A new machine learning based method for sampling virtual experiments and its effect on the parameter identification for anisotropic yield models

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Abstract. A new method for sampling virtual experiments on the initial yield surface is introduced for the plane stress state. The method is based on a machine learning technique called active learning, which can be used to adaptively sample a parameter space with respect to a certain criterion. For the evaluation of this new method, it is compared against a random sampling approach taken from literature and the effect of both methods on three different anisotropic yield models, namely Yld89, Yld2000-2d and Yld2004-18p (in-plane), is analysed. The results demonstrate that the active learning based sampling approach has advantages over the random sampling approach in terms of reliability and sample efficiency. Moreover, it is found that the effect of the sampling method on the resulting yield surface depends on the anisotropic yield model considered.

1. Introduction

An accurate description of plastic anisotropy by means of anisotropic yield models is essential for high-quality sheet metal forming simulations. To determine the parameters of these constitutive models, various mechanical experiments, e.g. uniaxial tensile tests in different directions with respect to the rolling direction (RD) or hydraulic bulge tests, are typically performed. As an extension to an experimental characterisation, virtual experiments based on crystal plasticity simulations are being used more and more in academic science [1]. Nonetheless, a generic approach for performing virtual experiments and thereby determining parameters for anisotropic yield models has not yet been established and, in particular, the procedure for sampling points on the initial yield surface differs within the literature. For instance, Barlat et al. [2] carried out four virtual experiments on AA2090-T3 and AA6111-T4 aluminium sheets to examine the resistance to shear in respect of the thickness direction of a sheet, and thus identified the out-of-plane parameters for the Yld2004-18p yield model. In comparison, Grytten et al. [3] calibrated all parameters for Yld2004-18p by conducting 690 virtual experiments within the full stress state for an AA5083-H116 aluminium alloy. By contrast, Zhang et al. [4] utilised an extension of the Miller indices proposed by Van Houtte et al. [5] to perform 201 virtual experiments on AA1050 in the full stress state and identified parameters for Yld2004-18p as well. Furthermore, Zhang et al. [6] applied only 125 randomly generated load cases to compute the parameters of Yld91, Yld2000-2d, Yld2004-18p and Yld2004-27p for a hot-band and a cold-rolled AA3104 aluminium sheet.
The present study seeks to improve the generation of points on the initial yield surface by introducing a new machine learning based sampling method for virtual experiments, and investigates the effect of different sampling methods on the parameter identification for anisotropic yield models. For simplicity, this study limits itself to the plane stress state only.

2. Crystal plasticity modelling

Virtual experiments were performed on DX56D deep drawing steel utilising the crystal plasticity finite element method (CPFEM). The simulations were conducted using the commercial finite element software Abaqus/Standard.

2.1. Constitutive model

The constitutive model was obtained by using a phenomenological crystal plasticity model and implemented into the finite element code through a UMAT user subroutine. The numerical implementation of the crystal plasticity model used was done by Pagenkopf et al. [7] and is based on an approach worked out by Kalidindi et al. [8]. Thus, the plastic shear rate for each slip system $\alpha$ is represented by a power-law type equation

$$\dot{\gamma}_{\alpha} = \gamma_0 \left| \frac{\tau_{\alpha}}{\tau_c} \right|^{1/m} \text{sgn}(\tau_{\alpha}),$$

(1)

with $\gamma_0$ and $m$ denoting the reference shear rate and the rate sensitivity of slip, respectively. The resolved shear stress $\tau_{\alpha}$, acting on a slip system $\alpha$, is approximated assuming an infinitesimal elastic elongation by Schmid’s law:

$$\tau_{\alpha} = \mathbf{T} \cdot \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha.$$

(2)

Here, $\mathbf{T}$ represents the second Piola-Kirchhoff stress tensor, and the two unit vectors $\mathbf{m}^\alpha$ and $\mathbf{n}^\alpha$ describe a certain slip system $\alpha$. For body-centered cubic materials, such as DX56D deep drawing steel, 24 slip systems crystallographically denoted as $\{110\} \langle 111 \rangle$ and $\{112\} \langle 111 \rangle$ are incorporated in the crystal plasticity model, which is in accordance with the literature [9-11]. In contrast to the suggested crystal plasticity implementation by Kalidindi et al. [8], the critical shear stress $\tau_c^\alpha$ of a slip system $\alpha$ is formulated according to Lebensohn et al. [12] by an extended Voce-type hardening law proposed by Tome et al. [13] as

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

(3)

with the hardening function

$$\Gamma = \int_0^\tau \frac{\dot{\gamma}_{\alpha}}{} = \Gamma$$

(4)

The quantities $\tau_0$, $\tau_1$, $\theta_0$, and $\theta_1$ are material constants and are assumed to be identical for each slip system. While $\tau_0$ is related to the initial yielding, the constant $\theta_0$ describes the initial hardening rate. The asymptotic hardening behaviour is characterised by $\tau_1$ and $\theta_1$. In equations (3) and (4), $\Gamma$ denotes the accumulated plastic shear strain over all slip systems $n$, and is expressed as

$$\Gamma = \int_0^\tau \frac{\dot{\gamma}_{\alpha}}{} = \Gamma.$$

(5)

Interactions between slip systems are taken into account by the interaction matrix $q^{\alpha\beta}$. This matrix represents the latent hardening behaviour of a single crystal and has the form:

$$q^{\alpha\beta} = \begin{bmatrix}
1 & q & \ldots & q \\
q & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & q \\
q & \ldots & q & 1
\end{bmatrix}.$$
The off-diagonal terms $q$ represent the ratio of the latent hardening to the self-hardening rate. Contrary to Kalidindi et al. [8], no distinction is made between coplanar and non-coplanar slip systems. Similar to Zhang et al. [4], the same latent hardening to self-hardening ratio is considered for all slip systems.

2.2. Representative volume element

Microstructure features were approximately reproduced in a statistically equivalent manner by a representative volume element (RVE). Based on earlier experience on a different batch of DX56D deep drawing steel [14-15], the RVE illustrated in figure 1 (a) was set up. It is a rectangular cuboid with an edge length of 1.0 and was generated using the software package Neper [16]. A total of 1000 grains were considered for the model setup by applying a Voronoi tessellation. Grains are slightly elongated towards the rolling direction, having an aspect ratio of 1.6. The polycrystal is discretised by 25x25x25 hexahedral elements with a linear shape function and reduced integration including hourglass control. To incorporate the crystallographic texture into the RVE, an electron backscatter diffraction (EBSD) analysis was performed on DX56D deep drawing steel. Based upon the outcome of the experimental measurement, the orientation distribution function (ODF) was reconstructed by means of 1000 discrete orientations using the MATLAB® toolbox MTEX [17] and each of the discrete orientations was assigned to one grain of the RVE.

![Figure 1.](image)

**Figure 1.** (a) RVE for DX56D deep drawing steel with 1000 grains and (b) a comparison between the experimental (each marker corresponds to one of three measurements) and the stress-strain curve of a uniaxial tensile test in RD as predicted by crystal plasticity simulations.

The parameters for the crystal plasticity model are summarised in table 2. They were partially taken from the literature, for example the elastic constants $C_{11}$, $C_{12}$ and $C_{44}$ for pure single crystalline iron. The rate sensitivity of slip $m$, which commonly varies between 0.01 and 0.05 in the literature [4, 6, 11], was set to 0.0125. The hardening parameters $\tau_0$, $\tau_1$, $\theta_0$ and $\theta_1$ were identified by a reverse engineering approach. This means that the hardening parameters were adjusted to match the experimental data of a uniaxial tensile test in RD, see figure 1 (b). Experimental results of uniaxial tensile tests at 22.5°, 45°, 67.5° and 90° with respect to RD were used to validate the hardening parameters.

**Table 1.** Crystal plasticity parameters utilised for DX56D deep drawing steel.

| Parameter | Value |
|-----------|-------|
| $C_{11}$  | 226   |
| $C_{12}$  | 140   |
| $C_{44}$  | 116   |
| $\gamma_0$ | 0.001 |
| $m$       | 0.0125|
| $\tau_0$ | 61.79 |
| $\tau_1$ | 43.71 |
| $\theta_0$ | 356.55 |
| $\theta_1$ | 42.73 |
| $q$       | 1.4   |

*Reference [18].

*Reference [4, 6].

*Reference [19].
For computing the macroscopic response of a virtual experiment, a numerical homogenisation approach suggested by Schmidt [20] was applied. Accordingly, the RVE was constrained by periodic boundary conditions and the loading was controlled by the use of three auxiliary nodes, each corresponding to one pair of opposite faces of the RVE.

2.3. Sampling points on the initial yield surface

To perform virtual experiments within the plane stress state, the loading history of the RVE needs to be prescribed. To do so, the deformation at the auxiliary nodes belonging to the x- and y-directions (corresponding to RD and TD of the sheet) was specified by a strain direction \((\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{xy})\), whereas the stress at the auxiliary node belonging to the z-direction (corresponding to ND of the sheet) was set to zero. This was done so as to ensure the strain rates are constant. Additionally, strain directions were also defined by means of two angles \(\varphi\) and \(\theta\) using spherical coordinates. Two different methods were applied for the definition of strain directions and hence sampling points on the initial yield surface.

2.3.1. Active learning based sampling

The first method is based on a machine learning technique called active learning. Generally, active learning models are designed to improve with experience and training in a continuous interactive learning process [21]. Here, a grey-box model, see for example [22], consisting of two models was used to set up this process: first, a data generating process, which corresponds to crystal plasticity simulations, and second, a regression model that learns the input-output relation of the data generating process and further provides a measure of the uncertainty of its own predictions. Here, the angles \(\varphi\) and \(\theta\) defining a strain direction serve as an input, and the corresponding yield point represents the output. The iterative process starts by training the regression model on an initial data set that, in this study, consisted of eleven pairs of angles \(\varphi\) and \(\theta\) and the corresponding yield points. After training, the \(\varphi\)-\(\theta\)-space is analysed for the location at which the prediction of the regression model is most uncertain. At this location, a new yield point is sampled using virtual experiments and added to the data base subsequently. Then the regression model is retrained and the process starts from the beginning.

The basis of the active learning approach is a Gaussian process regression model [23]. According to Rasmussen and Williams [24], a Gaussian process can be seen as a distribution over functions

\[
f(x) \sim GP(m(x), k(x, x'))
\]

in which \(m(x)\) denotes the mean function and \(k(x, x')\) represents the covariance function. For a discrete set of training data \(X, f\) and for unknown function values \(f_*\) at location \(X'\), the joint distribution for the noise-free case is written as follows:

\[
\begin{bmatrix} f \\ f_* \end{bmatrix} \sim \mathcal{N} \left( 0, \begin{bmatrix} K(X, X) & K(X, X') \\ K(X', X) & K(X', X') \end{bmatrix} \right)
\]

In this case, \(\mathcal{N}\) and \(K\) describe the Gaussian distribution and the kernel functions, respectively. Moreover, an additive composition of a radial basis function kernel and a Matérn kernel is used. The Gaussian process regression model considered was implemented via the Python package scikit-learn [25]. To search the input space for the location of maximum uncertainty, which is in this case the location of maximum variance, the Differential Evolution [26] global optimiser was utilised as it is implemented in the Python package SciPy [27].

2.3.2. Random sampling

The second method was a random sampling approach that has been applied in a similar manner by Zhang et al. [6] to carry out virtual experiments in the plane and full stress state. Here, the random sampling approach introduced by Muller [28], which was originally introduced to generate points uniformly on a \(n\)-dimensional sphere, was adapted to virtual experiments. Therefore, each component of a strain direction \((\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{xy})\) is described by

In this case, \(\mathcal{N}\) and \(K\) describe the Gaussian distribution and the kernel functions, respectively. Moreover, an additive composition of a radial basis function kernel and a Matérn kernel is used. The Gaussian process regression model considered was implemented via the Python package scikit-learn [25]. To search the input space for the location of maximum uncertainty, which is in this case the location of maximum variance, the Differential Evolution [26] global optimiser was utilised as it is implemented in the Python package SciPy [27].
where $x_1$, $x_2$ and $x_3$ are random samples from a normal Gaussian distribution. Since the random sampling approach generates strain directions at random, and the resulting points on the initial yield surface are not representative for a single iteration, the latter was repeated five times and thereby five individual sets of randomly sampled points were investigated. Further, to ensure comparability with the active learning based sampling approach, the same initial data set consisting of eleven yield points on the initial yield surface was also used for the random sampling approach.

3. Results

In total, 250 crystal plasticity simulations were carried out for the active learning based approach as well as for each data set of the random sampling approach. In the following, the results for the distribution of yield points, the convergence behaviour and the anisotropic yield surfaces are presented.

3.1. Distribution of points on the initial yield surface

Points on the initial yield surface were determined by using a specific plastic work per unit volume of 10.56 MPa, which corresponds to a uniaxial true plastic strain of 5.0% in RD. The points obtained for the active learning based sampling approach and two selected point sets of the random sampling approach are shown in figure 2 for three different stages.

![Figure 2](image_url)

**Figure 2.** The evolution of points on the initial yield surface (11 points, 50 points and 250 points from top to bottom) for (a) the active learning based sampling, and for (b) “set 1” and (c) “set 5” generated by the random sampling approach.
The top row shows the initial data consisting of eleven yield points and shared by all approaches. Nevertheless, there are differences within the point distribution of the two methods for 50 and 250 points and, in particular, in the simple and pure shear area. The active learning based sampling shows a higher density of points along the simple/pure shear line compared to the random sampling approach. Moreover, the comparison of the evolution of the two randomly sampled sets at a stage of 50 and 250 points shows that the variation between the data points at the same stage become less pronounced as the number of points on the initial yield surface increases.

3.2. Convergence behaviour

To study the convergence behaviour of the two sampling methods, parameters for Yld89, Yld2000-2d and Yld2004-18p (in-plane) were identified for different numbers of yield points, i.e. 20, 30, …, 100, 125, …, 250. Then, each of the parameters determined was used to calculate the respective error regarding the maximum number of 250 yield points, which serves as a reference. Finally, the results were normalised by the error corresponding to a total number of 250 yield points. It should be noted that for Yld2004-18p (in-plane), the parameters \( c_{12}' \) and \( c_{13}' \) were set to unity as proposed by van den Boogaard et al. [29], and therefore only 12 parameters were taken into account for the plane stress state considered here.

The results of this analysis are given in figure 3. Comparison between figure 3 (a) and (b) indicates that the convergence behaviour of the active learning based sampling approach is better than that of the averaged results of the random sampling method for the Yld89 and Yld2000-2d yield models. Approximately 75 to 100 yield points are necessary for the active learning based sampling approach to converge, whereas more than 100 yield points are needed for the random sampling approach. Further, there is a high level of variation in the averaged results of the random sampling approach. Here, the highest fluctuation is observed at “set 5”, which is illustrated in figure 3 (c). By contrast, the convergence behaviour for the Yld2004-18p (in-plane) yield model is similar for both sampling methods.

3.3. Anisotropic yield surfaces

Figure 4 compares the normalised yield surface, the normalised yield stress and the \( r \)-value with respect to RD for the active learning based and the random sampling approach. All results are based on a total number of 250 yield points to exclude the effect of a non-converging sampling method. Crystal plasticity simulations of uniaxial tensile tests at 0°, 22.5°, 45°, 67.5° and 90° with respect to RD serve as a reference. In contrast to the procedure described in section 2.3, these simulations were carried out based on a texture rotation of the RVE. Therefore, for each simulation the RVE was loaded in RD with the texture rotated at the respective angle.
With the Yld89 yield model, differences between the two sampling methods are visible in the normalised yield surface and especially in the simple shear area. Differences between the two sampling methods are also visible in the normalised yield stress and the r-value with respect to RD. This variation between the active learning based sampling approach and the random sampling approach is also apparent for the Yld2000-2d yield model, but less pronounced. In contrast to this, these differences between the two sampling methods are negligible for Yld2004-18p (in-plane).

Figure 4. Normalise yield surface (top), normalised yield stress (centre) and r-value with respect to RD (bottom) for (a) Yld89, (b) Yld2000-2d and (c) Yld2004-18p (in-plane).

Moreover, there are differences between the normalised yield stress and the r-value with respect to RD compared to the results of the uniaxial tensile test simulations serving as a reference. In this case, the error of the r-value regarding the reference results is more pronounced than that of the normalised yield stress – at least for Yld89 and Yld2000-2d. Further, the best match between the anisotropic yield models and the results of the five uniaxial tensile tests is found for Yld2004-18p (in-plane). In particular, the development of the r-value is captured precisely, even though parameters were identified by means of yield points only.
4. Discussion
The results presented in section 3 indicate that the newly introduced active learning based approach for sampling points on the initial yield surface is a promising approach for performing virtual experiments within the plane stress state. First, in contrast to the point distribution of the random sampling approach, that of the active learning based sampling approach shown in figure 2 seems to be more homogenous in the simple and pure shear area and, in particular, for smaller numbers of yield points, for example 50. This can be seen as an advantage since different stress states will be weighted more evenly for the identification of parameters for anisotropic yield models. Second, the active learning based sampling approach requires – at least for Yld89 and Yld2000-2d – a lower number of virtual experiments for convergence and is more robust compared to the random sampling approach, having a high level of fluctuation as indicated in figure 3 (b). In consequence, this means the active learning based sampling approach is more reliable and has better numerical efficiency. However, one major limitation of this study is that the effect of the initial data set for the active learning based sampling approach has not yet been considered. It is expected that the number and choice of initial yield points have a positive as well as a negative effect on the convergence behaviour.

Furthermore, the results shown in figure 4 highlight two important aspects of virtual experiments. First of all, different methods for sampling points on the initial yield surface can have an effect on the parameter identification for anisotropic yield models and hence on the resulting yield surfaces. This effect seems to depend on the anisotropic yield model considered, and becomes less pronounced for anisotropic yield models with a larger number of parameters, leading to greater flexibility. In the case of the DX56D deep drawing steel studied, the anisotropic yield model Yld2004-18p (in-plane) was flexible enough to handle large numbers of virtual experiments and therefore points on the initial yield surface without being affected by the sampling method. Secondly, the choice of anisotropic yield models has a big effect on the quality of the resulting yield surface and, in particular, on the r-value reflecting the curvature or rather the tangent planes of the yield surface. Again, for the DX56D deep drawing steel studied, the anisotropic yield model Yld2004-18p (in-plane) was sufficiently flexible to match yield stresses and r-values accurately, as illustrated in figure 4 (c). As a consequence of both statements, it can be hypothesised that by considering anisotropic yield models with satisfactory flexibility, the prediction accuracy of the virtual experiment approach, i.e. identifying parameters for anisotropic yield models based on crystal plasticity simulations, is mainly governed by the quality of the RVE. It should be mentioned here that, in this study, the quality of the RVE was validated by experimental results of uniaxial tensile tests at 22.5°, 45°, 67.5° and 90° with respect to RD only. To evaluate the quality of the RVE more extensively, further experimental measurements, such as hydraulic bulge tests, are desirable.

5. Conclusions
In summary, the following two conclusions can be drawn from the present work:

- The active learning based sampling approach introduced is a reasonable method for sampling points on the initial yield surface for the plane stress state. Compared to a random sampling approach taken from literature, the active learning based method has advantages in respect of a more homogenous distribution of points on the initial yield surface and sample efficiency. Furthermore, it is more reliable than the random sampling approach since strain directions are not generated at random.

- The sampling method for virtual experiments can have an effect on the parameter identification for anisotropic yield models and hence on the resulting yield surfaces. If a sufficiently flexible anisotropic yield model is considered, this effect becomes less distinct and rather becomes negligible. At the same time, anisotropic yield models with a greater number of parameters enhance the representation of the initial yield surface and, in particular, of the r-value or rather the tangent planes of the yield surface. In this study, the anisotropic yield model Yld2004-18p (in-plane) was adequate to account for both aspects.
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