As the complexity of the biological systems being studied increases, their spatial dimensions also approach sub-micrometer scale which is on the borderline between what one can see directly with microscopic and imaging techniques and what can be studied using diffraction and scattering [1]. Coherent X-ray diffraction imaging technique has become an exciting field of research as it holds the potential for high-resolution imaging of nonperiodic structures at diffraction-limited spatial resolution, without being limited by manufacturing defects of X-ray optics. In this talk we will provide an overview of the coherent diffraction imaging program at the APS. In particular, we present recent research and development on the concept of crystal guard aperture [2] as a way to eliminate parasitic-scattering backgrounds in coherent diffraction imaging experiments, which is crucial to achieving high signal-to-noise ratios at high diffraction resolution. We have applied this method to study metallic nanofoam formation in dealloying process. Recent experimental and phase-retrieval results will be presented. This work is performed at the Advanced Photon Source at Argonne National Laboratory which is supported by DOE BES under Contract No. W-31-109-ENG-38.

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Keywords: coherent diffraction imaging, phase problem, nanofoam structures

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Studies of silica aggregate structure and its dynamics in rubber using time-resolved USAXS and XPCS

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Rubber filled with silica particles shows reinforcement effect, which causes various changes in mechanical and viscoelastic behavior such as the increase of elastic modulus, tear strength, and tensile strength and hysteresis loss. Understanding of the physical mechanism of the reinforcement effect is one of the most important unsolved issues in the field of elastomers. In the present study, we focus on the role of silica aggregate structure on the reinforcement. By using time-resolved two-dimensional ultra-small- and small-angle X-ray scattering (2D USAXS-SAXS), we have obtained the structural change of silica aggregates in uniaxially deformed rubber in real time. The measured deformation behavior of aggregates qualitatively explains the stress-strain behavior of filled rubber. In addition, we performed X-ray photon correlation spectroscopy (XPCS) in order to elucidate the viscoelastic properties of filled rubber, in particular, the origin of energy loss. We obtained information on the structural fluctuation of silica aggregates in rubber by using XPCS. The results have revealed non-diffusive behavior of silica dynamics in rubber. Furthermore, XPCS measurement during vulcanization process of rubber clearly monitored the slowing process of silica accompanied with the cross-link of rubber polymers.

Keywords: time-resolved 2D-USAXS, XPCS, reinforcement effect

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Time-resolved monitoring of nanocomposite growth using grazing incidence small-angle scattering

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Nanocomposite organic-metallic materials are of crucial importance for many areas in modern technology. To name just a few, are biosensoring [1], solar cell applications [2] or organic electronics [3]. In order to design the structure-function relationship, one must tailor the interface metal - organic layer. This ranges from selective contacting [4] to exploiting the plasmon resonances of the nanostructured metal layer [5,6]. Deposition techniques include solution-casting [7,8], and vacuum deposition [5,6]. Therefore, understanding the growth kinetics of the nanocomposite during deposition is indispensable for tailoring the nanocomposites' properties [6]. Grazing incidence small-angle x-ray scattering (GISAXS) [5,9,10] allows for in-situ monitoring of the full three-dimensional structure and morphology of nanocomposite thin films in real time. We combined in-situ gold sputter-deposition on different organic multilayer substrates with GISAXS at the beamline BW4 / HASYLAB. Our real-time investigations allow for identifying the different kinetic growth regimes during sputter deposition and for deducing the changing structure of the polymer-metal interface with high time-resolution [11].

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Cctbx architecture and algorithms

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