medical importance. Both NMR spectroscopy and X-ray crystallography are used for protein structure determination. To accelerate the NMR analysis, we have constructed the large-scale NMR facility housing 40 high-field NMR spectrometers, and developed several key technologies such as a high-yield cell-free protein synthesis system for high-throughput and automated production, a software package, KUJIRA, for the systematic and interactive NMR data analysis, and the program CYANA for automated structure calculation. We determined 75 structures in 2002 fiscal year, and 207 structures in 2003 fiscal year, respectively, by NMR spectroscopy.

Keywords: NMR spectroscopy, structural proteomics, cell-free protein synthesis

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X-ray Microscopy Project at NSRRC

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Very recently, under the NSRRC X-ray Microscopy Project, we have installed a transmission X-ray microscope (TXM) to the BL01B end station of an advanced, high flux (3×10^{11} photon/s) and wide energy spectrum (7-23 keV), X-ray source generated by a superconducting wavelength shifter. The state-of-art TXM can provide 2D imaging and 3D tomography for imaging light materials such as biological specimens with a spatial resolution of 30-60 nm, using the Zernike-phase contrast capability with 8-11 keV hard X-ray. To our best knowledge, such resolution achieved is unprecedented in X-ray imaging up to date. In this presentation, we would like to share the scope and the prospective of the project as well as the progress of the TXM in our center. The impact of our TXM is expected in many imaging works for buried structures, including the analysis of failure mechanisms in microelectronic devices due to electromigration, thermal breakdown or inhomogeneity, or the characterization of porous materials such as soils and rock, and the transportation behavior in these porous structures. In addition, material failures due to induced strain, crack propagation or corrosion can be studied with our modern X-ray microscope of 2D and 3D imaging capability. Currently, we aim our unprecedented X-ray microscope at the research of cells in life science. With the 3-D "virtual sectioning" capacity to be matured, we intend to view either a single cell, cell clusters, or any region of a tissue. With labeling agents, for instance, gold, for contrast variation, in-situ imaging for specific cellular functions is possible with our TXM.

Keywords: X-ray imaging, X-ray microscopy, in-situ imaging

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Analysis of Liquid and Crystalline Proteins by Particle Induced X-ray Emission (PIXE)

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Unique identification of *metals* bound to macromolecules is an interesting challenge in structural biology, and an unambiguous assignment is often problematic. microPIXE (particle induced X-ray emission) with 2-3MeV protons on liquid and crystalline proteins has been used very successfully in both identifying elements and in measuring their stoichiometric ratio (calibrated per protein molecule by using the sulphur peak to give an internal normalisation of the sulphur atoms from the known cysteines and methioniones) to an accuracy of between 10 and 20% on over 50 samples [1,2].

Measurements using the technique have informed a wide range of questions, including the degree of seleno-methionine incorporation into a proteins destined for MAD structure determination, the identity of unexpected electron density in solved structures, identifying of metals bound to liquid protein samples to elucidate their function prior to structural studies, determining whether or not DNA is bound to a protein crystal (from the phosphorus to sulphur ratio), checking for paramagnetic species in proteins prior to NMR analysis, and analysing proteins before and after mutation of putative metal binding sites.

The method is now routine and may have potential as a high throughput screening tool in structural biology.

[1] Garman E., *Structure*, 1999, **7**, R291-R299. [2] Garman E.F., Grime G.W., *Progress in Biophysics and Molecular Biology*, 2005, *in press*.

Keywords: PIXE, proteins, trace-metal analysis

MS93 CRYSTALLOGRAPHY AND ENVIRONMENTAL SCIENCE

Chairpersons: Marcello Mellini, Mihaly Posfai

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Application of Natural Zeolites: Understanding the Properties at a Molecular Scale

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Natural zeolites are usually found as zeolite-rich rocks (zeolitites) which contain at least 50 wt% of zeolite phase. Italian zeolitites may contain phillipsite or chabazite with an overall content of zeolite phase as large as 70 wt%. Especially for agronomical and agricultural purposes, an important property is the adsorption and/or release of the ammonium ion. In this frame, the aim of this study is to present the structures of NH_4 exchanged chabazite and phillipsite and to explain the different behaviour of the two zeolites in agronomy and agriculture applications. It is shown that the knowledge of the local environment of NH_4^+ in the cavities of these zeolite species is extremely important. In chabazite, the ammonium ion with a monodentate local structural environment may be easily released or desorbed. NH_4-phillipsite [1] shows instead that the ammonium ion is in a tridentate local environment and it is consequently more difficult to be released or desorbed in solution. As a matter of fact, the zeolitite with NH_4-exchanged chabazite gave very encouraging results in agronomy applications. On the contrary, the zeolitite with NH_4-exchanged phillipsite gave very poor results for the same application [2].

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Keywords: natural zeolites, ammonium ion, application

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A Structural View of Carbonate Biomineralization by Bacteria

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Although it has been recognized for more than a century, biomineralization of carbonate minerals by prokaryotic organisms has been much less studied, from a structural point of view, than the formation of calcite and aragonite by eukaryotic cells. Formation of carbonates by bacteria and archaea has however a potential strong environmental significance, for example for immobilization of radionuclides under aridic conditions or for deep geological carbon dioxide mineral sequestration.

Investigation tools such as analytical transmission electron microscopy and synchrotron-based scanning transmission x- ray microscopy have allowed us to evidence, at nanometer scale, the well known, yet poorly understood, systematic relationship between bacterial extra-cellular polysaccharides and carbonates. We report examples from mineral (pyroxene) surface micro-habitats and from lacustrine carbonate microbialithes. Nanobacterial-like morphologies are characteristic of these carbonate crystals, the formation mechanism of which will be discussed.

A second mode of carbonate and phosphate biomineralization by bacteria has also been evidenced. It is radically different in that it involves intracellular, particularly periplasmic, components. Possible