Atlas of Yield Surfaces for Strongly Textured FCC Polycrystals

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Abstract. Discrete yield surfaces for several generic texture components, including randomness, found in aluminium alloys have been generated and used to calibrate the yield function Yld2004-18p. It is generally observed that the roundness of the corners of the yield surface increases, and the stress and strain ratios flatten towards isotropic values, as the ratio of random component increases. A short investigation on the effect of number of points and homogenization approach on calibration of the yield function seems to indicate that the number of points used in the calibration has a stronger effect than the homogenization approach. Furthermore, it is also shown that setting the exponent as a free parameter in calibrating the yield function could lead to better fits.

INTRODUCTION

It is well proven that the mechanical properties of sheets and extrusions of metals, typically aluminium alloys and steels, are strongly correlated with the microstructure and crystallographic texture – i.e. the size, shape and orientation of the crystals in the material – which in turn depend on the thermo-mechanical process history of the product. Most of the sheets and extrusions have predominant crystallographic orientations with small or large scatter around them. Post heat-treatment, e.g. annealing, may change the texture if recrystallization occurs in the material.

Textures are usually defined as composed of different generic texture components. Mechanical plastic anisotropy, geometrically represented by the shape of the yield surface, is sensitive to texture and grain shape. Many phenomenological yield criteria have been proposed, such as non-quadratic formulations, e.g. [1] or functions based on one or several linear transformations, e.g. [2]. These models are often calibrated using experimental data. Another complementary approach consists in using lower-scale models such as the crystal plasticity. To represent explicitly both microstructure and crystallographic texture, the latter is combined with the finite element method (CP-FEM). A discrete yield surface may then be generated by loading a representative volume element (RVE) along different strain paths. The aim of the study reported here is to generate discrete yield surfaces and calibrate the yield criterion Yld2004-18p for typical generic texture components found in aluminium alloys. To achieve this, a workflow has been established which consists in a texture generator, the open source software package DREAM.3D, a discrete yield surface generator using CP-FEM and a calibration software.

APPROACH

The objective is to obtain the parameters of yield criterion Yld2004-18p [3] for polycrystals having different generic strong textures. To achieve this, textures must be generated, representative volume elements (RVE) representing polycrystals with associated textures have to be made, discrete yield surfaces have to be built and Yld2004-18p has to be calibrated using the latter. Therefore, the workflow from texture generation to calibration of the yield criterion has been established as follows:

1. Generate user-defined texture (input texture),
2. Create simple RVE (polycrystal with 10x10x10 grains) with DREAM.3D using the generated texture,
3. Extract texture (output texture) from RVE generated by DREAM.3D,
4. Plot orientation distribution functions (ODF) for both input and output textures for comparison purposes,
5. Generate discrete yield surface,
6. Calibrate Yld2004-18p.

The open source, cross-platform and modular software package DREAM.3D [4] is used to generate the RVEs. A set of Python scripts has been developed that automates the above described workflow, from texture generation to calibration of a yield criterion. The following sections describe the different hypotheses used in this study.

Textures

The textures generated in this study are represented by a spread of orientations around an ideal component together with some randomness. The methodology used to generate such textures follows those described in [5-7]. In all textures generated, the spread of orientations follows a Gaussian distribution with a standard deviation of 10°, as a typical spread representing experimental observations [5], and assuming orthotropic symmetries. 10000 orientations are generated for each texture to obtain a better fit of the ODF with DREAM.3D. The misorientation distribution function (MDF) was defined in DREAM.3D as random.

The texture components investigated were taken from [6][8-9] and were Copper ($\{112\}\langle 11\bar{1}\rangle$), S ($\{123\}\langle 63\bar{4}\rangle$), Brass ($\{011\}\langle 2\bar{1}1\rangle$), Goss ($\{011\}\langle 100\rangle$), Cube ($\{001\}\langle 100\rangle$) and CubeND ($\{001\}\langle 110\rangle$), where CubeND signifies Cube rotated about the normal direction. For each texture component, different ratios of random component are added to provide a spectrum of textures going from being "strong/sharp" to "weak", i.e. 10, 20, 30, 40 and 50%.

Representative Volume Elements (RVEs)

The RVEs representing the polycrystal were of cubic shape with 1 mm side length, 10×10×10 elements and 1 element per cubical grain (i.e. 1000 grains), see Figure 1. The RVEs were modelled using solid linear eight-node "brick" elements with selectively reduced integration. Periodic boundary conditions were enforced in all directions. The RVEs were generated by running DREAM.3D that reads in the texture, generates an RVE, matches the ODF and MDF to the 1000 grains and creates all the input files necessary for the non-linear finite element code LS-DYNA [10]. The behaviour of each grain was described using crystal plasticity theory. The latter was implemented numerically using a rate-dependent formulation by use of a user material subroutine (UMAT) [11].

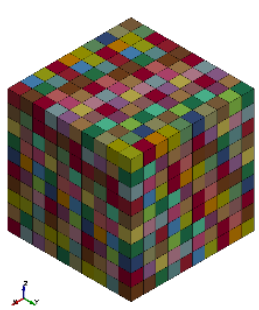

FIGURE 1. Normalized uniaxial yield stress, strain ratio and two selected contour plots of the calibrated Yld2004-18p yield function for Cube component with 50% randomness.

Discrete Yield Surfaces

The discrete yield surfaces were generated using a methodology similar to the one used when determining the yield surface of a material based on experimental tests: only a limited number of carefully selected tests is performed, i.e. uniaxial tension, plane-strain tension, shear, biaxial tension, disk compression, at different angles from the extrusion/rolling direction. The advantage of numerical analysis over experimental testing is that it is possible to choose any material plane, i.e. one may perform tests in the transverse direction-normal direction (TD-ND) plane. To load the RVE at any angle from the principal directions of the material – conventionally aligned with the coordinate system in which the RVE is built – the methodology proposed by Delannay et al. [12] has been implemented.

Yield surfaces are surfaces in stress space going through points at equivalent amounts of plastic work per unit volume obtained by proportional deformation in different directions. The reference value of plastic work adopted here corresponds to a plastic strain of 0.2% in a uniaxial tension test for a material with random texture.

Yield Criterion Yld2004-18p

After the generation of the discrete yield surfaces, the yield criterion Yld2004-18p is calibrated using all data available to obtain the full-component yield surfaces. Dependencies between the parameters of the yield criterion, as demonstrated in [13], are taken into account where $c_{1122}^{(1)}$ and $c_{1133}^{(1)}$ (or c'_{12} and c'_{13}) are set to unity. In all calibrations, the exponent of the yield criterion is fixed to 8, unless otherwise specified. All the other (16) parameters are set free.

RESULTS

Results will be provided here only for selected components. As an example, Figure 2 shows the normalized uniaxial yield stress and strain ratio from the CP-FEM simulations (red dots) and the calibrated Yld2004-18p (continuous line) together with contour plots of the yield surface for Cube component with 50% randomness. Figure 3, Figure 4 and Figure 5 show the same graphs for all yield surfaces built for Cube, Copper and Goss textures with different ratios of random component.

The main comments for all results relate to the increased roundness of the corners of the yield surface and flattening of the stress and strain ratios towards isotropic values, as the ratio of random component increases. This results in a better fit of the yield surface in the (RD-TD) plane as the ratio of random component increases. This is also reflected on the residual of the calibrations that is 10 to 20 times lower for the textures containing 50% random component compared to the ones containing 10%.

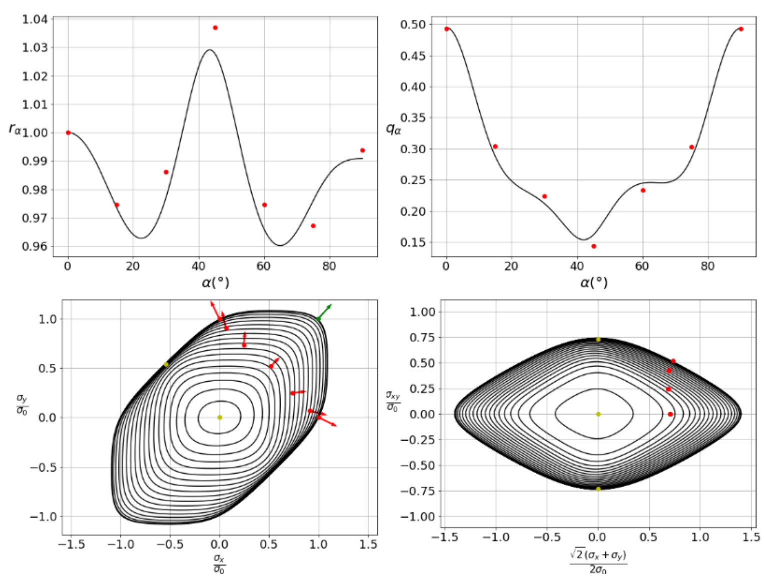

FIGURE 2. Normalized uniaxial yield stress, strain ratio and two selected contour plots of the calibrated Yld2004-18p yield function for Cube component with 50% randomness.

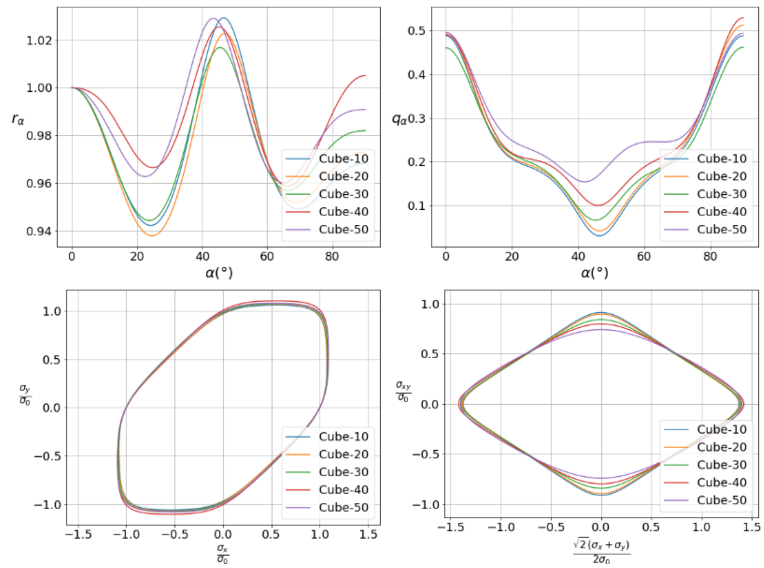

FIGURE 3. Normalized uniaxial yield stress, strain ratio and two selected contour plots of the calibrated Yld2004-18p yield function for Cube component, with different ratios of random component.

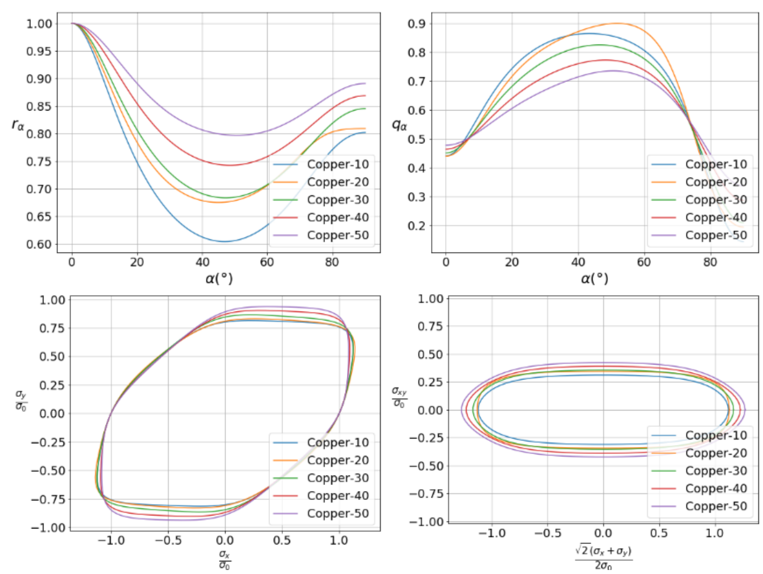

FIGURE 4. Normalized uniaxial yield stress, strain ratio and two selected contour plots of the calibrated Yld2004-18p yield function for Copper component, with different ratios of random component.

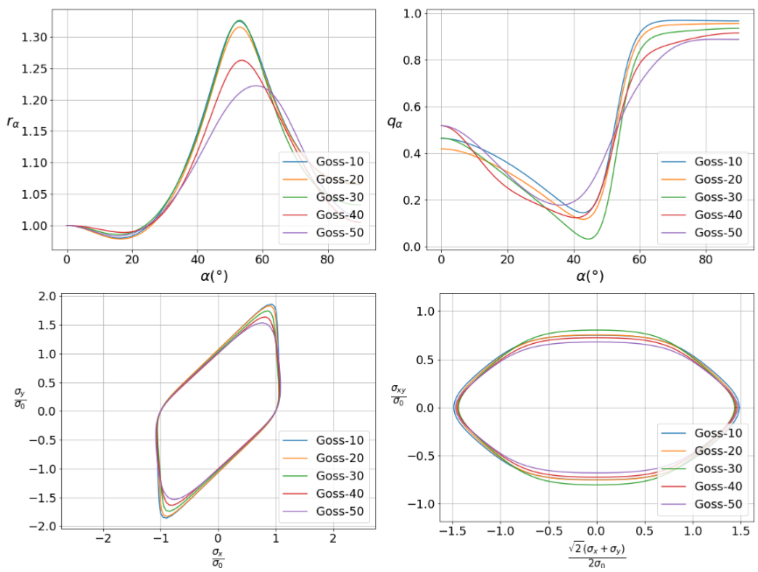

FIGURE 5. Normalized uniaxial yield stress, strain ratio and two selected contour plots of the calibrated Yld2004-18p yield function for Goss component, with different ratios of random component.

DISCUSSION

When generating yield surfaces and calibrating yield functions, many questions arise e.g.: what is the most accurate homogenization approach (CP-FEM, Taylor …) to be used? Should grains be discretised at all, i.e. does grain shape affect the results? How many points/simulations are required to have a good fit of the yield function? Do all these aspects depend on the texture/microstructure (i.e. on the alloy)?

To try to assess some of these questions one discrete yield surface was built using the Taylor approach rather than CP-FEM and calibration of Yld2004-18p was performed using only data available in the (RD-TD) plane. The texture chosen to perform the study is the one containing the Brass component with 50% randomness.

(a)

(b)

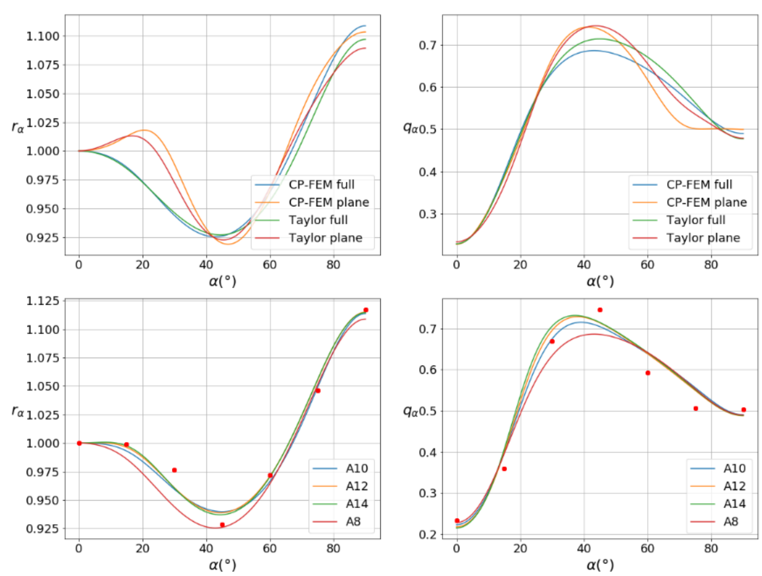

FIGURE 6. Normalized uniaxial yield stress and strain ratio for Brass component with 50% random component using (a) different homogenization and calibration approaches, and (b) for different values of the yield function's exponent.

Figure 6(a) shows the results; only normalized uniaxial yield stresses and strain ratios are shown. Comparing 'CP-FEM full' and 'CP-FEM plane' shows the effect of using only part of the data, i.e. 29 simulations in the full space versus 16 in the (RD-TD) plane. Here a noticeable effect is seen on the stress and strain ratios. Comparing 'CP-FEM full' versus Taylor full' and, 'CP-FEM plane' versus Taylor plane', shows the effect of the homogenization approach. It is observed that the number of simulations has a stronger effect than using CP-FEM or Taylor.

Finally, the effect of the exponent was assessed. The texture containing the Brass component with 50% random component is then calibrated setting the exponent *a* to either 10, 12 or 14. The comparison with the initial value of 8 and CP-FEM simulations (red dots) is shown in Figure 6(b). Increasing the exponent provides a better fit of the data; this is also reflected by a decrease of the residual. However, a too high exponent does not improve the calibration as observed when *a* is set to 14; the residual does actually increase. This means the optimal value of the exponent, i.e. the value providing the lowest residual for that specific texture, would be between 12 and 14.

CONCLUSION

A set, or atlas, of discrete yield surfaces has been generated for several generic texture components including different amounts of randomness. The yield function Yld2004-18p has been calibrated using these data and plots of stress and strain ratios as well as cross-sections of the yield surfaces have been generated and compared. It is generally observed that the roundness of the corners of the yield surface increases and the stress and strain ratios flatten towards isotropic values, as the ratio of random component increases.

A short investigation on the effect of number of points and homogenization approach on calibration of the yield function seems to indicate that the number of points used to calibrate the yield function has a stronger effect than the homogenization approach. Furthermore, it is also shown that setting the exponent as a free parameter in calibrating the yield function could lead to better fits. A more extensive study is required to confirm these conclusions.

Finally, an automated workflow has been built that allows calibrating any yield function for any user-defined texture using any type of modelling approach. This tool may be useful in providing sets of calibrated yield functions for generic realistic textures among which a user may choose the one fitting best available experimental data.

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