Abstract

This paper presents a new machine learning-based approach to investigate anisotropic yield surfaces of sheet metals by virtual experiments. The new sampling approach is based upon the machine learning technique active learning, which has been adapted to efficiently sample virtual experiments with respect to the full stress state in order to identify parameters of anisotropic yield models. The approach was employed to sample virtual experiments based on the crystal plasticity finite element method (CPFEM) for a DX56D deep drawing steel and compared with two state-of-the-art sampling methods taken from literature. The resulting points on the initial yield surface for all three sampling methods were then used to identify parameters of the anisotropic yield models Hill48, Yld91, Yld2004-18p, and Yld2004-27p. The results show that the new machine learning-based sampling approach has a higher sampling efficiency than the two state-of-the-art sampling methods. It was also discovered that the effect of the sampling method on the resulting yield surfaces for Hill48, Yld91, Yld2004-18p, and Yld2004-27p is less significant than the choice of the anisotropic yield model for a sufficiently large number of sampled yield points. In this respect, Yld2004-27p was identified as being sufficiently flexible to represent the anisotropic yield surface of DX56D within full stress state with reasonable accuracy.

Keyword: A. yield condition, B. anisotropic material, B. crystal plasticity, machine learning, adaptive sampling
1. Introduction

Sheet metal forming operations play an important role in various manufacturing industries, particularly in the automotive sector. In order to reduce development times, minimise costs and increase product quality of sheet metal parts, finite element simulations have become a state-of-the-art method to analyse and improve forming operations. One precondition for high-quality sheet metal forming simulations is an accurate description of the plastic material behaviour. Since sheet metal typically exhibits direction-dependent or rather anisotropic material properties due to its manufacturing process, the mathematical description of texture-induced plastic anisotropy by anisotropic yield models is essential (Banabic et al., 2010; Banabic et al., 2020, Tekkaya, 2000). Hence, many anisotropic yield models have been developed for plane and full stress states over the last decades. Apart from his well-known isotropic yield model (von Mises, 1913), von Mises (1928) also proposed the first anisotropic yield model for the plane and full stress state. This is a quadratic yield model and was initially introduced to describe the plastic anisotropy of single crystals. Using the concept of the plastic potential of von Mises (1928), Hill (1948) established a further anisotropic yield model, which can also be applied for the plane and full stress state. Hill’s quadratic yield model has six material parameters for the full stress state and is typically used for body-centred cubic (bcc) materials such as steel (Vegter and van den Boogaard, 2006). To increase flexibility, Hill (1979, 1990, 1993) subsequently developed three anisotropic yield models that focus on an enhanced representation of the anisotropic yield surface. Whereas the anisotropic yield models proposed by Hill (1990, 1993) are designed for the plane stress state, the Hill (1979) yield model takes the full stress state into account.

A further important group of anisotropic yield models that is relevant for the investigations in this study was developed by Barlat and co-workers. From the late 80s onwards, Barlat and Lian (1989) presented an anisotropic yield model for the plane stress state, which is often referred to as Yld89. This is based on the isotropic yield model introduced by Hershey (1954) and Hosford (1972) and has four material parameters. Two years later, Barlat et al. (1991) introduced the Yld91 yield model for the full stress state with six material parameters. The Yld91 yield model was then further developed, leading to the introduction of the two anisotropic yield models Yld94 (Barlat et al., 1997) and Yld96 (Barlat et al., 1997). The number of material parameters amounts to six and eight, respectively. In 2000, Barlat et al. (2003) also proposed the eight-parameter Yld2000-2d yield model for the plane stress state. Focussing on an enhanced representation of the plastic anisotropy for the full stress state, Barlat et al. (2005) established the Yld2004-18p yield model. This is based on two linear transformations of the deviatoric
stress tensor and contains 18 material parameters. Fourteen of these material parameters describe the in-plane behaviour, while the remaining four material parameters characterise the out-of-plane anisotropy. In addition, von den Boogaard et al. (2016) demonstrated that the Yld2004-18p yield model has only twelve independent material parameters for the in-plane behaviour and, thus, the number of independent parameters can be reduced to 16. Moreover, Aretz et al. (2010) introduced a modified version of the Yld2004-18p yield model by considering three linear transformations of the deviatoric stress tensor. In consequence, this anisotropic yield model has 27 material parameters and is referred to as Yld2004-27p. Of these 27 material parameters, 21 are related to the in-plane behaviour, while the remaining six parameters are associated with the out-of-plane behaviour. Additionally, Aretz and Barlat (2013) introduced two further anisotropic yield models, called Yld2011-18p and Yld2011-27p. Both anisotropic yield models have the same number of parameters compared to the Yld2004-18p and Yld2004-27p yield models, but represent rather complementary, i.e. different-shaped anisotropic yield surfaces.

Parameters of anisotropic yield models are typically identified by various mechanical tests such as uniaxial tensile tests, hydraulic bulge tests or plane strain tension tests (Banabic et al., 2010; Banabic et al., 2020). To extend the experimentally obtained data, virtual experiments based on crystal plasticity (CP) simulations are widely used to identify parameters of anisotropic yield models. With respect to single crystals, CP models to describe the deformation behaviour under external loading on the base of crystallographic slip were first developed by Peirce et al. (1982), Asaro (1983) and Peirce et al. (1983). However, the history of models for predicting the mechanical response of polycrystals goes back to the early 20th century, when Sachs (1929) proposed the first CP model assuming iso-stresses. Iso-stress means that the highest resolved stress acting on a slip system of a polycrystalline material is assumed for all grains within the polycrystal. In contrast to the iso-stress assumption, Taylor (1938) introduced a full-constraint (FC) CP model based on an iso-strain assumption. Later, this FC-Taylor model was enhanced by Bishop and Hill (1951) and renamed the Taylor-Bishop-Hill (TBH) model. Grain cluster models, like the LAMEL and the advanced LAMEL (ALAMEL) model by van Houtte et al. (1999, 2005), take grain interaction within the polycrystal aggregate into account. Viscoplastic self-consistent (VPSC) models, which were first introduced by Moliniari et al. (1987) and later extended by Lebensohn and Tomé (1993, 1994), are homogenisation schemes that treat each grain of the polycrystal as an ellipsoidal inclusion embedded in a homogeneous equivalent medium. In addition to these mean field CP models, full field CP models directly incorporate microstructural information of the polycrystal such as the grain morphology. Full field CP
models are typically employed in combination with the finite element method (FEM) or the fast Fourier transform (FFT). They were first used by Peirce et al. (1982) with a single crystal and then by several authors for a broad variety of material-related issues. An overview of different application examples appears in Roters et al. (2010). Nowadays, new types of CP models are emerging that utilise machine learning techniques like neural networks to relate stresses with strains. Examples of machine learning-based CP models are presented in Mozaffar et al. (2019), Bonatti et al. (2021), and Vlassis and Sun (2022).

Research has been steadily increasing into the use of virtual experiments to identify parameters of anisotropic yield models. Barlat et al. (2005) first performed virtual experiments to identify parameters of anisotropic yield models. Four virtual experiments using VPSC on AA2090-T3 and AA6111-T4 aluminium sheets were carried out to predict the resistance to shear relative to the thickness direction of the sheets, which cannot be measured experimentally. These results were then used to identify the out-of-plane parameters for the Yld2004-18p yield model. Similar approaches, where virtual experiments were performed as a substitute for real experiments, i.e. specific or rather experimentally realisable load cases were considered, were also conducted by Saai et al. (2013), Esmaeilpour et al. (2018), Han et al. (2020), Engler and Aretz (2021) and Liu and Pang (2021).

In contrast to replacing real experiments or carrying out virtual experiments with specifically defined load cases, further approaches can be found in literature that focus on an enhanced exploration of the plane and full stress state. This means that a larger number of virtual experiments is carried out by considering a certain sampling method to explore the entire initial yield surface. For instance, Grytten et al. (2008) sampled 690 virtual experiments based on a FC-Taylor model within the full stress state for AA5083-H116 aluminium sheets by considering a resolution of three points on the five axes of the five-dimensional strain rate space. Zhang et al. (2015) performed 201 virtual experiments on AA1050 aluminium sheets using an extension of the Miller indices as suggested by van Houtte et al. (2009) to identify parameters for the Yld2004-18p yield model. A random sampling approach was applied by Zhang et al. (2016) to perform 125 virtual experiments on a hot-band and a cold-rolled AA3104 aluminium sheet to calibrate parameters for the anisotropic yield models Yld91, Yld2000-2d, Yld2004-18p and Yld2004-27p.

Although different sampling methods are available in literature, there has been little research on the efficiency of these sampling methods and their impact on the parameter identification of anisotropic yield models for the full stress state. In a recent conference paper, Wessel et al.
(2021) introduced a machine learning-based sampling approach for the plane stress state, which is based on the active learning technique “uncertainty sampling” (cf. Settles et al., 2012). A comparison with a random sampling approach demonstrated that the active learning-based sampling approach is advantageous in terms of sample efficiency and reliability with respect to the plane stress state when sampling virtual experiments. Furthermore, the importance of developing new sampling methods for virtual experiments is also underlined by a recent publication by Shoghi and Hartmaier (2022). This shows that the sampling approach strongly affects the prediction quality of the data-driven yield model proposed by Hartmaier (2020).

Therefore, this study aims to improve the sampling of virtual experiments for the full stress state by introducing a new machine learning-based sampling approach. To this end, the concept of the machine learning-based sampling of virtual experiments to identify parameters of anisotropic yield models for the plane stress state as introduced by Wessel et al. (2021) is extended to the full stress state and enhanced using the active learning strategy called “query by committee” introduced by Burbidge et al. (2007). Query by committee is a committee-based approach, which has already been applied to efficiently explore microstructure-property spaces in Morand et al. (2022), for example. In this work, the query by committee approach is applied to actively learn mapping from linear load paths to corresponding points on the initial yield surface. Moreover, this paper focuses on the evaluation of the new machine learning-based sampling approach in comparison with two state-of-the-art sampling methods taken from literature, as well as on the analysis of the effect on parameter identification for anisotropic yield models for the full stress state. Additionally, an extensive material characterisation, including uniaxial tensile tests and hydraulic bulge tests, is performed to evaluate the prediction accuracy of the virtual experiment approach with respect to uniaxial and biaxial stress states.
2. Materials and methods

2.1. Experimental procedures

This study was performed using cold-rolled sheets made of a commercial IF steel (steel grade DX56D), which were supplied by thyssenkrupp Steel Europe AG. The sheets were hot-dip zinc coated and had a thickness of 1.5 mm. Their nominal chemical composition is summarised in Table 1.

Table 1: Nominal chemical composition of DX56D deep drawing steel shown as maximum values in wt.% as declared by thyssenkrupp Steel Europe AG.

|    | C   | Si  | Mn  | P   | S   | Ti  |
|----|-----|-----|-----|-----|-----|-----|
|    | 0.12| 0.50| 0.60| 0.10| 0.045| 0.30|

The mechanical characterisation of DX56D deep drawing steel was carried out in two different experiments. First, uniaxial tensile tests at 0°, 15°, 30°, 45°, 60°, 75° and 90° with respect to the rolling direction (RD) were performed on a ZwickRoell Kappa 50 DS uniaxial testing machine. The specimens were manufactured by water jet cutting and had a gauge length of 80 mm and gauge width of 20 mm in accordance with DIN EN ISO 6892, test piece type 2. All tensile tests were carried out until fracture using a constant engineering strain rate of 0.002 1/s. During the experiment, the change in the gauge length was measured in the longitudinal and transverse directions of the specimen using two tactile extensometers with accuracy class 0.5 according to EN ISO 9513. Three identical samples were tested for each direction. Second, hydraulic bulge tests with a diameter of 110.8 mm were conducted on a ZwickRoell BUP 600 sheet metal testing machine. The tests were performed with a constant engineering strain rate of approximately 0.002 1/s following the procedure suggested by Jocham et al. (2017). In the experiment, the oil pressure was directly measured in the chamber by a pressure sensor, while the strain field was determined by a GOM Aramis digital image correction (DIC) system. The measurement frequency of the DIC system was set to its maximum value of 40 Hz. Three hydraulic bulge tests were carried out in line with the uniaxial tensile tests. For post-processing, hydraulic bulge data was analysed in accordance with DIN EN ISO 16808 using GOM Aramis Professional 2017 software.

Crystallographic orientations and further microstructural information were obtained by electron backscatter diffraction (EBSD) measurements of the longitudinal and transverse cross-sections. Scans were conducted in a Zeiss Supra 40VP scanning electron microscope (SEM) equipped...
with an EDAX-TSL EBSD system and OIM Data Collect 5.31 software. An accelerating voltage of 20 kV was used to scan an area of 850 μm x 850 μm using a hexagonal grid with a step size of 1.5 μm. The EBSD data was analysed using the Matlab toolbox MTEX 5.1.1 (Bachmann et al., 2010). Only measurement points with a confidence index greater than 0.1 were considered for post-processing, as recommended by Field (1997). A misorientation of 5° was used for grain reconstruction and only grains with a minimum of 10 measurement points were considered in the analysis.

2.2. Virtual experiments

2.2.1. Crystal plasticity model

Virtual experiments were performed using a CP constitutive model implemented in the commercial finite element software Abaqus/Standard. The phenomenological CP model used in this study is based on the work of Asaro (1983) and on the numerical framework presented in Kalidindi et al. (1992). The CP model was implemented in the finite element code through a UMAT user subroutine developed for the studies presented in Pagenkopf et al. (2016). The basis of the CP model is the multiplicative decomposition of the deformation gradient \( \mathbf{F} \) into its elastic and plastic parts, assuming finite deformations according to the idea of Kröner (Kröner, 1959; Lee and Liu, 1967):

\[
\mathbf{F} = \mathbf{F}_e \mathbf{F}_p.  
\]

The elastic part of the deformation gradient \( \mathbf{F}_e \) represents the reversible deformation behaviour of the crystal lattice due to external loads and displacements, while the irreversible permanent response remaining after removing external loads and displacements is described by the plastic deformation gradient \( \mathbf{F}_p \). Due to the definition of the spatial velocity gradient

\[
\mathbf{L} = \hat{\mathbf{F}} \mathbf{F}^{-1} = \hat{\mathbf{F}}_e \mathbf{F}_e^{-1} + \mathbf{F}_e \hat{\mathbf{F}}_p \mathbf{F}_p^{-1} \mathbf{F}_e^{-1},
\]

the evolution of plastic deformation is defined by the plastic part of the velocity gradient \( \mathbf{L}_p \) and expressed in terms of

\[
\mathbf{L}_p = \hat{\mathbf{F}}_p \mathbf{F}_p^{-1}.
\]

\( \mathbf{L}_p \), the result of crystallographic slip, is in turn defined as the sum of the shear rates \( \dot{\gamma}^\alpha \) acting on every slip system \( \alpha \):

\[
\mathbf{L}_p = \sum_{\alpha=1}^{n} \dot{\gamma}^\alpha \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha.
\]
The unit vectors $\mathbf{m}^\alpha$ and $\mathbf{n}^\alpha$ are the slip plane direction and the slip normal of the slip system, respectively. The parameter $n$ represents the total number of slip systems. Body-centred cubic materials like steel grade DX56D have a total of 48 slip systems. In accordance with literature (Asaro, 1983; Franciosi, 1983; Raphanel and van Houwte, 1985; Raabe et al., 2005; Baiker et al., 2014), only 24 slip systems, crystallographically called $\{110\} \{111\}$ and $\{112\} \{111\}$, are incorporated in the crystal plasticity model. In order to formulate the evolution of the plastic shear rate $\dot{\gamma}^\alpha$ in Eq. (4), a phenomenological approach is considered using a critical resolved shear stress $\tau_c^\alpha$ for each slip system $\alpha$ as a state variable. Therefore, the plastic shear rate is derived by

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left|\frac{\tau_c^\alpha}{\tau_c^\alpha}\right|^{1/m} \text{sign}(\tau_c^\alpha)$$

as a power law-type equation where $\dot{\gamma}_0$ and $m$ are the reference shear rate and the rate sensitivity of slip respectively. The resolved shear stress $\tau_c^\alpha$ acting on a slip system $\alpha$ is calculated by

$$\tau_c^\alpha = (\mathbf{F}_0^T \mathbf{F}_0 \mathbf{S}) \cdot (\mathbf{m}^\alpha \otimes \mathbf{n}^\alpha),$$

where $\mathbf{S}$ denotes the second Piola-Kirchhoff stress tensor in the intermediate configuration. Assuming an infinitesimal elongation, the second Piola-Kirchhoff stress tensor is, in turn, given by the generalised Hooke's law

$$\mathbf{S} = \mathbb{C} : \mathbf{E}_e,$$

where $\mathbb{C}$ and $\mathbf{E}_e$ represent the fourth-order elasticity tensor and the elastic part of the Green-Lagrange strain tensor respectively. The elasticity tensor is characterised by three independent parameters, namely $C_{11}$, $C_{12}$ and $C_{44}$ in Voigt notation, for materials with a cubic crystal symmetry like DX56D deep drawing steel.

Unlike the approach suggested by Asaro (1983) and Kalidindi et al. (1992), the critical shear stress $\tau_c^\alpha$ of a slip system $\alpha$ is described according to Lebensohn et al. (2007), Prakash and Lebensohn (2009) and Zhang et al. (2015) by

$$\dot{\tau}_c^\alpha = \frac{d\tau}{dt} \sum_{\beta=1}^{n} q^{\alpha\beta} |\gamma^\beta|$$

with the extended Voce type hardening law according to Tomé et al. (1984):

$$\tau^\alpha = \tau_0 + (\tau_1 + \theta_1 \Gamma) \left[1 - \exp\left(-\frac{\tau_0}{\tau_1}\right)\right].$$

The quantities $\tau_0$, $\tau_1$, $\theta_0$ and $\theta_1$ are material-dependent parameters and are assumed to be identical for all slip systems. While $\tau_0$ and $\theta_0$ describe the initial yield stress and initial
hardening rate in the grain, the asymptotic hardening behaviour for large strains is characterised by $\tau_1$ and $\theta_1$. In Eq. (8) and (9), $\Gamma$ is the accumulated plastic shear strain over all slip systems $n$, which is expressed as

$$\Gamma = \int_0^t \sum_{\alpha=1}^n |\dot{\gamma}^\alpha| \, dt. \quad (10)$$

Interaction between two different slip systems $\alpha$ and $\beta$ is incorporated by the interaction matrix $q^{\alpha\beta}$. The interaction matrix represents the latent hardening behaviour of a crystal and has the form:

$$q^{\alpha\beta} = \begin{bmatrix} 1 & q & \ldots & q \\ q & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & q \\ q & \ldots & q & 1 \end{bmatrix}. \quad (11)$$

The off-diagonal parameter $q$ defines the ratio of the latent to self-hardening rate. In line with Zhang et al. (2015), the same latent to self-hardening ratio is considered for all slip systems.

2.2.2. Representative volume element

The representative volume element (RVE), which is assumed to be representative for DX56D deep drawing steel, was set up using the software package Neper 3.5.2 (Quey, 2011). A rectangular cuboid with a normalised edge length of 1.0 and a total number of 1000 grains was considered for the model setup of the RVE. Grain elongation as obtained by EBSD measurements was also taken into account. Additionally, the polycrystal was discretised by 40x40x40 eight-node hexahedral elements with linear shape functions and full integration (element C3D8 in Abaqus). In order to incorporate the crystallographic texture of DX56D deep drawing steel into the RVE, the experimental results of the EBSD measurements were used to derive the orientation density function (ODF). The ODF was reconstructed considering 1000 orientations using the Matlab toolbox MTEX 5.1.1. Each of the obtained crystallographic orientations were assigned to one grain of the RVE.

Crystal plasticity parameters, which were taken from literature, are summarised in Table 2. In this context, the data for pure crystalline iron published by Frederikse (2014) was chosen as elastic constants $C_{11}$, $C_{12}$ and $C_{44}$ for DX56D deep drawing steel. The parameter for the rate sensitivity of slip $m$, which commonly varies between 0.01 and 0.05 (Raabe et al., 2005), (Zhang et al., 2014), (Zhang et al., 2015), (Zhang et al., 2016), was set to a relatively low value of 0.0125. This was done to minimise the strain rate dependency of the crystal plasticity model. Conversely, the hardening parameters $\tau_0$, $\tau_1$, $\theta_0$, and $\theta_1$ were identified by a reverse engineering
approach using the commercial software LS-OPT. Thus, the hardening parameters were
determined by fitting the effective stress-strain curve of the microstructural model to the
corresponding experimental stress-strain curve, considering a uniaxial loading at 0° with
respect to RD. Afterwards, the experimental stress-strain curves, the normalised yield stresses
and r-values of the uniaxial tensile tests at 15°, 30°, 45°, 60°, 75° and 90° as well as the results
of the hydraulic bulge tests were used to validate the hardening parameters. In this connection,
virtual experiments for the uniaxial tensile tests were carried out at 15°, 30°, 45°, 60°, 75° and
90° with respect to RD based on a texture rotation of the RVE. Since texture rotation does not
account for the grain morphology incorporated in RVEs, it can lead to errors. An additional
uniaxial tensile test was performed at 90° with respect to RD by directly applying a load in the
y-direction to access this error.

Table 2: Crystal plasticity parameters taken from literature as representative for DX56D deep drawing steel.

| CP parameter | Unit | Value | Reference                        |
|--------------|------|-------|----------------------------------|
| $C_{11}$     | GPa  | 226   | Frederikse (2014)               |
| $C_{12}$     | GPa  | 140   | Frederikse (2014)               |
| $C_{44}$     | GPa  | 116   | Frederikse (2014)               |
| $\dot{\gamma}_0$ | -    | 0.001 | Raabe et al. (2005), Zhang et al. (2015), Zhang et al. (2016) |
| $m$          | -    | 0.0125| Pagenkopf et al. (2016)         |
| $q$          | -    | 1.4   | Kocks (1970)                    |

The numerical homogenisation scheme introduced by Schmidt (2011) was used to derive
macroscopic quantities of the RVE. Thus, periodic boundary conditions were applied to the
RVE by introducing three auxiliary nodes – one for each pair of opposite faces. In addition, a
fourth auxiliary node was implemented to impede rigid body rotations. The translational
degrees of freedom of one arbitrary node of the RVE were fixed to prevent rigid body
translations.

2.2.3. Machine learning-based sampling of virtual experiments

Active learning is a machine learning technique that can be understood as an interactive process
to train machine learning models (cf. Settles et al., 2012). This means that a machine learning
model is trained on an initial data set and new data points are generated iteratively at locations
at which the model’s prediction quality is supposed to be worst. With respect to virtual
experiments, active learning is applied to sample proportional strain paths in order to obtain points on the anisotropic yield surface. For a definition of the proportional strain paths with respect to the full strain space, the three-dimensional deformation history of the RVE is defined by the use of a six-dimensional strain rate vector ($\dot{\varepsilon}_{xx}, \dot{\varepsilon}_{yy}, \dot{\varepsilon}_{zz}, \dot{\varepsilon}_{yz}, \dot{\varepsilon}_{xz}, \dot{\varepsilon}_{xx}$). Assuming plastic incompressibility, this six-dimensional vector is transformed to five-dimensions as suggested by Van Houtte et al. (1992):

$$
\begin{align*}
\dot{\varepsilon}_1 &= \frac{\sqrt{2}}{2} (\dot{\varepsilon}_{xx} - \dot{\varepsilon}_{yy}), \\
\dot{\varepsilon}_2 &= \frac{\sqrt{2}}{2} (\dot{\varepsilon}_{xx} + \dot{\varepsilon}_{yy}), \\
\dot{\varepsilon}_3 &= \sqrt{2} \dot{\varepsilon}_{yz}, \\
\dot{\varepsilon}_4 &= \sqrt{2} \dot{\varepsilon}_{xz}, \\
\dot{\varepsilon}_5 &= \sqrt{2} \dot{\varepsilon}_{xx}
\end{align*}
$$

(12)

The corresponding components of the original six-dimensional strain rate vector follow from the inversion of Eq. (12) and are:

$$
\begin{align*}
\dot{\varepsilon}_{xx} &= \frac{\sqrt{6} \dot{\varepsilon}_2 + 3 \sqrt{2} \dot{\varepsilon}_1}{6}, \\
\dot{\varepsilon}_{yy} &= \frac{\sqrt{6} \dot{\varepsilon}_2 - 3 \sqrt{2} \dot{\varepsilon}_1}{6}, \\
\dot{\varepsilon}_{zz} &= -\frac{2}{3} \dot{\varepsilon}_2, \\
\dot{\varepsilon}_{yz} &= \frac{2}{\sqrt{2}} \dot{\varepsilon}_3, \\
\dot{\varepsilon}_{xz} &= \frac{2}{\sqrt{2}} \dot{\varepsilon}_4, \\
\dot{\varepsilon}_{xx} &= \frac{2}{\sqrt{2}} \dot{\varepsilon}_5
\end{align*}
$$

(13)

This transformation is based on the introduction of a five-dimensional orthogonal base system and was already used by Grytten et al. (2008) and Zhang et al. (2015) to perform virtual experiments with respect to the full stress state. The five-dimensional strain rate vector in Eq. (12) also serves as a starting point for the active learning-based sampling approach and the two state-of-the-art sampling methods presented hereinafter. With respect to the boundary conditions of the RVE, the five-dimensional strain rate vector is scaled according to a reference strain rate so as to ensure constant strain rates and is then applied to the three auxiliary nodes of the RVE as a displacement gradient.

The active learning strategy query by committee is applied in this study. As the output space for sampling points on the initial yield surface is continuous, the approach introduced in Burbidge et al. (2007) for regression problems is deployed. In that respect, the input-output relation for the mapping to be learned is defined by
\[
\sigma_i = f(\dot{\varepsilon}_i),
\]  
(14)

where \(\dot{\varepsilon}_i\) and \(\sigma_i\) define the proportional strain path given by the five-dimensional strain rate vector in Eq. (12) and the corresponding point on the six-dimensional yield surface respectively. It is assumed that well-sampled data points for the mapping in Eq. (14) are also well suited to describe the anisotropic yield surface.

The general concept of the query by committee approach applied here is shown in Fig. 1. It is based on a committee of \(n\) regression models that learn the input-output relation in Eq. (14). When the regression models are trained, the input space is searched for the location, i.e. a five-dimensional strain rate vector \(\dot{\varepsilon}^*_i\), at which the committee disagrees the most. The disagreement is measured by the variance \(s^2\), which is expressed according to Krogh and Vedelsby (1995) as

\[
s^2(\dot{\varepsilon}_i) = \sum_{\eta=1}^{n} \left( \tilde{\sigma}^{(\eta)}_i(\dot{\varepsilon}_i) - \bar{\sigma}_i(\dot{\varepsilon}_i) \right)^2.
\]  
(15)

Here, \(\tilde{\sigma}^{(\eta)}_i\) denotes the prediction of the \(\eta\)th regression model and \(\bar{\sigma}_i\) describes the mean overall predictions. New strain rate vectors \(\dot{\varepsilon}^*_i\) are identified by solving the optimisation problem

\[
\dot{\varepsilon}^*_i = \arg \max_{\dot{\varepsilon}_i} s^2(\dot{\varepsilon}_i).
\]  
(16)

To ensure that the norm of the strain rate vector equals unity, a soft constraint is incorporated into Eq. (16). Therefore, the optimisation problem yields

\[
\dot{\varepsilon}^*_i = \arg \max_{\dot{\varepsilon}_i} \left( s^2(\dot{\varepsilon}_i) + W^* \left( 1 - \text{norm}(\dot{\varepsilon}_i) \right)^2 \right),
\]  
(17)

where \(W^*\) is a factor to weight the soft constraint. After solving the optimisation problem in Eq. (17), a new virtual experiment is performed that considers the new strain rate vector \(\dot{\varepsilon}^*_i\) in order to determine the corresponding yield point \(\sigma^*_i\). The new generated data tuple \((\dot{\varepsilon}^*_i, \sigma^*_i)\) is then added to the training data set and the active learning loop is repeated.
In this study, the committee of regression models were realised by five neural networks, which were implemented using the Python package scikit-learn (Pedregosa et al., 2011). The neural networks consisted of three hidden layers with five, ten and ten neurons respectively. All of them use rectifiers as activation functions. The models were trained using the limited memory BFGS optimiser (Liu and Nocedal 1989). Early stopping (Prechelt, 1998) was used for training as well as an L2-regularisation (Krogh and Hertz 1992) with a regularisation parameter of 0.00001. The differential evolution algorithm of Storn and Price (1997) as implemented in the Python package SciPy (Virtanen et al., 2020) was applied to solve the optimisation problem in Eq. (17) considering a weighting factor $W^*$ of 1000.

To assess the performance of the machine learning-based sampling approach, it was compared to two state-of-the-art sampling methods from literature. The first state-of-the-art method is a random sampling approach that was first used by Zhang et al. (2016). The random sampling approach used in this study is based on the work of Mueller (1959) and was originally introduced to generate uniformly distributed points on a hypersphere. Therefore, the five-dimensional strain rate vector described in Eq. (12) is defined by

$$\dot{\varepsilon}_i = \frac{x_i}{\sqrt{x_1^2+x_2^2+x_3^2+x_4^2+x_5^2}} \quad (18)$$

The values $x_i$ are drawn randomly from a Gaussian distribution with a mean of 0.0 and a standard deviation of 1.0 to sample five-dimensional strain rate vectors.
The second state-of-the-art sampling method was originally introduced by Van Houtte et al. (2009) and is based on an extension of the Miller indices. This means that the three Miller indices \([h_1, h_2, h_3]\) are extended to five dimensions \([h_1, h_2, h_3, h_4, h_5]\) and then used to define strain rate directions within the five-dimensional strain rate space. In that respect, the five-dimensional strain rate vector in Eq. (12) is defined as:

\[
\dot{\varepsilon}_i = \frac{h_i}{\sqrt{h_1^2 + h_2^2 + h_3^2 + h_4^2 + h_5^2}}
\]  

(19)

As suggested by Zhang et al. (2015), the following sets of five-dimensional Miller indices were considered: \([0 0 0 0 1]\), \([0 0 0 1 1]\), \([0 0 1 1 1]\), \([0 1 1 1 1]\), \([1 1 1 1 1]\) and \([1 1 1 1 3]\), including all permutations and changes of sign. This results in a total of 402 virtual experiments, which were carried out for the Miller indices-based sampling approach.

Since sampling that uses the active learning-based as well as the random sampling approach is not the same with multiple repetitions, i.e. the sampling sequence is not unique, both sampling methods were repeated five times. Five individual sets of sampled points were thus investigated for both sampling methods. 402 virtual experiments were performed for each of these sets so that they could be compared to the Miller indices-based sampling approach.

2.2.4. Parameter identification for anisotropic yield models

Virtual experiments were evaluated using a specific plastic work per unit volume of 24.58 MPa, corresponding to a uniaxial true plastic strain of 0.1 in RD, to obtain points on the initial yield surface. This value was chosen to ensure a nearly constant ratio of plastic anisotropy between uniaxial tensile tests and hydraulic bulge tests, see Section 3.1 and 3.2. The yield points were then used to identify parameters for anisotropic yield models by minimising the error function:

\[
E(\mathbf{c}) = \sum_{n=1}^{N}(\frac{\bar{\sigma}(\sigma^n, \mathbf{c}) - \sigma_{ref}}{\sigma_{ref}} - 1)^2.
\]  

(20)

In this case, \(\sigma^n\) and \(\bar{\sigma}\) are the stress tensor as predicted by a virtual experiment and the corresponding equivalent stress for a specific anisotropic yield model respectively. \(N\) is the total number of yield points and \(\mathbf{c}\) denotes a vector containing the parameters of the anisotropic yield model under consideration. The flow stress of the virtual tensile test in RD was taken a reference stress \(\sigma_{ref}\). Eq. (20) was minimised by using the Sequential Least Squares Programming (SLSQP) algorithm as implemented in the Python package SciPy (Virtanen et al., 2020). In addition, the error function in Eq. (20) was constrained so that the normalised equivalent stress in RD predicted by the anisotropic yield model is equal to 1.
The anisotropic yield models Hill48 (Hill, 1948), Yld91 (Barlat et al., 1991), Yld2004-18p (Barlat et al., 2005), and Yld2004-27p (Aretz et al., 2008) were considered to represent the full stress state for parameter identification. Since two parameters of the Yld2004-18p yield model are known to be dependent, the parameters $c_{12}'$ and $c_{13}'$ were set to unity as suggested by van den Boogaard et al. (2016). Hence, only 16 parameters were taken into account for the parameter identification of Yld2004-18p.

Parameters of the Yld2004-18p yield model were also identified as an in-plane version to study the accuracy of these anisotropic yield models with respect to in-plane anisotropy. To this end, the machine learning-based sampling method as originally introduced by Wessel et al. (2021) was used to carry out 100 virtual experiments with respect to the plane stress state. Only parameters relating to the plane stress state were then identified by minimising the error function in Eq. (20). Again, as suggested by van den Boogaard et al. (2016) the parameters $c_{12}'$ and $c_{13}'$ were set to unity so that only 12 independent parameters were considered for the in-plane version of Yld2004-18p.
3. Results

3.1 Material characterisation

The representative stress-strain curves of the uniaxial tensile tests at 0°, 15°, 30°, 45°, 60°, 75°, and 90° with respect to RD in Fig. 2 (a) demonstrate a direction-dependent plastic material behaviour for DX56D deep drawing steel. The stress-strain curves were highest at 45° and lowest at 90° with respect to RD. In addition, the results of the hydraulic bulge tests in Fig. 2 (b) illustrate a high formability with an average (± standard error) of 0.63 ± 0.02 for the maximum true strain before localisation.

The ratios of normalised yield stresses in Fig. 3 illustrate that the plastic anisotropy of the hydraulic bulge test relative to the uniaxial tensile test at 0° with respect to RD is not constant during deformation, but changes continuously until a constant value is reached. In that respect, normalised yield stresses determined by hydraulic bulge tests saturate at around 24.58 to 40.6 MPa specific plastic work, corresponding to an average true plastic strain in RD of 0.10 to 0.15 respectively. Conversely, normalised yield stresses of the uniaxial tensile tests at 15°, 30°, 45°, 60°, 75°, and 90° with respect to RD stay constant from the beginning.

![Fig. 2: Representative stress-strain curves of (a) uniaxial tensile tests at 0°, 15°, 30°, 45°, 60°, 75° and 90° with respect to the rolling direction (RD) and (b) hydraulic bulge tests considering a biaxial stress state for DX56D deep drawing steel. Only one of three repetitions is illustrated as an example.](image-url)
Fig. 3: Evaluation of the plastic anisotropy for DX56D deep drawing steel. Yield stresses were normalised by the average yield stress of the uniaxial tensile tests at 0° with respect to RD. Each data point represents the average of three repetitions. Due to artefacts of the elastic material behaviour, the specific plastic work is illustrated from 5.75 MPa upwards.

Evaluated material properties of the uniaxial tensile tests and the hydraulic bulge tests are summarised in Table 3. Similar to the stress-strain curves in Fig. 2 (a), the results of the yield stress, yield strength and r-value demonstrate a pronounced plastic anisotropy for DX56D deep drawing steel.

Table 3: Mechanical properties (mean ± standard error) of DX56D deep drawing steel obtained by uniaxial tensile tests in different directions with respect to RD and hydraulic bulge tests considering a biaxial stress state.

| Direction | Flow stress\textsuperscript{a} (MPa) | Yield strength\textsuperscript{b} (MPa) | Uniform elong.\textsuperscript{b} (%) | r-value\textsuperscript{c} (-) |
|-----------|----------------------------------|----------------------------------|----------------------------------|----------------------------------|
| 0°        | 303.7 ± 0.8                      | 294.3 ± 0.9                      | 27.0 ± 0.1                       | 2.15 ± 0.04                      |
| 15°       | 306.1 ± 0.1                      | 296.8 ± 0.2                      | 26.2 ± 0.2                       | 2.02 ± 0.02                      |
| 30°       | 310.8 ± 0.1                      | 300.6 ± 0.1                      | 25.3 ± 0.1                       | 1.77 ± 0.01                      |
| 45°       | 314.0 ± 0.3                      | 303.2 ± 0.4                      | 24.4 ± 0.1                       | 1.74 ± 0.02                      |
| 60°       | 312.3 ± 0.2                      | 301.5 ± 0.2                      | 24.8 ± 0.1                       | 1.97 ± 0.02                      |
| 75°       | 305.8 ± 0.1                      | 295.3 ± 0.2                      | 25.6 ± 0.1                       | 2.46 ± 0.01                      |
| 90°       | 302.1 ± 0.5                      | 291.5 ± 0.6                      | 26.2 ± 0.1                       | 2.60 ± 0.05                      |
| biaxial   | 363.4 ± 0.2                      | -                                | -                                | -                                |

\textsuperscript{a} True stress at a specific plastic work of 24.58 MPa (corresponds to the average of 0.1 true plastic strain in RD)
\textsuperscript{b} Engineering value
\textsuperscript{c} Analysed between 0.1 and 0.2 true plastic strain according to DIN EN 10346
The inverse pole figure (IPF) maps of the longitudinal and transverse cross-section in Fig. 4 show that <111> crystal axes are preferably orientated perpendicular to the normal direction of the sheet metal and that DX56D thus has a pronounced γ-fiber. As to the grain morphology, both IPF maps contain a total of 5452 grains in the longitudinal and 5670 grains in the transverse cross-section. The shape of the grains is slightly elongated towards RD, with an aspect ratio of approximately 1.6. Their average size accounts for roughly 133 μm² and 128 μm² in the longitudinal and transverse direction respectively.

![Fig. 4: Inverse pole figures (IPF) of the (a) longitudinal and (b) transverse cross-section of DX56D deep drawing steel. IPFs were plotted with respect to the normal direction (ND).](image)

Fig. 5 illustrates the ODF of DX56D deep drawing steel in the reduced Euler space with $0° \leq \varphi_1, \Phi, \varphi_2 \leq 90°$. In accordance with Fig. 4, a pronounced γ-fiber with a dominant crystallographic orientation (111) [1\(\overline{2}1\)] is visible. The maximum intensity for the longitudinal and traverse cross-section amounts to 11 multiples of a random density (MRD).
3.2 Microstructural model

The representative volume element generated for DX56D deep drawing steel is illustrated in Fig. 6. Based on the results of the EBSD measurements in Section 3.1, grains were replicated by incorporating an elongation towards RD with an aspect ratio of 1.6.

Fig. 5: Orientation density function (ODF) of DX56D deep drawing steel in the (a) longitudinal and (b) transverse cross-section. Shown as $\varphi_2$-sections from 0° to 90° in steps of 5° through the reduced Euler space.

Fig. 6: Microstructure of DX56D deep drawing steel shown as a representative volume element (RVE). Grains are elongated towards RD using an aspect ratio of 1.6 as determined by electron backscatter diffraction (EBSD) measurements.
The hardening parameters of the crystal plasticity model obtained by the reverse engineering approach are shown in Table 4. The corresponding stress-strain curve for the uniaxial tensile test in RD in Fig. 7 correlates well with the experimental data.

Table 4: Hardening parameters of the crystal plasticity model identified for DX56D deep drawing steel using a reverse engineering approach. Values are given in MPa.

| $\tau_0$ | $\tau_1$ | $\theta_0$ | $\theta_1$ |
|----------|----------|------------|------------|
| 62.19    | 48.19    | 356.84     | 37.44      |

Fig. 7: Comparison of experimental (each marker represents one of three repetitions) and stress-strain curve of a uniaxial tensile test in RD as predicted by a virtual experiment.

The results of the validation in Fig. 8 show that virtual experiments match the experimental normalised yield stresses and the r-values at 15°, 30°, 45°, 60°, 75° and 90° with respect to RD. However, compared to the reference solution obtained by direct loading in the $y$-direction, the virtual experiment based on a rotation of the texture leads to a lower normalised yield stress. The error amounts to roughly 1.6% with respect to the reference solution. In Fig. 8 (b), the texture rotation causes an overestimation of the r-value of approximately 4.7% with respect to the reference solution.
Fig. 8: Validation results of the (a) normalised yield stresses and (b) r-values with respect to RD. Yield stresses were determined considering a specific plastic work of 24.58 MPa. Results in RD are not part of the validation as these results were adjusted by a reverse engineering approach to match the experimental data.

The validation results of the hydraulic bulge test in Fig. 9 (a) show a good match between the virtual experiment and the experimental data for true strains up to 0.1. The stress-strain curve as predicted by the virtual experiment slightly underestimates the experimental data for strains higher than 0.1. Additionally, Fig. 9 (b) demonstrates that the microstructural model is able to reproduce the experimental verified change in the biaxial yield stress in Figure 3 at a slightly lower level. The maximum error between both curves amounts to approximately 3.4% with respect to the experiment.
Fig. 9: a) Comparison of the experimental stress-strain curve (each marker represents one of three repetitions) of the hydraulic bulge test and as predicted by a virtual experiment. b) Normalised yield stresses obtained by crystal plasticity simulations at different levels of specific plastic work. Yield stresses were normalised by the uniaxial yield stress at 0° with respect to RD. The experimental results of the biaxial yield stress taken from Fig. 3 are also shown for comparison.

3.3 Convergence of sampling methods

The Miller indices-based sampling approach is based on a predefined number of 402 virtual experiments, whereas the active learning-based and the random sampling approach allow sampling of variable numbers of yield points. The convergence behaviour of both sampling methods was studied to assess the necessity of those 402 virtual experiments for the active learning-based and the random sampling approach. Fig. 10 illustrates the evolution of anisotropic yield surfaces by representing the normalised error with respect to the reference state of 402 yield points. The results show that all anisotropic yield surfaces can be approximated with respect to the reference state using fewer than 402 virtual experiments. With respect to the Hill48, Yld91 and Yld2004-18p yield models, the normalised error for the active learning-based sampling approach decreases faster compared to the random sampling approach. This means that parameters of anisotropic yield models – considering a deviation of 10.0% with respect to the reference state for example – can be identified with an even lower number of virtual experiments. No significant differences between the active learning-based and the random sampling approach are visible for Yld2004-27p. However, the standard error, i.e. the variances between the five repetitions for both sampling methods considering less than 100 virtual experiments, is lower for the active learning-based than the random sampling approach.
Fig. 10: Normalised error for the active learning-based and the random sampling approach (mean ± standard error of 5 data sets in each case) with respect to the anisotropic yield models (a) Hill48, (b) Yld91, (c) Yld2004-18p and (d) Yld2004-27p. In order to determine the normalised error, the error of each parameter set identified for a certain number of points ($n = 10, 20, \ldots 100, 125, 400, 402$) was determined with respect to the maximum number of 402 yield points. Errors were normalised by the error corresponding to a total number of 402 yield points.

In the following, parameters of the anisotropic yield models Hill48, Yld91, Yld2004-18p, and Yld2004-27p were identified for the active learning-based and the random sampling approach considering a 5% deviation of the normalised error. Table 5 summaries the corresponding number of yield points used in the parameter identification for all five data sets of the active learning-based and the random sampling approach.
Anisotropic yield surfaces as identified by the number of yield points in Table 5 and the maximum number of 402 yield points serving as a reference are compared in Fig. 11 for Hill48 and Fig. 12 for Yld2004-27p, considering two exemplary data sets of the active learning-based and the random sampling approach. The anisotropic yield surfaces correlate well with the reference state of 402 yield points.

![Anisotropic yield surfaces](image)

**Fig. 11:** Anisotropic yield surface for the Hill48 yield model as identified by 60 and 402 yield points of the active learning-based sampling approach data set 3. Representation of normalised yield surface with respect to (a) the RD-TD plane, (b) the TD-ND plane, (c) the ND-RD plane, and (d) normalised yield stresses as well as (e) r-values with respect to RD. Normalised shear contours shown in increments of 0.1 from 0.0 to 0.5.
Fig. 12: Anisotropic yield surface for the Yld2004-27p yield model as identified by 250 and 402 yield points of the random sampling approach data set 5. Representation of normalised yield surface with respect to (a) the RD-TD plane, (b) the TD-ND plane, (c) the ND-RD plane, and (d) normalised yield stresses as well as (e) r-values with respect to RD. Normalised shear contours shown in increments of 0.1 from 0.0 to 0.5.

3.4 Evaluation of anisotropic yield surfaces

To assess the effect of the three sampling methods on the parameter identification of anisotropic yield models for the full stress state when a sufficiently large amount of yield points is sampled, Fig. 13 to 16 compare the normalised yield surfaces, the normalised yield stresses and the r-values for all three sampling methods. Yield surfaces of the active learning-based and the random sampling approach were identified according to Table 5 and averaged by computing the arithmetic mean of the five individual yield surfaces. All 402 points were utilised to identify parameters for the Hill48, Yld91, Yld2004-18p, and Yld2004-27p yield models for the Miller indices-based sampling approach. The comparison of the anisotropic yield surfaces demonstrates that the effect of the three sampling methods is rather small compared to the effect of the choice of the anisotropic yield models. For example, differences between the three yield surfaces for Hill48 in Fig. 13 and Yld2004-27p in Fig. 16 are less pronounced compared to the change between these two anisotropic yield models. In addition, the results for Yld2004-27p show the best agreement with respect to the virtual experiments of the uniaxial tensile tests from Section 3.2, which were not part of the parameter identification and serve as a reference.
Fig. 13: Hill48 yield surface as identified by the active learning-based, random and Miller indices-based sampling approach: Normalised yield surface with respect to (a) the RD-TD plane, (b) the TD-ND plane, (c) the ND-RD plane, and (d) normalised yield stresses as well as (e) r-values with respect to RD. Normalised shear contours shown in increments of 0.1 from 0.0 to 0.5. Yield surfaces identified by active learning-based and random sampling approach were averaged by calculating the arithmetic mean.

Fig. 14: Yld91 yield surface as identified by the active learning-based, random and Miller indices-based sampling approach: Normalised yield surface with respect to (a) the RD-TD plane, (b) the TD-ND plane, (c) the ND-RD plane, and (d) normalised yield stresses as well as (e) r-values with respect to RD. Normalised shear contours shown in increments of 0.1 from 0.0 to 0.5. Yield surfaces identified by active learning-based and random sampling approach were averaged by calculating the arithmetic mean.
Fig. 15: Yld2004-18p yield surface as identified by the active learning-based, random and Miller indices-based sampling approach: Normalised yield surface with respect to (a) the RD-TD plane, (b) the TD-ND plane, (c) the ND-RD plane, and (d) normalised yield stresses as well as (e) r-values with respect to RD. Normalised shear contours shown in increments of 0.1 from 0.0 to 0.5. Yield surfaces identified by active learning-based and random sampling approach were averaged by calculating the arithmetic mean.

Fig. 16: Yld2004-27p yield surface as identified by the active learning-based, random and Miller indices-based sampling approach: Normalised yield surface with respect to (a) the RD-TD plane, (b) the TD-ND plane, (c) the ND-RD plane, and (d) normalised yield stresses as well as (e) r-values with respect to RD. Normalised shear contours shown in increments of 0.1 from 0.0 to 0.5. Yield surfaces identified by active learning-based and random sampling approach were averaged by calculating the arithmetic mean.
As the reference results of the uniaxial tensile tests at 0°, 15°, 30°, 45°, 60°, 75°, and 90° with respect to RD in Fig. 13 to 16 only represent a small area of the anisotropic yield surface, the error of an anisotropic yield surface with respect to the 402 yield points sampled by a different sampling method was determined using the least squares method. This procedure was repeated for each anisotropic yield surface with respect to the yield points of each sampling method, including all data sets. The resulting errors are illustrated in Fig. 17. In accordance with the findings in Fig. 13 to 16, the results show that there are differences between the anisotropic yield surfaces identified by different sampling methods. However, these differences are minor compared to the effect of the anisotropic yield model. For instance, the minimum and maximum error for the Hill48 yield surface in Fig. 16 (a) accounts for 0.16 and 0.33 respectively. In contrast, the minimum error for the Yld2004-27p yield surface in Fig. 16 (d) is 0.05 and the maximum error 0.08, and thus is lower than the minimum error of all Hill48 yield surfaces.
Fig. 17: Error of the yield surfaces for (a) Hill48, (b) Yld91, (c) Yld2004-18p and (d) Yld2004-27p as identified by different sampling methods in accordance with Section 3.3 with respect to the total number of 402 yield points of each data set. Diagonal error squares represent the error of a yield surface for all yield points of its own data set. Sampling methods and data sets are abbreviated as follows: AL – active learning-based sampling approach, RND – random sampling approach, numbers 1 to 5 define the respective data set.

Fig. 18 compares the normalised yield surfaces of Hill48, Yld91, Yld2004-18p, and Yld2004-27p as identified by the active learning-based sampling approach to the Yld2004-18p (in-plane) yield model. The parameters for Yld2004-18p (in-plane) were identified by sampling virtual experiments with respect to the plane stress state and therefore serve as a reference for the in-plane behaviour. Overall, the best match between the reference solution and the anisotropic yield models is found for Yld2004-27p. Similar results were also detected for the anisotropy yield models determined by the random and Miller indices-based sampling approaches.
Fig. 18: (a) Normalised yield surface with respect to the RD-TD plane, (b) normalised yield stresses and (c) r-values with respect to RD for the active learning-based sampling approach compared to the reference solution. Reference solution is given by Yld2004-18p (in-plane) yield models, whose parameters were determined using virtual experiments considering the plane stress state. Normalised shear contours shown in increments of 0.1 from 0.0 to 0.5.
4. Discussion

Both the mechanical and crystallographic results in Section 3.1 demonstrate that the DX56D deep drawing steel under investigation has a strong plastic anisotropy. The mechanical material properties generally correspond with the technical delivery conditions as given in DIN EN 10346 and are consistent with the mechanical and crystallographic results reported by Butz et al. (2019) for a different batch of DX56D. The results of the hydraulic bulge tests are in accordance with Sigvant et al. (2009). In addition, the results for the evaluation of the plastic anisotropy in Fig. 3 demonstrate that plastic anisotropy under uniaxial and biaxial loading changes during deformation and only remains constant for strains above 10 to 15%. A similar behaviour for plastic anisotropy was observed by Volk et al. (2011) for a DX54D steel grade. According to Hill and Hutchinson (1992), this phenomenon of an evolution of plastic anisotropy, or rather hardening behaviour under proportional monotonic loading conditions, is defined as differential work hardening. As differential work hardening is generally known in IF and low-carbon steel grades, see Kuwabara et al. (1998) and Eyckens et al. (2015) for example, it would appear to be the most likely explanation for the differences observed with respect to the plastic anisotropy or hardening behaviour. Additionally, physical mechanisms for differential work hardening include texture development and strain heterogeneity at grain length scale, which is why crystal plasticity models are generally able to capture differential work hardening (Eyckens et al., 2015). The results in Fig. 9 (b) furnish evidence that the phenomenological crystal plasticity model used in this study can predict differential work hardening for commercial IF steels like DX56D with reasonable accuracy.

The results of the microstructural model in Section 3.2 indicate two important aspects of the virtual experiment approach. First, due to the good match between experimentally and virtually determined yield stresses and r-values in Fig. 8, virtual experiments are well suited to predict the plastic anisotropy of sheet metals like DX56D deep drawing steel. Similar results have already been reported by Zhang et al. (2015), Zhang et al. (2016), Butz et al. (2019), Liu et al. (2020) and Engler and Aretz (2021), considering multiple stress states, i.e. uniaxial tensile tests, plane strain tension tests and pure shear tests, and different aluminium alloys as well as different steel grades. The results in Fig. 9 demonstrate that the experimental biaxial flow stress of hydraulic bulge tests can also be predicted with a reasonable error of 3 to 4% by virtual experiments. Second, the results in Fig. 8 illustrate that simulating uniaxial tensile test in different directions with respect to RD on the basis of a texture rotation – which is often done in literature, cf. Zhang et al. (2015), Zhang et al. (2016) – can cause a noticeable error for microstructures with elongated grains. This error was expected by the authors and is due to the
The fact that texture rotation excludes any effect of the grain morphology. Elongated grains with an aspect ratio 1.6 were incorporated into the RVE for DX56D deep drawing steel. With respect to the result for the normalised yield stress in TD in Fig. 8 (a), this led to an error of roughly 1.6% compared to the reference solution without rotating the texture. This error is still considered reasonable. However, as this error is expected to be governed by the size of the grain elongation, i.e. the error increases as the aspect ratio incorporated into the RVE rises, it should be taken into account for microstructures with higher grain elongation.

The comparison of the four anisotropic yield surfaces Hill48, Yld91, Yld2004-18p, and Yld2004-27p in Section 3.4 demonstrates the following aspects with respect to virtual experiments and anisotropic yield models: firstly, the sampling approach affects the resulting yield surface, as seen in Fig. 13 to 17. However, the effect of sampling seems to be of minor relevance compared to the choice of the anisotropic yield model – assuming enough yield points were sampled. Secondly, only anisotropic yield models with a sufficient number of parameters are able to represent the anisotropic plastic material behaviour with reasonable accuracy. With regard to DX56D, only Yld2004-27p was flexible enough to describe the anisotropic plastic material behaviour with respect to the in- and out-of-plane behaviour. This contradicts the results of Zhang et al. (2015), where the Yld2004-18p yield model was assessed to be sufficiently flexible to match the yield points predicted by virtual experiments of an AA1050 aluminium alloy for the full stress state. Furthermore, Zhang et al. (2016) reported that both Yld2004-18p and Yld2004-27p presented the anisotropic yield surface of a AA3014 aluminium alloy for the full stress state with reasonable accuracy. This discrepancy with literature can most likely be explained by the different levels of plastic anisotropy of the analysed materials. Compared to the AA1050 and AA3104 aluminium alloys, DX56D deep drawing steel has a stronger plastic anisotropy with respect to the r-values. Hence, anisotropic yield models with greater flexibility, like Yld2004-27p, are necessary to represent the plastic anisotropy for the in-plane and out-of-plane behaviour of DX56D precisely. Furthermore, anisotropic yield models with sufficient flexibility are able to match the yield points predicted by virtual experiments very accurately. As a consequence, the prediction accuracy of the virtual experiment approach, i.e. identifying parameters for anisotropic yield models based on crystal plasticity simulations, is mainly affected by the quality of the RVE when enough flexible anisotropic yield models are applied. Therefore, further research should focus on an improved setup of microstructural models for the virtual experiment approach.

In addition, the results of the anisotropic yield surfaces in Fig. 18 reveal an important aspect of the Yld2004-18p and Yld2004-27p yield models. Assuming that the anisotropic yield model
Yld2004-18p is flexible enough to represent the plastic anisotropy of DX56D for the plane stress state accurately, as was shown in a previous work by the authors (Wessel et al., 2021), a consideration of the out-of-plane plastic anisotropy would appear to lead to a degradation of the in-plane accuracy. Therefore, it is thought that the improved representation of the anisotropic yield surface for Yld2004-27p is mainly governed by the increase in out-of-plane parameters. In comparison with Yld2004-18p, the anisotropic yield model Yld2004-27p has seven additional parameters to describe the in-plane and two for the out-of-plane behaviour. In that respect, the two additional parameters associated with the out-of-plane behaviour are expected to be more relevant than the seven additional in-plane parameters. Since van den Boogaard et al. (2016) has already verified the existence of dependencies between in-plane parameters for Yld2004-18p, it can also be expected that a parameter reduction for Yld2004-27p is highly probable.

Finally, the results presented in Sections 3.3 and 3.4 demonstrate that the new active learning-based sampling approach is suitable for virtual experiments with respect to the full stress state in a data efficient manner. In comparison with the Miller indices-based sampling approach, parameters for all anisotropic yield models considered could be identified with fewer virtual experiments. This advantage also applies for the random sampling approach, but is less significant compared to an active learning-based sampling approach in view of the results for Hill48, Yld91, and Yld2004-18p in Fig. 10. Differences regarding the sampling efficiency of both sampling methods seem to be negligible for the Yld2004-27p yield model. This can be explained by the high number of parameters for Yld2004-27p, which leads to a larger number of required yield points for parameter identification. It could be shown that the active learning-based sampling approach improves the sampling of points on the initial yield surface, particularly when the number of virtual experiments to be performed is limited – e.g. due to limited computational recourses. Since the number of virtual experiments performed increases, this advantage vanishes compared to the random sampling approach so that no differences are visible for anisotropic yield models like Yld2004-27p. Moreover, the results for the active learning learning-based sampling approach in Fig. 10 show a lower standard error compared to the random sampling approach, which can be regarded as being beneficial for repeatability. In conclusion, the active learning-based sampling approach is a data-efficient and reliable sampling method if the full stress state is taken into account. Both findings are consistent with the results of Wessel et al. (2021) for applying the active learning-based approach uncertainty sampling and considering the plane stress state. Nevertheless, this study does not investigate the behaviour of the active learning-based sampling approach in detail. For example, the choice
of the initial yield points and hyperparameters of the active learning approach is expected to have a great effect on the sampling efficiency and repeatability in both a positive and negative way. The authors generally believe that there is a high potential for the use of active learning to train data-driven models in materials sciences more efficiently. Future work will therefore concentrate on the application of the active learning-based sampling approach to data-driven models such as recurrent neural networks.
5. Conclusions

This study introduces a new machine learning-based sampling approach based on active learning to perform virtual experiments with respect to the full stress state and also analyses the effect of different sampling methods on identifying the parameters for anisotropy yield models. To this end, virtual experiments were carried out for a DX56D deep drawing steel using the new active learning-based sampling approach and two state-of-the-art sampling methods taken from literature by way of comparison. In summary, the following conclusions can be drawn from the present work:

- The new active learning-based sampling approach is a suitable method to sample points on the initial yield surface with respect to the full stress state in a data-efficient manner. Compared with two state-of-the-art sampling approaches taken from literature, this new sampling method shows an improved sampling efficiency and repeatability.

- Assuming enough sampled yield points, the effect of different sampling methods on the resulting yield surface is less significant than the choice of the anisotropic yield model itself. In that respect, anisotropic yield models with a high number of parameters offer the advantage of representing the plastic anisotropy for the in-plane as well as out-of-plane behaviour with sufficient accuracy. The anisotropic yield model Yld2004-27p was flexible enough to represent the full stress state with reasonable accuracy for DX56D deep drawing steel.

- The rotation of the texture causes an error for sheet metals with elongated grains when simulating tensile tests at different directions with respect to RD by means of virtual experiments. In connection with the DX56D deep drawing steel under consideration, the grains of the RVE had an aspect ratio of 1.6, which led to an error of 1.6% with respect to the normalised yield stress in TD.
CRediT authorship contribution statement

Alexander Wessel: Conceptualisation, Funding acquisition, Investigation, Methodology, Software, Writing – original draft, Visualisation. Lukas Morand: Methodology, Software, Writing – original draft, Visualisation. Alexander Butz: Funding acquisition, Writing – review & editing, Supervision. Dirk Helm: Funding acquisition, Writing – review & editing, Supervision. Wolfram Volk: Writing – review & editing, Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Research data

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