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On the prediction of yield loci based on crystal plasticity models and the spectral solver framework

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Abstract. Prediction of the yield loci based on crystal plasticity material models in combination with an efficient solver, the FFT-based spectral solver, is the main focus of this study. Results of the CP-based yield locus modeling are compared with the well-established macroscopic model YLD2000-2d for various materials; steel as well as aluminum alloys. For this purpose, uniaxial tensile tests in various directions as well as biaxial tests were performed. Further, the influence of grain size in crystal plasticity simulations is often neglected due to the fact that most grains are assumed to have similar size or the influence of grain size is directly mapped within material parameters. For materials containing significantly different grain sizes, this approach does not apply and therefore, a suitable model for crystal plasticity laws is needed. In the framework of this research, an adapted Hall-Petch phenomenological model is implemented in the crystal plasticity open-source code DAMASK. The spectral solver in combination with the phenomenological constitutive laws allows computing of numerical results in short time, which is a key factor for the development of new materials and industrial research.

1. Introduction
The need and requirements for more safe and light structures has led to developing of new materials. Nowadays, most metal forming process like e.g. deep drawing, are simulated using various finite element software. In this context, the focus of the research is the development of material models, enabling the optimization of material properties as well as developing new materials. However, due to the complexity of the available models, a small number of them are established in the industry. In addition, the effort of the parameter determination has increased too, making them not appropriate for the practical use in the industry, because of the required complex experiments and their evaluation. Further, some experiments are very difficult to perform e.g. the plane stress biaxial compression test. The aim of this study is to highlight the possibility for replacing costly and time consuming macroscopic experiments with virtual experiments based on crystal plasticity models and efficient solvers. The presented strategy is validated on four deep drawing materials: DC05 steel, two 6xxx- and a 4xxx-Aluminum alloy for linear as well as non-linear strain paths.

2. Crystal plasticity model
All RVE simulations of this publication are carried out with the DAMASK kit [1] and its implemented phenomenological crystal plasticity model, which is briefly outlined hereinafter.
In this study, only plastic deformation due to dislocation slip is considered. Thus, the plastic velocity gradient reads

$$\mathbf{L}_p = \dot{\mathbf{F}}_p \mathbf{F}_p^{-1} = \sum_{\alpha=1}^{N_{\text{slip}}} \dot{\gamma}_\alpha (\mathbf{m}_\alpha \otimes \mathbf{n}_\alpha)$$

(1)

This relationship requires the shear strain rate $\dot{\gamma}_\alpha$ of a slip system described by the slip direction $\mathbf{m}_\alpha$ and its normal $\mathbf{n}_\alpha$. The evolution equation for $\dot{\gamma}_\alpha$ is given by

$$\dot{\gamma}_\alpha = \dot{\gamma}_0 \frac{\tau_\alpha}{\tau_c} \frac{1}{\tau_c} \cdot \text{sgn}(\tau_\alpha)$$

(2)

where $\tau_\alpha$ and $\tau_c$ are the actual resolved shear stress and the critical resolved shear stress, respectively. A popular evolution equation for the critical shear stress is given by (3)

$$\dot{\tau}_c = \sum_{\beta=1}^{N_{\text{slip}}} h_{\alpha\beta} |\dot{\gamma}_\beta|$$

(3)

with the interaction matrix components $h_{\alpha\beta}$ between the slip systems $\alpha$ and $\beta$

$$h_{\alpha\beta} = q^{\alpha\beta} \left[ h_0 \left( 1 - \frac{\tau_c}{\tau_{\text{sat}}} \right) \right]$$

(4)

In general, $q^{\alpha\beta}$ is set to 1, if $\alpha$ and $\beta$ are coplanar. Otherwise, $q^{\alpha\beta} = 1.4$.

2.1. RVE-modeling in the framework of FFT-solver

The major input for the RVE computation is the ODF (Oriented Distribution Function), computed from the measured pole figures. Texture analyses have been carried out by X-ray diffraction (XRD). The number of measured orientations is in general very high and has to be reduced to some representative orientations, in order to enable RVE computations in a reasonable time. For this purpose, the algorithm published by [2] has been used. However reduction of the measured ODF can have a significant influence in the CP based material modeling. The major discrepancies arise when in the reduced texture additional components appear or some of the significant components vanish. For the investigated materials, measured ODFs are shown in figures 5, 6, 7 and 8, for DC05, AA6016-T4, AA6xxx and AA4xxx, respectively. A RVE discretization by $16^3$ for DC05 [3] and AA6016 [4] has been used, whereas for AA6xxx and AA4xxx the number of FFT points is set to $32^3$. Due to the finer resolution in space more orientations can be considered.

3. Calculation of yield loci without pre-straining of the material

Various biaxial stress ratios between $\sigma_2$ and $\sigma_1$ have been chosen to generate virtual experiments for the investigated materials. The resulting CP-yield points (see model parameters in table 2) are compared with the well established macroscopic yield loci YLD2000-2d (model parameters in table 3). The results are shown in figures 1 to 4. Yield loci based on CP simulations show a good agreement for the most investigated alloys. However, some discrepancies could be observed especially for the very soft AA4xxx aluminum alloy.
Table 1. Normalized material properties

<table>
<thead>
<tr>
<th>Material</th>
<th>$\sigma_0/\sigma_0$</th>
<th>$\sigma_{45}/\sigma_0$</th>
<th>$\sigma_{90}/\sigma_0$</th>
<th>$\sigma_b/\sigma_0$</th>
<th>$r_0$</th>
<th>$r_{45}$</th>
<th>$r_{90}$</th>
<th>$r_b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DC05</td>
<td>1.00</td>
<td>1.05</td>
<td>1.04</td>
<td>1.14</td>
<td>2.00</td>
<td>1.47</td>
<td>2.52</td>
<td>0.85</td>
</tr>
<tr>
<td>AA6016-T4</td>
<td>1.00</td>
<td>0.96</td>
<td>0.98</td>
<td>0.99</td>
<td>0.69</td>
<td>0.50</td>
<td>0.67</td>
<td>1.00</td>
</tr>
<tr>
<td>AA6xxx</td>
<td>1.00</td>
<td>0.97</td>
<td>0.99</td>
<td>1.03</td>
<td>0.53</td>
<td>0.51</td>
<td>0.56</td>
<td>1.00</td>
</tr>
<tr>
<td>AA4xxx</td>
<td>1.00</td>
<td>0.98</td>
<td>0.97</td>
<td>1.10</td>
<td>0.67</td>
<td>0.60</td>
<td>0.64</td>
<td>1.00</td>
</tr>
</tbody>
</table>

Table 2. Hardening parameters for the CP model

<table>
<thead>
<tr>
<th>Material</th>
<th>$\tau_{c,0}$</th>
<th>$\tau_{sat}$</th>
<th>$h_0$</th>
<th>$a$</th>
<th>$n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DC05</td>
<td>58.00 MPa</td>
<td>151.0 MPa</td>
<td>900.0 MPa</td>
<td>2.1</td>
<td>60</td>
</tr>
<tr>
<td>AA6016-T4</td>
<td>42.85 MPa</td>
<td>120.8 MPa</td>
<td>503.3 MPa</td>
<td>1.3</td>
<td>50</td>
</tr>
<tr>
<td>AA6xxx</td>
<td>49.75 MPa</td>
<td>140.6 MPa</td>
<td>947.2 MPa</td>
<td>2.0</td>
<td>50</td>
</tr>
<tr>
<td>AA4xxx</td>
<td>33.36 MPa</td>
<td>87.51 MPa</td>
<td>571.8 MPa</td>
<td>2.0</td>
<td>50</td>
</tr>
</tbody>
</table>

Table 3. Fitted Yld2000-2d parameters

<table>
<thead>
<tr>
<th>Material</th>
<th>$a$</th>
<th>$\alpha_1$</th>
<th>$\alpha_2$</th>
<th>$\alpha_3$</th>
<th>$\alpha_4$</th>
<th>$\alpha_5$</th>
<th>$\alpha_6$</th>
<th>$\alpha_7$</th>
<th>$\alpha_8$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DC05</td>
<td>6</td>
<td>1.084</td>
<td>0.982</td>
<td>0.846</td>
<td>0.881</td>
<td>0.908</td>
<td>0.836</td>
<td>0.972</td>
<td>0.975</td>
</tr>
<tr>
<td>AA6016-T4</td>
<td>8</td>
<td>0.947</td>
<td>1.107</td>
<td>0.961</td>
<td>1.032</td>
<td>1.021</td>
<td>1.013</td>
<td>0.967</td>
<td>1.153</td>
</tr>
<tr>
<td>AA6xxx</td>
<td>8</td>
<td>0.923</td>
<td>0.962</td>
<td>0.894</td>
<td>1.010</td>
<td>1.008</td>
<td>0.900</td>
<td>0.949</td>
<td>1.186</td>
</tr>
<tr>
<td>AA4xxx</td>
<td>8</td>
<td>0.929</td>
<td>0.972</td>
<td>0.725</td>
<td>0.992</td>
<td>0.977</td>
<td>0.785</td>
<td>0.941</td>
<td>1.237</td>
</tr>
</tbody>
</table>

The CP based prediction of yielding compared to the macroscopic yield locus YLD2000-2d can be summarized as follows:

- DC05: A negligible small deviation in the second and fourth quadrant has been observed. Otherwise, practically no difference exists between the models.
- AA6016: An excellent agreement between the models is observed.
- AA6xxx: A good agreement in the shear range, whereas in the plane strain and equibiaxial a small deviation could be observed.
- AA4xxx: Similar to AA6xxx. Additionally, a bigger difference in the biaxial range could be observed.

It can be concluded that the CP-prediction of the equibiaxial point, for the aluminum alloys with a specifically sharp yield locus, the difference between the models is the biggest. One of the reasons could be the way how the measured ODF is reduced to a smaller number of orientations. For this purpose, especially the intensity of the RC (Rotated Cube) components of the reduced ODF were increased. As a result, the equibiaxial point could been moved to the correct direction, see figure 4. It is also worth mentioning that the macroscopic model is a fit of the experimental data in uniaxial tension ($0^\circ, 45^\circ, 90^\circ$) and the biaxial deformation, including the corresponding R-values. In contrast to that, the CP results shown here are model predictions based just on the measured texture.
4. Calculation of yield loci for the pre-strained material
An accurate modeling of forming processes requires also the consideration of nonlinear strain paths. For this purpose, the DC05 material was prestrained in rolling direction to $\epsilon_{11} = 0.15$ followed by a transverse uniaxial test as well as a biaxial deformation. Prediction of yielding based on the introduced RVE-methodology has been compared with the experimental data and a very good agreement could be observed, see figure 9. Further, a slightly anisotropic hardening of the CP-prediction could be observed, see for further details [3].
Figure 5. ODF of DC05.

Figure 6. ODF of AA6016-T4.

Figure 7. ODF of AA6xxx.

Figure 8. ODF of AA4xxx.

Figure 9. Comparison of the CP-prediction and the YLD2000-2d model for the prestrained material of $\varepsilon_{11} = 0.15$ in rolling direction [3].
5. **Further aspects in the microstructure modeling - grain size effects**

It is well established that the Hall-Petch relation can be used to describe the grain size influences on the hardening behavior of the material. However, most of the crystal plasticity codes do not consider this phenomenon explicitly. In the framework of this study, a similar model as presented by [5] was implemented in DAMASK. The main equations are given in (5) and (6)

\[
\tilde{\tau}_{c,0} = \tau_{c,0} + k_1 \frac{1}{\sqrt{d}} \quad (5)
\]

\[
\tilde{\tau}_{sat} = \tau_{sat} + k_2 \frac{1}{\sqrt{d}} \quad (6)
\]

where \(d\) is the average grain diameter and \(k_1, k_2\) are material constants. The influence of the grain size on the uniaxial hardening behavior of a generic material is shown in figure 10. However, to quantify the hardening behavior for a specific material, the presented model has to be validated with experimental results.

![Figure 10](image_url)

**Figure 10.** Influence of the grain size on the hardening behavior of a generic material. Yield point as well as saturation value can be modeled independently.

6. **Conclusions and outlook**

A RVE-based methodology to predict yield loci for steel and aluminum has been presented. A comparison with the well established macroscopic yield locus YLD200-2d showed good agreement with the crystal plasticity model. The strongest difference between the models could be observed in the equibiaxial yield point for the very soft 4xxx aluminum alloy. In the macroscopic yield locus the plane strain and the equibiaxial point are very close to each other and therefore, the yield locus is very sharp. Reduction of the measured ODF to a smaller number of orientations has to be carried out in an appropriate way such that the representative components of the ODF are captured correctly. Further, the influence of the grain size on the hardening behavior has been implemented in the open source code DAMASK. This will enable one to consider the grain size influence also in the prediction of the yield loci.

**References**