

REVERSE MONTE CARLO MODELING OF AMORPHOUS ALLOYS AND COVALENT GLASSES

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It will be demonstrated, on the example of amorphous silicon, that for proper interpretation of diffraction data taken on disordered materials, structural modeling cannot be avoided. One particular suitable technique, reverse Monte Carlo (RMC) modeling, will be described. Many examples, including two- and three component metallic glasses, amorphous semiconductors and other glassy materials will be presented where RMC modeling revealed essential details of the structure.

Keywords: DISORDERED STRUCTURES COMPUTER MODELING DIFFRACTION DATA

HYDROGEN AND HYDRATION IN PROTEINS OBSERVED BY HIGH RESOLUTION NEUTRON CRYSTALLOGRAPHY

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One of the most important fields today is structural genomics, in which the functions of proteins are analyzed using the results from synchrotron X-ray and NMR protein structure analysis. However, it is difficult in an NMR or X-ray crystallographic analysis of a protein to identify all of the hydrogen atoms and the water molecules of hydration, even though they play important roles in innumerable biological processes. In contrast, the neutron diffraction method has the ability to locate hydrogen position absolutely. We have recently developed a neutron imaging plate (NIP) and a neutron monochromator, and have successfully applied them to construct a neutron diffractometer dedicated for biological macromolecules (BIX-2, BIX-3, BIX-4) in the JRR-3M reactor. The performance of BIX type diffractometer has been certified as one of the best in the world. By using BIX type diffractometer, all the hydrogen atoms and most of the solvent molecules of hydration of lysozyme (Hen Egg-white L. at different pH, Human L.), insulin, myoglobin and rubredoxin (wild type and mutant), which are small but fundamentally important proteins, have been unambiguously identified in 1.5 Å resolution. These structural results have provided new and important discoveries such as the bifurcated hydrogen bonds in α -helices, the fine structure of methyl group, details of hydrogen/deuterium exchange reactions, the role of hydrogen atoms in enzyme reaction and the dynamic behavior of hydration in proteins.

Keywords: HYDROGEN HYDRATION NEUTRON DIFFRACTION

AMORPHOUS STRUCTURES STUDIED BY HIGH-ENERGY X-RAY DIFFRACTION AND RESONANT SCATTERING

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The structure determination of amorphous solids containing three or more elements is still a difficult task. One of the major problems is the precise and accurate determination of interatomic distances and the identification of the corresponding correlations. Without this information no reliable values for bond angles and coordination numbers can be calculated.

It shall be demonstrated that the determination and identification of interatomic distances can essentially be facilitated by the combination of high-energy synchrotron X-ray diffraction (HXD) [1] and anomalous wide angle X-ray diffraction (AWAXS) [2] experiments. Latest results on multicomponent amorphous solids in the compositional ranges Ba-Si-O [3], Ba-Ge-O, Si-Ge-O, K-Ge-O, Te-Br-J, Ba-Zr-F, Ba-La-Zr-F and Ni-Na-P-O will be presented. The intention is to illustrate that by the combination of HXD- and AWAXS-results more experimental information about the short-range and the medium-range orders can be obtained. Therefore HXD-experiments at $E = 100-150$ keV were performed as well as AWAXS-experiments near the Ge K-, Zr K- and Ba K-absorption edge, respectively. Hard X-rays were used, because a high resolution in direct space can be achieved. The AWAXS-data were analyzed in terms of differential anomalous scattering [2,4], which permits the calculation of differential structure factors from data collected at two or three different energies.

References

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Keywords: AMORPHOUS SOLID, X-RAY DIFFRACTION, RESONANT SCATTERING

STRUCTURE AND DYNAMICS OF HYDROGEN ATOMS AND WATER MOLECULES IN/ AROUND LYSOZYME: A COMBINED NEUTRON CRYSTALLOGRAPHY/INCOHERENT QUASI-ELASTIC NEUTRON SCATTERING STUDY

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Cells are highly macromolecular crowded media, and a precise knowledge of the water properties around macromolecules is necessary in order to understand various biological mechanisms. This presentation reports a combined study of the structure and dynamics of water in triclinic crystal of hen-egg white lysozyme. A model of the dynamics of water around lysozyme, in a highly crowded environment, under about 500 pa and at 300 K, is proposed.

Neutron diffraction data were collected with a resolution of 1.7 Å on LADI diffractometer (ILL/EMBL). A model with all hydrogen or deuterium atoms on the protein, and 244 out of the 310 water molecules theoretically present in the unit cell was constructed. Interesting characteristics about the disorder of the interfacial water, the structure of water around apolar parts of the protein, the presence of water in apolar cavities within the protein were observed.

The single-particle diffusive dynamics study by IQNS shows that all water molecules have their dynamics affected by the presence of the protein. Two populations of water molecules were observed. One mainly corresponds to the first hydration shell, in which water molecules reorient themselves 5 to 10 fold slower than in bulk solvent, and jumps from hydration site to hydration site. The self-diffusion constant is reduced 5 fold compared to bulk solvent. The second group corresponds to few water in the second hydration shell, confined between hydrated macromolecules. Within the time scale probed these undergo a translation diffusion, with a self-diffusion constant reduced about 50-fold compared to bulk solvent.

Keywords: SOLVENT STRUCTURE DYNAMICS