

**PS23.01.13 PLASTIC MODELS OF PROTEINS AND NUCLEIC ACIDS FOR EDUCATION.** Marilyn D. Yoder, University of Missouri-Kansas City, School of Biological Sciences, Kansas City, MO 64110 USA and Robert E. Smith, Allied Signal, Kansas City, MO 64141 USA

A method to manufacture plastic models of proteins and nucleic acids of known three-dimensional structure has been developed for both research and educational purposes. The plastic models were made using stereolithography (SL) and selective laser sintering (SLS) techniques. Ball-and-stick, a-carbon backbone, solvent accessible surface, and ribbon models have been constructed.

The technique has been adapted from the automotive and aerospace industries where SL and SLS are commonly used to prototype manufacturing designs as plastic models. A computer-directed laser maps out the topology of the biopolymer at the surface of either a light sensitive resin (in the case of SL) or a block of nylon powder (in the case of SLS). Upon irradiation by the laser, either the light sensitive resin is converted to a solid polymer, or the nylon powder is fused, or sintered. The laser is controlled by an ISO 9001 compatible computer file, the stl file, that contains the topology of the biopolymer represented as a set of triangles. The normals of each triangle must be pointed outward and the vertices listed in counterclockwise order when looking at the object from the outside. The stl data are used by a slicing algorithm to determine the cross sectional areas of the model to be built. A library of stl files has been calculated from structural data from the Brookhaven PDB and stored on CD-ROM for distribution.

The plastic models are approximately 10 cm in the longest dimension and are lightweight and very portable. They have been used in classroom instruction for students from the sixth grade (approximately 12 years of age) to the graduate school level. A stainless steel casting of a SL model of subtilisin was made for the Science in American Life exhibit in the Smithsonian Institution's Museum of American History (Washington, D.C. USA) and is used with an interactive computer to teach the principles of protein docking.

**PS23.01.14 COMPUTER SOFTWARE FOR INTERACTIVE MANIPULATION OF REPRESENTATION SURFACES FOR HIGHER-RANK TENSOR PROPERTIES** Andrew F. Stark<sup>1</sup>, James S. Miller<sup>1</sup> and Bernhardt J. Wuensch<sup>2</sup>, <sup>1</sup>Artificial Intelligence Laboratory, <sup>2</sup>Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

We have found it useful, in teaching crystallography to students of materials science, to couple the development of symmetry theory with demonstration of the consequences of symmetry on the physical behavior of materials. An appropriate set of topics is tensor description of crystal properties, derivation of the restrictions that symmetry imposes on tensor elements, and the nature of the resulting anisotropy in physical properties. No single representation surface is adequate for third and higher-rank tensor properties, but the dependence on crystallographic direction (specified by direction cosines  $l_i$ ) of important scalar moduli can be specified. Examples are Young's modulus  $E = s_{11}/e_{11} = 1/(l_m l_n l_p l_q S_{mnpq})$  that relates tensile stress  $s_{11}$  to tensile strain  $e_{11}$  in the same direction, and the longitudinal piezoelectric modulus  $d = P_{11}/s_{11} = l_m l_n l_p d_{mnp}$  that provides the component of the polarization vector along the direction in which a uniaxial stress is applied. These two moduli are given by very complex polynomials that, for triclinic crystals, include 21 and 18 terms, respectively. A fast, interactive program with high-quality graphics has been developed to display the associated representation surfaces. The viewing perspective may be varied to convey appreciation of both the shape of the surface and that it conforms to the point group of the crystal. The magnitude of any tensor element in the polynomial may be "zoomed" up or down to show its contribution to the shape of the surface.

The software and accompanying documentation are publicly available over the World Wide Web at <http://www-swiss.ai.mit.edu/~astark/crystal.html>. Users need a UNIX workstation and a copy of the mathematical software MAPLE for Xwindows.

**PS23.01.15 THE ROLE OF CRYSTALLOMORPHOLOGY IN EVALUATION OF FLUORITE ORE DEPOSITION IN TAJIKISTAN** A.R.Fajziev Tajik State University, Dushanbe, Tajikistan.

It is known that Tajikistan is among the regions with fluorite ore deposition. Tajikistan also poses mining enterprise which work out this ore from different deposits. Crystallography along with other means played an important role in investigation and evaluation of new fluorite deposits in Tajikistan. In the veining deposits we found the following vertical zones and distribution of habitus forms of fluorite crystals: in the upper horizons the crystals have cubic habitus, in the middle cubic octohedral and rhombododecahedral and in the lower horizons octohedral. The utilysation of the zonal system made it possible to oversee the prospectivity (unprospectivity) of a number of fluorite features. Here are also two examples:

Our investigation in Kara-jilga (Eastern Pamir) showed that the fluoride crystals on the surface are always of cubic forms, with additional  $\{211\}$ ,  $\{311\}$ ,  $\{731\}$  facets.

An opinion was expressed on this basis about not deep eroze section veins existing in this deposit and thus prospectivity of ore deposition in the deapth, which later on was proved by the results of our investigation: in the galleries of middle and lower horizons deposits, in the veins of crystals of fluorite of rhombododecahedral and octobedrical habitus types were found.

In the ores of Fayzabad region (Central Tajikistan) the crystals of fluorite are only of octohedral habitus types and it proves that the crystals here represent underroot parts (according to the scheme of changing the forms of crystals).

As it is really was found out during our future investigation compartively large veins ( tile 3 meters) and which are situated not very deep (35 - 40 meters) change into small veins and then completly wedge in.

**PS23.01.16 THE CALIFORNIA STATE UNIVERSITY CENTER FOR MOLECULAR STRUCTURE** Katherine Kantardjieff, Department of Chemistry and Biochemistry, California State University, Fullerton, CA 92634

The California State University Center for Molecular Structure is a core research and training facility that serves the largest four-year and Masters' degree-granting public university system in the United States. The Center, the first of its kind at an institution not granting the Ph.D. degree, provides faculty and students throughout the CSU access to a Siemens HISTAR system for macromolecular structure determination, a scintillation detector and, soon, a Siemens SMART system for small molecule applications. A Silicon Graphics computer laboratory of Indigo and Extreme workstations and Challenge L server provides computational power and an extensive library of software for molecular structure analysis. Studies at the Center that will be discussed include: 1) bacterial toxins, 2) bovine ceruloplasmin, 3) glycyL- tRNA synthetase from E. coli, 4) ADP Glucose Pyrophosphorylase from photosynthetic bacteria, 5) cytochromes from photosynthetic bacteria, 6) novel organometallic compounds, 7) organotin-based polymer systems, 8) oxyallyl cation chemistry. The use of computers and x-ray instrumentation and innovative applications have been integrated into the undergraduate and graduate curriculum. The Center aspires to combine the best qualities of teaching and research universities where actively engaged students, faculty and staff work in close collaboration to expand knowledge. Support for the Center is generously provided by NSF-ILI-DUE, NSF-ARI-BIR, the State of California, CSUPERB, the Camille and Henry Dreyfus Foundation and pending, the W.M. Keck Foundation.