Acta Cryst. (2002). A**58** (Supplement), C34

STRUCTURAL CHEMISTRY OF NATURAL NANOPARTICLES VIA SYNCHROTRON MICRO-SXRF, -SXRD, AND -EXAFS

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The partitioning of potentially-toxic metals into coexisting minerals, the difficulty of identifying the mineral species to which these elements are bound, and the multiplicity of sorption mechanisms are key problems in understanding how metals interact at the molecular level with environmental nanoparticles. These long-standing impediments are now yielding to investigations by X-ray techniques developed at 3rd generation synchrotron facilities. We shall show that these problems can be overcome without disrupting the heterogeneous matrix by combining scanning X-ray fluorescence (SRXF) and diffraction (SXRD), and extended X-ray absorption fine structure (EXAFS) spectroscopy at micrometer-scale of resolution. First, micro-SXRF and micro-SXRD are used to identify the host solid phase by mapping the distributions of elements and solid species, respectively. Micro-EXAFS spectroscopy is then used to determine the mechanism of trace element binding by the host phase at the molecular scale. To illustrate the complementary application of these three techniques, we studied how nickel is sequestered in soil ferromanganese nodules, a hellishly complex natural matrix consisting of submicrometer to nanometer-sized particles with varying structure and chemical composition. We showed that nickel substitutes for Mn (III) in the manganese layer of the $MnO^{2-}Al(OH)_3$ mixed-layer oxide lithiophorite. The affinity of Ni for lithiophorite was characteristic of micronodules sampled from soils across the USA and Europe. Since many natural and synthetic materials are heterogeneous at nanometer to micrometer scales, the synergistic use of micro-SXRF, micro-SXRD, and micro-EXAFS is expected to have broad applications to earth and materials science.

Keywords: SYNCHROTRON XRD EXAFS

Acta Cryst. (2002). A**58** (Supplement), C34

UNIAXIAL PLASTIC DEFORMATION OF POLYCRYSTALLINE Cu AND Al THIN FILMS STUDIED ON A GRAIN-BY-GRAIN BASIS UTILIZING X-RAY MICRODIFFRATION

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We have discovered that grain-to-grain interactions dominate the plasticity of Al and Cu thin films and that the influence of these interactions establishes effective length scales for the phenomena that can be even smaller than the grain size. We have examined the large grain-to-grain strain distributions and their changes with added plastic strain in 1.5 mm Al 0.5% Cu films using a 0.8 micron diameter white x-ray probe at the ALS.
The strain distributions arise not only from the distribution of grain sizes and orientation as previously believed to be the key parameters, but also the differences in grain shape and the stress environment of a grain as imposed by neighboring grains across their boundaries. Multiple active glide plane domains have been found within single grains. Large grains, hence, behave like multiple smaller grains since their stress state is strongly influenced by their neighbors.

Keywords: MICRODIFFRACTION, PLASTICITY, THIN FILMS

Acta Cryst. (2002). A**58** (Supplement), C34

THE INFLUENZA VIRUS ANTIGEN, NEURAMINIDASE

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The description of the 3-D structure of influenza virus neuraminidase and its complex with two different monoclonal antibodies led to a number of insights into antibody recognition of protein antigens.
The antigenic structure of the neuraminidase is an almost continuous surface surrounding the catalytic site. Although very small changes in the antigenic structure can be selected with monoclonal antibodies, examples are known of non-conservative amino acid substitutions being tolerated at the antibody-antigen interface. Two monoclonal antibodies binding a largely common surface structure on the antigen are unrelated and utilize different substructures within that surface to produce their binding energy. These observations have implications for the mechanisms by which viruses 'protect' functionally important structural elements from antibody surveillance.
Many new neuraminidase sequences are being reported as part of the global surveillance established to monitor the emergence of drug resistance to the recently registered neuraminidase inhibitors.

Keywords: NEURAMINIDASE

Acta Cryst. (2002). A**58** (Supplement), C34

THE MHC FAMILY OF PROTEINS IN IMMUNE AND NON-IMMUNE RECOGNITION

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The three dimensional structures of MHC molecules seem to be ideally suited for their function in antigen presentation in the cellular immune response. A large groove located between two α-helices accommodates short peptides, which are examined by T cell receptors that simultaneously contact the peptide and the MHC protein, rationalizing the dual recognition properties of T cell receptors. Although it might appear that the MHC fold evolved specifically for antigen presentation, a number of other proteins have adapted the same basic fold to perform widely different roles within and outside of the immune system. These include an immunoglobulin G receptor (FcRn); the protein mutated in the iron storage disease hereditary hemochromatosis (HFE), a protein that stimulates lipid catabolism (Zn-α2-glycoprotein; ZAG), and virally encoded class I MHC homologues (UL18 and m144 from human and murine cytomegalovirus). These molecules illustrate the versatility of the MHC fold and raise intriguing questions about the ancestral function of MHC-related proteins and the evolution of the adaptive immune response.

Keywords: MHC PROTEINS, FC RECEPTORS, IRON METABOLISM