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Morphological parameters in supramolecular structure of new IPP/PLA fibers using saxs

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ABSTRACT

Using small angle X-ray scattering (SAXS) data recorded by E.Wojciechowska et al.[1] for iPP/PLA fibers, we have computed microstructural parameters by simulating SAXS pattern employing one-dimensional Hosemann's paracrystalline model. For this purpose we have used the SAXS data of the fibers containing 100wt% of iPP and 40wt% of PLA. The supramolecular structure of fibers was correlated in terms crystalline and amorphous phase lengths. It is observed that there are significant changes in phase lengths owing to the presence of biodegradable PLA when compared to polypropylene fibers.

INTRODUCTION

Polypropylene fibers are synthetic fibers which are widely used in the textile industry because of their abrasion resistance, resistance to chemical and biological agents. Also it has good heat-insulating properties and of low manufacturing cost[2,3]. The main drawback of these fibers is non-biodegradability. In view of this earlier investigators have made an extensive work to obtain modified polypropylene fibers that would be partly biodegradable[4,5]. The polylactide (PLA) is a component in polypropylene fibers which has biodegradability. Adding of PLA to polypropylene with different composition it was observed that there is significant change in biodegradability and their properties[6,7]. Extensive work on SAXS study of iPP (melt of polypropylene)/ PLA (polylactide) fibers [Slovnaft isotactic polypropylene TATREN TI 992 with MFI 309/10 min (230C/ 2.16 Kg) and poly(L-lactide) RESOMER^R L 207 produced by Boehringer Ingelheim Pharma GmbH were used] were carried out by E.Wojciechowska et al.[1].

Using one-dimensional linear paracrystalline Hosemann's model we have carried out SAXS profile analysis of different composition iPP/PLA fibers, and were able to compute and quantify the composition of PLA in iPP on the basis of phase lengths, long periodicity and distribution functions in terms of biodegradability.

THEORY

The linear paracrystalline model of polymer morphology like synthetic fiber comprises of stacks containing a finite number of crystalline lamellae separated by amorphous segments. The thickness of successive lamellae along a stack is randomly selected from a certain probability density function, as the length of amorphous segment, although they may be distributed according to a different function. If it is assumed that the transverse width of a stack is infinite and that the lamellae boundaries are flat and normal to the axis, then the X-ray beam normal to stack axis will be scattered along a line in reciprocal space parallel to the stack axis on the distribution of intensity along this will be given at small angles. The equation is given by[8].

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$$\frac{2I(\pi S)^2}{\Delta\rho^2} = Re[\frac{(1-H_Y)}{(1-H_YJ_Z)}\{N(1-J_Z)+ \frac{J_Z(1-H_Y)(1-H_YJ_Z)^N}{(1-H_YJ_Z)}\}] \quad (1)$$

where H_Y and J_Z are respectively the Fourier transforms of the normalized distribution function of lengths Y and Z of the amorphous and crystalline phase segments, $S(=2\sin\theta/\lambda)$ is the scattering vector, 2θ is the scattering angle and λ is the wavelength of radiation (CuKα, $\lambda=1.542$Å), N(=20 units) is the number of repeating units in a stack, $\Delta\rho$ is the difference between the electron densities of the phases and I(s) is the scattering intensity as a function of scattering angle parallel to stack axis. If it is assumed that the fiber comprises of parallel stacks, incoherently arranged, there will be distribution of intensity scattered by fiber. A correction of broadening of intensity profile has been reported[9] and incorporated here.

Using exponential distributions for H_Y and J_Z, Hosemann's equation (1) is expressed in a form which is amenable to computational analysis and is given by

$$\frac{2I(\pi S)^2}{\Delta\rho^2} = \frac{C}{F} + \frac{(D+E)}{F^2} \quad (2)$$

where

$$F = 1 + A^2B^2 - 2AB\cos X \quad (3)$$

$$C = N\{1 - A^2B^2 - A(1-B^2)\cos\phi - B(1-A^2)\cos\chi\} \quad (4)$$

$$D = \frac{B[(1-A^2)(1-A^2B^2)\sin X\sin\phi + \{(1+A^2B^2)\cos X - 2AB\}\{(1+A^2)\cos\phi - 2A\}]}{G} \quad (5)$$

$$G = 1 - A^NB^N\cos NX \quad (6)$$

$$E = A^NB^{N+1}\sin NX[(1-A^2B^2)\{(1+A^2)\cos\phi - 2A\} \sin X - (1-A^2)\times\{(1+A^2B^2)\cos X - 2AB\}\sin\phi] \quad (7)$$

For given values of A, B, χ and ϕ, I(S) can be evaluating from the equations (2) to (7). A, B, χ and ϕ are the values of Fourier transforms of the probability distributions of the amorphous and crystalline phase lengths. A and χ are related to the distribution of phase-Y segment lengths and B and ϕ to that of phase-Z segment lengths[10].

EXPERIMENTAL

SAXS data of iPP/PLA fibers collected using Philips PW1830 X-ray generator of $\lambda=1.542$Å and reported by E.Wojiechowska et al.[1]. was used in this paper.

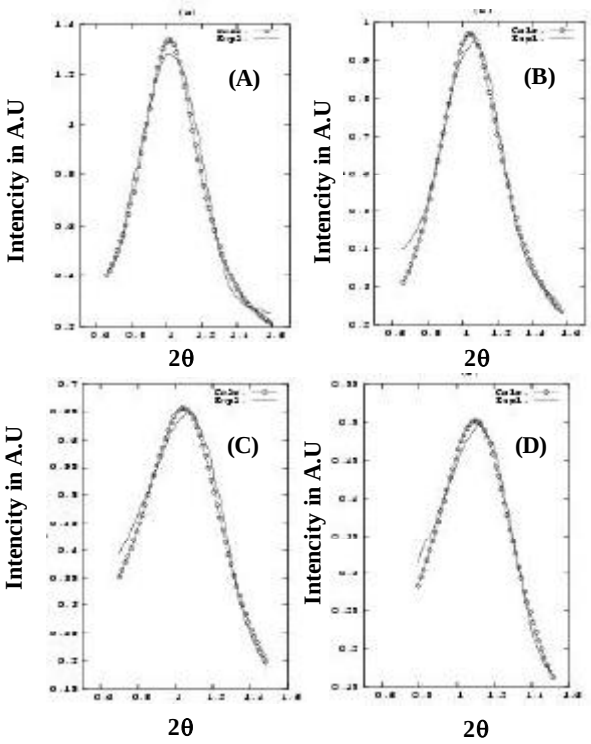

Figure 1: Exponential and simulated SAXS profiles using paracrystalline model (a) iPP/PLA composition of (100/0), (b) iPP/PLA composition of (90/10), (c) iPP/PLA composition of (80/20) and (d) iPP/PLA composition of (60/40)

RESULT AND DISCUSSIONS

Figure 1(a-d) show the simulated and experimental small angle X-ray scattering profile of supramolecular structure of melt iPP/PLA fibers of composition (100/0, 90/10, 80/20 and 60/40). The values of $<\chi^2>$ (goodness of fit) averaged over 10 successive points are also shown in the figure 1. The objective of this investigation has been to establish the general validity of the paracrystalline model and also to investigate the detailed changes in morphology due to biodegradable property of different composition of melt iPP/PLA fibers. Figure 2(a-b) shows the normalized exponential probability distribution function of the lengths of the phases crystalline (γ_Z) and amorphous (γ_Y). The values of morphological parameters like long period (L), phase length (<Y> and <Z>), phase ratio (Y/Z) and probability distribution of the phases (γ_Z and γ_Y) for different composition of iPP/PLA fiber given in the TABLE 1. Here the long period significantly decreases with increase of composition of polylactide in polypropylene. The phase ratio also in-

TABLE 1: Morphological parameters of supramolecular structure of iPP/PLA fibers

Composition iPP/PLA	Long period in Å	Phase ratio (Y/Z)	γ_Y	γ_Z	<Y> in Å	<Z> in Å	Crystallanity <Z>/<Y>+<Z>	N	$<\chi^2>$
100/0	104.0	0.30	0.031	0.250	31.2	72.8	0.70	20	0.004
90/10	101.0	0.25	0.110	0.235	25.2	75.8	0.75	20	0.001
80/20	91.9	0.30	0.280	0.200	27.2	64.3	0.70	20	0.001
60/40	87.0	0.35	0.255	0.200	30.5	56.5	0.65	20	0.001

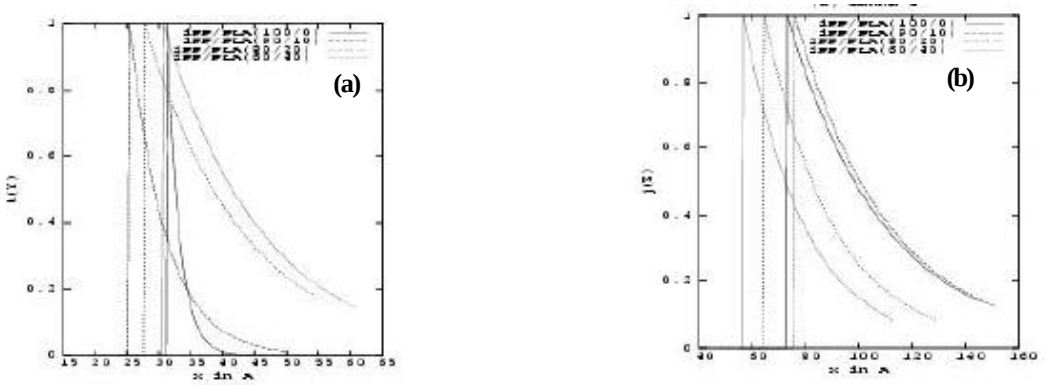

Figure 2: The normalized exponential distribution function of the lengths of the phases (a) Gamma-Y (amorphous) and (b) Gamma-Z (crystalline) of iPP/PLA composition of (100/0), (90/10), (80/20), (60/40) respectively

creases with iPP/PLA composition. The probability distribution function for amorphous region also increases significantly for the same compositions. The amorphous phase length increases with the composition of PLA in iPP, but the crystalline length and the crystallanity decreases with the increase of PLA composition in iPP. It is evident from TABLE 1 that, there are significant changes in the morphological parameters due to the fact that there is a change in the polymer network in a scale of the order 100 to 500Å. Changes of this magnitude normally facilitates biodegradable ability since these changes are attributed to the presence of weak hydrogen bonds.

CONCLUSIONS

Simulated small angle X-ray scattering pattern for different composition of iPP/PLA filament using Hosemann's linear paracrystalline model fits very well with experimental data and the changes in morphological parameters are due to compositional as well as organizational differences which influence the rearrangement of the crystalline and amorphous regions[11]. We observe from these studies that as PLA components increase in iPP, there is an increase of amorphous lengths and decrease of crystalline phase lengths facilitating the biodegradability.

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