**Parametric study of unconstrained high-pressure torsion-Finite element analysis**

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**Abstract.** The high-pressure torsion (HPT) experiments have been investigated numerically. An axisymmetric model with twist was developed with commercial finite element software (Abaqus) to study locally the specificity of the stress and strain history within the transformed layers produced during HPT processing. The material local behaviour law in the plastic domain was modelled. A parametric study highlights the role of the imposed parameters (friction coefficient at the interfaces anvil surfaces/sample, imposed pressure) on the stress/strain distribution in the sample bulk for two materials: ultra-high purity iron and steel grade R260. The present modelling provides a tool to investigate and to analyse the effect of pressure and friction on the local stress and strain history during the HPT process and to couple with experimental results.

**1. Introduction**

In most cases metallic contact wear studies reveal structural changes occurring at the near surface layer for sliding conditions: these transformations are one of the most common and natural responses of materials to tribological stresses, i.e. temperature, hydrostatic pressure and shearing gradients. This response is known as tribological transformation of surface (TTS) [1–3]. Understanding and controlling the formation of TTS faces the considerable difficulty of placing instruments inside contacts. High pressure Torsion (HPT) tests reproduce conditions that are close to those found inside contacts, i.e. high shearing, high shearing gradients and pressure conditions [4, 5, 6]. Thus carrying out HPT tests seems to be an efficient means of investigating TTS initiation mechanisms under severe shearing conditions and simultaneously analyzing and controlling their formation under conditions that can be controlled with greater precision than in a contact. To overcome the difficulties of
instrumenting the contact, a finite element model was developed to simulate the HPT tests and study the specific characteristics of the stress and strain loading cycles within sample volume. Despite a wide range of interests for HPT test, only a few numbers of studies exist that focus on these specific local strain stress history. Up to now very few finite element analysis have been done for unconstrained HPT [6-9] and quasi-constrained HPT [10-15]. Most of them focus on copper [8-11], a few on iron [7, 14], ZnSe [13] and high-density polyethylene [15]. To calculate significant stress and strain cycles, this model has to take into account both for the contact conditions/friction (at the sample/anvil interfaces) and for the material behavior law in the pertinent range of pressure and stresses (local contact pressures can reach several GPa). In this study the results of an elasto-plastic finite element analysis during unconstrained HPT tests are presented. The knowledge of internal stress and strain distributions and cycles is important in order to investigate the process of grain size refinement and thus better understand the deformation behavior during HPT process and in the longer term tribological processes.

2. Finite element model

2.1. Model
The anvil geometry used in these simulations was based on the unconstrained HPT set-up geometry (figure 1a). In previous work, stress and strain results obtained with a 3D model used to simulate the tests were shown to be axisymmetric [6]. An axisymmetric model with twist (figure 1b) was developed with commercial software (Abaqus 6.9) to simulate the cylindrical sample compressed and sheared between two anvils. This development provided a more refined mesh and reduced computing times. The two cylindrical WC anvils were considered to be elastic with a Young Modulus of 630 GPa and a Poisson coefficient of 0.293. Real HPT anvils contain sufficient roughness on the flat surfaces in the aim to increase the adherence with the samples and thus to limit the slippage of the sample during processing. In the simulations the anvils were smooth. The sample was 6 mm in diameter and 0.5 mm thick. The model parts were meshed with 4 noded-10 µm elements (CGAX4R elements) for the samples and 30 µm elements for the anvils. The simulations, through a quasi-static analysis, were used to examine the processing operation up to one half turn of the bottom anvil.
2.2. Material behavior and friction coefficient

Two materials were studied: an ultra-high purity iron Fe and a standard grade steel R260. For the ultra-high purity iron and for the steel, the Young’s modulus E is 210 GPa, a Poisson ratio \( \nu \) is 0.3. The material plastic behaviour law was not known under the test conditions, i.e. coupling between high pressures and strong shear deformation. Thus, in this work, the material behaviour was based on flow curve determined experimentally through compression tests under hydrostatic pressure up to 0.9 GPa. The stress–strain curves used are plotted in figure 2. In real HPT process, slippage occurs between the anvils and the sample [6, 7, 16]. The difficulty is that the friction coefficient is unknown during a real test. The present modelling provides a tool to analyse the effect of friction at the interface anvils/sample during the experimental process. Two Coulomb friction coefficient values were studied, 0.2 and 0.5, for the two materials.

2.3. Description of a simulation
In the first load step, the target vertical load (kN) was applied via the bottom anvil through a vertical displacement along X2 (in exactly the same way as in the experiment). In order to simulate conditions associated with different pressures, simulations were conducted using loads of 28 kN, 84 kN and 112 kN, corresponding to nominal pressures P, on a circular 6 mm diameter disk of respectively 1, 3 and 4 GPa.

Throughout the simulation, the top anvil was prevented from moving or rotating. In the second step, the vertical displacement was stopped and the normal load was maintained constant while small incremental rotation around the axis (X2) was imposed on the bottom anvil. In the last step the rotation was applied up to the target rotation angle.

3. Results and discussion

3.1 Presentation of the numerical results

The global numerical results, i.e. the calculated torques and sample thicknesses were plotted versus the anvil rotation angle. Preliminary results [7, 16] show that the transformed layers exhibiting the finest microstructures were produced in a specific sample volume linked with sliding/adhesion contact conditions (figure 3a). The surface conditions thus govern the location of material transformation in the bulk. Different paths (a path is composed of consecutive nodes) were defined to study the strain and the stress along radius at a given rotation angle. The stresses and strains could thus be calculated during a simulation at different depths within the sample following these paths. In the present paper the results at path h1 located at the interfaces sample/anvils (surface) (figures 1c, 1d) were presented.

The evolution of contact conditions was calculated at the interface. The contact pressure was calculated along radius on the path h1 for the different angles of rotation. The relative sliding between the anvil and the sample was also quantified along path h1 by using the cumulative sliding distance in radial direction and θ-direction (respectively variables CSlip1 and CSlip2 in Abaqus software). An adhesion zone could thus be highlighted (figure 1e, figure 3b). The adhesion zone was characterized by a radius \( r_A \). The evolution of \( r_A \) was followed versus the rotation angle. The history of the Von Mises equivalent plastic strains \( \bar{\varepsilon} \) (variable PEEQ used in Abaqus software) was also plotted along radius r for path h1 for different anvil rotation angle, measuring the evolution of material distortion within the first layer just below the surface.
3.2. The effect of the nominal pressure
The calculations performed on R260 steel showed that an increasing applied pressure led to an increase of torque (figure 4). The effect of the pressure on the $r_A$ was plotted figure 5. $r_A$ increased with increasing pressure at a given rotation angle. $r_A$ also decreased with rotation angles, particularly for low pressure conditions. For the 1GPa case, $r_A$ even became null after 5° rotation for the lowest pressure, illustrating preponderance of sliding at interface for this case. Some experimental results highlighted that slippage decreased with increasing applied pressure in the case of quasi constrained HPT tests [17].

During HPT tests, there are simultaneously both surface phenomena (sliding) and volume phenomena (transformation). The torque obtained during a test is the sum of the torque necessary to shear the bulk of the sample and the torque due to friction at the interface sample/anvils. In present work, the objective is to study material transformation in volume; some adherence is required to achieve such transformation. Thus, a nominal pressure of 3GPa is chosen for R260 steel and of 1GPa is chosen for Iron. It also can be checked that the radius $r_A$ is almost equal to the radial location of maximal equivalent strain, as will be more illustrated next section.

3.3. The effect of friction coefficient $\mu$ at the interface sample/anvils
Case of the ultra-high-purity iron

In this section, the results are presented for high purity iron obtained with 1GPa of nominal pressure and with friction coefficients of 0.2 or 0.5 at (1) the beginning of the torsion (θ=13°) and (2) the end of rotation (θ=162°). Whatever the friction coefficient, the torque continuously increased with the rotation angle (figure 6a). The torque and the slope were higher with a friction coefficient of 0.5 than with 0.2. It appears that friction had a significant effect on the torque evolution such that the torque doubled when friction increased. For the friction coefficient of 0.5 the thickness decreased less than for 0.2 during the compression step. During torsion the difference between both thickness (with 0.2 and 0.5 friction coefficient) was almost the same as well as the slope. (figure 6b). The central region of the sample (r < 1.5 mm) exhibited a contact pressure higher than 1 GPa (figure 7). In the centre the contact pressure was higher for a friction of 0.2 than for 0.5.

![Figure 6](image1.png)

Figure 6. Pure iron, 1 GPa, effect of friction on (a) Torque, (b) sample thickness evolution

![Figure 7](image2.png)

Figure 7. Pure iron, 1 GPa, pressure function of friction coefficient

Concerning the slippage at the interface it has been observed that at low rotation angle the tangential slippages CSlip2 had almost the same maximal values for both friction coefficients; the radial slippage CSlip1 had a higher maximal value for friction coefficient of 0.2 than for friction coefficient 0.5.
Slippages were located in a circumferential rim: $r > 2.5 \text{mm}$ for friction coefficient of 0.5 and $r > 1.3 \text{mm}$ for friction coefficient of 0.2. When the rotation angle increased the maximal value of $CSlip_1$ tended to stabilize for friction coefficient of 0.5 but still increased for friction coefficient of 0.2. The maximal value of $CSlip_2$ increased for both friction coefficient but the sliding area increased drastically for friction coefficient of 0.2 while it tended to stabilize for friction coefficient of 0.5. Slippage has been highlighted experimentally for iron in the case of unconstrained HPT tests conducted in the same conditions of pressure than the simulations (figure 9a); but also in previous work [7, 16]. This has also been measured in the case of quasi constrained HPT tests with three materials included iron [17].

The figure 8c plotted the evolution of the adhesion zone radius $r_A$. $r_A$ decreased when the rotation angle increased but was different function of the friction value. After 90° of rotation, $r_A$ tended to reach a constant for friction coefficient of 0.5 and approached zero for friction coefficient of 0.2. Without focusing exclusively on the friction coefficient value, the existence and this kind of evolution of the adhesion/sliding areas have been highlighted experimentally in previous works [7, 16].

For both friction values, the strains $\varepsilon$ were low at the centre of the sample and at the periphery, but reached a maximum value (figures 10a, 10b) and their radial positions draw closer to the transition area between the adhesion and the sliding zones, i.e around $r_A$. For a friction coefficient of 0.5 and 0.2 the maximal value of $\varepsilon$ increased as the rotation angle increases but greater for 0.5 than 0.2 (figure 10c). Between 90 and 162° $\varepsilon$ doubled for 0.5 of friction whereas it increased by 30% for 0.2 of friction coefficient. For the highest friction coefficient, a very high level of strain ($\varepsilon > 20$) and strain gradients can be identified around $r_A$. These very high mesh distortions lead to convergence problems around these numerical singularities.

![Figure 8](image-url)

**Figure 8.** Radial ($CSlip_1$) and tangential ($CSlip_2$) cumulative slippage distances after (a) 13° and (b) 162° of rotation, (c) adhesion radius $r_A$ versus rotation angle. For iron, at 1GPa, versus $\mu$. 
Figure 9. Radial and tangential sliding on surface samples after HPT tests, for (a) high-purity iron, (b) steel grade R260 (Secondary electron images in a scanning electron microscope FEI Quanta600).

Figure 10. Pure iron, 1 GPa, effect of friction, (a) and (b) equivalent strain evolution function of rotation angle, (c) evolution of the maximal value of equivalent strain versus angle rotation

Case of grade steel
In the case of the steel the calculations have diverged after 30° of rotation at 3 GPa for friction of 0.5 (very high mesh distortion and numerical singularities). Only results up to 26° will be presented.

The global trends were the same than for iron for the torques, the thicknesses versus the rotation anvil (figure 11). The central region of the sample (r < 1.3 mm) exhibited a contact pressure higher than 3 GPa, except in the case of a friction coefficient of 0.5 at the end of the compression step (figure 12). This was due to the deformation of the anvil.

Figure 11. Steel, 3GPa, effect of friction on (a) torque, (b) sample thickness
One of the main differences between the two materials was for the slippage: CSlip1 and Cslip2 maximal values had the same values (figures 13a, 13b). Slippage has been highlighted experimentally in the case of unconstrained HPT for steel after tests conducted in the same conditions of pressure (figure 9b). As already written, further investigation is needed to analyze the relative importance of both sliding directions. \( r_A \) decreased drastically in the case of friction coefficient of 0.2 at the beginning of the torsion (figure 13c). The behavior was the same than iron. The present results showed that strong effects arised from the friction between the sample and the anvils. Thus, a low friction coefficient made easier the flow of material between the anvils. This led to an early reduction in the overall thickness of the sample. A high friction coefficient reduced the material flow between the anvils and increased the torque required to rotate the anvils and thus to shear the bulk of the sample. Experimentally, one of the great challenge is to control the adhesion between the sample and the anvils.

For both friction values, the strains \( \varepsilon \) were low at the centre of the sample and reached a maximum value close to the periphery of the contact (figures 14a, 14b) and their radial positions are around \( r_A \).

For a friction coefficient of 0.5 and 0.2 the maximal value of \( \varepsilon \) increased as the rotation angle increases but greater for 0.5 than 0.2 (figure 14c).
4. Conclusions

FEM simulations were used to estimate the stress and strain history within the sample but also at the interface between the sample and anvils during HPT processing. The history of the calculated global parameters (torque and sample thickness) and local parameters (strain and stress) was investigated versus the friction coefficient at the interfaces and versus the imposed pressure. The influence of the flow law was also investigated as two materials were tested: an ultra-high purity iron and steel grade R260. Analysis was focused on a specific sample “depth” corresponding to the interface between sample/anvils (surface) and to the first layer of the sample just below surface as preliminary results [7, 16] showed that the transformed layers exhibiting the finest microstructures could locate in such sample volume. This parametric study highlights the role of the imposed parameters (friction coefficient at the interfaces anvil surfaces/sample, imposed pressure). In particular the friction coefficient controls the stress/strain distribution in the sample bulk for the two tested materials. As was already suggested [7, 16], this work confirms that the surface conditions govern the location and the level of material strain, strain gradients and pressure in the bulk.

The present modelling provides thus a tool to investigate and to analyze the effect of mechanical parameters such as pressure and friction on the local stress and strain history during the HPT process and to couple with experimental results. However numerical difficulties appear for high strength material or for high friction coefficient or high pressure. To overcome numerical difficulties associated with strong distortions of mesh, high pressure and strong contact conditions leading to numerical singularities, some new developments of the model are under progress. Experimentally, one of the great challenge is to control the adhesion between the sample and the anvils.

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