

Numerical Simulation of Severe Plastic Deformation during High Pressure Torsion Processing

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Abstract: The principle of achieving high strength and superior properties in metal alloys through the application of severe plastic deformation has been exploited in the metal processing industry for many decades. The High Pressure Torsion (HPT) process is one of the most promising techniques for imposing very high strains to a bulk solid without introducing a significant change in sample dimensions. The HPT process involves large shear and compressive plastic deformations, and offers the possibility to deform the material under very high hydrostatic pressures (up to several GPa), with continuous control of the degree of deformation. This process can produce exceptional levels of grain refinement, and provides a corresponding improvement in mechanical properties. It is of paramount importance that the shape of the sample is retained during the high pressure torsion process, by means of special tool geometries which effectively prevent free flow of the metal to obtain high hydrostatic pressures. The design of the mold geometry and the corresponding sample dimensions is an iterative process, which is governed by the constitutive behavior of the metal alloy under investigation. In this paper, we highlight the added value of Abaqus as a powerful numerical tool to assist in the design of high pressure torsion experiments.

Keywords: High Pressure Torsion, plastic deformation, metal plasticity, design optimization

1. Introduction

Nanocrystalline materials (NCM) represent a whole generation of solids with new atomic structures and properties by utilizing the atomic arrangements in the cores of defects such as grain boundaries, interphase boundaries or dislocations. Severe plastic deformation (SPD) achieves very fine crystals by the use of severe straining and deforming the material under high pressure to prevent the material from failing. SPD processing is defined in (Zhilyaev, 2008) as any method of metal forming under an extensive hydrostatic pressure that may be used to impart a very high strain to a bulk solid without the introduction of any significant change in the overall dimensions of the sample and having the ability to produce exceptional grain refinement. The most important methods to achieve SPD are Equal Channel Angular Pressing (ECAP) and high pressure torsion.

During a HPT process a disk-like specimen, with a height around 1mm and a diameter between 10 and 20mm, is compressed between two anvils. The pressure varies from 1GPa up to 10GPa. Once the pressure is applied, one anvil is rotated with respect to the other.

Due to friction in contact surfaces between the specimen and the anvils, the specimen is deformed by shear force. The main volume of the specimen is strained under hydrostatic compression because of the applied pressure and the pressure of the outer layers of the sample.

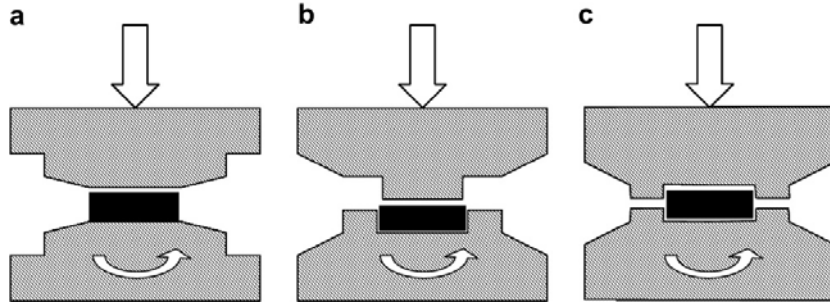


Figure 1. Unconstrained (a), constrained (b) and semi-constrained (c) HPT

Two distinct types of high pressure torsion exist, each with its own features. The first type, see figure 1a (Zhilyaev, 2008), is called *unconstrained*. The sample is placed between two flat anvils during the test. This type has the advantage of a simple anvil design. The downside of this technique is the difficulty to accomplish a hydrostatic pressure throughout the specimen. When the pressure is applied, and the work piece is rotated, nothing obstructs the outward flow of material at the edges. As a result, the diameter of the sample increases while in the center the backpressure due to friction is large, and no outward flow is possible. As a result, the thickness varies as function of the radius, with inhomogeneous properties as a result.

The second type is represented in figure 1b and is called *constrained*. The sample is placed within the mold, which prevents outward flow completely. The hydrostatic pressure is constant throughout the specimen with more homogeneous properties after processing. The difficulty lies in the mold: designing the geometry and selection of appropriate materials is a difficult challenge. When the compression force is applied, both the specimen and the mold decrease in height. As a result, it is likely that the molds will come into contact and introduce high friction forces and wear rates in the contact surface.

A compromise is found when using the quasi-constrained geometry. The outward flow is partially prohibited by placing the specimen in depressions in the anvils. However, the height of the specimen is larger than the depth of the depressions. This will result in large friction forces at the edges, ensuring hydrostatic pressure in the specimen, and lower wear rates in the anvils. This is the kind of HPT found in most literature.

The grain refinement and the corresponding enhancement of mechanical properties obtained by a HPT process are to a large extent dependent on the pressure and strain imposed to the material. The distribution of the strain and the pressure in a sample are determined by the geometry and material of both the mold and the sample, and the friction between mold and sample. Numerical simulations have been used to study the conditions of the HPT process.

In (Draï, 2013), the 3D deformation behaviour of a high density polyethylene (HDPE) sample during an unconstrained high pressure torsion process is simulated using MSC.Marc. The initial dimensions of the cylindrical sample are a diameter of 20 mm and a height 10 mm. The sample is meshed with 34 992 eight-node isoparametric hexahedral elements. The upper and lower anvils are assumed to be rigid bodies. A vertical displacement is imposed to the upper anvil in the compressive direction, and is maintained during torsion.

In (Yoon, 2008), the DEFORM finite element code is used to perform isothermal simulations of the unconstrained HPT for pure copper. The initial dimensions of the copper work piece are 20 mm in diameter and 10 mm in height. The anvils are modelled as rigid bodies, and are assumed to be tied to the deforming sample. (Kim, 2001) and (Kim, 2003) report isothermal finite element simulations of unconstrained HPT for pure copper using Abaqus. The cylindrical specimen with diameter 20 mm and height 0.7 mm is modelled using four-node generalised axisymmetric elements with twist (CGAX4). These elements allow for displacements in the circumferential direction that vary with radius and height.

In this paper, the added value of Abaqus in simulating HPT processes for metal alloys is highlighted. First, the use of adaptive remeshing techniques is demonstrated to cope with the large deformation and corresponding mesh distortion that occurs during severe plastic deformation. Then, the versatility of Abaqus/CAE is exploited in the parametric design of the tool geometry, where Abaqus offers an integrated interface to optimize the shape of the sample and the dimensions of the mold. At the end of this paper, the use of axisymmetric elements with twist (CGAX4) is introduced as an elegant and computationally efficient way to simulate high pressure torsion.

2. Mesh control during severe plastic deformation

For the analyses, presented here, a disk shaped specimen with diameter $D = 10$ mm and thickness $H = 1.0$ mm is used. The mold geometry is shown on Figure 2. Initially, the die is modelled as a rigid body by applying a *RIGID BODY constraint.

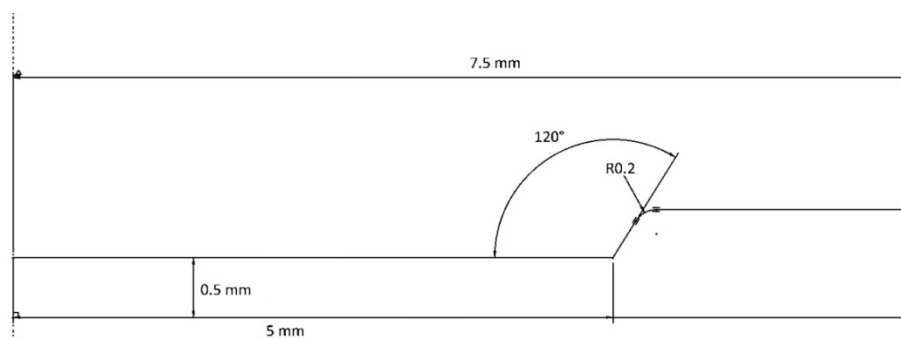


Figure 2. Geometry and dimensions of an axisymmetric section of the die

The sample is modelled as soft steel, with a Young's modulus $E = 210$ GPa and a Poisson coefficient $\nu = 0.3$. The elastoplastic properties are defined by a yield stress $\sigma_y = 100$ MPa, and a small-slope hardening curve that allows for severe plastic deformation (up to 500% strain).

Coulomb frictional contact conditions (with a friction coefficient $\mu = 0.1$) are applied at the interface between the steel sample and the rigid die. The sample is meshed with 50×10 CAX4 (four node bilinear axisymmetric quadrilateral) elements, a mesh density suggested by (Kim, 2001).

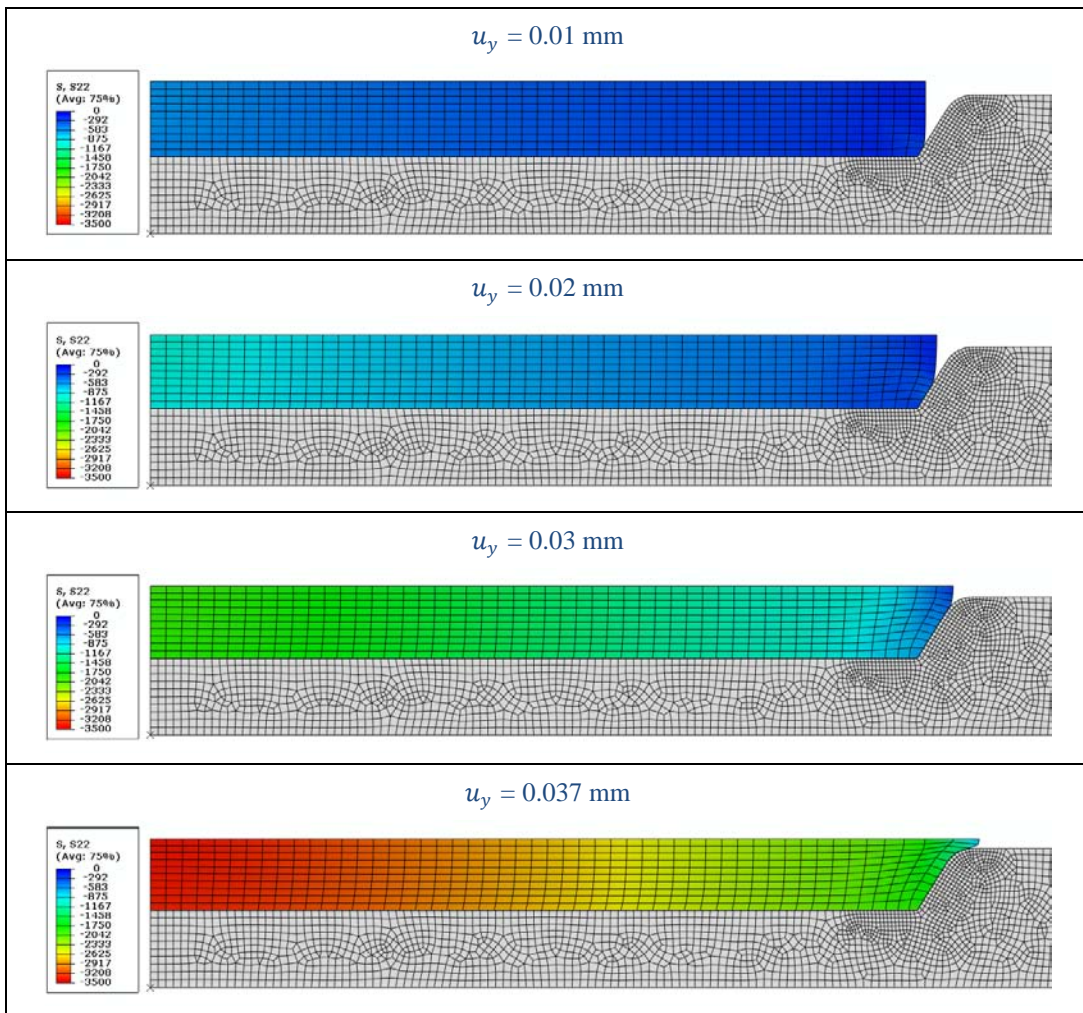


Figure 3. Mesh distortion during application of compressive load

In a first step, a vertical displacement $u_y = 0.04$ mm is imposed on the reference point of the rigid die, to simulate compressive loading of the steel specimen. The deformation of the sample, and the corresponding compressive stresses, are shown on Figure 3. At (very) high levels of compressive strain (up to 3.5 GPa), however, the simulation seems to suffer from mesh distortion. The soft steel sample cannot cope with the extreme plastic deformation at the extremity, and convergence during a subsequent torsion loading step is judged unlikely.

Abaqus offers several tools to improve mesh quality in simulations where severe mesh distortion can be expected. The strategy, pursued in our analysis, involved

- Partitioning the outer edge of the die, to introduce more elements in the vicinity of the inclined shoulder. A higher mesh density in this critical area of the master surface improves the stability of the contact algorithm
- Using a biased mesh over the thickness of the sample, to anticipate to large deformations at the extremity of the sample
- Applying adaptive remeshing to maintain reasonable element shapes and aspect ratios whilst the shape of the sample is evolving.

In Figure 4, the initial simulation is compared with an enhanced mesh strategy, indicating that the latter solution can cope with extreme plastic deformation.

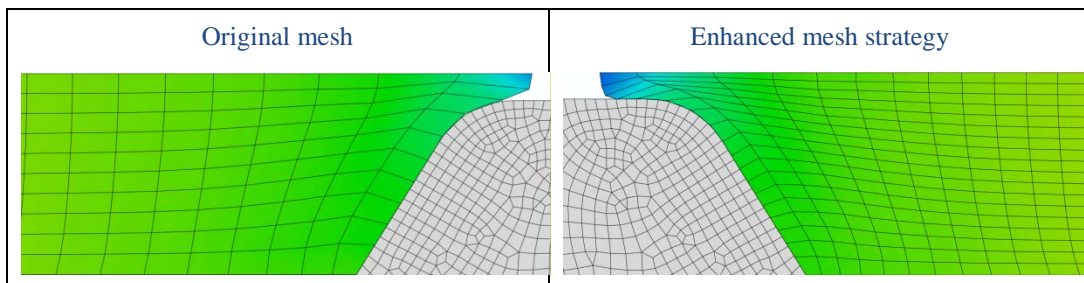


Figure 4. Mesh control during severe plastic deformation

3. Parametric design optimization

The shape of the mold and material sample, to a large extent determine the homogeneity of the stresses and the distribution of the strains in the sample. The depth of the cavities in the symmetric molds in a semi-constrained configuration has to be large enough to guarantee radial containment of the sample, on the other hand a too large depth can result in an undesirable contact of the molds at the end of the compression stage and/or during torsion. The depth of the sample cavity in the molds is chosen to be 0.3mm, which allows for a maximum sample compression of 0.4mm (1-2x0.3). Next to the depth of the mold cavity, also the inclination of the lateral boundary is important, since it affects both the level of hydrostatic pressure and strain distribution.

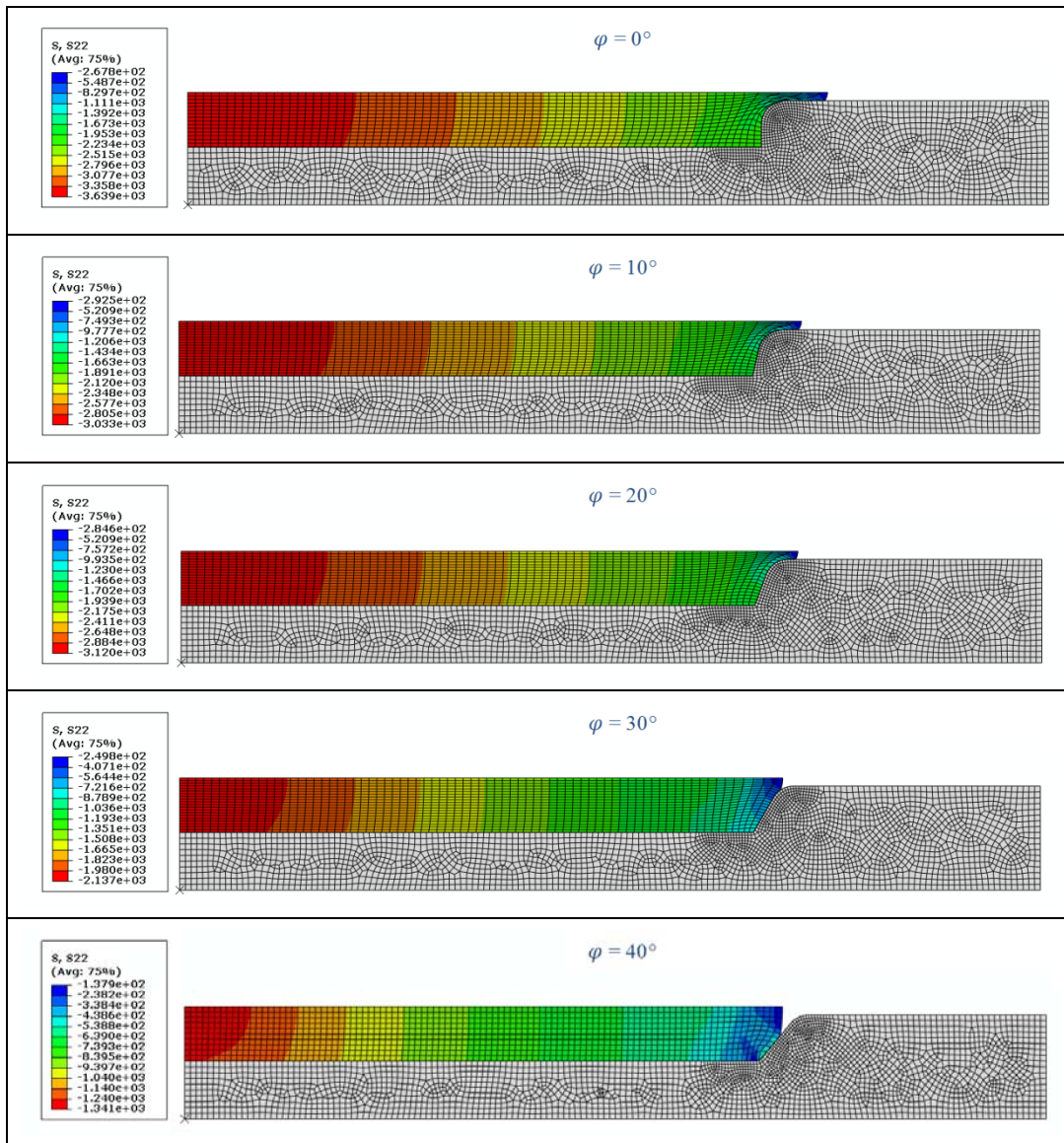


Figure 5. Influence of inclination on deformation and compressive stress state

The Abaqus/CAE integrated interface to enable the parametric design of the tool geometry was used to study the effect of specimen and mold dimensions. On Figure 5, the influence of the inclination on the sample deformation and the induced compressive stress state is clearly visible.

Based on the tool dimensions, suggested by the designer, a Python script can be launched to subsequently

- (i) Construct the die geometry
- (ii) Partition the edges to facilitate biased seeding
- (iii) Mesh the rigid die
- (iv) Write the input file

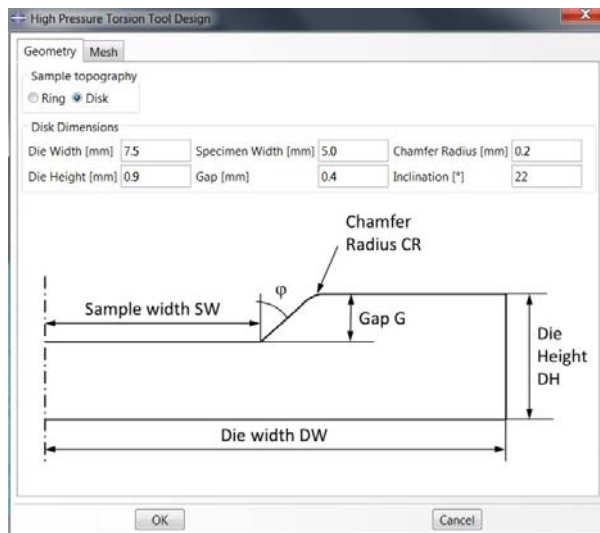


Figure 6. Python plug-in for the parametric tool design

The development of such a geometric plug-in, like shown in Figure 6, enables a fast and straightforward optimization of the die geometry.

4. Simulation of High Pressure Torsion

The CGAX4 element is useful for the analysis of structures that are axially symmetric, but can twist about their symmetric axis, as is the case in high pressure torsion processes. Indeed, the CGAX4 element allows displacements in the circumferential (θ) direction that vary with the radius and the height, but not with θ .

In Figure 7, the results of a HPT simulation using CGAX4 elements are shown, where the soft steel specimen has been subjected to a compressive load (corresponding to an 0.04 mm vertical die displacement), followed by a 30° rotation of the die.

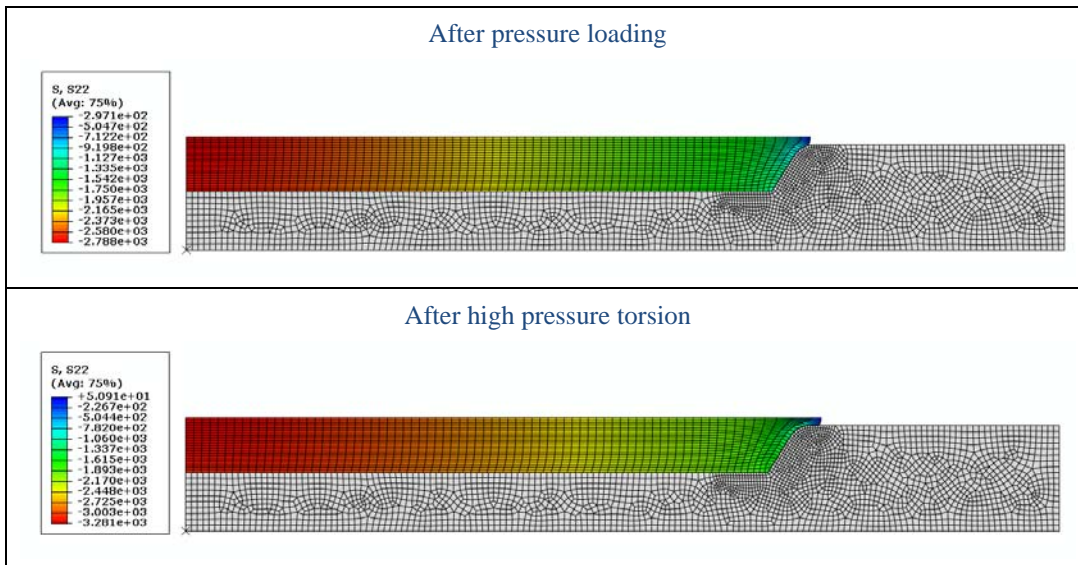


Figure 7. Sample deformation during high pressure torsion processing

Note, however, that axisymmetric solid elements with twist should be used with caution within rigid bodies, as incorrect results may be obtained under large rotations, as stated in the output .dat file. To mitigate this risk, the die can be modelled as a deformable body with high stiffness and yield strength. On Figure 8, the predicted sample shape after high pressure torsion is shown using this 'deformable die' approach.

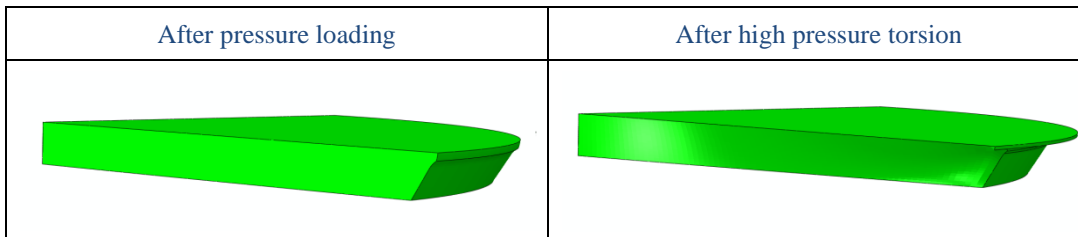


Figure 8. Prediction of the deformed sample shape

5. Conclusions

In this contribution simulations of the high pressure torsion process using the finite element code Abaqus are presented. The adaptive remeshing capabilities were used to cope with element distortion at very high levels of equivalent plastic strain. The integrated Abaqus CAE interface was used for the parametric design of the tool and specimen geometry, and dimensions. In addition, the extensive library of constitutive models for metal plasticity allowed us to come to an in-depth understanding of the sample response during severe plastic deformation.

6. References

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