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3D modeling of unconstrained HPT process: role of strain gradient on high deformed microstructure formation

A Ben Kaabar¹, A Aoufi², S Descartes¹, C Desrayaud²

¹ Univ Lyon, INSA-Lyon, CNRS, UMR5259 LaMCoS, F-69621 Villeurbanne, France

² Univ Lyon, Ecole des Mines de Saint-Etienne, CNRS, UMR 5307 Laboratoire Georges Friedel, F-42023 Saint-Etienne, France

Corresponding author: sylvie.descartes@insa-lyon.fr

Abstract. During tribological contact's life, different deformation paths lead to the formation of high deformed microstructure, in the near-surface layers of the bodies. The mechanical conditions (high pressure, shear) occurring under contact, are reproduced through unconstrained High Pressure Torsion configuration. A 3D finite element model of this HPT test is developed to study the local deformation history leading to high deformed microstructure with nominal pressure and friction coefficient. For the present numerical study the friction coefficient at the interface sample/anvils is kept constant at 0.3; the material used is high purity iron. The strain distribution in the sample bulk, as well as the main components of the strain gradients according to the spatial coordinates are investigated, with rotation angle of the anvil.

1. Introduction

During tribological contact's life, different deformation paths lead to the formation of high deformed microstructure in the near-surface layers of the bodies. Those structural changes occurring at the near surface are one of the natural responses of materials to tribological stresses, i.e. temperature, hydrostatic pressure and shearing gradients. This response is named Tribologically Transformed Structures (TTS) [1–3]. In most cases, the TTS are often described as submicrometric structured nearsurface layers produced at contacts [1-5]. Initially attributed to flash temperatures generated by frictional heating at the contact zone, followed by subsequent quenching [5, 6], several studies have shown that the temperature increase was often too low to explain these phase transformations [7-10]. Thus these transformations could result from high strain under high hydrostatic pressure [9-12] and even at low temperatures. In parallel, among the Severe Plastic Deformation (SPD) processes [13], High-Pressure Torsion (HPT) experiments are efficient to obtain materials with ultra-fine structures [14-17] or phase transformations in materials. 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.

Furthermore, in the case of the unconstrained version of HPT, previous experimental work [18, 19] has shown the development of a refined structure after only one revolution, for two carbon steels materials and high purity iron (Fe 99.9999%) tested on such apparatus, at room temperature. The evolution of the microstructure has been correlated with the contact conditions (localization of the

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sliding or adhesion zones between sample and anvil surfaces) [20, 21]. In the present work, the unconstrained HPT process simulates numerically the HPT tests. The material is a high purity iron (Fe 99.9999%). The 3D finite element model developed allows to study locally the specificity of the stress and strain loading cycles within the areas where TTS are formed during these tests. To calculate significant stress and strain cycles in the right range of tribological conditions, this modeling takes into account both the contact conditions (friction at the sample / anvil interfaces) and the material behavior law in an adequate range of pressure and stresses.

2. 3D finite element model

2.1. Model geometry

In order to investigate the stress and strain results but also the strain gradients in the sample volume, a 3D model (figure 1) was developed with commercial software (Abaqus 6.9) to simulate the cylindrical sample compressed and sheared between two anvils. The two cylindrical tungsten carbide (WC) anvils were considered to be rigid, with mass and inertial moment. The anvil geometry used in these simulations was based on the unconstrained HPT set-up geometry. The anvils were smooth with a diameter of 3.2mm. The sample was 3.0 mm in diameter and 0.5 mm thick. The model parts were meshed with 8 noded-50 μ m elements (C3D8R elements) for the samples and 100 μ m elements for the anvils. The simulations, through a quasi-static analysis, were used to examine the processing operation up to a quarter revolution of the bottom anvil. The model was assuming an ALE (Arbitrary Lagrangien Eulerien) numerical scheme providing the displacement variable as the sum of both the material and the grid motion in order to:

- satisfy the mechanical balance equilibrium,
- minimize the mesh distortion according to criteria defined on aspect ratios and angles of the elements of the mesh.

Practically in the explicit version of the Abaqus software, a smooth procedure of the mesh is processed at a frequency of 10 increments (default value) to respect the limit defined in terms of distortion of the elements which the topology was constant during whole the calculation. The explicit formulation of the problem implied an averaging procedure of the output variables to avoid numerical noise in the solution. Finally the mass scaling procedure applied in the prescribed range enabled to decrease significantly the CPU time at completion.



Figure 1: (a) Schematics of HPT model, (b) 3D view, (c) Behaviour law for pure iron

2.2. Material behaviour and boundary conditions

An ultra-high purity iron Fe was studied: the Young's modulus E was 210 GPa, the Poisson ratio v was 0.3, the density was 8.7 10^{-9} t/mm³ and the yield stress was 120 MPa. 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 elasto-plastic and based on flow curve determined experimentally through compression tests under hydrostatic pressure up to 0.8 GPa. The stress–strain curves used are plotted in figure 2. In real HPT process, slippage occurs

between the anvils and the sample. One Coulomb friction coefficient value was chosen and equal to 0.3, based on previous results [20-21].

2.3. Description of a numerical test

In the first load step, the target vertical load (3.5kN) was applied via the bottom anvil through a vertical displacement along Y (in exactly the same way as in the experiment). This load corresponds to a nominal pressure P of 1 GPa, on a circular 3 mm diameter disk. 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 (Y) was imposed on the bottom anvil. In the last step the rotation was applied up to the 3 target rotation angles: 1°, 30° and 90° of anvil rotation.

3. Results and discussion

Previous experimental results [18, 20] have shown that the transformed layers exhibiting the finest microstructures were produced in a specific sample volume linked with sliding/adhesion contact conditions (Figures 2a, 2b). The adhesion zone was characterized by a radius rA. The surface conditions thus govern the location of material transformation in the bulk. Different paths (a path is composed of consecutive nodes) were thus defined, in relation to previous experimental work highlighting the TTS location within the sample [18, 20] (Figure 2c). The stresses and strains could thus be calculated during a simulation at different depths and along radius within the sample following these paths, at a given rotation angle.



Figure 2: Sliding/adhesion contact. (a) The adhesion radius rA decreases with increased φ (b)
Schematics evolution of the microstructure refinement (pink) based on previous experimental results,
(c) Location of the chosen paths for the present numerical model

The evolution of contact conditions was calculated at the interface. The contact pressure distribution (CPress in abaqus software) was presented for 90° of anvil rotation (Figure 3a). For 3 different angles of rotation, the relative sliding between the anvil and the sample was quantified along "path-sup surface". An adhesion zone could thus be highlighted (Figure 3b); it decreased with increasing of $\varphi(^{\circ})$.

The history of the Von Mises equivalent plastic strains ε (variable PEEQ used in Abaqus software) was also plotted along radius r and through thickness of the sample, for the different paths and for different anvil rotation angle (Figure 4). For a given depth, these strain were low at the centre of the sample and at the periphery, but reached a maximum value around a radial position close to the transition area between the adhesion and the sliding zones. The radial location of the maximum approached the centre of the sample when the angle increases. For a given radius, the strain values are maximal in the skin.

During the unconstrained HPT process pure shear strain $(\varepsilon_{z\theta})$ occurred but also a shearing strain $(\varepsilon_{r\theta})$ at the frontier between the sliding and the adhesion zones, considering that elongation was possible in the radial direction. Thus those strain components were plotted along the different paths (Figures 5, 6, 7). The strain components reached a maximum value and their radial positions draw

closer to the transition area between the adhesion and the sliding zones. While $\varepsilon_{\theta z}$ evolution stabilized between 30° and 90° of anvil rotation (Figure 5), $\varepsilon_{r\theta}$ values increased with increase of $\varphi(^{\circ})$, especially in the near-surface layer (Figure 6). The increase was closely linked to rA evolution. ε_{rr} increased continuously along the different paths r- with increase of φ (Figure 7) in the whole sample.



Figure 3: (a) Contact pressure distribution for $\varphi = 90^{\circ}$, (b) Evolution of the adhesion zone



Figure 4: Von Mises equivalent plastic strain for 3 angles of rotation 1°, 30° and 90°, along different paths (see figure 2c)



Figure 5: Plastic strain $\mathcal{E}_{\theta z}$ for 3 angles of rotation 1°, 30° and 90°, along different paths (see figure 2c)

Previous work [20] highlighted strong equivalent plastic strain values coupled with large equivalent strain gradients in both radial and axial directions, where TTS were located. To go further in the mechanical analysis, the main components of the strain gradients according to the spatial coordinates were calculated in the present work (tables in the figure 8). The gradients were obtained as the average values of the strain variation ($\Delta PE_{r\theta}$, $\Delta PE_{z\theta}$, ΔPE_{rr}) along the considered coordinates (r or h). These table provided an estimation of the curvature. The strain gradients (i. e. components of the curvatures tensor) were maximal in the areas in which "TTS" were observed (Figure 8). The gradients of $\mathcal{E}_{r\theta}$ were the highest ones within whole the sample, especially in the axial direction, and below the adhesion zone. Maximal gradients of \mathcal{E}_{rr} values were linked with the edge sliding/adhesion zones. Nevertheless

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the accurate values can be obtained by the calculation of second gradients of the displacements (i.e. curvature) [22], $\alpha_{ii} = \varepsilon_{ikl} \frac{\partial \beta_{li}^{p}}{2}$ (m/m²); this work is in progress.







Figure 7: Plastic strain \mathcal{E}_{rr} for 3 angles of rotation 1°, 30° and 90°, along different paths (figure 2c)

4. Conclusion

The objective of the present work was to investigate numerically the unconstrained HPT process through a 3D finite element model. Gradients of the strain components in both radial and axial directions have been highlighted. Those gradients coupled with high strain seem to be a condition necessary to form TTS. This model will allow to investigate in an accurate way the strain paths and curvatures, in relation with the developed microstructures during a test and their localization in the sample.

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Figure 8: Strain gradients components

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