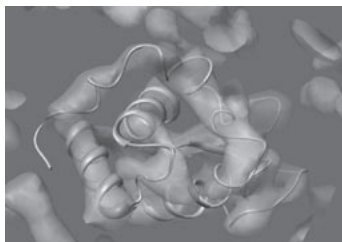


crystallography. Recently, an interest has grown for protein powder diffraction which is becoming a well-established method in the field of structure refinement and molecular replacement. With the use of two examples it is shown that de novo solutions to the phase problem can be obtained at low resolution via phasing methods such as the isomorphous replacement method. Using synchrotron radiation, high quality protein powder patterns have been collected in which pH- and radiation-induced anisotropic lattice changes were exploited in order to reduce the challenging and powder specific problem of overlapping reflections. The Single Isomorphous Replacement method enabled the computation of molecular envelopes and the mapping out of the solvent channels in the crystal. Electron density maps in which features of the secondary structure of the lysozyme protein molecule can be discerned, were then obtained using the Multiple Isomorphous Replacement method (as illustrated in the image).



Keywords: powder diffraction, protein structure determination, isomorphous replacement

MS.09.5

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Characterization of spider silks weaved by different species living in the Black sea region of Turkey

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Spider silks have attracted many researchers on account of their superior (Physical, chemical, biological and pharmacological) properties [1-4]. Our research group has begun to investigate spider silks with a project (TUBITAK, TBAG-107T017) after pre-studies[5]. The aims of this project are structural investigation of spider silk samples (in dragline and cocoon forms) and obtaining some systematical information according to the different species(habitats, feeding and type of silk, etc.) First of all, our biologist group started to look for endemic species in The Backsea region of Turkey. They are indicating that, this geographic region is including very different spider species. During these researches, a lot of species, their draglines and egg-cocoons were collected from their natural habitats. On the other hand, several living cavities (simulating their natural habitats) for the collected species were also constructed by our biologists in laboratory conditions. After these studies, a lot of silk samples produced by different species from Araneidae and Gnaphosidae familia were available. With this presentation, we would like to summarize our studies about structural investigation and characterization of the mentioned silks. Approximately, 15 samples were chosen and studied by using SEM, TEM, SWAXS, and XRD experimental methods. Alanine and glycine regions can be detected in XRD and SWAXS patterns due to their nanostructured and crystalline aggregations. XRD and SWAXS data have shown

that the majority of these silks contain beta-plated sheet crystals that form from bilateral repeated aminoacid sequences rich in small aminoacid residues. At the end of the presentation, structural views, stabilizations and crystallinities of the samples will be compared.

Keywords: spider silk, Black Sea region, nanostructures, SWAXS, XRD, Araneidae, Gnaphosidae

MS.10.1

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Automation of the APS 11-BM high-resolution and high-throughput powder diffractometer

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The 11-BM powder diffractometer at the Argonne Advanced Photon Source operates with resolution on the order of 2×10^{-4} delta-Q/Q and collects an average diffraction pattern in ~1 hour. Equipped with a robotic sample changer, we expect this instrument to collect 20 or more datasets per day, primarily for remote users. Managing this level of use with minimal staffing has required that we optimize handling of sample metadata, as well as instrument control and data reduction. This talk will outline the database and web interface for 11-BM, which interfaces to the APS proposal and safety approval systems, as well as the instrument control system. A description of how users supply sample information and retrieve diffraction data via the web will be presented. The current instrument control software, which automatically calibrates the instrument, as well as streamlines data reduction, will also be discussed. Other topics to be presented include our current development plans, which will implement publication tracking and simplify sample storage and return/disposal. Progress on methods for automated review of diffraction data for internal consistency will also be presented.

Keywords: synchrotron powder diffraction, robots, automated data collection

MS.10.2

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Start to finish: Algorithms and parameters for successful robotic data collection

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Data acquisition automation implies robotics, and the appearance of new commercial robotic systems (such as the Rigaku ACTOR-SM) for small-molecule samples now requires algorithms that are robust and reliable but also flexible. To achieve fully automated crystal mounting, centering, data collection and processing (and optionally structure solution and refinement), a large number of parameters are necessary. Also, the system should be able to make intelligent decisions about whether to keep a given sample or to move on to the next one. These decisions can be made by applying the technique of *ranking* in order to aid in the decision process, for example to choose the best crystal from a group or to avoid wasting time collecting data on a sample that is unlikely to provide viable results. The choice of a minimum rank will depend on the purpose of the experiment;