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.

1. Stroud W. J. and Millane R. P. (1995). Acta Cryst. A51, 771—790.
2. Stroud W. J. and Millane R. P. (1996). Proc. R. Soc. Lond. 452, 151—173.
3. Stroud W. J. and Millane R. P. (1995). Acta Cryst. Submitted.
4. Stroud W. J. and Millane R. P. (1995). Acta Cryst. A51, 790—880.

Fiber III
Fiber Diffraction of Biological Polymers

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