NOTE

About the Ambiguity of the Quantitative Assessment of Crystalline Orientation in Uniaxially Drawn Pet

INTRODUCTION

The triclinic lattice of PET crystallites[1] and the occurrence of the inclined axial texture (tilted orientation) in uniaxially drawn PET specimens (fiber, filaments)[2] entail that the X-ray reflexes 010, $1\bar{1}0$, and 100 are not strictly single aquatorial reflexes but, in fact, doublets of reflexes slightly shifted symmetrically above and below the aquator.

This shift depends on the tilting angle of the texture. For specimens with high orientation, i.e., drawn to the draw ratio higher than $R = 3, 0x$, the tilting angle is less than 6°. As a result, a partial overlap of the above-mentioned reflexes is brought about. This overlap leads to a slight azimuthal extension and simultaneously to a slight alteration of the azimuthal intensity distribution within the aquatorial reflexes. These effects are usually neglected in X-ray diffraction methods commonly used in the quantitative appraisal of the crystallite axes' orientation based on considering the aquatorial reflexes.

As is known, the second possible method of assessing the crystallite axes orientation in PET samples consists of evaluating the $\bar{1}05$ reflex. In the case of this reflex, there occurs a similar effect as in the case of aquatorial reflexes. In fact, the meridional reflex $\bar{1}05$ is a superposition of two adjacents shifted slightly apart from other reflexes. The resulting partial overlap of the reflexes brings about an extension and alteration of the azimuthal intensity distribution within the $\bar{1}05$ diffraction. Because of the very small value of the shifting of both reflexes, the overlapping effect is always neglected.

Journal of Applied Polymer Science, Vol. 51, 201–202 (1994)
 CCC 0021-8995/94/010201-02

Both of the approaches mentioned applied in the evaluation of the crystallite orientation of uniaxially drawn PET samples can bring about differences in assessment. To verify the resulting ambiguities in the assessment of orientation, measurements on PET filaments stretched at the draw ratio $R = 3, 2x$, and $R = 4, 4x$ have been carried out. Four different X-ray evaluation methods have been applied: one following the direct approach method, i.e., the method that relies on evaluation of the azimuthal intensity distribution of the meridional $\bar{1}05$ diffraction and three different indirect approach methods, which are based on considering the aquatorial reflexes 010, $1\bar{1}0$, and 110. These last three composed the method introduced by Gupta and Satish Kumar[3] and two modifications applied by Buchneva and Perepetchko,[4] versions in which the virtual and the Gaussian approximated intensity distribution within the aquatorial reflections 010, $1\bar{1}0$, and 100 are regarded correspondingly.

RESULTS AND DISCUSSION

The ascertained results of the investigations carried out are compiled in Table I. The results obtained enable the following conclusions to be drawn:

1. The direct-approach method based on considering the meridional diffraction $\bar{1}05$ brings about relatively low values of crystallite axes' orientation coefficients, which, consequently, leads to an underestimation of the crystalline orientation. It seems that the underestimation of orientation is a result of the partial overlap of the adjacent $\bar{1}05$ reflexes.

Table I Results of Direct- and Indirect-Approach Methods

Crystallite Axes Orientation Coefficients	Direct-approach Method $\bar{1}05$ Reflex		Indirect-approach Method 100, $1\bar{1}0$, and 100 Reflexes					
			Gupta–Satish Kumar		Buchneva–Perepetchko			
					Virtual Distribution		Gauss Distribution	
	$R = 3, 2x$	$R = 4, 4x$	$R = 3, 2x$	$R = 4, 4x$	$R = 3, 2x$	$R = 4, 4x$	$R = 3, 2x$	$R = 4, 4x$
$\langle\cos^2\phi\rangle$	0.630	0.709	0.953	0.956	0.968	0.988	0.953	0.975
f_x	0.445	0.563	0.929	0.935	0.952	0.982	0.930	0.963

f_x = Hermann's orientation function $f_x = \frac{1}{2} \cdot (3\langle\cos^2\phi\rangle - 1)$.

2. The indirect-approach methods lead, in general, to orientation coefficients of a higher value than those of the direct approach method. They should be regarded as more adequately assessing the crystallite orientation.
3. The respective indirect-approach methods considered deliver different results according to the method used. The lowest values refer to the Gupta–Satish Kumar method, and the highest, to the Buchneva–Perepetchko method, by regarding the virtual azimuthal intensity distribution within the aquatorial reflections.

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Received June 4, 1993
Accepted June 15, 1993