DS-12.03.04 WIDE ANGLE XRD STUDY OF THE EFFECT OF PROCESSING CONDITIONS ON POLY(V-PHENYLENE BENZOBISTHIAZOLE) BY E. Garstein* and Y. Cohen , "Department of Physics and Department of Chemical Engineering, Technion, Haifa 32000, Israel.

Fibers and films exhibiting exceptional mechanical properties have been developed from rigid rod polymers by processing from solution in a way which provides very high alignment of the rigid chains. The success in translating the molecular strength and stiffness of the individual rigid chains to macroscopic properties relies on unique morphology on the supramolecular scale, and it is therefore important to characterize the microstructure on this scale.

In addition to microfibrous characterization, in the SAXS study (Cohen and Garstein, 1990) of polymer fibers formed in a supercellular drug by drawing the fibers at high temperature through the surface at 600°C for 10 sec., additional scans (in the direction of fiber axis) were carried out employing symmetrical transmission technique and equatorial scans (perpendicular to the fiber axis) employing symmetrical reflection technique. The presence of the multiple equatorial reflections pointed to a good orientation of the molecules, as well as to the high degree of axial order. From the WAXS photographs recorded using Siemens camera, the preferred orientation was found to improve according to the azimuthal angle a=0°-20° to a=20°-28° for the -CO2-dried and the heat treated films, respectively. The equatorial scans showed that the 3 D crystallography improved with heat treatment, since the overlapping reflections became better resolved. The lateral size of the crystals is estimated from the breadth of the equatorial peaks using the Scherrer formula increased from 4 nm to 11 nm, making it comparable to the microfibrous diameter as a result of better chain packing. The observed shift of the one-dimensional reflections with heat treatment also indicated the possible combination of the reduction of the disorder and/or increase in the crystal size.

It is much of interest now to apply the paracrystallinity models for the detailed interpretation of the diffraction spectra.


DS-12.03.05 FRX-XRSA FOR INVESTIGATION OF CRYSTALLINITY AND ORIENTATION OF PREPARED ORIENTATION POLYMERS. By J.C. Hu*, Department of Materials Science, Fudan University, Shanghai, China.

A new theoretical analysis. Full Reciprocal Space X-Ray Scattering Analysis (FRX-XRSA) is suggested by the author. This method can be used to investigate and characterize the crystallinity and orientation distribution of crystallites (ODC) of various preferred orientation polymers. Based on the FRX-XRSA conservation principle (FRX-XRSA C), we first obtain the X-ray crystallinity of the non-oriented examined samples. Based on the crystallography geometry principle (CGP), we establish a series of basic relationships between crystallographic system and sample coordinate system of various orientation samples, which can simplify the deduction of ODC greatly and in principle. Pole Figures of most of main (hkl) planes concerned can be obtained by one FRX-XRSA measurement. FRX-XRSA eliminates the interference of amorphous scattering and heavy overlap of (hkl) planes' projection by means of Compton Peak Resolution (CPR), so the results of FRX-XRSA are more reasonable than that of traditional Pole Figure Method. Furthermore, in contrast with Orientation Distribution Function Analysis (ODFA), because FRX-XRSA is a direct method, no ghost texture occurs in FRX-XRSA. Therefore, FRX-XRSA is preferable to the traditional Powder Method. Pole Figure Method and ODFA to investigate and characterize the crystallinity and orientation of the preferred orientation polymers.

DS-12.03.06 THE DETERMINATION OF TOPOLOGICAL CONNECTIVITY PARAMETERS BY B. Müller, Institute of Physical Chemistry, Friedrich-Schiller-University of Jena, Germany

The complex and complicated structures of glasses, gels, polymers, melts, amorphous semiconductors, thin layers etc. determined by a great structure variety on the different structure levels, mostly in thermodynamic non-equilibrium, gives practically the result that both their structure analysis and their structure theory represent a scientific problem till now. In this paper, a contribution is given to the structure theory and analysis of amorphous matter based on both homomorphic and connective automorphisms on cellular systems. Therefore, the topological connective structure description is very fit for a description of chemical bond structure (B. Müller, in Physical Research: Amorphous Structures, Berlin, Akademie-Verlag 1990, 292-306). The structure elements of these topological connective configuration are realized as k-celloids with different dimension k (k=0, 1, ..., 0) on a (d+n)-dimensional configuration space. Each of the k-celloids represents a k-dimensional figure bounded at least k+1 (k+1)-celloids (k≥1). The β-celloids fill utterly and completely the d-dimensional configuration space. Therefore, the configuration space for itself has a structure. A complete determination of all topological connective invariant of a configuration represented by means of the connective mean value parameters Nk is possible, if the atomic coordinates are known as those in crystalline structures or in structure models of amorphous matter. The mean Nk of called also connective parameter, characterizes the number of linkoid connective relations of a typical k-celloid regarding its t-celloids. The algorithm of our FORTRAN computing program NWS (R. Schubert, B. Müller, Computer Program NWS, Rechenzentrum, Friedrich-Schiller-University of Jena, Germany) is described in this paper. Generally, the program NWS can compute the structure parameters of a connective configuration given as follows: (i) k-celloids (vertices): In our case of structures in atomic systems the atoms given as a point set represent the β-celloids. The program generated a list of atoms differed in the atomic and binding kind, which contains the k-celloids m[k] of (ii) t-celloids (edges): The bonds existing between neighboring atoms represent t-celloids of configuration. Depending on the aim of bonding several kinds of binding may be used in order to declare the t-celloids mt of and the connective matrix M(t) of the linkoid connective relations m(t) of. The t-celloids represent spatial correlation functions of 2 order into the configuration space. (iii) 3-celloids (faces): The edges of cellular systems may be free cycles also called rings or loops. Only such rings are faces, which separate two neighboring polyhedra. Search of all possible rings contained in the connective matrix M(t) and discrimination of the faces m(t) which are generally the smallest rings, and specification of the connective matrix M(t) by means of the connectivity of the faces. (iv) Evaluation of the connective distribution functions and the connective parameters with help of the connective matrices (M(t)) and (M(l)) of 3-celloids (polyhedra): The 3-celloids will be formed by faces and represent spatial correlation functions of 4 order and characterize the connective structure of the complete configuration. Several applications of the computer program NWS in order to evaluate the topological connective parameters of zeolites, feldspars, the various crystalline phases of SiO2, and of few models of amorphous SiO2, respectively, are shown in the paper.