DS-12.03.05 WIDE ANGLE XRD STUDY OF THE EFFECT OF PROCESSING CONDITIONS ON POLY(P-PHENYLENE BENZO[THIAZOLE]) BY E. Garsstein 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 variable morphology on the supramolecular scale, and it is therefore important to characterize the microstructure on this scale.

In addition to microfibril characterization in the SAXS study (Cohen and Garsstein, 1990) of polymer wet films dried in a supercritical fluid, we also submitted heat treatment by drawing hot steam through the furnace at 600°C for 10 sec, accord, enabling symmetrical transmission technique and equatorial scans (perpendicular to the fiber axis) employing symmetrical reflection technique. The presence of the multiple mesodimensional reflections pointed to a good orientation of the monofibrils, as well as to the high degree of axial order. From the WAXS photographs recorded using a Siemens camera, the preferred orientation was found to improve according to the azimuthal angle α = 0° - 30° to α = 25° - 28° for the as-CO2 dried and the heat treated films, respectively. The equatorial scans showed that the 3-D crystallinity improved with heat treatments since the overlapping reflections became better resolved. The lateral size of the crystallites estimated from the breadth of the equatorial peaks using the Scherrer formula increases from 8 nm to 11 nm, making it comparable to the microscopic diameter of a result of better chain packing. The observed value of the mesodimensional reflections with heat treatment also indicated on the possible combination of the reduction of the disorder and/or increase in the crystalline size.

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


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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, 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 structural representation is a scientific problem till now. In this paper, a contribution is given to the structure theory and analysis of amorphous matter based on both homomorphous 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+1) dimensional space configuration. Each of the k-celloids represents a k-dimensional figure bounded at least k-1 (k=0) celloids (k=1). The 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 called also connective parameter, characterizes the number of linkable 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 computing program NWS can compute the structure parameters of a connective configuration given as follows: (i) V-celloids (vertices): In our case of structures in atomic systems the atoms given as a point set represent the V-celloids. The program generated a list of atoms differed in the atomic and binding kind, which contains the V-celloids mVL / (ii) l-celloids (edges): The bonds existing between neighboring atoms represent l-celloids of configuration. Depending on the aim of bonding several kinds of binding may be used in order to declare l-celloids (mL): The edges of cellular systems may be for cycles also called rings or loops. Only such rings are faces, which separate two neighboring polyhedron. Search of all possible rings contained in the connective matrix (ML) and determine of the faces mL, which are generally the smallest rings, and specification of the connective matrix (M(12)) by means of the connectivity of the faces. (vi) Evaluation of the connective distribution functions and the connective parameters with help of the connective matrices (M(12)) and (M(12)). (vii) V-celloids (polyhedrons): The 3-celloids will be formed by faces and represent spatial correlation functions of 4th 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, foams, the various crystalline phases of SiO2, and of few models of amorphous SiO2, respectively, are shown in the paper.