ESSENTIAL WORK OF FRACTURE CONCEPT IN POLYMERS

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Abstract

Plane-stress fracture toughness of amorphous copolyester (COP) sheets of different composition and molecular mass characteristics was determined by the essential work of fracture (EWF) concept using tensile-loaded deeply double-edge notched (DDEN-T) specimens. It was determined that these COPs meet the basic requirement of the EWF concept since their yielding along the full ligament preceded crack growth. A drop in load in the corresponding load-displacement (F–x) curves indicated yielding and allowed us to split both the specific essential and non-essential work of fracture (w_e and w_p, respectively) into their contributing terms based on yielding (w_y) and necking including fracture (w_n). Development and size of the plastic zone were studied by light microscopy (LM) and infrared thermography (IT).

Keywords: essential work, fracture mechanics, infrared thermography, non-essential work, plastic work, polyethylene terephthalate.

1. Introduction

The assessment of fracture toughness of ductile polymers by concepts of fracture mechanics is a great challenge. Linear elastic fracture mechanics (LEFM) fails to provide us with proper fracture toughness values for ductile polymers due to the large plastic zone created at the crack tip of the specimens. In order to overcome this difficulty, the methods of the non-linear fracture mechanics (denoted also as ductile, elastoplastic or post-yield fracture mechanics) have gained considerable attention. Although several approaches of the latter were proposed to consider the large-scale plastic deformation during loading (as listed e.g. in [1]), only two of them have become widely used: the J-integral ([1]–[4] and references within) and the essential work of fracture (EWF) theory ([1], [3]–[6] and references within).

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The curves used for data reduction by both methods are quite similar since they reflect the material resistance to stable crack growth. The basic difference between them is the determination of the material parameter representing the fracture toughness. In the case of the multiple-specimen J-integral technique, for example, the critical value under mode I deformation, $J_{Ic}$, is defined by the intercept of the blunting line or its offset with the $J$ versus $\Delta a$ ($J_R$) curve, where $\Delta a$ designates the crack growth \[1\]–[4]. Since direct experimental evidence for crack tip blunting in the form of a stretch width zone is rather seldom [7], and the intercept of the blunting line with the $J_R$-curve can be determined by different methods, $J_{Ic}$ alone can hardly represent an inherent toughness parameter. The situation seems to be more simple with the EWF concept, which differentiates between the essential work required to fracture the polymer in its process zone, $W_e$, and the non-essential or plastic work consumed by various deformation mechanisms in the plastic zone, $W_p$, as indicated in Fig. 1. The total work of fracture, $W_f$, is composed of the two above terms:

$$W_f = W_e + W_p.$$  \hspace{1cm} (1)

Fig. 1. Designation and size of the specimens used

Taking into consideration that $W_e$ is surface-related, whereas $W_p$ is volume-related, $W_f$ can be given by the related specific work terms (i.e. $w_e$ and $w_p$, respectively):

$$W_f = w_e \cdot l \cdot t + \beta \cdot w_p \cdot l^2 \cdot t,$$  \hspace{1cm} (2)

$$w_f = \frac{W_f}{l \cdot t} = w_e + \beta \cdot w_p \cdot l,$$  \hspace{1cm} (3)
where \( l \) is the ligament length, \( t \) is the thickness of the specimen and \( \beta \) is a shape factor related to the form of the plastic zone. Based on Eq. (3) the specific essential work of fracture \((w_e)\) can easily be determined by reading the ordinate intercept of the linear plot \( w_f \text{ vs } l \).

It is noteworthy that \( J_{Ic} \) and \( w_e \) should be identical or very similar, as was indeed corroborated by several authors [3], [4], [6], [8]. The basic question with \( w_e \) is, however, how far this parameter represents the inherent material toughness. Although it has been shown by several groups [3], [9], [10], that \( w_e \) is independent of the specimen geometry, which is a fundamental criterion for a material parameter, the above question still remained. Let us consider only two aspects in connection to the EWF. It should be kept in mind that for the reliable application of the EWF, the ligament must yield prior to tearing at the notch tip. Contrary to this requirement, it was observed [4], [9], [11] that tearing may start before the full ligament is yielded. In addition, none of the load-displacement \((F - x)\) curves displayed in the literature [3], [4], [9]–[12] shows any yielding prior to tearing. Yielding should be discernible in the related \( F - x \) curves as clearly as in case of a standard tensile test, where yielding precedes necking. A further problem with using \( w_e \), as material parameter, is that until now no correlation between \( w_e \) and material characteristics, such as molecular mass, molecular weight between entanglements and similar values has been disclosed. These open questions triggered the study outlined below.

The objective of this work was to determine the fracture toughness of amorphous copolyester (COP) sheets that meet the application requirement of the EWF concept, i.e. they are thin enough so that plane stress condition prevails and they undergo full ligament necking prior to crack growth.

2. Experimentals

2.1. Materials

Two amorphous copolyesters were supplied by Eastman Chemical Company, Kingsport, TN, USA. The copolyesters were synthesized from dimethyl terephthalate (DMT), and two diols ethylene glycol (EG) and 1,4-cyclohexane dimethanol (CHDM). The copolyesters contained either 31 mole, CHDM (COP31) or 68 mole % CHDM (COP68).

2.2. Mechanical Testing

All mechanical tests reported here were performed at room temperature (RT) on a Zwick Z020 universal testing machine using a crosshead speed of 1 mm/min. Tensile E-modulus \((E)\), yield strength, \( \sigma_y \), and elongation at yield, \( \varepsilon_y \), were determined (cf. Table 1) by using dumbbell specimens (No.3 according to DIN 53 455).
On Table 1 IV is the inherent viscosity, \( T_g \) is the glass temperature and \( M_e \) is the molecular weight between entanglements.

### Table 1. Basic molecular and mechanical characteristics of the COPs studied

<table>
<thead>
<tr>
<th>Material</th>
<th>IV [dl/g]</th>
<th>( T_g ) [°C]</th>
<th>( M_e ) [g/mol]</th>
<th>E-modulus [GPa]</th>
<th>( \sigma_y ) [MPa]</th>
<th>( \varepsilon_y ) [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>COP 31</td>
<td>0.689</td>
<td>89</td>
<td>3260</td>
<td>2.36</td>
<td>51</td>
<td>2.8</td>
</tr>
<tr>
<td>COP 68</td>
<td>0.705</td>
<td>96</td>
<td>4710</td>
<td>1.98</td>
<td>41</td>
<td>2.9</td>
</tr>
</tbody>
</table>

For determination of the specific plastic work, \( w_p \), another dumbbell specimen (S3A according to DIN 53 504) was used. Dimensions of these specimens can be taken from Fig. 1.

For the EWF study, double deeply edge-notched tensile (DDENT-T) specimens with a width of 35 and overall length of 100 mm (clamped length 70 mm; cf. Fig. 1) were selected. The free ligament length, \( l \), was set in the range \( l = 5 \) to 20 mm. At every ligament length, at least 3 specimens were investigated. Data reduction (cf. Eq. (3)) followed the recommendations of the ESIS TC-4 group [13].

The non-essential or plastic work (\( w_p \)) was derived by two methods: directly from tensile tests on small dumbbells, and indirectly by assessing the shape of the plastic zone (cf. Fig. 1) using light microscopy (LM) and infrared thermography (IT, Hughes) [11]. For the former case, \( w_p \) is given directly by the ratio of the total energy to failure (calculated from the area beneath the load-displacement curves) to the energy up to the onset of necking. For the latter case, the shape parameter (\( \beta \)) of the plastic zone should be considered [11], [13]. Viewing of the plastic zone by LM occurred after breaking the DDENT-T specimens. On the other hand, IT frames were taken during loading either continuously by a videotape or at selected points of the loading curve. IT was aimed at mapping the relative temperature rise in the ligament region, so that an arbitrarily chosen emission factor \( E = 0.9 \) was set. IT pictures served for determination of both shape and extension of the plastic zone.

### 3. Results and Discussion

Figs. 2 and 3 depict the load-displacement \( (F - x) \) curves of DDENT-T specimens at various ligaments for COP 31 and COP 68, respectively. It is very striking that the \( F - x \) curves at different ligament length are similar to one another, so that the basic requirement of the EWF theory is met. A more important phenomenon in respect to the \( F - x \) curves is related to a load drop, indicated by arrows in Figs. 2 and 3, that identifies where yielding, or the onset of necking, take place. At this point the entire ligament yields instantaneously. The full ligament yielding is followed by a necking stage up to the final fracture, as illustrated in Fig. 4.
Fig. 2. The $F - x$ curves of DDEN-T specimens at different ligament lengths ($l = 5, 10, 15$ and $20$ mm) for COP 31.

Fig. 3. The $F - x$ curves of DDEN-T specimens at different ligament lengths ($l = 5, 10, 15$ and $20$ mm) for COP 68.
Fig. 4. Light microscopic picture taken on the necked ligament of a DDEN-T specimen of COP 68 with \( l = 20 \text{ mm} \)

Fig. 5. The serial IT frames of a DDEN-T specimen with \( l = 20 \text{ mm} \) of COP 31 taken during loading. Note: taking position of the IT frames is indicated in the \( F - x \) curve in Fig. 7

IT frames taken during loading (cf. Figs. 5 and 6) confirm, in fact, the full ligament yielding at the load drop. The temperatures of the COP 3l and COP
68 specimens increase by 4 and 3 °C, respectively, due to instantaneous yielding. Figs. 7 and 8 show the $F - x$ curves belonging to IT frames. The serial IT pictures in Figs. 5 and 6 portray the development of the temperature field in the ligament area, and thus indicate the formation of the plastic zone (cf. Fig. 1) in the necking stage. The cursor points 1 to 4 on the IT frames were positioned as follows: 1 – showing the reference temperature; 2 and 3 – at the necking borderline of the upper and lower parts of the DDEN-T specimens, respectively, and 4 – in the mid ligament range or at hottest spot. The IT frames before final separation of the specimens hint for the development a shallow, diamond-like plastic zone (cf. pictures D in Figs. 5 and 6). This is in harmony with the LM observation (cf. Fig. 4).

Figs. 9 and 10 depict the $w_f$ vs $l$ curves for the DDEN-T specimens of COP 31 and COP 68, respectively. $w_f$ was computed from the area beneath the $F - x$ curves registered (cf. Figs. 3, 4, 5 and 6). According to Eq. (3), the essential work of fracture ($w_e$) was read from the intercept of the linear regression line with the ordinate and is reported in Table 2. Table 2 contains also the slope value, $\beta w_p$, (Eq. (3)) and the correlation coefficients of the related regression lines.

The appearance of the $F - x$ curves of COPs allowed us to differentiate between the specific work of fracture required for yielding ($w_y$) and that consumed
Fig. 7. The $F - x$ curves of a DDEN-T specimen with $l = 20$ mm of COP 31 taken during loading.

Fig. 8. The $F - x$ curves of a DDEN-T specimen with $l = 20$ mm of COP 68 taken during loading.
**Fig. 9.** Total specific work of fracture \((w_f)\) and its contributing terms (yielding, \(w_y\) and necking and fracture, \(w_n\)) versus ligament length \((l)\) for the DDEN-T specimens of COP 31

**Fig. 10.** Total specific work of fracture \((w_f)\) and its contributing terms (yielding, \(w_y\) and necking and fracture, \(w_n\)) versus ligament length \((l)\) for the DDEN-T specimens of COP 68
Fig. 11. Total height of the plastic zone ($h$) determined by LM and IT techniques versus ligament length ($l$) for DDEN-T specimens of COP 31 (a) and COP 68 (b), respectively.

by necking and fracture ($w_n$). Figs. 9 and 10 make obvious the contribution of $w_y$ and $w_n$ with respect to the essential work of fracture ($w_{e,y}$ and $w_{e,n}$). The slope of $w_y$, i.e. $\beta_l w_{p,y}$, can be well estimated by the term $\sigma_y \varepsilon_y$. For COP 31 and COP 68 this approach (cf. Table 2) yields 1.43 and 1.19 MJ/m$^3$, which are closely matched to the experimental results (1.98 and 1.49 MJ/m$^3$, respectively).

Before starting with the explicit determination of the non-essential or plastic work ($w_p$), let us consider the usual size criteria of the EWF tests. The validity range of the EWF is generally given by $[5], [6], [9]–[12]$

$$(3 - 5)t \leq l \leq \min(b/3 \text{ or } 2r_p),$$

where $b$ is the width of the specimen (35 mm; cf. Fig. 1) and $2r_p$ is the size of the plastic zone:

$$2 \cdot r_p \frac{1}{\pi} \cdot \frac{E \cdot w_e}{\sigma_z^2}.$$ (5)

The plastic zone calculated by inserting the following mechanical data: $E = 2.3$ GPa, $w_e = 35$ kJ/m$^2$ and $\sigma_z = 45$ MPa, yielded $2r_p \approx 13$ mm. This size is very close to the alternative width criterion; i.e. $B/3 = 12$ mm. Based on the self-similarity of the $F - x$ curves in the ligament range up to $l = 20$ mm, one can claim, however, that both above criteria for the upper ligament length are definitely too conservative for the COPs studied.
It is instructive to compare our data with those reported for an amorphous PET [10] having an analogous mechanical response \( E = 2.3 \) GPa and \( \sigma_y = 40 \) MPa. For this PET, \( w_e \) and \( \beta w_p \) were 54 kJ/m\(^2\) and 12.7 MJ/m\(^3\), respectively, using DDEN-T specimens. Both values lay considerably higher than ours. The difference in slope may be attributable to a more circular shaped plastic zone, whereas the difference in \( w_e \) may be due to some strain-induced crystallization in PET.

The calculation of the plastic work dissipated per unit volume, \( w_p \), in uni-axial tensile tests on small dumbbells (cf. Fig. 1) was performed according to the recommendations of the ESIS group [13]. Recalling that the slope of the plot of \( w_f vs l \) is equal to \( \beta w_p \), the shape parameter of the plastic zone, \( \beta \), was determined and is reported in Table 2.

Attempts were made to estimate indirectly \( \beta \) from the shape of the necked region by light microscopy (post-mortem) and from the IT heat maps taken during loading of the DDEN-T specimens (in-situ). Fig. 11 demonstrates a good agreement between the \( \beta \) parameters derived from IT and LM, respectively. The shape of the plastic zone can be well approached by a shallow diamondlike form for which

\[
\beta = \frac{1}{2} \cdot \frac{h}{l}
\]

holds [13]. Taking a mean \( \beta \) value of 0.08 for the COPs investigated, a \( w_p \) range between 67 (COP 68) and 100 MJ/m\(^3\) (COP 31) can be computed (Table 2).

Table 2. Essential work \( (w_e) \), non-essential or plastic work \( (w_p) \) along with their contributing terms and correlation coefficients (\( R^2 \)), and shape parameter of the plastic zone \( (\beta) \) defined by different approaches for the COPs studied

<table>
<thead>
<tr>
<th>Material</th>
<th>( w_e )</th>
<th>( R^2 )</th>
<th>( w_{e,y} )</th>
<th>( R^2 )</th>
<th>( w_{e,n} )</th>
<th>( R^2 )</th>
<th>( \beta w_p )</th>
<th>( \beta_1 w_{p,y} )</th>
<th>( \beta_2 w_{p,n} )</th>
<th>Shape parameter</th>
<th>Tensile test</th>
<th>LM</th>
<th>IT</th>
</tr>
</thead>
<tbody>
<tr>
<td>COP 31</td>
<td>30.28</td>
<td>0.993</td>
<td>12.76</td>
<td>0.979</td>
<td>17.52</td>
<td>0.992</td>
<td>7.68</td>
<td>1.98</td>
<td>5.71</td>
<td>0.085</td>
<td>0.078</td>
<td>0.079</td>
<td></td>
</tr>
<tr>
<td>COP 38</td>
<td>36.11</td>
<td>0.975</td>
<td>14.52</td>
<td>0.949</td>
<td>21.59</td>
<td>0.974</td>
<td>5.36</td>
<td>1.49</td>
<td>3.87</td>
<td>0.067</td>
<td>0.077</td>
<td>0.075</td>
<td></td>
</tr>
</tbody>
</table>

4. Conclusions

The plane stress ductile fracture behaviour of amorphous copolyesters (COPs) was studied by the essential work of fracture (EWF) method using deeply double-edge notched tensile (DDEN-T) specimens. Based on this study the following conclusions can be drawn.
Amorphous COPs are likely the ideal polymers for EWF tests, since they undergo full ligament yielding prior the onset of crack growth. In addition, due to the clear indication of yielding in the load-displacement curve, it is possible to distinguish the specific essential and non-essential parts of work of fracture required for yielding ($w_{e,y}$ and $w_{p,y}$) and for subsequent necking and fracture ($w_{e,n}$ and $w_{p,n}$) [14]–[17].

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References