PS14.01.10 DETERMINATION OF 3D VIRAL STRUCTURE FROM SOLUTION X-RAY SCATTERING. Yibin Zheng, Peter C. Doerschuk, School of Electrical and Computer Eng., Purdue Univ., West Lafayette, IN 47907 USA, John E. Johnson, Dept. of Molecular Biology, The Scripps Research Inst., La Jolla, CA 92037 USA, yibin@ecn.purdue.edu, doerschu@ecn.purdue.edu, jackj @scripps.edu

A new method for determining the low-resolution 3D structure of icosahedrally-symmetric viruses from solution x-ray scattering is proposed and demonstrated on cowpea mosaic virus (CpMV) data. In spherical coordinates, the electron density $\rho(\vec{x})$ is represented as a sum of icosahedral harmonics $T_{l,n}(\theta,\phi)$ with radially-dependent weights $A_{l,n}(r)$. The $T_{l,n}(\theta,\phi)$ are used because, for any choice of $A_{l,n}(r)$, the resulting $\rho(\vec{x})$ is icosahedrally-symmetric. The $A_{l,n}(r)$ are represented as a sum of spherical Bessel functions $z_l(\alpha_{l,p}r)$ with weights $c_{l,n,p}$. The $z_l(\alpha_{l,p}r)$ are used because the Fourier transform of $z_l(\alpha_{l,p}r)$ can be computed analytically. Linear combinations of $z_l(\alpha_{l,p}r)$ are used such that $\rho(\vec{x})$ is non-zero only between fixed inner (R_-) and outer (R_+) radii where the inner radius can be non-zero (e.g., empty particles). The two radii $(R_-$ and $R_+)$ and the weights $c_{l,n,p}$ are the only parameters in the model and the model can represent any icosahedrally-symmetric $\rho(\vec{x})$. The major short-coming of this representation is that it does not restrict $\rho(\vec{x})$ to be positive. To determine the parameters from the experimental data, we use the Levenberg-Marquardt method to minimize $\int k^8 |I(k) - \hat{I}(k)|^2 dk$ where $I(k)$ is the experimental data and $\hat{I}(k)$ is the predicted scattering pattern as a function of $c_{l,n,p}$. We have applied this method to experimental data (0.004279-0.020853Å⁻¹) for CpMV resulting in 3D reconstructions at 30Å resolution which accurately follow the known atomic resolution structures. In comparison to our previous work (ACA-95 Abstract W155; *Biophysical J.* 69(2):619-639, August 1995), the optimization required here is easier to compute and the model can represent a general $\rho(\vec{x})$. This work was supported by NSF grant BIR9513594.

Small Angle Scattering II
Applications

MS14.02.01 POLARIZED NEUTRON SCATTERING FROM POLARIZED NUCLEAR SPINS. H. B. Stuhrmann[1], B. van den Brandt[2], P. Hautle[2], J. A. Konter[2], S. Mango[2], T. O. Niinikoski[3], M. Schmitt[1], R. Willumeit[1], J. Zhao[1], K. H. Nierhaus[4], [1]GKSS Forschungszentrum D-21502 Geesthacht, Germany, [2]Paul Scherrer Institut, CH-5232 Villigen, Switzerland, [3]T. O. Niinikoski, CERN-PPE, CH-1211 Geneva, Switzerland, [4]K. H. Nierhaus, MPI für Molekulare Genetik, D-14195 Berlin, Germany

The scattering amplitude of neutron scattering by protons is known for its strong dependence on the polarization direction of the interacting spins. Polarized deuterons show a much weaker effect. This is the basis for nuclear spin contrast variation which is applied to the study of the *in situ* structure of macromolecular components of complex assemblies (1). Results of polarized neutron scattering from protonated tRNA in a deuterated ribosome clearly differentiate between the pretranslocational and the postranslocational state of the functional complex. Moreover the site of a small protonated mRNA fragment (14 kD) bound to the completely deuterated functional complex of the ribosome could be identified.

The alternative to ‚pre-contrasting' by isotopic substitution is the creation of contrast by selective nuclear spin depolarization or even better by reversal of nuclear spin polarization using the method of adiabatic fast passage. In dynamically polarized targets a frequency limited rf scan across the NMR profile acts preferentially on nuclei which are not close to the paramagnetic centers. The polarization of the nuclear spins near unpaired electrons remains unchanged. The size and the lifetime of the electronic spin label bound nuclear polarization domains appears to be largely spin diffusion controlled.

(1) H. B. Stuhrmann, N. Burkhardt, G. Dietrich, R. Jünemann, W. Meerwinck, M. Schmitt, J. Wadzack, R. Willumeit, J. Zhao, K. H. Nierhaus (1995) *Nucl. Instr. and Methods* A 356 124-132

MS14.02.02 CRYSTALS OF DEFECTS IN CHIRAL THERMOTROPIC MESOGENS: PERIODIC ARRAYS OF TWIST GRAIN BOUNDARIES. A.-M. Levelut, Laboratoire de Physique des Solides, Université Paris-Sud, F91405 Orsay Cédex, France

Crystals of defects form a distinct class of mesophases in which a periodic array of defects such as disclinations or dislocations coexist with the fluid organization at a molecular scale. These periodic networks are an intermediate step in a process where intrinsic bending or twisting forces tend to destroy the nematic or smectic organization [1].

Recently crystals of defects with a tetragonal lattice have been put in evidence in some chiral mesogenic molecules [2]. The tetragonal phase is obtained directly by cooling the isotropic liquid state. At lower temperature the only possible mesophase-mesophase transformation is toward a smectic (lamellar) mesophase with antiferroelectric properties. Finally the temperature range of existence of the tetragonal mesophase in a binary mixture decreases as the optical activity decreases so that this phase was never detected in racemic mixtures or in achiral compounds. X ray diffraction studies have been performed on single crystals of the tetragonal mesophase of several compounds. First of all the liquid ordering at a molecular scale is asserted by a wide angle isotropic diffuse ring. At small angle a set of sharp Bragg spots corresponds to a tetragonal tridimensional lattice. The unit cell contains about 500 molecules which confirms the "crystal of defects" nature of the mesophase. The lattice constants compare to the layer periodicity of the smectic antiferroelectric phase. In fact three different space groups have been identified : I4, I 4_1, P 4_1.

A description of the tetragonal phases as crystalline arrays of twist grain boundaries [3] (which can form a triply periodic minimal surface) inside an antiferroelectric structure is proposed. The twist grain boundaries perpendicular to the smectic planes divide the smectic structure in narrow sheets, the smectic planes are twisted by an angle of $\pi/2$ on each side of a boundary and the successive sheets correspond one each other by a 4_1 or a 4_2 helical axis.

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