10.1–1 A NEW TREATMENT OF THE THEORY FOR SMALL-ANGLE X-RAY SCATTERING WITH APPLICATIONS TO POLYSTYRENE CRAZES.* By M.-Y. Tang and J. F. Fellers, The University of Tennessee, Knoxville, Tennessee 37996-2200, and J. S. Lin, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831.

Surface scattering phenomenon of electromagnetic waves by single or multiple layers of films are reviewed and a special treatment for the total reflection of x-rays is developed. This theory is applied to the analysis of the surface scattering observed in SAXS studies of two-phase matter in polymers having lamella stacks or a flat interfacial boundary structure. Important features of this vector theory are the ability to calculate the surface scattering invariant, the absolute scattering intensity, and surface roughness that gives rise to dispersion of specular reflection from perfectly smooth surfaces. By considering the interfacial surface roughness of polystyrene crazes, the surface scattering spectrum is calculated theoretically and compared to some experimental results. Also the theory is presented in such a way as to compare surface scattering to volume scattering, i.e. both two and three dimensional scattering events can be simultaneously treated. This gives rise to a new quantitative analysis of crazes in polystyrene.

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10.1–2 AN INTERPRETATION OF THE DYNAMICS MORPHOLOGICAL CHARACTER OF POLYSTYRENE CRAZES USING SMALL-ANGLE X-RAY SURFACE AND VOLUME SCATTERING THEORY.* By M.-Y. Tang, P. A. Westbrook, J. F. Fellers, The University of Tennessee, Knoxville, Tennessee, 37996-2200 and J. S. Lin, Oak Ridge National Laboratory, Oak Ridge, 37831

A study of the dependence of polystyrene craze morphology with respect to molecular weight parameters and stress history was performed at the National Center for Small-Angle Scattering Research. Small-angle x-ray scattering (SAXS) patterns are analyzed using reflection theory for the tensile axis scattering and volume scattering theory for the non-tensile axis, as prescribed from analysis of earlier work. Morphological characteristics such as the surface scattering invariant, surface correlation distance, volume scattering invariant, microvoid fraction, and microvoid average size can now be determined from the statistical parameters contained in the fitted distribution function. Important information about the stress and time dependence of internal surface creation compared to microvoid creation can now be deduced from this analysis of the scattering function. Also the normalized scattering intensity of post fracture crazes is shown to be molecular weight dependent. Additionally, the crack propagation mechanism within the crazed material discussed by Kambour that the crack jumps back and forth across the craze is confirmed and calculated by the theory to be approximately 5 μm in steplength as experimentally observed by Behan and Hull.

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10.2–1 THE CRYSTAL STRUCTURES OF SOME POLYESTERS USING X-RAY AND ELECTRON DIFFRACTION.

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The structures of a family of related polyesters, poly(hexamethylene terephthalate) or poly(6GT), poly(1,4-trans-cyclohexanediyldimethylene terephthalate) and the parent succinate, [poly(t-CDT) and poly(t-CDS) respectively], have been established using X-ray fiber diffraction as well as electron diffraction of micro single crystals of these polyesters. As revealed by electron microscopy and electron diffraction, poly(6GT) is at least dimorphic, one form being triclinic, the other, monoclinic. However, in both cases, the hexamethylene sequence is in the fully extented conformation. The various unit cells observed for poly(6GT) arise from different packing modes. The X-ray fiber diagram of poly(6GT) is made up of diffraction spots from both the triclinic and the monoclinic forms. Poly(t-CDT) and poly (t-CDS) are triclinic and monoclinic respectively. The crystal structures were confirmed using X-ray fiber diffraction for the former and by three dimensional electron diffraction for the latter. The trans-cyclohexanedimethylene section of the polyesters have the same stretched conformation and both the terephthaloyl and the succinate groups are planar. The conformations and the packing of the above polyesters will be discussed and compared.

10.2–2 INVESTIGATIONS OF THE CRYSTAL STRUCTURES OF SOME nT NYLONS.

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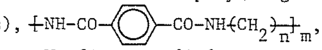
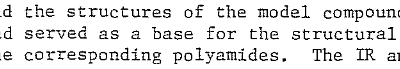
We have undertaken to determine the crystal structures of the series of poly(oligomethylene terephthalamides), , better known as nT Nylons. We first studied a series of model compounds chosen for their chemical similarity with the nT Nylons. These compounds, the N,N'-oligomethylene dibenzamides, or nDBN, , have been synthesized and characterized by IR spectroscopy and single crystal X-ray diffraction for n=2 to 10. The structures were established by direct methods. We therefore gained access to detailed information on the bond distances and angles, the conformations of the methylenic sequences as well as the hydrogen bonding schemes, as the number of CH_2 groups increased from 2 to 10. The structure of 6T Nylon was then investigated making use of both X-ray fiber diffraction diagrams and electron diffraction patterns obtained from micro single crystals of this polyamide. The correlations noted between the IR spectra and the structures of the model compounds were extended and served as a base for the structural determination of the corresponding polyamides. The IR and the structural features of the model compounds and their relations to the parent polyamides will be discussed.