

Table 1 Some parameters of the structural unit element for PET samples investigated (see also ref. 1)^a

Sample	<i>L</i> (nm)	<i>A</i> (nm ²)	<i>L_c/L</i>	<i>n</i>	<i>e</i>	<i>β</i>
2	14.5	11.9	0.26	48	0.35	0.093
3	14.7	13.3	0.27	53	0.35	0.103
4	15.7	13.3	0.33	53	0.37	0.108
5	14.7	12.1	0.28	48	0.35	0.097
9	12.7	11.0	0.39	44	0.30	0.070

^aSee text for notation

PET molecule for the given number average molecular weight $\bar{M}_n = 15\,000$ ($L_0 = (\bar{M}_n/192)1.075$ nm). As shown in Table 1, *e* is about 0.35 and thus much greater than for ultra-high modulus PE fibres²⁻⁴. Neglecting chain entanglements (i.e. considering only \bar{M}_n) there could be achieved a maximum relative content of taut tie molecules $\beta_{\max} = 0.65$ by drawing. On the other hand the maximum attainable linear degree of order (L_c/L_{\max}) seems to be about 0.4 for our material (note that L_c is the average length of the crystalline portion of the structural unit element with $L_c \approx L_{105}$; see ref. 1 and Table 1). Using $\beta = 0.65$ and $(L_c/L) = 0.4$ the maximum attainable longitudinal modulus of our PET samples ($\bar{M}_w \approx 20\,000$, $\bar{M}_n = 15\,000$) can be calculated using^{1,5}:

$$E \approx E_c \beta / (1 - (L_c/L)(1 - \beta)) \quad (2)$$

to $E_{\max} = 83$ GPa. This value is considerably greater than the maximum value of about 28 GPa calculated by Postema and Smith for drawn PET of $\bar{M}_w = 20\,000$. That means that for semicrystalline (i.e. hot zone drawn or fast cold drawn) PET samples the finite chain length of the molecules is not of the same importance for the maximum attainable longitudinal modulus as in the case of slow and cold drawn PET where the assumptions of Postema and Smith are fully valid.

In our paper¹ we assumed that the total relative fraction of tie molecules is nearly equal to the maximum obtained relative content of taut tie molecules β in a non-crystalline region which was about 0.11 (see ref. 1 and Table 1). That means 89% of

molecular sections in such a region have to be chain ends or to be included in chain entanglements. Since there are about 35% chain ends (see Table 1), 54% of the molecular sections are assumed to take part in entanglements. Then the average number *i* of entanglements per molecule is $i = (0.54L_0)/L$ (see refs 2 and 3). Using a typical *L* value of 14.5 nm, $i = 3.2$ is obtained.

Conclusion

The results presented in this reply show that for semicrystalline PET samples the maximum attainable longitudinal modulus does not only depend on the molecular weight (i.e. on the chain-end density) but also on the degree of crystallinity and the density of chain entanglements in the sample. The model of Postema and Smith, however, is especially suited for the discussion of cold and slow drawn PET fibres.

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References

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Corrigendum

'Kinetic theory of directional isomerism in polymer chains: 1. Polymer microstructure'

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Polymer 1988, **29**, 1858-1866

Equations (17) to (21) should read as follows:

$$x = \int_0^t [\text{HT}] dt \quad (17)$$

$$\sum_{n=1}^{\infty} P_n^* = I_0 k_{\text{th}} \left(\frac{c}{K_1} + \alpha_1 e^{-K_1 x} + \frac{\beta}{K_1 - K_3} e^{-K_3 x} - \frac{c + \beta}{K_1 - K_4} e^{-K_4 x} \right) \quad (18)$$

$$\sum_{n=1}^{\infty} Q_n^* = I_0 k_{\text{th}} \left(\frac{1-c}{K_2} + \alpha_2 e^{-K_2 x} - \frac{\beta}{K_2 - K_3} e^{-K_3 x} - \frac{1-c-\beta}{K_2 - K_4} e^{-K_4 x} \right) \quad (19)$$

$$B^* = I_0 k_{\text{th}} \left[\frac{1-c}{K_1} + \left(\frac{K_4}{K_1(K_1 - K_4)} - \alpha_1 \right) e^{-K_1 x} - \frac{\beta}{K_1 - K_3} e^{-K_3 x} - \frac{1-c-\beta}{K_1 - K_4} e^{-K_4 x} \right] \quad (20)$$

$$D^* = I_0 k_{\text{th}} \left[\frac{c}{K_2} + \left(\frac{K_4}{K_2(K_2 - K_4)} - \alpha_2 \right) e^{-K_2 x} + \frac{\beta}{K_2 - K_3} e^{-K_3 x} - \frac{c + \beta}{K_2 - K_4} e^{-K_4 x} \right] \quad (21)$$

Equations (44) and (45) should read as follows:

$$f(\text{H-H}) = \frac{D}{B + D + \sum_{n=1}^{\infty} n(P_n + Q_n)} = k_{\text{th}} [cK_3K_4x - K_4\beta(e^{-K_3x} - 1) + K_3(c + \beta)(e^{-K_4x} - 1)] / \{ [K_2 + (K_1 - K_2)c]K_3K_4x + K_4\beta(K_2 - K_1) \times (e^{-K_3x} - 1) + [K_2 + (K_1 - K_2)(c + \beta)]K_3(e^{-K_4x} - 1) \} \quad (44)$$

$$f(\text{T-T}) = \frac{B}{B + D + \sum_{n=1}^{\infty} n(P_n + Q_n)} = k_{\text{th}} [(1-c)K_3K_4x + K_4\beta(e^{-K_3x} - 1) + K_3(1-c-\beta)(e^{-K_4x} - 1)] / \{ [K_2 + (K_1 - K_2)c]K_3K_4x + K_4\beta(K_2 - K_1) \times (e^{-K_3x} - 1) + [K_2 + (K_1 - K_2)(c + \beta)]K_3(e^{-K_4x} - 1) \} \quad (45)$$