Crystal plasticity as complementary modelling technique for improved simulations results of anisotropic sheet metal behaviour in forming processes

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**Abstract.** The accuracy of the simulation results in terms of metal sheet forming strongly depends on the capability of modelling the anisotropic material behaviour. In addition, predictive capabilities of the models are strongly influenced by the way how the constitutive model parameters are calibrated. Macroscopic models lean towards to become more complex in order to map the material behaviour more precisely. As consequence the amount and complexity of the experiments is increasing as well. In addition, it is well known that, some of the experiments, for example the equibiaxial compression test, are difficult to perform and therefore, a reasonable coupling of crystal plasticity (CP) modelling and macroscopic models is proposed. It is worth to mention that, in the domain of CP, arbitrary load cases are possible and therefore, any stress ratio of the yield criterion can be used for calibration. Prediction of anisotropic material behaviour of AA6016-T4 and DC05 sheets based on CP simulations were previously presented and compared with the macroscopic Yld2000-2d model. Their data set is now used for the calibration of the parameters of the macroscopic model, where in contrast to the classical procedure, the exponent of the yield locus is defined as a fitting parameter. The strain distributions predicted by the models have been compared with DIC-measurements of Nakajima samples. The predictive capabilities of the CP-based fitting procedure, compared to the classical fitting, are highlighted. Additionally, a comparison of the strain distribution prediction between all model variants is performed on a cruciform shaped deep drawing part. It underlines the importance of the correct prediction of the yield normal, as it is given by the crystal plasticity computation.

1. Introduction

In the era of climate change and increased sensibility for material efficiency the demand and requirements for more safe and light structures has led to more sophisticated material models and simulation tools. Nowadays it is state of art for most metal forming process like e.g. deep drawing, to use numerical simulations based on finite element software. In this context the complexity of the available constitutive models has increased a lot but only a small number of them are actually established in industry. In addition, the effort of the parameter determination has increased too, making them not appropriate for the daily use in industry, because of the required complex experiments and their evaluation. In this context, the focus of the research is...
the development of a new methodology of incorporating texture data into the set of available experimental data. It was already shown [1, 2] that proper calibrated CP models can be used to predict the metal sheet anisotropy. In this work we use the virtually created simulation results by CP to improve the model parameter estimation. This methodology is exemplary shown for two different commonly used metal sheets in industry. To be precise, the method is applied on the aluminium alloy AA6016-T4 with dominant Cube texture \{001\}\{100\}. The second material is a deep drawing steel, labeled with DC05 and has a strong \(\gamma\)-fiber \{111\}//ND texture. The novel methodology to calibrate the constitutive model parameters is tested in the prediction of strain distribution for selected Nakajima samples. DC05 is additionally validated by predicting strain patterns on a deep drawn part.

2. Numerical methods
For the CP calculations the physically motivated phenomenological model from DAMASK [3] is used. For this work, dislocation glide is considered as exclusive source of plasticity.

2.1. Phenomenological crystal plasticity
The plastic velocity gradient \(L_p\) is expressed in the sense of [4] as a product of the plastic shear rate \(\dot{\gamma}\) with the slip system projection tensor by

\[
L_p = \sum_{\alpha \in A} \dot{\gamma}^\alpha m^\alpha \otimes n^\alpha.
\]  
In equation (1), \(A\) denotes all active slip systems \(\alpha\)'s with \(|\dot{\gamma}^\alpha| > 0\) and \(N_s\) the amount of theoretically possible slip systems for the specific unit cell type. The vector \(m^\alpha\) represents the direction of slip and \(n^\alpha\) the plane normal of the slip plane respectively. The evolution of the shear rate is modelled with a power-law after [5] with

\[
\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{\xi^\alpha} \right|^{m_{\text{slip}}} \cdot \text{sgn}(\tau^\alpha).
\] 
In equation (2) the shear stress \(\tau\) acting on the slip system \(\alpha\) acts as driving force for the phenomenological description of dislocation glide. The exponent \(m_{\text{slip}}\) describes the strain rate sensitivity (SRS) behaviour of the slip systems and the value of \(\xi^\alpha\) denotes the strength or necessary resolved shear stress to start a dislocation. In the plastic domain, metals usually show a nonlinear work hardening behaviour. This process is phenomenologically described in the sense of CP with

\[
\dot{\xi}^\alpha = h_{0,\text{slip-slip}} \sum_{\alpha' = 1}^{N_s} \dot{\gamma}^{\alpha'} \left| 1 - \frac{\xi^{\alpha'}}{\xi^{\alpha}} \right|^{a} \cdot \text{sgn} \left( 1 - \frac{\xi^{\alpha'}}{\xi^{\alpha}} \right) h_{\alpha\alpha'}.
\] 
Due to the nature of equation (3), the value of \(\xi^\alpha\) asymptotically increases until it reaches the saturation value of slip resistance \(\xi^{\alpha}_{\infty}\). The slope of this increase is controlled by several coefficients. \(h_{0,\text{slip-slip}}\) is the reference slip-slip hardening parameter, it denotes the minimum stress increase of the interaction of two slip systems. \(h_{\alpha\alpha'}\) is dimensionless latent hardening factor, which denotes the specific stress increase factor by the interaction of two distinct slip systems. The value of this interaction is usually taken with \(h_{\alpha\alpha'} = 1.0\) for a coplanar slip system interactions and \(h_{\alpha\alpha'} = 1.4\) for non-coplanar interactions [6].
2.2. Mechanical boundary problem solver

To numerically solve the conservation of linear momentum for a representative volume element (RVE), the highly efficient spectral solver of DAMASK is used. This solver is based on the fast Fourier transformation (FFT) and is considerably faster than the finite element method (FEM) [7]. FFT requires that the applied boundary conditions on the RVE are of periodic nature, as the FFT only works for periodic functions.

3. Calibration of macroscopic yield criteria by virtual experiments

Based on calibrated CP models for AA6016-T4 and DC05, virtual experiments with varying boundary conditions are performed. Details about the calibration of the phenomenological CP parameters are given in [8]. In the plane stress yield domain 72 biaxial simulations are performed. In addition 18 RVE simulations loaded by uniaxial tension and with rotated texture between rolling and transverse direction are performed. For all simulations the stress state $\sigma$ and the plastic strain rate tensor $D_p$ are extracted at the same level of plastic strain energy density. The obtained simulation data is then used in a least squares method to calibrate the Yld2000-2d [9] model parameters. The classical calibration of Yld2000-2d is done by only using the experimental data of three uniaxial tensile tests ($\sigma_0$, $\sigma_{45}$, $\sigma_{90}$) and an equibiaxial experiment ($\sigma_b$), in combination with their measured plastic strain anisotropy values ($r_0$, $r_{45}$, $r_{90}$, $r_b$). These values are used to estimate the values of $\alpha_1 - \alpha_8$, where the exponent $a$ is fixed with respect to crystalline structure (fcc: $a = 8$, bcc: $a = 6$). To calibrate all constitutive model parameters simultaneously, including the exponent $a$, the equation (4) is introduced.

$$
\epsilon_{\text{Calibration}}(\alpha_i, W_{pl}) = w_\sigma \left\| \frac{\sigma(\alpha, W_{pl}) - \langle \sigma \rangle(W_{pl})}{\sigma_0} \right\|_2
+ w_r \left\| \frac{\sigma_0 - \langle \sigma \rangle(W_{pl})}{\sigma_0} \right\|_2
+ w_\theta \left\| \frac{\sigma_0 - \langle \sigma \rangle(W_{pl})}{\sigma_0} \right\|_2
+ w_{\text{dir}} \left\| \frac{d\varepsilon_2}{d\varepsilon_1}(\alpha, W_{pl}) - \langle \frac{d\varepsilon_2}{d\varepsilon_1} \rangle(W_{pl}) \right\|_2
$$

Please note, that $\langle \bullet \rangle$, denotes the volume average value of the RVE quantity $\bullet$. Equation (4) contains four terms, where the first one describes the error of the biaxial stress results. The second term takes the plastic strain ratios into account. The third one quantifies the error of the observed uniaxial flow stresses in different sheet directions. The novel fourth term, takes the plastic flow direction on the yield surface into account. All terms can be individually weighted ($w_i$), however for the sake of simplicity all weights were chosen to be identical. The results of the CP simulations and the novel calibrated constitutive model for AA6016-T4 at a level of $\varepsilon_{pl} = 0.0219$ are illustrated in Figure 1, where the results are compared to the classical macroscopically model variant of [10]. The calculated stress points (Fig. 1a) from the CP simulations show small deviations compared to the macroscopically calibrated constitutive model, whereas the experimental data is properly matched. Most pronounced are the differences in the shape of the yield locus itself, which can be observed in the diagram for the plastic flow direction (Fig. 1c). This also applies to the prediction of the plastic strain anisotropy (Fig. 1b), where the predicted shape is similar to the macroscopic one but at slightly higher values. In terms of model parameters (Tab. 1), it can be observed that the biggest difference is given in the value of the exponent $a$. The same methodology has been applied for DC05. The results at a level of $\varepsilon_{pl} = 0.0274$ are illustrated with Figure 2. It can be observed that the error for the plastic strain anisotropy (Fig. 2b) is slightly bigger than previously seen in AA6016-T4. The yield locus and the plastic flow direction show almost no difference. In terms of anisotropy
coefficients Table 2 shows that no big differences between the macroscopic and CP based variant exist. The assumption of an exponent value of \(a = 6\) seems to be sufficiently good. For DC05 also the Yld2000-2d model variants with strain dependent coefficients as introduced in [11, 12], were calibrated. For the sake of brevity their results in terms of yield locus prediction are not
presented in this work, however they can be accessed in [8]. The performance of the strain-dependent Yld2000-2d variants can be summarized as being able to represent the deformation of the yield locus more accurately at higher plastic strains, since the anisotropic strain hardening effect in DC05 is significant.

4. Validation
The calibrated macroscopic yield criteria are validated in terms of strain distribution prediction in finite element (FE) simulations. FE simulations of a standardized ductility test for metal sheets [13] with so-called Nakajima specimens are used. Experimental strain distribution was gathered for AA6016-T4 by [10] and for DC05 by [11]. Their results and the performance of the classically derived model parameters will be compared to the ones obtained by the virtual experiments. The FE simulation is set-up in LS-DYNA\(^1\) using standard fully integrated shell element for the blank discretization, while having seven integration points over the sheet thickness. For both materials, the model performance is additionally validated using a deep drawing process with a cruciform shaped die geometry. The setup of the deep drawing process is illustrated in Figure 3.

4.1. Major strain distribution on Nakajima specimens
The strain distribution is exclusively analysed on the sample types of B20, B100 and B200. For the sake of brevity only the simulation results of major strain ($\varepsilon_1$) are presented. The strain distributions are evaluated at several punch heights, along the center line of the sample itself. The results for AA6016-T4 (Fig. 4) clearly show the improved strain prediction of the

\begin{table}
\centering
\begin{tabular}{|c|c|c|c|c|c|c|c|c|}
\hline
Type & $a$ & $\alpha_1$ & $\alpha_2$ & $\alpha_3$ & $\alpha_4$ & $\alpha_5$ & $\alpha_6$ & $\alpha_7$ & $\alpha_8$ \\
\hline
Macroscopic & 6 & 1.084 & 0.982 & 0.846 & 0.881 & 0.908 & 0.836 & 0.972 & 0.975 \\
CP based & 5.454 & 1.030 & 1.095 & 0.875 & 0.871 & 0.880 & 0.781 & 0.983 & 0.979 \\
\hline
\end{tabular}
\caption{Yld2000-2d parameters for DC05.}
\end{table}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{Model illustration of deep drawing processes with a cruciform geometry, with faded out blankholder.}
\end{figure}

\(^1\) www.lstc.com
CP based model coefficients. In particular, the results for the B200 sample (Fig. 4c) show the substantially better performance. In the other two sample types the differences between the model variants are smaller. The results for DC05 (Fig. 5) show a more complex behaviour. For B20 no differences are observable, for the B100 it can be seen that at the highest punch level the model with strain dependent coefficients works best. Similar results can be seen in the B200 sample. However the experimental data is suffering from strain localization outside the specimen center.

**Figure 4.** Major strain $\varepsilon_1$ distribution evaluated at several punch levels for AA6016-T4 [14].

**Figure 5.** Major strain $\varepsilon_1$ distribution evaluated at several punch levels for DC05 [14].
4.2. Strain distribution of the drawn cruciform profile along a section
Simulations results are compared with experimental data at a parallel cut to the base of the
drawn part, at a height of 5mm. Unfortunately for AA6016-T4 no experimental data is available,
therefore only a qualitative comparison is made. It is seen for both materials, that the biggest
differences occur when the minor strain component is positive. This coincidences with the range,
where the predicted plastic flow direction on the yield locus has the biggest difference between
both model variants.

Figure 6. Simulation results for AA6016-T4 from a section parallel to punch head surface,
5.0mm above the base.

Figure 7. Simulation results for DC05 from a section parallel to punch head surface, 5.0mm
above the base.
5. Conclusion
The presented work illustrates the importance of an accurate description of the plastic flow direction in macroscopic constitutive models. CP simulations based on EBSD data allow us to consider the influence of grain orientations on plastic flow. Therefore, a more accurate calculation of the plastic flow direction is given if standard, not highly flexible flow criteria such as the Yld2000-2d criterion are still used. A fitting methodology was presented to determine the anisotropic parameters as well as the yield locus exponent while additionally using the information of plastic flow direction, predicted by CP calculations. Based on this methodology, it was shown that it is not recommended to use an exponent of 8 for aluminum alloys, whereas the suggestions for steel with $a = 6$ is sufficiently appropriate.

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