352   12-Amorphous, Imperfectly Ordered and Quasi-periodic Materials

DS–12.03.04 WIDE ANGLE XRD STUDY OF THE EFFECT OF PROCESSING CONDITIONS ON POLY(P-PHENYLENE BENZOBISTHIAZOLE) By E. Gartstein* 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 the stiffness of the individual rigid chains to macroscopic properties relies on suitable morphology on the supramolecular scale, and it is therefore important to characterize the microstructure on this scale.

In addition to microfibrillar characterization in the SAXS study (Cohen and Gartstein, 1990) of polymer wet films dried in a supercritical CO_2 and also subjected to heat treatment by drawing through the furnace at 600° for 10 sec., meridional 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 meridional 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 Statton camera, the preferred orientation was found to improve according to the azimuthal angle $\alpha=27°$ -30° to $\alpha=22°$-25° for the as-CO_2 dried and the heat treated films, respectively. The equatorial scans showed that the 3-D crystallinity improved with heat treatment, since the overlapping reflections became better resolved. The lateral size of the crystallites estimated from the breadths of the equatorial peaks using the Scherrer formula increased from 4 nm to 11 nm, making it comparable to the microfibrillar diameter as a result of better chain packing. The observed sharpening of the meridional reflections with heat treatment also indicated on the possible combination of the reduction of the disorder and/or increase in the crystallite size.

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

1. Y Cohen and E. Gartstein, (1990) Proc. 5th Isr. Mater. Sci. Soc.; Haifa, p. 259, eds. M. Bumberger and M Schorr, Freund Publishing House, Ltd.

DS–12.03.05   FRS–XRSA FOR INVESTIGATION OF CRYSTALLINITY AND ORIENTATION OF PREFERRED 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 (FRS-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 FRS-XRS conservation principle (FRS-XRSCP), we at first obtain the X-ray crystallinity of the non-powdered orientated samples. Based on crystallography geometry principle (CGP), we establish a series of basic relationships between crystallite coordinate 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 FRS-XRS measurement. FRS-XRSA eliminates the interferences of amorphous scattering and heavy overlap of (hkl) planes' diffraction by means of Computer Peak Resolution (CPR), so the results of FRS-XRSA are more reasonable than that of traditional Pole Figure Method. Furthermore, in contrast with Orientation Distribution Function Analysis (ODFA), because FRS-XRSA is a direct method, no ghost texture occurs in FRS-XRSA. Therefore, FRS-XRSA is preferabe 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 CONNECTIVE STRUCTURE PARAMETERS. By B. Müller, Institute of Physical Chemistry, Friedrich-Schiller-University of Jena, Germany

The complex and complicated structures of glasses, gels, polymeres, 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 homeomorphic 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, 293-306). The structure elements of these topological connective configuration are realized as k-celloids with different dimension k ($k = 0, 1, ..., d$) on a $(d+1)$ dimensional configuration space. Each of the k-celloids represents a k-dimensional figure bounded at least k+1 $(k-1)$-celloids ($k \geq 1$). The d-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 invariants of a configuration represented by means of the connective mean value parameters N^{kl} is possible, if the atomic coordinates are know as those in crystalline structures or in structure models of amorphous matter. The mean N^{kl} called also connective parameter, characterizes the number of limboide connective relations of a typical k-celloid regarding its l-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) 0-celloids (vertices): In our case of structures in atomic systems the atoms given as a point set represent the 0-celloids. The program generated a list of atoms differed in the atomic and binding kind, which contains the 0-celloids m^0_p. (ii) 1-celloids (edges): The bonds existing between neighbouring atoms represent 1-celloids of configuration. Depending on the aim of bonding several kinds of binding may be used in order to declarare 1-celloids m^1_q and the connective matrix (M^{01}) of the limboide connective relations m^{01}_{pq} The 1-celloids represent spatial correlation functions of 2. order into the configuration space. (iii) 2-celloids (faces): The edges of cellular systems may be form cycles also called rings or loops. Only such rings are faces, which seperate two neighbouring polyhedra. Search of all possible rings contained in the connective matrix (M^{01}) and discrimination of the faces m^2_r which are generally the smallest rings, and specification of the connective matrix (M^{12}) by means of the connectivity of the faces. (iv) Evaluation of the connective distribution functions and the connective parameters with help of the connective matrizes (M^{01}) and (M^{12}). (v) 3-celloids (polyhedra): The 3-celloids will be formed by faces and represent spatial correlation functions of 4. order and characterize the connective structur 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 SiO_2, and of few models of amorphous SiO_2, respectively, are shown in the paper.