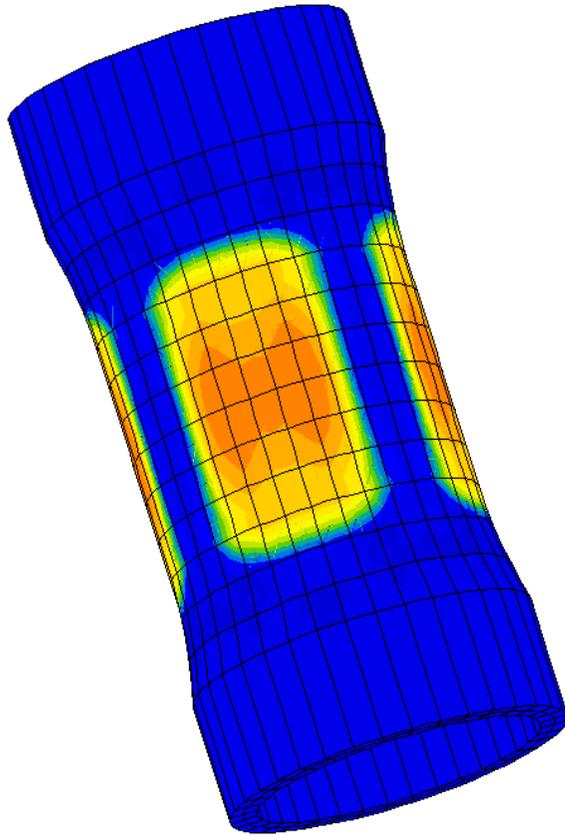


Tension–torsion of a single crystal tube



Macroscopic yield loci derived from crystal plasticity cannot be reduced to a classical macroscopic model expressed by means of invariants. The purpose of this mini-project is to illustrate this fact, by using a single crystal tube loaded in torsion, tension, and combined tension–torsion.

There is two tracks, labelled *A* and *B* in the present document. Students are free to choose one of them. . . or both !

An experimental and numerical study on a single crystal tube can be found in [1]. The students will be asked to reproduce the main aspects of the numerical simulations, using a finite element code, a driver of constitutive equations for plotting yield surfaces, and also analytical solutions, derived by hand. The following directories are provided:

- BIBLIO, a directory containing the paper in reference, and a tutorial detailing the construction of yield surfaces for a single crystal;
- TORSION, a directory containing mesh and input files needed to run a computation under torsion loading;
- TENSION, a directory containing mesh and input files needed to run a computation under tension loading;
- SURFACE, a directory containing input files needed to compute and plot yield loci.

The students will have to run the computations in pure torsion for a $\langle 001 \rangle$ oriented tube. The resulting stress and plastic strain fields will be carefully analysed, on a global (loading curves) and local level (stress and plastic strain fields, strain localisation). These results will be consolidated by using the simulation of the yield surfaces in tension and shear, in the SURFACE directory. As an extension of this first part, other load cases can be investigated. The project *A* will add tension cases and combined in-phase tension–torsion on the same tube, meanwhile project *B* considers a $\langle 111 \rangle$ oriented tube.

Keywords: *Tension–torsion loadings; crystal plasticity; yield surfaces; octahedral and cube slip systems*

Before starting the project, the students are invited to go in the directory BIBLIO, to have a quick look to [1]. They will then read carefully the file SX.pdf, which provides a short overview of the plasticity mechanisms attached to slip system theory, and shows the resulting yield surfaces in various planes, for the case of octahedral slip systems.

1 Yield surface plots

Tracks (A) and (B) Go to directory SURFACE

In the mini-project, slip will be also considered on cube planes. Six slip systems can then be defined. Like for octahedral slip, the slip directions are the six diagonals of the cube, but now the slip planes are the planes of the cube, so that the systems are:

$$\begin{array}{ll} \text{E5: } < 001 > \{ \bar{1}10 \} & \text{E6: } < 001 > \{ 110 \} \\ \text{F1: } < 100 > \{ 011 \} & \text{F2: } < 100 > \{ 0\bar{1}1 \} \\ \text{G4: } < 010 > \{ \bar{1}01 \} & \text{G3: } < 010 > \{ 101 \} \end{array}$$

As a first step, it is proposed to reproduce the yield surface in tension and shear for a point located on the $\bar{1}00$ crystal axis. This can be made by means of the command

```
Zrun surf001
```

(please have a look to the data file surf001.inp, and to the material files *001.mat before running the code). The present computation is made with an initial resolved shear stress of 100 MPa. The result is in the files s001*.test, and can be plotted by means of the command

```
./D001
```

Check that the result is in agreement with the equations provided in the tutorial file SX.dat for octahedral slip, and with the values obtained for cube slip. Check that the result is the same for other types of tension–shear planes (like $\sigma_{11}-\sigma_{31}$ for instance). Change the value to reproduce exactly the figures 1a and 1b in [1] (the resolved shear stress was calibrated to have an initial yield in tension equal to 1000 MPa for octahedral slip, and the same value for cube slip).

In order to reproduce the figures 1c and 1d of the paper, it is now necessary to change the relative orientation of the crystal and of the loading. This will be made by rotating the crystal with respect to the loading frame. As a result, there are only little changes in the input file surf011.inp. The material file is cube011.mat. Check that the slip systems are now defined in a frame obtained by a rotation of 45 degrees around the x_3 axis, which is also the $< 001 >$ crystal axis. Of course, the various shears are no longer equivalent in this case, and the surface search must be performed in the $\sigma_{11}-\sigma_{31}$. Run the code by means of

```
Zrun surf011
```

and draw the result by means of

```
./D011
```

What is the ratio between the previous value and the present one ?

Track A

For octahedral slip, the file octa011.mat needs to be documented. So, apply the previously defined rotation to the octahedral slip systems, and run the calculation, using again the surf011.inp file, where the first occurrence of the line ****return will be commented. Use again D011 file to draw the result.

Track B In order to be prepared for a tube with a $< 111 >$ axis, give the expression of the various slip systems in a frame where the x_1 load axis coincide with the $< 1\bar{1}0 >$ and the x_2 axis with the $< 111 >$ direction. How many "soft" zones are expected from this computation ?

2 Classical results for a tube under torsion loading (A and B)

The following classical results will be used to obtain estimations of the stress and strain levels in the tube. They are valid for a tube whose internal and external radii are r_i and r_e . The elasticity of the material is supposed to be cubic, and the axis of the tube coincides with one of the cube axes. The inelastic behaviour is represented by a perfectly plastic model.

The angle per unit length is denoted by α . The resulting angle for a total length L will then be $\beta = L\alpha$. The section of the tube remains flat, and the only component of the strain tensor in a cylindrical referential is the shear strain $\varepsilon_{z\theta} = \gamma/2$, that is proportional to the radius, $\gamma = \alpha r$. If an angle β is applied to a tube of length L , the resulting shear will then be $\gamma = \beta r/L$. For the case of cubic elasticity with a shear modulus C_{44} , the shear stress τ in the tube is related to the shear strain γ by $\tau = C_{44}\gamma = C_{44}\alpha r$. The torque applied to the tube in these conditions is obtained by integrating the stress on the section of the tube:

$$C = \int_0^{2\pi} \int_{r_i}^{r_e} (r\tau)(rdrd\theta) = D\alpha \quad \text{with } D = \frac{1}{2}\pi C_{44}(r_e^4 - r_i^4)$$

The resistance to torsion is characterized by D , which depends on the geometry of the tube and on the elastic properties of the material. The onset of plasticity is reached when the shear strain meets the plasticity criterion. This happens at the external radius of the tube. For the case of a von Mises material with an initial yield of σ_y , the corresponding value of the torque, C_e , is obtained when $\tau = \sigma_y/\sqrt{3}$:

$$C_e = \frac{\pi}{2\sqrt{3}} \sigma_y \frac{r_e^4 - r_i^4}{r_e}$$

The plastic zone will extend from r_e to r_i if the applied torque (or the angle) still increases. For a perfectly plastic material, the final value of τ is equal to $\sigma_y/\sqrt{3}$ everywhere in the section, so that the maximum torque that

can be applied is

$$C_m = \int_0^{2\pi} \int_{r_i}^{r_e} \left(r \frac{\sigma_y}{\sqrt{3}}\right)(rdrd\theta) = \frac{2\pi}{3\sqrt{3}} \sigma_y (r_e^3 - r_i^3)$$

3 Computation of the tube under torsion loading (A and B)

Go to directory `TORSION`

The following files are available to run the computation:

- `torsion.geof`, the geometry file, including nodes, and elements and groups (the cylindrical part of the specimen has an internal radius of 12 mm, and an external radius of 13 mm, and a length of 20 mm. The total length of the specimen is 60 mm); this 3D mesh has been generated by a sweep operation applied to the 2D mesh `tors2d.geof`, which can be seen also by using the command

`Zmaster tor2d.geof`

- `cyl2.inp`, the input file, that allows the user to define the algorithm and the convergence parameters, to prescribe the applied load (a rotation of 2 degrees), to manage the outputs and to point toward the material file;
- `j21d.mat`, the material file, that defines the single crystal behaviour, with a cubic elasticity, and two slip system families, octahedral and cube slip. The viscosity defined by the model is low; the initial resolved shear stresses are respectively 375 MPa for octahedral planes and 490 MPa for the cubic planes, in agreement with the paper in reference. There is also a low isotropic hardening.

The computation has to be run by means of the command:

`Zrun torsion`

To perform the graphical analysis of the calculation, check the results by means of the command:

`Zmaster torsion`

First analysis

The analysis will be made by following the suggestions below:

- Use `Results` option to plot a map of the equivalent von Mises stress, of the contribution of the two slip system families (`evcum i` for the i th slip system of the octahedral family, `cui` for the i th slip system of the cube family, `evgeq` and `cugeq` for the sum of the plastic slip for each slip system family).
- Check the evolution of the inelastic zones during the loading.
- Use the `Plot` option to draw the global loading curve. This can be made by means of the `Add/Del` button, then the `nset_sum` choice, which allows to introduce the name of the elset `top` as the name of the node collection used for computing the torque. Ask for a curve that combines `time` and `torque2` to get the torque on the top section. Put the name `torque.txt` in the `Curve` output box to get the numerical results in the file `torque.txt` for future plot with `gnuplot`. It can be a good idea to close `Zmaster` for a while, and to use the command `DRAW_global` to draw the previous result together with some elastic responses. The plot can be obtained by the command

`./DRAW_global`

- . Please edit `DRAW_global`, and give an explanation of the various curves of the graph.
- Use the `Plot` option to draw the variation of the same variables as a function of space along lines like `circ-ext`, `circ-int`, `long001-int`, `long011-int`. The location of these lines can be checked by highlighting them in the `Mesh` option of the graphical postprocessor, and by reading the data file used for their generation

(section `****mesher` at the end of the file `tension.inp`). The `****mesher` section of the input file can be invoked by means of the command

`Zrun -m torsion`

. It is suggested to save the curves in text files by providing a file name in the `Curve` output box, and to compare the various data on the internal radius and the external radius of the tube.

- In addition to equivalent stresses and plastic strains, it is recommended to plot the evolution of the stress and displacement fields. This should allow to understand the global behaviour of the tube, including the stress redistributions, and to investigate the perturbation due to the strong boundary condition imposed of the `bottom` section of the tube.

More details

The batch post-processing can be used to manipulate the results of the analysis. Two computations are proposed in the section `****post_processing` of the file `tension.inp`, a computation of `tau`, the shear stress in the section of the tube, and of `displ`, the displacement in the same section. The treatment can be run by means of the command

`Zrun -pp torsion`

This command will generate new files, which can be read by the graphical post-processor, and analyzed by using

`Zmaster torsion`

Please perform with these variables the type of analysis already applied to the initial data. This graphical analysis should allow to verify that the stress τ and the shear γ are uniform along the circumference in the elastic regime.

In order to avoid the perturbation due to the encastred section, try to find a softer way to attach the `bottom` section of the tube.

Output of this section

The analysis of the results of the computations must at least answer the following questions:

- What is the value of the torque at the onset of plastic flow ?
- What are the active slip systems in each case ?
- What is the location of the initial plastic flow, and the value of the angle reached at that time ?
- How is distributed the shear stress along the circumference, for the internal and for the external radius, in the middle of the tube ?
- Does a current section remain flat ?
- Compare these data with the reference solution (von Mises criterion, perfect plasticity)
- What is the distribution of these variables along the vertical lines `long001-int`, `long011-int`.

4 Tension and tension–torsion on a tube with a crystal axis $\langle 001 \rangle$ (A)

Go to directory TENSION

Check the file `tension.inp`, to determine the active boundary conditions, run the computation, using

`Zrun tension`

then use `Zmaster` to analyse the results. According to crystal plasticity theory, strain should now be uniform in the section of the tube. Is it the

case ? Provide a detailed discussion, following the requests of the previous section (macroscopic curve, onset of plastic flow, active slip systems, ...).

As a last step of this track, one would like to demonstrate that plastic flow may appear first in the central section of the tube, in the $\langle 001 \rangle$ zones, for some combinations of in-phase tension and torsion (and not in the $\langle 011 \rangle$ zones, like for the torsion case). In order to find the proper boundary conditions, please refer to figure 10 in [1]. The intersection between the two hexagonal surface must first be characterised. The ratio between the maximum angle and the maximum axial displacement must then be found. A new input file (`tentor.inp`) will then be used to compute cases with in-phase tension and torsion. After running the problem, check the results by following the precedures already used for the first case.

5 Tube with a crystal axis $\langle 111 \rangle$ (B)

Instead of having a $\langle 001 \rangle$ axis, it is now proposed to consider a tube of axis $\langle 111 \rangle$. The only change to be made in the file `torsion.inp` is to add

```
*rotation x1 1. -1. 0. x2 1. 1. 1.
```

in the `***material` section. This is made in the file `torsion111.inp`.

Run this problem, and check the results by following the procedures already used for the first case.

Any other rotation of the material could then be used as well. The two first attempts ($\langle 001 \rangle$ and $\langle 111 \rangle$) where *high symmetry* conditions. The next orientation could be for instance $\langle 011 \rangle$.

References

- [1] D. Nouailhas and G. Cailletaud. Tension-torsion behavior of single-crystal superalloys: experiment and finite element analysis. *Int. J. of Plasticity*, 11(4):451–470, 1995.