We have assessed the relative information content of a number of bulk solvent models using cross-validation. The real R approach was generalized to study the quality of the fit for all reflections as opposed to a single test set. We compared the single homogeneous solvent map model (Wang, B.-C., Methods Enzymol. 115, 90-112, 1985), the multiple-shell model (Schoenborn, B.P., J. Mol. Biol. 201, 741-749, 1988; Cheng, X.D. and Schoenborn, B.P., Acta Cryst. B46, 155-208, 1991), and the difference map (Badger, J. and Caspar, D.L.D., Proc. Natl. Acad. Sci. 82, 323-326, 1991). The relative merit of these models will be discussed.

PS-02.07.09 PHASE DETERMINATION OF MACROMOLECULAR CRYSTALS FROM MULTIPLE X-RAY DIFFRACTION USING A CONVENTIONAL LABORATORY SOURCE. By Mao-Tai Kuang, Chien-Mei Wang, and Shih-Lin Chang. Department of Physics, National Tsing Hua University, Hsinchu, Taiwan

Coherent interaction among diffracted waves in x-ray multiple diffraction has been successfully utilized in determining phases of structure-factor multiplets for organic crystals. For macromolecular crystals, synchrotron radiation is generally believed to be the only indispensable source for phasing the structure factors in multi-beam experiments, because the signal-to-noise ratio of the multiply diffracted intensities is usually very small. However, the limited synchrotron beam time and the fast deterioration of crystals under high photon flux are the disadvantages of using synchrotron radiation. To overcome this difficulty, we have used a rotating-anode x-ray generator together with a 2-axis four-circle diffractometer to carry out multiple diffraction experiments. The z-axis is a vertical arm for the detector mounted perpendicular to the diffracting plane. Secondary reflections can therefore be easily detected. We have applied this geometry to observe the intensities of many 3-beam and 4-beam diffractions for lysozyme crystals. The associated phases are correctly determined. The condition of observing the weak multi-beam intensities is derived and the difficulties encountered in the experiments are discussed.

PS-02.07.10 COMPARISON OF REAL-SPACE AND RECIPROCAL SPACE CRITERIA TO ASSESS THE ACCURACY OF MACRO-MOLECULAR CRYSTAL STRUCTURES. By J.-S. Jiang, R.B. Hubbard and A.T. Brunger. Department of Molecular Biophysics and Biochemistry, Yale University, U.S.A.

A number of real-space and reciprocal space criteria to assess the quality of atomic models has been compared. Among the criteria are the free R value (Brunger, A.T., Nature 355, 472-474, 1992), the real space R value (Branden, C.I. and Jones, T.A., Nature 343, 687-689, 1990), contiguity of density maps (Emsley, P.A. and Ruben, R., Acta Cryst. A47, 392-400, 1991) and satisfaction of geometric and stereochemical restraints. We have also generalized the real space R value to measure the agreement between atomic shapes of observed and computed density maps.

PS-02.07.11 CONNECTIVITY AND THE PHASE PROBLEM IN MACROMOLECULAR CRYSTALLOGRAPHY. By D Baker, B Buskirk, A Krakowski, C Wilson and D Agard. Department of Biochemistry and Biophysics, UCSF

The crystallographic phase problem is indeterminate in the absence of additional chemical information. The commonly employed chemical constraints—positivity, atomicity, and a solvent boundary—leave the phase problem (as determined for Fourier data sets at moderate (2.5-3.0 Å) resolution. A successful ab initio approach must make use of high resolution Fourier data and/or stronger chemical constraints. Such constraints can be exploited by the connective of the macroscopic. We have developed a rapid algorithm for measuring the connectivity of a map which promises in reducing the multiplicity of solutions to the phase problem. We have also developed a refinement method (PRSM) which exploits the connectivity constraint to iteratively improve phases. An initial electron density map is generated with accurate phases derived from a partial structure or from isomorphous replacement. A linear connected skeleton is then constructed from the map using a modified version of Green's algorithm and a new map is created from the skeleton. This "skeltonized" map is Fourier transformed to obtain new phases, which are combined with any starting phase information and the experimental structure factor amplitudes to produce a new map. The procedure is iterated until convergence is reached. The method has been applied to problems with starting phase information from either molecular replacement or isomorphous replacement and appears to be a significant improvement over solvent flattening in both cases.


Multiple isomorphous derivatives tested against the native x-ray diffraction pattern, were used to phase the h, k, l reflections and produce an electron density map of the collagen fiber. This allows conclusions to be drawn about the molecular packing in native fibrils and the molecular conformation of the telopeptides which contain the inter-molecular crosslinks.