MS13.02.06 FULL-PATTERN PARAMETERIZATION OF TWO-DIMENSIONAL DIFFRACTION AND SCATTERING DATA FROM ORIENTED POLYMERS. N.S. Murthy[1], K. Zero[1] and D.T. Grubb[2], [1]AlliedSignal Inc., Morristown New Jersey; [2]Cornell University, Ithaca, New York

Two-dimensional wide-angle diffraction data and small-angle scattering data from uniaxially oriented polymers are profile fitted by describing the intensity distribution as a product of two orthogonal functions in a suitable coordinate system. Whereas polar coordinates are appropriate for wide-angle data, elliptical coordinates for found to best describe the small-angle data. The parameters of the fit from the wide-angle data are used to describe the structure in terms of amorphous and crystalline orientation, crystallinity and crystallite size. The essential features fitted in the small-angle data include the equatorial streak, lamellar reflections and the interfibrillar interference peak. These parameters are used to describe the fibrillar and lamellar structures. The analysis is illustrated with wide-angle diffraction (x-ray) data, small-angle scattering (x-ray and neutron) data from a series of nylon 6 fibers. The results are compared with those from a previous analysis of a series of one-dimensional scans.

MS13.02.07 THE PROGRESS OF FULL-RECIPROCAL-SPACE X-RAY SCATTERING ANALYSIS IN STUDYING THE ORIENTED POLYMERS. Jia-Cong, Hu*, Department of Macromolecular Science, Fudan University, Shanghai, China 200433

Full-Reciprocal-Space X-Ray Scattering Analysis (FRS-XRSA), suggested by the author, is a new theoretical analysis, which can be used to investigate and characterize the crystallinity and orientation texture of various oriented polymers. FRS-XRSA is preferable to the traditional Power Method(PM), Pole Figure Method (PF), Azimuthal Angle Scanning Method (AAS) and Orientation Distribution Function Analysis (ODFA) to investigate the preferred orientation polymers, the reason had been discussed in my original papers. In the present work, the main progress is how to apply FRS-XRSA in studying the oriented fiber, oriented film and strained polymers. For example, the crystallinity and orientation texture of uniaxially oriented hard elastic iso-poly (- propylene) fiber (HEPP) and biaxially stretched poly (- ethylene terephthalate) film(PET) were measured by FRS-XRSA procedure. The results show that the crystallinities, not only of the original samples but also of the on-line stretching samples, obtained by FRS-XRSA are more reasonable than that by PM, and all of the orientation textures and average orientations of a set of (hkl) planes, for HDEPP e.g. (040), (110), (130) and (111) planes; for PET e.g. (011), (110), (021) (010), (100), (113), (101), (121) and (105) planes, and various crystal axes, e. g. a, b and c, can be obtained by FRS-XRSA easily. The distribution of cristallite size in FRS can also be gained uniquely by this procedure. Because the crystal systems of i-PP and PET belong to the most complex two systems, i. e. monoclinic and triclinic systems respectively, now we deal with them successfully, so the other systems in crystalline polymers would be handled more easily. We think that FRS XRSA can be an alternative new procedure to study the crystallinity and orientation texture of various oriented polymers simultaneously and effectively.

MS13.02.08 MEASURING DISORDER IN POLYNUCLEOTIDE FIBERS. W. J. Stroud and R. P. Millane, Whistler Center for Carbohydrate Research, Purdue University, West Lafayette, Indiana 47907-1160, U.S.A.

Diffraction patterns from oriented polycrystalline fibers of some biopolymers show both Bragg and continuous layer line intensities as the result of disorder within the crystalline domains of the fibers. Diagnosing this disorder and quantitatively accounting for its effects on diffraction, is essential for accurate structure determinationusing data measured from these patterns.

We have developed a general statistical model of disorder in fibers along with expressions that describe the effects of disorder on cylindrically averaged intensities [1,2,3]. To demonstrate the utility and applicability of our model, we have used it to quantitatively analyze the disorder in two polynucleotide fibers. The disorder in each fiber was diagnosed by matching features of diffraction patterns calculated from models to key features of the observed diffraction patterns. For both fibers, this lead to a unique description of the disorder present [4]. Initially only uncorrelated disorder was considered, but subsequent inclusionof correlations in the lattice disorder model significantly improved the match between the calculated and observed reflection profiles and continuous intensity distributions for one of the specimens. Comparison of the disorder parameters estimated for the models with correlated and uncorrelated lattice disorder showed that both models describe the same type and degree of local disorder.

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MS13.03.01 STRUCTURAL BASE OF ASSEMBLY AND POLYMORPHISM OF BACTERIAL FLAGELLAR FILAMENT. Keiichi Namba, Yuko Mimori, Ichiro Yamashita, Ferenc Vonderviszt, International Institute for Advanced Research, Matsushita Electric Industrial Co., Ltd., 3-4 Hikaridai, Seika 619-02 Japan

A complementary use of X-ray fiber diffraction and electron cryomicroscopy has allowed us to deduce the domain structure of flagellin subunit in the flagellar filament, which reveals overall folding of flagellin and direct interaction of the termini in the very inner core of the filament. Flagellar filaments are formed by self-assembly process and are known to be polymorphic, being able to take various supercoiled forms as well as the two distinct straight forms. To understand the mechanisms of self-assembly and polymorphism, structure analysis toward atomic resolution is underway. Electron cryomicroscopy and helical image reconstruction were used to analyze the structures of various straight filaments at around 10 Å resolution. The layer-line spacings and symmetries of the filaments used in the EM analyses were obtained from X-ray fiber diffraction patterns of well oriented sols with disorientation angles less than 1 degree, which were prepared by liquid crystallization and magnetic orientation of flagellar sols. By carefully comparing the filaments of intact flagellins with those reconstituted with various flagellins of terminal truncations and central deletions, structural domains were assigned to sequence positions. In particular, a direct terminal interaction was found essential for the correct folding of large terminal regions that form the very inner core of the filament, which is in turn essential for the polymorphic ability.

A two-dimensional extension of the angular deconvolution

method was applied to process X-ray diffraction patterns from well-oriented sols, which allowed us to extract layer-line amplitude distribution reliably. The phase data from the EM analyses were combined with X-ray amplitudes from the native and heavy atom derivatives of the filament to locate heavy atom binding positions in difference Fourier maps. The multiple isomorphous replacement phasing procedure is being applied to deduce electron density maps at higher resolution available in the X-ray data.

MS13.03.02 REFINEMENT OF THE F-ACTIN STRUCTURE AGAINST FIBER DIFFRACTION DATA. M. M. Tirion, K.C. Holmes, M. Lorenz. Department of Membrane Research and Biophysics, weizmann Institute of Science, Rehovot, Israel.

The crystal structure of G-actin permits development of atomic models of F-actin based on X-ray fiber diffraction images from aligned filaments. The initial atomic model of F-actin, obtained using only 4 structural parameters, reproduced most features of the X-ray and electron-microscopic data. However, the 7Å resolution X-ray fiber diffraction images contain sufficient data to refine more than 4 structural parameters. Refinement at atomic level is too fine-grained and would overfit the diffraction data. The challenge therefore, is to identify appropriate structural parameters which reduce the fiber diffraction residual while preserving the stereochemistry of actin.

We present two different methods: use of slow, normal modes of G-actin as structural refinement parameters, and a Monte-Carlo method to select appropriate subdomains in G-actin, for the refinement of F-actin. Both methods resulted in a significant reduction of the residual and showed similar trends in the structural changes from G- to F-actin, including the closure of the nucleotide binding pocket between the large and small domains. This finds strong support from biochemical experiments which show that polymerization of actin inhibits the nucleotide exchange rate.

MS13.03.03 STRUCTURE OF MUSCLE IN THE RELAXED STATE AND RIGOR LABELLED WITH MYOSIN S-1: IMPLICATIONS ABOUT FORCE PRODUCTION. Harford, J. J., Hudson, L., Denny, R., Squire, I. M., Biophysics Section, Imperial College, Prince Consort Rd, London, UK

The purpose of this project is to solve the structure of the A-band unit cell in relaxed fish muscle and to use this to follow the molecular movements in active muscle regulation and force generation. The first frame, relaxed muscle, has now been solved. Time-resolved X-ray diffraction patterns from contracting plaice fin muscle have been recorded at 1ms or 5ms time-intervals (depending on the region being studied) and these are then processed using CCP13 software and modelled using the known myosin head shape and actin filament structure. The solution for the first frame has revealed the organisation of myosin heads around the actin filaments in the hexagonal A-band unit cell. This frame is now being used as a starting structure to model successive frames through the time-series, thus producing a 'Movie' of the molecular processes involved in contraction. Already, from analysis of the resting and rigor muscle structures, it has been shown that myosin heads need to swing axially on actin by about 5 to 15nm in order to proceed from the resting to rigor states. It is presumed that the heads need to do this in active force generation as well. More recently we have recorded X-ray diffraction patterns to a resolution of about 1nm from chemically skinned plaice muscle in the rigor state labelled with exogenous myosin S-1 heads. Modelling of these patterns, now in progress, is revealing in much greater detail the changes in conformation of the myosin heads that accompany this transition from the relaxed to the rigor state.

MS13.03.04 STRUCTURAL DIVERSITY IN FILAMENTOUS BACTERIOPHAGES. Makowski, L., Institute of Molecular Biophysics, Florida State University, Tallahassee, FL 32306-3015, USA

X-ray and neutron diffraction data have been used to study the structure of filamentous bacteriophage M13 and Pf1, and chemically and genetically constructed variants of these particles. Ambiguity is intrinsic to the analysis of the structure of macromolecular assemblies using fiber diffraction. The ratio of data-to-model parameters for fiber diffraction is substantially lower than for x-ray crystallography. Even when the number of isomorphous derivatives are available, it may be not possible to obtain a unique structural solution from fiber diffraction data. Consequently, after a number of years, there continues to be substantial controversy in the literature about the filamentous bacteriophages M13 and Pf1. Differences among the molecular models for the viruses have substantial implications for our understanding of their membrane-mediated assembly, and for their use in phage display technology. It is now possible to obtain fiber diffraction data from a wide range of structural variants of filamentous bacteriophages that can provide rigorous tests of competing structural models. The relative positions and fidelity with which known structural features of the variants are reproduced in difference maps calculated on the basis of competing structural models provides a significant test of the competing models. The use of this strategy for exploring competing models of the coat proteins of filamentous bacteriophages Pf1 and M13 is demonstrated.

MS13.03.05 MOLECULAR DYNAMICS REFINEMENT WITHOUT DECONVOLUTION IN FIBER DIFFRACTION OF BIOLOGICAL POLYMERS. Gerald Stubbs and Hong Wang, Department of Molecular Biology, Vanderbilt University, Nashville, Tennessee 37235

There is useful information in a fiber diffraction pattern even beyond the resolution at which layer lines overlap. Most fiber diffraction studies involving large monomers have been limited to the non-overlapping region of the pattern, since objective determination of a molecular structure depends on complete phasing of separated diffraction intensities. Once a model has been constructed, however, there is no reason to discard higher resolution data. Makowski has shown that beyond the point where layer lines can be deconvoluted, the information content of a diffraction pattern continues to increase with resolution, although only linearly. The most powerful method of refinement of macromolecular structures currently available is molecular dynamics refinement, for example as used in our adaptation of the program X-PLOR to use fiber diffraction data. We have further modified X-PLOR to handle undeconvoluted data. In addition to atomic coordinates, global parameters such as specimen disorientation are refined. Testing so far has been against simulated and real helical virus data. Supported by NSF grant MCB 9506204.