Parameter identification of 3D yield functions based on a virtual material testing procedure

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Abstract. The parameter identification of anisotropic 3D yield functions for sheet metals based on experimental data is very difficult, because material properties associated to the out-of-plane stress states cannot be directly measured. An alternative and promising approach for identifying parameters of anisotropic yield models, and particularly for 3D yield models, is the concept of virtual testing. Within the presented work, a full-field microstructure simulation framework based on a crystal plasticity (CP) model is used to determine macroscopic mechanical properties of a ferritic deep drawing steel DX56 within 3D stress space. The results are utilized to identify the parameter of anisotropic 2D and 3D yield models according to Hill [1] and Barlat [2, 3].

1. Introduction
For the simulation of sheet metal forming processes it is important to incorporate an accurate description of the plastic material behavior using anisotropic yield functions. For most sheet metal forming simulations, a reduced stress state (\(\sigma_{11}, \sigma_{22}, \sigma_{12}\)), in combination with an anisotropic 2D yield function, is typically taken into consideration. However, for some applications like bending with small radii, thick sheets, special forming processes (hemming, wall ironing or sheet-bulk forming) or for the description of local stress and strain fields after necking, a full 3D stress state as well as a 3D yield function has to be taken into account to obtain accurate and reliable results.

In contrast to 2D yield functions, identifying parameters of anisotropic 3D yield models and in particular those related to out-of-plane properties based on solely experimental data is extremely challenging. This is because experiments, such as tensile tests, cannot be realized in the thickness direction of sheet. As a result, the concept of virtual testing has become a commonly used method for identifying parameters of anisotropic 3D yield functions in academic science [4, 5]. Nevertheless, a fixed strategy to determine the 3D stress space virtually has not yet been established.

2. Virtual material testing for DX56 deep drawing steel
The basic idea of “virtual material testing” is to describe the material on the micro-scale using the crystal plasticity finite element method (CPFEM), so that macroscopic properties like flow curve, r-values or points on the yield surface can be calculated by a numerical homogenization scheme. Microstructural features like the specific microstructure morphology and the crystallographic texture of the sheet metal are taken into account in the crystal plasticity model to represent the plastic anisotropy. A general overview of the approach can be found in [6]. Since the workflow of the virtual testing procedure must be accurate as well as efficient, the proposed virtual testing procedure is divided into three steps according to Figure 1.
2.1. Generation, calibration and validation of the microstructure model

For the virtual testing procedure, a relatively small set of experimental data is needed. To calibrate and validate the mechanical properties of the microstructure model, tensile tests in 0, 45 and 90 degrees to the rolling direction of the sheet are used. Additional, electron backscatter diffraction (EBSD) is necessary to characterize the crystallographic texture and the grain structure of the material. The corresponding EBSD measurements for the ferritic deep drawing steel DX56 are illustrated in Figure 2 and were used to create a microstructure model representing the grain structure of the steel. Based on former studies [7], approximately 1000 slightly elongated grains have been assessed as sufficient for DX56. An initial orientation of the bcc crystal lattice was assigned to each grain. This initial texture of the microstructure model fits well to the experimentally measured texture as illustrated in Figure 2.

Figure 2. Microstructure model. Generation of a unit cell model and representative texture from EBSD measurements [12].
Moreover, a full field crystal plasticity finite element method (CPFEM) modelling approach is used. The elasto-plastic deformation on grain scale is described by a single crystal plasticity material model that was implemented as user subroutine into the finite element software Abaqus/Standard. Therefore, the numerical framework proposed by [9] was applied. The major equations of the crystal plasticity material used in this work are given in the following paragraph.

Schmidt’s law is used to calculate the shear stress $\tau^{(\alpha)}$ on the slip system ($\alpha$) from the stress tensor $\sigma_{ij}$. The vectors $s_i^{(\alpha)}$ and $m_j^{(\alpha)}$ correspond to the slip direction of the slip plane and the normal vector on the slip plane

$$\tau^{(\alpha)} = s_i^{(\alpha)} \sigma_{ij} m_j^{(\alpha)}. \quad (1)$$

The shear rate $\dot{\gamma}^{(\alpha)}$ of a slip system $(\alpha)$ is defined by the following equation

$$\dot{\gamma}^{(\alpha)} = \dot{a} \text{sign}(\tau^{(\alpha)}) \left[\frac{\tau^{(\alpha)}}{g^{(\alpha)}}\right]^{1/M} . \quad (2)$$

Here, $\dot{a}$ denotes the reference shear rate, $M$ is the strain rate sensitivity exponent and $g^{(\alpha)}$ is the critical shear stress of the slip system $(\alpha)$. The rate of $g^{(\alpha)}$ is defined as

$$\dot{g}^{(\alpha)} = \frac{d\tau^{(\alpha)}}{d\Gamma} \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^{(\beta)} \quad \text{with} \quad \dot{\Gamma} = \sum_{\alpha} \dot{\gamma}^{(\alpha)} . \quad (3)$$

In Equation (3) $\Gamma$ describes the accumulated shear over all slip systems. The hardening matrix $h_{\alpha\beta}$ describes the interaction between the slip systems [10]. It allows the slip of one slip system to be taken into account, which also impedes the slip on other slip systems due to the distortion of the crystal lattice. The hardening function $\dot{\tau}^{(\alpha)}$ of one slip system $(\alpha)$ is defined as a function of the accumulated shear $\Gamma$ and is given by an extended Voce law [11] as follows

$$\dot{\tau}^{(\alpha)}(\Gamma) = \tau_0^{(\alpha)} + (\tau_1^{(\alpha)} + \theta_0^{(\alpha)} \Gamma) \left[1 - \exp\left(-\frac{\theta_0^{(\alpha)}}{\tau_1^{(\alpha)}} \Gamma\right)\right] . \quad (4)$$

The quantities $\tau_0^{(\alpha)}$, $\tau_1^{(\alpha)}$, $\theta_0^{(\alpha)}$ and $\theta_0^{(\alpha)}$ in Equation 4 are the model parameters which have to be determined. For this reason, an inverse parameter identification procedure of the uniaxial tensile test in rolling direction was applied. The parameters were optimized until the homogenized stress strain curve of the microstructure model fits the experimental data. The result of the final fit is illustrated in Figure 3 on the left hand side. A good fit of the uniaxial tensile test in rolling direction can be obtained with the calibrated microstructure model.

**Figure 3.** Results of the model calibration (left) and the model validation (centre and right)
In the next step, the calibrated material model was validated by a comparison with tensile test data at 90 degrees and with r-values in 0, 45 and 90 degrees. It is mentioned that these data sets were not used for model calibration. The results are illustrated in Figure 3. Both the predicted initial yield strength and the r-values are in good agreement with the experimental data.

2.2. Virtual testing

The validated microstructure model can now be used for virtual testing procedure. This includes the definition of the load case, the CPFEM simulation and the homogenization of the resulting stress and strain fields. To provide a sufficient large number of virtual tests for the subsequent parameter identification (see Section 3) a systematic and automatized approach for the virtual testing procedure is needed.

2D yield functions in combination with shell elements consider a reduced stress space with the components $\sigma_{11}$, $\sigma_{22}$ and $\sigma_{12}$. In that case, the stress space can be scanned by prescribing the macroscopic strain components $\varepsilon_{11}$, $\varepsilon_{22}$ and $\varepsilon_{12}$ as boundary conditions for virtual testing. By definition of two angles $\varphi$ and $\theta$ any combination of the three strain components can be defined. This approach is illustrated in Figure 4. The strain component $\varepsilon_{33}$ follows from the plane stress condition that the macroscopic stress component $\sigma_{33}$ has to be zero. Since the crystal plasticity material model is based on a strain rate dependent formulation, it is also important to ensure that the equivalent strain rate is the same for each simulated load case. Hence, for each virtual material test the equivalent strain rate is calculated from the principle values. Then the strain components were scaled to obtain the reference strain rate given by the setup of the tensile tests.

![Figure 4](image)

**Figure 4.** From left to right: Definition of the strain path by two angles, set of strains paths for the virtual testing, corresponding effective stresses and resulting points on the yield surface.

For an accurate parameter identification of 3D yield functions the whole stress space consisting of six components should be considered. However, a systematic scan of the stress space is not feasible since the number of virtual test would become too large. For this reason, a simplified approach based on the procedure for a reduced stress state ($\sigma_{11}$, $\sigma_{22}$, $\sigma_{12}$) was used in this work. As a consequence, the 3D stress space was subdivided into the three following subspaces:

- subspace 1: $\sigma_{11}$, $\sigma_{22}$, $\sigma_{12}$
- subspace 2: $\sigma_{22}$, $\sigma_{33}$, $\sigma_{23}$
- subspace 3: $\sigma_{33}$, $\sigma_{11}$, $\sigma_{31}$

Each of these three subspaces takes two normal stress components and the corresponding shear stress component into account. Subspace 1 corresponds to the plane stress state which is also considered in the case of 2D yield functions. To take advantage of the possibilities of virtual material testing and to improve the characterization of the yield surface, a large quantity of virtual tests were performed. The number of virtual tests carried out in subspaces 1, 2 and 3 were 128, 64 and 64, respectively.
2.3. Post processing/generation of points on the yield surface

To determine the points on the yield surface, the homogenized data from the microstructure simulations have to be further processed. It is assumed that stress states with the same amount of plastic work belong to the same yield surface. With respect to the crystal plasticity material model, the plastic work $\Delta W_{pl}$ in one load increment is defined as

$$\Delta W_{pl} = \sum \tau^\alpha \Delta \gamma^\alpha .$$

(5)

Within this work, a specific plastic work of 1.755 MPa was considered as reference value for determining points on the yield surface. This corresponds to a true plastic strain of 0.01 in the experimental uniaxial tension test in rolling direction. From experiments it was found that the yield stress ratios $\sigma_{45}/\sigma_0$ and $\sigma_{90}/\sigma_0$ are not constant for small strains [12]. Therefore, a higher plastic strain value than $R_{p0.2}$ was chosen to determine the points on the yield surface.

The obtained points on the yield-surface are illustrated in Figure 5 for all three subspaces. Subspace 1 corresponds to the plane stress state which is typically used to fit 2D yield functions. One can clearly see that the shape in subspaces 2 and 3 significantly differs from that in subspace 1. This corresponds to similar findings reported by [3] for aluminum sheet metals. Nevertheless, the results have to be considered carefully since no experimental data regarding the thickness direction is available.

![Figure 5](image_url)

**Figure 5.** Determined points on the yield surface for all three subspaces

3. Fitting of yield surface models

Compared to experiments, the virtual testing provides significantly more data points for the parameter identification of the yield function. Therefore, an optimization was applied to identify the parameter of the yield function. The following error function was minimized:

$$RMSD = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left( \frac{\sigma_i}{\sigma_y} - 1 \right)^2}$$

(6)

Here, $n$ denotes the number of data points (virtual tests), $\overline{\sigma}$ is the effective stress as a function of the stress tensor $\sigma_{ij}$ and $\sigma_y$ is the yield stress. The 2D and 3D yield functions which were compared in this study as well as the corresponding RMSD-error are given in Table 1. Regarding Yld2004-18p three different cases were considered: the original Yld2004-18p having 18 parameters and an exponent $m$ equaling 6.0 for bcc metals, a second case where the out-of-plane properties were set to unity ($\alpha_7 = \alpha_8 = \alpha_{16} = \alpha_{17} = 1$) and a third case where $m$ was treated as an additional fitting parameter.
Table 1: Overview of the yield functions and the RMSD-error of the fitting procedure

| Fitting strategy | RMSD-error |
|------------------|------------|
| **2D yield function** (parameter fitting in plane stress state) | |
| Hill48 – 2D | 0.015977 |
| Barlat YLD2000-2D | 0.005704 |
| **3D yield functions** (parameter fitting in plane stress state) | |
| Barlat YLD2004-18p (14p): Out of plane parameter set to 1 | 0.001504 |
| **3D yield functions** (parameter fitting in 3D stress state) | |
| Hill48 – 3D | 0.022840 |
| Barlat YLD2004-18p | 0.007560 |
| Barlat YLD2004-18p (19p): Exponent m as additional fitting parameter | 0.007284 |

Figure 6 illustrates the yield surfaces for different yield functions in the plane stress space ($\sigma_{11}, \sigma_{22}, \sigma_{12}$). Compared to both of the Hill48 yield functions the Barlat-type yield functions are in better agreement with the data points from the virtual testing. This can be explained by the lower number of parameters of the Hill48 yield functions. The difference becomes more pronounced with increasing shear component. Furthermore, a slight difference can be observed between the YLD2000-2d and the YLD2004-18 yield functions. Both functions differ in the number of parameters and in the underlying data set used for the parameter fitting.

Figure 6. Comparison of the yield surface of different yield functions in the plane stress space

A more detailed analysis was performed for the yield function YLD2004-18p considering two additional fittings strategies. The resulting yield surfaces are plotted in Figure 7 for each of the three sub spaces. The shapes of the yield surfaces for the same yield function significantly differ in the three stress spaces, which is in agreement with Figure 5. In the plane stress space ($\sigma_{11}, \sigma_{22}, \sigma_{12}$), which is
typically applied in sheet metal forming simulations, the influence of the different 3D yield models seems to be relatively low. In contrast to this, the difference becomes much more important if the yield surface is plotted in the two other sub spaces. Especially, the fitting approach Yld2004-18p (14p), which uses a simplified assumption for the out-of-plane parameters, deviates considerably from the other two variants. This observation is in agreement with [3] indicating that the simplified assumption ($\alpha_7 = \alpha_8 = \alpha_{16} = \alpha_{17} = 1$) for Barlat Yld2004-18p is limited to applications where a plane stress state dominates.

**Figure 7.** Different fitting approaches for the Barlat YLD2004-18p yield function. Representation of normalized shear contours in 0.1 increments from 0 to 0.5.

Figure 8 shows the comparison between the experimental results for the yield stress analyzed at a specific plastic work of 1.755 MPa and the r-values against the prediction of the yield function. The Hill48 yield functions have little agreement with the experimental data. In particular, the curve-shape of the experimental r-values is not predicted at all. This can be most likely explained by the lower number of parameters used in the Hill48 yield functions, as the agreement increases with a higher quantity of parameters. The best match is found for the Yld2004-18p (19p) approach, pointing out that the consideration of exponent $m$ as an additional parameter can increase the accuracy of yield models. In this specific case $m$ was fitted to approximately 5.57, which is slightly lower than the standard value of 6.0 for bcc metals. Similar findings have been made in a former study for Barlat Yld2000-2d [12].

**Figure 8.** Predicted yield stress (at a true plastic strain of 0.01) and r-value as function of the angle to rolling direction for different yield functions.

However, even for the Yld2004-18p (19p) fitting approach there is still some difference compared to the experimental data. This difference can be explained to the most extent by the initial differences.
between the experiments and the calibrated microstructure model. The r-values which were predicted by the fitted Yld2004-18p (19p) yield function are very close to the values which were directly calculated by CPFEM as illustrated in Figure 3.

Furthermore, the proposed fitting strategy aims to provide a good average fit of the yield function over a large part of the 3D stress space. As a consequence, some deviations between the given points in the stress space and the fitted yield function have to be taken into account. This is especially the case for yield function with a lower number of parameters like the Hill48 yield functions.

In addition, in the authors’ opinion, the comparison shown in Figure 8 is valuable to assess the accuracy yield functions but it is not sufficient. It considers only a small part of the yield function in the (plane) stress space. The accuracy of other stress states cannot be estimated. The example of the Yld2004-18p (14p) fitting approach shows this clearly. The parameter fit gives good results for the comparison shown in Figure 8, but it shows significant differences in other stress spaces as illustrated in Figure 7. Consequently, additional analyses which allow assessing yield functions in a three-dimensional stress state are required.

4. Conclusion
The virtual testing procedure can be used for parameter fitting of complex yield functions. Based on an automatized workflow, an efficient virtual testing procedure can be realized. The results for the three Barlat Yld2004-18p are in good agreement with experiments for the considered DX56 steel material, depending on the fitting approach. In this context, it was shown that the consideration of the exponent m as a further free parameter can improve the accuracy of the Yld2004-18p yield model predicted by a large number of virtual material tests. Simplified fitting strategies of three dimensional yield functions which do not consider out of plane stress states should be carefully analyzed.

Further work will concentrate on the development of more efficient sampling strategies for the virtual tests and on the development of alternative criteria for the assessment of the quality of 3D yield functions. Moreover, it is planned to analyze an aluminum alloy.

Acknowledgments
The research was supported by the AiF (grant ID 18810BG and grant ID 19707N) within the program for promoting the Industrial Collective Research (IGF) of the German Ministry of Economics and Energy (BMWi).

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