Analysis of the temperature effect on the behavior of high density polyethylene during high pressure torsion process

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Abstract:
The High Pressure Torsion (HPT) is an effective tool for obtaining nanomaterials with high performance by severe plastic deformation. This work is focused to highlight the plastic strain distribution in the deformed material according to different HPT parameters, such as, the applied pressure, the rotation angle and the temperature of the deformed material. A typical thermoplastic polymer (HDPE) was tested. To this end, the material parameters of an elasto-viscoplastic model were derived from compressive tests at different temperatures and strain rates. Then, the distributions of the effective plastic strain were analyzed by three-dimensional finite element. Recommendations on process conditions were proclaimed according to the obtained numerical results.

Mots clefs: HPT; Eléments finis; PEHD ; Modélisation ; Déformation plastique

1 Introduction
Severe Plastic Deformation (SPD) method has become a recognized technique in the materials treatment. Since the pilot experiences of Bridgman in 1952 on a process of combining the torsion with compression to create shear deformations, the progress in the domain has been strongly related to the development of the super plastic deformation technique. A considerable interest has been given to the materials treatment by SPD in order to confer to the material a high tenacity by producing an ultrafine microstructure [1].

Among the SPD processes that have known more scientific production in the literature, we find the equal channel angular extrusion (ECAE) and high pressure torsion process (HPT). The first involves the extrusion of a sample through a die which is composed of two channels with equal sections intersecting at an angle generally between 90° and 135° [2]. The second process, which is the subject of this work, consists of putting a disc-shaped sample under the simultaneous action of high compression and torsion, using two anvils as shown in figure 1. Previous experimental data on metallic materials have proven that the HPT is more effective than the ECAE to produce exceptionally weak sized grains [3,4]. By against, in the case of polymeric materials, ECAE process has been some developments which have allowed identifying the shear plastic extruded material [5-12]. But in the case of HPT, to date very limited studies have been devoted to evaluate the potential of this process on the orientation of the microstructure [13]. Therefore, further work on the HPT process appears to be very promising for improving the mechanical properties of polymers by severe plastic deformation. Indeed, the HPT process is very easy to implementing saw that only two key parameters must be taken into consideration: (i) the imposed pressure (compression) and (ii) the torsion angle applied on the sample.

In order to highlight the plastic deformation distribution in the sample during the HPT process, the finite element method appears to be a crucial tool for accurately quantifying the displacements, strains and stresses at any point of the sample [14, 15].
In this study, a three-dimensional finite element analysis of a thermoplastic polymer (high density polyethylene (HDPE)) behavior during HPT process has been conducted. Our particular attention has been focused on the effects of the material temperature and the process scenarios on the plastic strain distribution in order to optimize the operating conditions of HPT process.

![Diagram of HPT process](image)

**FIG. 1 – Principle of HPT process.**

## 2 Constitutive model

The large strain behavior of the polymer under study (HDPE) is characterized by a strain rate dependent yield followed by a strain hardening. Various viscoplastic models, basing on physical or purely phenomenological considerations \[16,17\], were developed to intend to describe the particular mechanical behavior of polymers. In this paper, a phenomenological constitutive model, detailed in this section, is used to describe specific behavior of the studied material \[9\].

The strain rate tensor $\mathbf{d}$ is decomposed into an elastic part $\mathbf{d}^e$ and a viscoplastic part $\mathbf{d}^{vp}$ as:

$$
\mathbf{d} = \mathbf{d}^e + \mathbf{d}^{vp}
$$

(1)

The elastic strain rate tensor $\mathbf{d}^e$ is given by the hypo-elastic law:

$$
\mathbf{d}^e = C^{-1} \dot{\mathbf{e}}
$$

(2)

Where $\dot{\mathbf{e}} = \dot{\mathbf{e}} - \mathbf{W}\sigma + \sigma\mathbf{W}$ is the Jaumann derivative of the Cauchy stress tensor $\sigma$ based upon the spin tensor $\mathbf{W}$ and $C$ is the fourth-order isotropic elastic modulus tensor:

$$
C_{ijkl} = \frac{E}{2(1+\nu)} \left( \delta_i\delta_j + \delta_j\delta_i \right) + \frac{2\nu}{1-2\nu} \delta_i\delta_j
$$

(3)

In Eq. (3), $E$, $\nu$ and $\delta$ are respectively Young’s modulus, Poisson’s ratio and Kronecker-delta symbol.

The viscoplastic strain rate tensor $\mathbf{d}^{vp}$ can be given by the following Norton-type power law equation:

$$
\mathbf{d}^{vp} = \frac{3}{2} \left( \frac{\sigma - R}{\sigma} \right)^n \mathbf{d}^e
$$

(4)

Where $\sigma' = \sigma - tr(\sigma)/3I$ is the deviatoric stress tensor, $\sigma_c = \sqrt{3/2\sigma'^2}$ is the equivalent stress, $K$ and $n$ are the viscosity parameters and $R$ is the isotropic hardening defined by a simple phenomenological evolution law:

$$
R = h \left( 1 + \frac{\varepsilon^{vp}}{\varepsilon_0} \right)^m
$$

(5)

In relation (5), $\varepsilon^{vp} = \int_0^t \dot{\varepsilon} d\tau = \int_0^t \sqrt{2/3\mathbf{d}^{vp}\mathbf{d}^{vp}} d\tau$ is the equivalent viscoplastic strain, $\varepsilon_0$ is the initial yield strain, $m$ and $h$ are the hardening parameters.

## 3 Identification of behavior law by compression tests

### 3.1 Materials used

In this study a semi-crystalline polymer (high density polyethylene HDPE) has been selected. This polymer was provided by the Goodfellow Company. The mechanical properties are given in table 1. The choice of HDPE is based on three considerations:
They preserve a ductile behavior at high strain rate;

They enabled us to easily follow the evolution of the microstructures (crystalline phases, plates) during the deformation;

They are easy to be handled at ambient temperature.

### Mechanical Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>PEHD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (g cm(^{-3}))</td>
<td>0.95</td>
</tr>
<tr>
<td>Coefficient of friction</td>
<td>0.29</td>
</tr>
<tr>
<td>Hardness – Rockwell</td>
<td>D60-73</td>
</tr>
<tr>
<td>Izod impact strength</td>
<td>20-210</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.46</td>
</tr>
<tr>
<td>Tensile modulus</td>
<td>0.5-1.2</td>
</tr>
<tr>
<td>Tensile strength</td>
<td>15-40</td>
</tr>
</tbody>
</table>

**TAB. 1 – Mechanical properties of high density polyethylene (HDPE).**

The compressive tests have been performed on an electromechanical Instron test machine on cylindrical samples of 8mm (diameter) × 16mm (length). A loading cell of 10KN was used to carry out these tests at different temperatures T={room temperature, 40, 60 and 80°C}, and constant strain rates ranging from 10\(^{-5}\) to 10\(^{-1}\)/s. Noting that the plates of the testing machine were well lubricated so that the effect of friction at the contact surfaces with the sample is negligible. During the tests, the displacement values, loads and time were recorded by the computer using Bluehill software.

### 3.2 Identification of the constitutive law

The constitutive equations presented in the previous section were used to predict the nonlinear behavior of HDPE with large deformations. In addition to the Young's modulus and Poisson's ratio, the constitutive equations contain four parameters to be determined: \(K\), \(n\), \(m\) and \(h\). The experimental results were used to determine the parameters of the elastic-viscoplastic model presented in the previous section. Young’s modulus \(E\) was obtained at low stresses and strains and Poisson’s ratio \(\nu\) was fixed to 0.38. The parameters \(K\), \(n\), \(h\) and \(m\) were determined using a least squares regression fitting as shown in figure 2 and their values are summarized in table 2.

<table>
<thead>
<tr>
<th>(T) (°C)</th>
<th>(E) (Mpa)</th>
<th>(K) (Mpa)</th>
<th>(n)</th>
<th>(h) (Mpa)</th>
<th>(m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>500</td>
<td>31.2</td>
<td>7.8</td>
<td>3.15</td>
<td>0.88</td>
</tr>
<tr>
<td>40</td>
<td>280</td>
<td>20</td>
<td>8.3</td>
<td>5</td>
<td>0.7</td>
</tr>
<tr>
<td>60</td>
<td>150</td>
<td>10.7</td>
<td>10.2</td>
<td>5.5</td>
<td>0.65</td>
</tr>
<tr>
<td>80</td>
<td>130</td>
<td>5.7</td>
<td>11.17</td>
<td>6</td>
<td>0.45</td>
</tr>
</tbody>
</table>

**TAB. 2 – The material parameters for HDPE at different temperatures.**

From figure 2, it can be noted that there is a good agreement between the experimental data and the elasto-viscoplastic constitutive model.

**FIG 2 – Stress-strain curves of HDPE for various temperatures:**

(a) room temperature (25 °C), (b) 40 °C, (c) 60 °C, (d) 80 °C.
4 Finite element simulation of the HPT process

The simulations were carried out using the finite element code MSC.Marc, with a mesh of 34,992 elements. It should be noted that the mesh size used is largely sufficient to show accurately the distribution of localized plastic strain within the samples. The sample used is a cylindrical disc of 20 mm in diameter and 10 mm in thickness (figure 3). The upper and lower anvils were taken as rigid bodies in the finite element simulations.

FIG. 3 – Finite element discretization of a cylindrical sample (disc).

4.1 Sequence effect

In most practical cases, we can distinguish two major scenarios to perform the HPT process. The first is to apply a compression followed by torsion using the upper anvil (scenario 1). In the second, the sample is subjected simultaneously to compression-torsion (scenario 2). In order to make a comparison between the both scenarios finite element simulations have been conducted. Figure 4 shows a comparison between the obtained results for the distributions of the total equivalent plastic strain using the both scenarios. One can easily observe that the plastic strain induced by the first scenario is higher than that of the second one. This result can be confirmed by plotting the distribution of the equivalent plastic strain along the diameter of the disc at the top surface as shown in figure 5. Indeed, in the first scenario, the maximum equivalent plastic strain is 2.82, while in the second scenario, it is 2.03. Therefore, it is advised to use the first scenario in order to obtain a large plastic strain.

FIG. 4 – Illustration of the plastic strain distribution under the sequence effect of HPT process in the case of: (a) Scenario 1 and (b) Scenario 2.

FIG. 5 – Evolution of the total equivalent plastic strain during the HPT process using the two scenarios: (a) along the radial distance at the end of the process and (b) during the different process phases at a radial distance of 10 mm.
4.2 Temperature effect

The behavior of polymers depends strongly on the temperature. They are the seat of transition behavior that can be associated with different molecular relaxations, i.e. activation of local conformational changes. In order to study the dependence of the polymer behavior during HPT process under temperature effect, a series of numerical computations under isothermal conditions was carried out on a high-density polyethylene by varying the temperature from 25°C to 80°C. An imposed vertical displacement of 2.5 mm with a speed of 0.5 mm/s and a rotation of 30° with an angular velocity of 0.2618 rad/s were applied to the upper anvil. In order to highlight the deformation state into the HDPE sample, the distribution of the equivalent plastic strain contours plots for the four different temperatures are shown in figure 6. It may be remarked that the equivalent plastic strain decreases with the increase of the temperature and the most important values of plastic strain are localized at the periphery of the disc.

![Image](image_url)

**FIG. 6** – Illustration of the plastic deformation distribution on the sample during the HPT process under the temperature effect: (a) 25 °C, (b) 40 °C, (c) 60 °C and (d) 80 °C.

Figure 7 shows the evolution of the total equivalent plastic strain along the radial distance of the disc according to the variation in temperature after the compression phase (figure 7.a) and at the end of HPT process (figure 7.b). It may be noted that in both cases, the equivalent plastic strain decreases with the increase of the material temperature.

![Image](image_url)

**FIG. 7** – Evolution of the total equivalent plastic strain along the diametrical distance of the disc according to the variation of temperature: (a) after the compression phase and (b) at the end of HPT process.
5 Conclusion

In this study the results of the analysis of the scenario and temperature effects on the behavior of high density polyethylene during high pressure torsion process were presented. The following conclusions can be drawn:

- The first scenario which comprises applying a compression followed by torsion gives better results than the second scenario where the compression and torsion are applied simultaneously.
- The equivalent plastic strain decreases with the increase of the material temperature.
- To confirm the presented results and to highlight the evolution of mechanical properties and orientation aspect of the microstructure, an experimental analysis of the HPT process is under investigation.

References