Crystal plasticity finite element method calculation of formability limit diagram

DUANCHENG MA

LKR Leichtmetallkompetenzzentrum Ranshofen GmbH, AIT Austrian Institute of Technology,
Lamprechtshausenerstraße 61, Postfach 26, 5282 Ranshofen-Braunau, Austria
duancheng.ma@ait.ac.at

Abstract

This study is inspired by the recent development of “virtual material testing laboratory” in which the main equipment is a full field crystal plasticity modelling tool. Ample examples have demonstrated its applications to sheet forming operations. In those applications, the mechanical anisotropy originated from the crystallographic texture can be adequately described, such as r-values and earing. Formability is also another very important property in sheet metal forming, which yet have not been equipped in these virtual laboratories. Though theoretical models for formability can be dated back to 1885 due to Considère, all popular models at the moment suffer from their respective limitations. In this study, we explore the feasibility of applying full field crystal plasticity model for calculating formability limit diagram, avoiding using additional assumptions or models for determining the formability limits. The focus is placed on the texture dependence of the formability limit diagram.

I. Introduction

i. Formability limit diagram

In sheet metal forming, it is popular to use formability limit diagrams (FLDs) to guide the forming operation. A schematics of FLD is shown in Fig. 1a pioneered by Keeler [1] and Goodwin [2]. A FLD basically maps “safe” and “failure” areas of the applied principle strains, \( \varepsilon_{\text{major}} \) and \( \varepsilon_{\text{minor}} \), along certain strain paths (see Fig. 1b). In Fig. 1a, the safe area is below the critical strain and the failure area is above it. The critical strain in Fig. 1a is not the strain for fracture, but the strain at which the localized necking occurs. The strain for fracture is usually above the localized necking, and approximately linearly depends on \( \varepsilon_{\text{minor}} \) with a negative slope [3]. When the strain path is close to \( \varepsilon_{\text{major}} = \varepsilon_{\text{minor}} \), fracture might occur without any localized necking event [4].

Fig. 1 is a strain based FLD and only valid when the strain path is not changed. If the strain path is changed, the FLD will shift [5, 6]. When the shape of the formed component is to be complex or it undergoes multiple forming steps, ignoring the effect of the strain path change gives an inaccurate measure of the formability. This limitation of the strain based FLD gives rise to the development of stress-based FLD [6, 7, 8], in which the critical stress for localized necking is not sensitive to the strain path change. Despite the advantage of the stress based FLD over the conventional strain based FLD, accurately measuring stress is rather challenging, whereas measuring strain can be very accurate. Thus, the use of stress based FLD has not yet become a common engineering practice.

ii. Theoretical models for formability

Theoretically modeling FLD has been an active topic, and there are three popular families of theoretical models, i.e. the maximum force criteria (MFC), the Marciniak-Kuczynski model (MK), and the bifurcation theory (BT). Comprehensive reviews can be found in [9, 10, 11, 12]. Here, we give a brief sketch of them.

ii.1 Maximum force criteria (MFC)

Among the maximum force criteria (MFC) family, the first model can be traced back to Considère [13] who proposed the well-known Considère criterion, specifically for uniaxial tensile deformation, i.e.

\[
\frac{df_1}{d \varepsilon_1} = 0 \quad (1a)
\]

or

\[
\frac{d \sigma_1}{d \varepsilon_1} = \sigma_1 \quad (1b)
\]

where \( f_1 \) is the force in the tensile direction; and \( \sigma_1 \) and \( \varepsilon_1 \) are the corresponding respective Cauchy stress and strain.

This 1D formulation by Considère was later adopted by Swift [14], and extended to 2D case, i.e. biaxial loading, which is more relevant to sheet metal forming. Swift’s hypothesis reads:

\[
\frac{df_1}{d \varepsilon_1} = 0 \quad \text{and} \quad \frac{df_2}{d \varepsilon_2} = 0 \quad (2a)
\]

or

\[
\frac{d \sigma_1}{d \varepsilon_1} = \sigma_1 \quad \text{and} \quad \frac{d \sigma_2}{d \varepsilon_2} = \sigma_2 \quad (2b)
\]
Swift’s hypothesis is, however, rarely supported by experimental observations [11]. Both Considère and Swift’s criteria consider the case of diffuse necking. Also based on Considère’s idea, Hill proposed a criteria for localized necking [15]. In Hill’s criterion, two conditions should be fulfilled when a localized necking occurs. The first condition is that the direction of the band where localized necking occurs is the same to the direction where the elongation is zero; the second condition is that in the normal direction of the localized band the force becomes extremum. These two conditions read:

$$d\varepsilon_{tt} = 0 \quad (3a)$$

and

$$df_n = 0 \quad \text{or} \quad \frac{d\varepsilon_n}{d\varepsilon_n} = \sigma_n \quad (3b)$$

where \(n\) and \(t\) are the normal direction of the band and the direction along the band, respectively.

The MFC were further brought forward by Hora and co-workers [16, 17] based on the fact that localized necking takes place in plane strain condition. At the onset of localized necking, the deformation path represented by the incremental strain ratio should become zero, namely:

$$\beta = \frac{d\varepsilon_2}{d\varepsilon_1} = 0 \quad (4)$$

Thus the criterion is

$$\frac{\partial \varepsilon_1}{\partial \varepsilon_1} + \frac{\partial \varepsilon_1}{\partial \beta} \frac{d\beta}{d\varepsilon_1} = \sigma_1 \quad (5)$$

Though there are the numerical issues with Hora’s criterion when straight line segments exist on the yield surface [18], they are not directly caused by Hora’s criterion itself, but by the yield surface description [19]. Recently, Hora’s criterion has been reformulated to be more flexible with the yield functions, also extended to include strain rate sensitivity and anisotropic hardening effects [19].

ii.2 Marciniak-Kuczyński model (MK-model)

The Marciniak-Kuczyński model (MK-model) [20] is physically intuitive. It assumes a pre-existing geometrical imperfection in the sheet metal, and it gradually evolves to localized necking as the deformation progresses. The imperfection is usually modeled as a thin band, and geometrically characterized by (i) its orientation relative to the principle directions of the sheet metal and (ii) its reduced thickness [21].

The basic assumption in the MK-model implicitly separates the sheet metal into two regions, i.e. the region inside the band and the region outside the band. During deformation, two conditions are to be fulfilled [22]: (i) the continuity of the strain rate along the band; (ii) the mechanical equilibrium on the interface between the above mentioned two regions.

Localized necking occurs when a criterion (usually empirical) is met by comparing the kinematic evolutions in those two regions. This criterion can be the ratio of the strain rates in the major principal direction or the thickness direction, or the ratio of the equivalent strain rates [11], and it can also be the ratio of the principal strains [21].

Since those criteria which detect the occurrence of localized necking only involve the kinematic evolution, the constitutive law is independent of the localized necking.
Hence, the MK-model can be coupled with any constitutive laws, which lets the MK-model gain its flexibility in terms of modeling.

The postulate of a pre-existing geometrical imperfection in the MK-model is often criticized for being arbitrary, and the prediction is very sensitive to the two assumed geometrical characteristics of the pre-existing geometrical imperfection. The numerical value of the band orientation can be chosen in such a way that it corresponds to the minimum formability for a given strain path, and those minimum corresponding formability limits have been shown to be in good agreement with experiments (see for example in Ref. [23]). The value of the reduced thickness, on the other hand, can never be chosen in such a systematical way, and usually it is obtained by fitting the experiments. Even by fitting the same experiments, the obtained reduced thickness depends on the employed constitutive law [23], indicating the reduced thickness is hardly a physical quantity.

ii.3 Bifurcation theory (BT)

The bifurcation theory (BT) is theoretically and mathematically rigorous and sound [24]. Its essence is to inspect the stiffness matrix. It has certain similarities to the MK-model that a localized necking occurs also in a thin band rendering two regions inside and outside the band. The occurrence of the band and its geometrical characteristics are the predictions of BT, whereas in MK-model, the geometrical characters are assumed as model parameters.

Due to the similarities between BT and the MK-model, BT has shown to be the upper limit of MK-model, i.e. when the thicknesses inside and outside the band are the same [11]. This actually implies that the prediction by BT is likely to be overestimated, if assuming a reduced thickness would allow a good agreement with experiments.

In principle, BT can be coupled with any constitutive laws. Coupling with rate dependent constitutive laws would, however, gives an unrealistic prediction, e.g. the stress level when the localized necking occurs could be unrealistically high [25]. An interested reader can also refer to Appendix A for the mathematical origin that coupling BT with a rate dependent constitutive law would give an unrealistic prediction.

iii. Previous studies of using crystal plasticity for FLD prediction

According to the methods of realizing polycrystal simulations, the previous studies can be further cast into two groups: mean field and full field models.

iii.1 By mean field models

In the group of mean field models, the classical Taylor model [26, 27, 28, 29, 30, 31, 32, 33, 25] and the viscoplastic self-consistent model [34, 23, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44] are often applied. Essentially, a crystal plasticity formulation together with a numerical homogenization scheme provides the stress-strain relation of a polycrystalline material, i.e. a constitutive description. As mentioned above, both the MK-model and BT are very flexible in terms of the constitutive law. Hence, these mean field polycrystal models are usually coupled with the MK-model [26, 27, 28, 29, 30, 31, 32, 33, 25, 34, 23, 35, 37, 36, 38, 39, 42, 40, 41, 43, 44] or BT [25, 42, 44].

iii.2 By full field models

As for the group of the full field model, it has been so far exclusively based on crystal plasticity finite element method [45, 46, 47, 48, 49], and applying full field crystal plasticity models for FLD prediction deserves some discussion.

It should be firstly pointed out that the primary purpose of applying any full field models is to reveal physical processes at a lower length scale. In the case simulating the localized deformation, the element size should be in general smaller than the volume of the localized deformation. On the other hand, MFC and BT are both at the length scale of the components. It is in principle feasible to apply the MFC and BT in conjunction with the full field model, but it may lose all the essence of applying the full field models in the first place.

For sheet metal forming, it might be tempting to use 2D model with plane stress condition, but it should be noted that the single crystalline crystal plasticity formulation is not compatible with plane stress condition (see Section 8.3 in Ref. [50] for more detailed clarification). Hence, even for sheet metal forming simulations, it is more appropriate to use 3D crystal plasticity models with proper boundary conditions to fulfill macroscopic plane stress condition.

In the previous studies with 3D models [47, 48, 49], full field crystal plasticity models are usually coupled with the MK-model, i.e. introducing a geometrical imperfection in a finite element mesh. Direct coupling the MK-model with finite element method is rather straightforward, but this kind of simulations requires considerable computational resources as shown in [47]. Hence, simplifications are sometimes made to reduce the computational effort [48, 49].

iv. Motivation and scope of this study

The idea of introducing a geometrical imperfection in those above mentioned previous studies [47, 48, 49] is
to trigger a localization event. On the other hand, a localization event can also be triggered by microstructural heterogeneity, and polycrystalline materials are intrinsically heterogeneous. Hence, without a geometrical imperfection, a localized deformation event should naturally take place in a full field crystal plasticity simulation of a polycrystalline material, as already observed in many previous studies, e.g. in 2D plane strain simulations [51, 52, 53, 54, 55, 56, 57] or 3D uniaxial tension simulations [58, 59].

To simulate localized deformation, it is not necessary to introduce an initial geometrical imperfection to prompt localized deformation when using full field crystal plasticity models. More importantly, the geometrical characteristics of the initial imperfection assumed in the MK-model are not measurable quantities, whereas microstructure can be always measured and characterized by modern analytic techniques.

In this study, the primary aim is at assessing the feasibility of using full field polycrystalline crystal plasticity models for the prediction of FLD. The localization event is to be triggered by microstructural heterogeneity, instead of an initial geometrical imperfection.

We confine our focus in this study on (i) the right hand side of the FLD, (ii) the texture dependence, and (iii) face centered cubic (fcc) metals.

The rest of the text is organized as the follows: in Section II, we describe the employed crystal plasticity finite element method, the simulation setup, and the assumed initial orientation distributions; in Section i, the measurement of quantifying deformation localization employed in this study will be presented, as well as the evolution of the localized deformation at different strain paths; a criterion for the formability limit is to be proposed in Section ii; the calculated FLDs for different initial orientation distributions are presented in Section iii; in Section iv, some limitations of this study are discussed; we summarize this study in Section IV.

II. METHODOLOGY

i. Crystal plasticity

In this study, crystal plasticity finite element method (CP-FEM) is applied. CP is to incorporate the microscopic plastic deformation mechanisms into continuum mechanics, and CP-FEM is to use FEM as a numerical solver to solve mechanical equilibrium equations for the solids whose constitutive behavior is formulated by CP. The subject of CP-FEM is very well documented in [50, 60], here a brief description is provided.

i.1 Kinematics

In the present crystal plasticity formulation, the deformation gradient, \( F \), is decomposed into a plastic part and an elastic part,

\[
F = F_e F_p
\]

where \( F_p \) is the plastic deformation gradient, and \( F_e \) is the elastic deformation gradient. The above decomposition is to firstly deform the solid to an intermediate configuration transformed by \( F_p \) from the reference configuration. During this transformation, the solid is deformed plastically, thus being stress free. For convenience, \( F_p \) contains a rotation part which is equivalent to the rotation matrix of the crystallographic orientation. Consequently, the intermediate configuration corresponds to the crystal frame.

The transformation from the intermediate configuration to the current configuration is carried by \( F_e \). It contains the elastic stretching and a rotation part. The elastic stretching part is very close to a unity tensor for metals. The rotation part is to transform from the crystal frame to the sample frame. Thus, the rotation part in \( F_e \) is the inverse of the rotation matrix of the crystallographic orientation.

With Eq. (6), it is easy to show that

\[
L = L_e + \frac{F_e}{F_p} F_p^{-1}
\]

where \( L \) is the velocity gradient corresponding to \( F \), and \( L_e \) and \( L_p \) are the respective velocity gradients for \( F_e \) and \( F_p \). The plastic velocity gradient, \( L_p \), is a function of the stress measure at the intermediate configuration and the current microstructure,

\[
L_p = f (S, S_1, S_2, \cdots) \tag{8}
\]

where \( S \) is the second Piola-Kirchhoff stress, and \( S_i \) are the state variables describing the microstructure. Eq. (8) is essentially a constitutive law, and a specific form of it employed in this study will be given in the next section.

i.2 Constitutive law

In this study, we confine ourselves with the fcc crystal structure and only consider the dislocation slip as the plastic deformation mechanism. In this case, the specific form of Eq. (8) is

\[
L_p = \sum_{a=1}^{12} \gamma^a (m^a \otimes n^a) \tag{9}
\]

where \( \gamma^a \) is the shear rate on the slip system \( a \), and its shear direction is \( m^a \), shear plane normal is \( n^a \). The dyadic product, \( m^a \otimes n^a \), is termed as Schmid tensor.
As proposed by Peirce, Asaro, and Needleman [61], \( \dot{\gamma}_0 \) depends on the resolved shear stress, \( \tau^a \) on the shear plane, and the shear resistance, \( \tau_c^a \), of this slip system,

\[
\dot{\gamma}^a = \dot{\gamma}_0 \left| \frac{\tau^a}{\tau_c^a} \right| \text{sgn} (\tau^a)
\]  

(10)

where \( \dot{\gamma}_0 \) and \( a \) are material parameters.

\( \tau^a \) is obtained by projecting \( S \) on the corresponding Schmid tensor,

\[
\tau^a = S : (\mathbf{m}^a \otimes \mathbf{n}^a)
\]  

(11)

in which \( S \) is related to the elastic deformation gradient, \( F_e \), by

\[
S = C : (F_e^T F_e - I)/2
\]  

(12)

where \( C \) is the elastic stiffness tensor.

In this constitutive description, the microstructure is solely characterized by the slip resistance on the slip system, \( \tau_c^a \), and it saturates towards \( \tau_c^a \) due to slip activity on systems \( \beta \),

\[
\dot{\tau}^a_c = h_0 \left( 1 - \frac{\tau^a}{\tau_c^a} \right)^w h_{a\beta} \left| \dot{\gamma}^\beta \right|
\]  

(13)

where \( h_{a\beta} \) is a 12×12 matrix in which 1.0 is for the case when \( a \) and \( \beta \) are coplanar slip systems, and 1.4 otherwise. \( h_0 \) and \( w \) are material parameters.

Material parameters in Eqs. (10), (12) and (13) used in this study are listed in Table 1.

### Table 1: Material parameters used in Eqs. (10), (12) and (13). Note \( a = 1, \ldots, 12 \). \( \tau_0^a \) is the initial shear resistance of the slip system \( a \). * if \( a \) and \( \beta \) are coplanar slip systems. ** if \( a \) and \( \beta \) are not coplanar slip systems.

| \( \tau_0^a \) | \( \tau_0^a \) | \( \dot{\gamma}_0 \) | \( a \) | \( C_{11} \) | \( C_{12} \) | \( C_{44} \) |
|---|---|---|---|---|---|---|
| 31 MPa | 64 MPa | 0.001 | 20 | 106.75 GPa | 60.41 GPa | 28.34 GPa |
| \( w \) | 2.25 | 1.0* | | | | |
| \( h_0 \) | 75 MPa | | | | | |
| \( h_{a\beta} \) | 1.0* | | | | | |
| \( 1.4^{**} \) | | | | | | |

At the beginning, LS-Dyna passes a new deformation gradient, \( F \) and a new time step, \( \Delta t \) into the user defined material subroutine. By using a guessed \( F_p \) and Eq. (6), the elastic deformation gradient, \( F_e \), is obtained, which in turn is used to evaluate the second Piola-Kirchhoff stress, \( S \) (Eq. (12)). Then, a \( L_p \) is obtained by using the constitutive law described in the preceding section together with the newly evaluated \( S \). With the knowledge of \( L_p \), the guessed \( F_p \) is updated by using its rate, i.e. \( F_p = L_p F_p \) and the given \( \Delta t \). The updated \( F_p \) is then used to update \( S \), then update \( L_p \), which goes on to make a new update on \( F_p \). This loop continues until the variables, \( F_p, S \), and \( L_p \), are consistent with each other for the given \( F \) and the given time step \( \Delta t \).

Besides the above consistent loop, another consistent loop is also performed during the process of obtaining \( L_p \) by using the given \( S \). With the specific constitutive law in the preceding section, \( \dot{\gamma}^a \) and \( \dot{\tau}^a_c \) are to be consistent with each other at the end of this consistent loop. In general, the obtained \( L_p \) is to be consistent with the state variable \( S_i \) in Eq. (8) for any given constitutive laws at a given \( S \).

At the end of these consistent loops, the newly updated \( S \) and \( F_p \) are used to obtain the first Piola-Kirchhoff stress, \( P \), by

\[
P = FF_p^{-1}SF_p^{-T}
\]  

(14)

One may notice that the above expression is different from the usual conversion between \( P \) and \( S \), which is simply \( P = FS \). As described in Section i.1, \( S \) is the stress measure in the intermediate configuration transformed from the reference configuration by \( F_p \). Thus, \( S \) should be firstly transformed back from the intermediate configuration to the reference configuration.

Afterwards, the Cauchy stress, \( \sigma_e \), can be easily obtained by the usual conversion between \( P \) and \( \sigma_e \).

\[
\sigma_e = \frac{1}{\det(F)}PF^T
\]  

(15)

Then \( \sigma_e \) is returned to LS-Dyna.

### ii. Simulation setup

Sheet metals under biaxial tension is modeled. We use two meshes as shown in Fig. 2. The dimensions of the meshes are 4 mm × 4 mm × 1 mm and 8 mm × 8 mm × 1 mm (width × breadth × thickness). The element size is 0.2 mm × 0.2 mm × 0.2 mm, which renders the total number of elements to be 20 × 20 × 5 = 2000, and 40 × 40 × 5 = 8000, respectively. Full integration element with 8 integration points is used. A single orientation is
assigned to each integration point, and a certain orientation distribution is followed which is to be described in the next subsection (Section iii).

In this study, a periodic boundary condition (PBC) is applied to the above meshes to mimic an infinitive sheet metal under biaxial tension in x and y directions (see Fig. 2 for the coordinate system). PBC is applied to the faces normal to x or y axis. The PBC is described as follows [66, 67]:

- PBC on x-y plane: in Fig. 3a, the nodes A, B, D, and C are on an arbitrary plane whose normal is parallel to the z axis. The node \( N_{AB} \) is an arbitrary node on A–B, and its equivalent node on C–D is \( N_{CD} \). The node \( N_{AC} \) is another arbitrary node on A–C, and its equivalent node on B–D is \( N_{BD} \). The displacements, \( u \), of these nodes should fulfill the following relations:

\[
\begin{align*}
    u_{N_{AB}} - u_A &= u_{N_{CD}} - u_C \\
    u_{N_{AC}} - u_A &= u_{N_{BD}} - u_B \\
    u_B - u_A &= u_D - u_C
\end{align*}
\]  

(16a, 16b, 16c)

- PBC on z-x plane: in Fig. 3b, the nodes E, F, H, and G are on an arbitrary plane whose normal is parallel to the y axis. The node \( N_{EG} \) is an arbitrary node on E–G, and its equivalent node on H–F is \( N_{FH} \). The displacements, \( u \), of these nodes should fulfill the following relations:

\[
\begin{align*}
    u_{N_{EG}} - u_E &= u_{N_{FH}} - u_H \\
    u_G - u_E &= u_H - u_F
\end{align*}
\]  

(17a, 17b)

Since the simulation is meant for sheet metals, nodes on E–F are not equivalent to the nodes on G–H.

- PBC on y-z plane: in Fig. 3c, the nodes are constrained by the following conditions,

\[
\begin{align*}
    u_{N_{IK}} - u_I &= u_{N_{JL}} - u_J \\
    u_K - u_I &= u_L - u_J
\end{align*}
\]  

(18a, 18b)

Fig. 3d shows three control nodes, O, X, and Y. The translation and rotation of O is fully constrained. Prescribed displacements are applied to the nodes X and Y along the respective x and y position directions. The prescribed displacements on X and Y follow the relation that

\[
u_Y = L_0 \left( 1 + \frac{u_X}{L_0} \right)^\rho - L_0
\]  

(19)

where \( L_0 \) is the initial width or breadth of sheet unit cell (see Fig. 2). This leads to

\[
\ln \left( \frac{u_Y}{L_0} + 1 \right) = \ln \left( \frac{u_X}{L_0} + 1 \right)^\rho
\]  

(20)

\[
\varepsilon_{\text{minor}} = \rho \cdot \varepsilon_{\text{major}}
\]

where \( \rho = 0.0, 0.2, 0.4, 0.6, 0.8, \) and 1.0 for the mesh \( 20 \times 20 \times 5 \), and \( \rho = 0.0, 0.25, 0.5, 0.75, \) and 1.0 for \( 40 \times 40 \times 5 \).

iii. Initial texture

Six orientation distributions are considered: random, cube, Goss, copper, brass, and S. The latter five texture components are scattered around their ideal orientation by 15°, as shown in Fig. 4. For each texture component, five instances are created for each mesh. In Fig. 4, only one instance is shown for each mesh. All other instances can be found in Appendix B.

III. RESULTS AND DISCUSSION

i. Monitoring localized deformation

Strictly speaking, there is no quantitative measure for localized deformation or necking. Thus, in this section, we first discuss the measure employed in this study for quantifying localized deformation.

The localized deformation is quantified in this study from a statistical point of view. To illustrate, we show two examples for a random texture distribution instance.
III RESULTS AND DISCUSSION

(i) Monitoring localized deformation

(a) Periodic boundary condition on $x-y$ plane

(b) Periodic boundary condition on $z-x$ plane

(c) Periodic boundary condition on $y-z$ plane

(d) Locations of control nodes

Figure 3: Periodic boundary condition applied on (a) $x-y$ (see Eq. (16)), (b) $z-x$ (see Eq. (17)), and (c) $y-z$ (see Eq. (18)) planes, and (d) three control nodes.

In Figs. 5 and 6, where the evolutions of the cumulative probability functions (CPFs) of $\varepsilon_{11}$ and $\varepsilon_{22}$ are shown.

In Fig. 5a when $\rho = 0.0$ (see Eq. (20)), at early stage of deformation, the distribution of $\varepsilon_{11}$ approximately follows the normal distribution. This is because the mean value, $\varepsilon_{11}^{\text{mean}}$, is approximately the same to the median value, $\varepsilon_{11}^{\text{median}}$. As the deformation progresses, $\varepsilon_{11}^{\text{mean}}$ and $\varepsilon_{11}^{\text{median}}$ deviate from each other, indicating the distribution becomes more and more asymmetric. As $\varepsilon_{11}^{\text{mean}}$ and $\varepsilon_{11}^{\text{median}}$ deviates apart, the distribution of $\varepsilon_{11}$ below $\varepsilon_{11}^{\text{median}}$ starts to evolve slowly, but the distribution above it advances quickly. Eventually, $\varepsilon_{11}^{\text{mean}}$ is mainly driven by the population above $\varepsilon_{11}^{\text{median}}$. These observations are consistent with the formation of a localized deformation in the direction of $\varepsilon_{11}$ (see the contour plots of $\varepsilon_{11}$ accompanying Fig. 5a). Fig. 5b shows that $\varepsilon_{22}^{\text{mean}}$ and $\varepsilon_{22}^{\text{median}}$ are always close to zero, which is consistent with the boundary condition of the plane strain tension ($\rho = 0.0$). Though, as the deformation progresses, the distribution of $\varepsilon_{22}$ becomes wider, yet there is no indication of localized deformation.

In Fig. 6 for $\rho = 1.0$, the mean values of $\varepsilon_{11}$ and $\varepsilon_{22}$ both deviate from their respective median values. In comparison with Fig. 5a, the deviations of the mean from the median values start at the earlier stage of the deformation.

Based on the observations in Figs. 5 and 6, we use the ratios, $\varepsilon_{ii}^{\text{mean}}/\varepsilon_{ii}^{\text{median}}$ ($i=1$ or 2), as the measure for observing the evolution of localized deformation. As illustrated in Figs. 5 and 6, $\varepsilon_{ii}^{\text{mean}}/\varepsilon_{ii}^{\text{median}} = 1$ indicates (approximately) homogenous deformation, and when it deviates from 1, the deformation becomes localized.
Figure 4: Orientation distributions in the simulations: (a) random, (b) cube, (c) Goss, (d) copper, (e) brass, and (f) S. The texture components are with 15° scatter. RD (rolling direction) coincides with x, and TD (transverse direction) coincides with y in Figs. 2 and 3. Note that 5 distribution instances for each orientation distribution and each mesh are used, and here we only show 1 instance for each mesh as examples. All the instances are shown in the Appendix B. The orientation generation was realized by using the method described in [68, 69, 70].

Figure 5: Evolution of the cumulative probability functions of (a) $\varepsilon_{11}$ and (b) $\varepsilon_{22}$ under plane strain tension, i.e. $\rho = 0.0$ (see Eq. (20)). The orientation distribution is random and the mesh is $20 \times 20 \times 5$.

$\varepsilon_{\text{mean}} / \varepsilon_{\text{median}}$ and $\varepsilon_{\text{mean}}^1 / \varepsilon_{\text{median}}^1 vs. \varepsilon_{\text{major}}$ are shown in Fig. 7. In most cases, at the early stage of deformation, the deformation is homogenous. At some point, the localized deformation takes place, indicated by a slope change from $\sim 0$ to nearly infinitive. This transition in slope is not sudden, but gradually.

There are some special cases that $\varepsilon_{22} / \varepsilon_{22}$ deviates from 1 almost instantaneously when the load is imposed, mostly notably in Fig. 7a for random, Fig. 7c for Goss and Fig. 7e for brass when $\rho$ is small, e.g. $\rho = 0.2$ and $\rho = 0.25$. The deformation in the direction of $\varepsilon_{22}$, however, is not mainly carried by those localizations, as there is only slight change in the slope. Only when the localization takes place in $\varepsilon_{11}$, the slope of $\varepsilon_{22}^\text{mean} / \varepsilon_{22}^\text{median}$ starts to increase quickly.

Fig. 7 reveals strong texture dependence of the localization evolution, still they can be put into two groups. The first group consists of random in Fig. 7a, cube in Fig. 7b, copper in Fig. 7d, and S in Fig. 7f. In this group, the localized deformation primarily occurs in the direction of $\varepsilon_{11}$, except for $\rho = 1.0$. In this group,
ii. Determination of formability limit

Fig. 8 shows $\Sigma_{11}$ vs. $\varepsilon_{11}^\text{mean}/\varepsilon_{11}^\text{median}$ and $\Sigma_{22}$ vs. $\varepsilon_{22}^\text{mean}/\varepsilon_{22}^\text{median}$. Note that $\Sigma_{11}$ and $\Sigma_{22}$ are global quantities obtained by averaging over all integration points. It shows that a decrease in $\Sigma_{11}$ or $\Sigma_{22}$ is always associated with localized deformation, when their respective $\varepsilon_{ii}^\text{mean}/\varepsilon_{ii}^\text{median}$ starts to deviate from 1. On the other hand, however, a localization does not necessarily cause a decrease in $\Sigma_{ii}$. An obvious example is $\Sigma_{22}$ in Fig. 8e for brass when $\rho = 0.2$ and 0.25 that even there is localization, and the magnitude of the localization is maintained and $\Sigma_{22}$ still continues to rise.

It should be noted that the texture evolution could possibly cause stress softening. Though the texture evolution is not analyzed in this study, based on the observations in Fig. 8, it seems localization is the predominant factor for the stress softening effect.

According to the observations in Fig. 8, we propose the formability limit criteria in this study to be the strains when either $\Sigma_{11}$ or $\Sigma_{22}$ reaches its maximum in their respective stress-strain curves. This criteria is essentially equivalent to Drucker’s stability criterion [71, 72].

This criterion is probably only applicable in a full field simulation, if there is no softening effect in the constitutive description of the materials. The stress decrease is a natural outcome of the simulation due to localized deformation as shown in Fig. 8. It should be mentioned that it is not new to apply this criterion to identify the formability limit, and it has been used in [73, 46].

Fig. 9 shows $\Sigma_{11}$, $\Sigma_{22}$, and other $\Sigma_{ij}$ vs. $\varepsilon_{\text{major}}$. The solid circles mark the locations of the maximum stress of $\Sigma_{11}$ or $\Sigma_{22}$ which is at a smaller $\varepsilon_{\text{major}}$ than the other. For copper in Fig. 9d, only $\Sigma_{11}$ exhibits softening effect, while there is no softening with $\Sigma_{22}$, which is consistent with Fig. 8d. For random in Fig. 9a, cube in Fig. 9b, and S in Fig. 9f, the softening effect of $\Sigma_{11}$ can be always observed, and the softening of $\Sigma_{22}$ can be observed when $\rho$ becomes larger.

For Goss in Fig. 9c and brass in Fig. 9e, above a certain $\rho$ value, $\Sigma_{11}$ starts to exhibits less softening effect than $\Sigma_{22}$. It is more pronounced for Goss that when $\rho$ is larger than 0.4, there is almost no softening in $\Sigma_{11}$.

There is an interesting observation in Fig. 9 that a stronger strain hardening is not always associated with a better formability. For example, when $\rho = 1.0$, the strain hardening of cube seems to be the lowest, yet it has the best formability. In the constitutive description in this study (see Section i.2), the true strain hardening capacity lies in individual slip systems (see Eq. (13) in Section i.2).
Figure 7: $\frac{\varepsilon_{\text{mean}}}{\varepsilon_{\text{median}}} / \varepsilon_{\text{median}}$ and $\frac{\varepsilon_{\text{mean}}}{\varepsilon_{\text{median}}}$ vs. $\varepsilon_{\text{major}}$ for different orientation distributions: (a) random, (b) cube, (c) Goss, (d) copper, (e) brass, and (f) S. For each orientation distribution, the results from the mesh $20 \times 20 \times 5$ are shown at the top row, and $40 \times 40 \times 5$ are at the bottom row. Each line corresponds to an orientation distribution instance. $\rho$ represents the strain path that $\varepsilon_{\text{minor}} = \rho \cdot \varepsilon_{\text{major}}$ (see Eq. (20)).
III RESULTS AND DISCUSSION

ii Determination of formability limit

Figure 7 (continued)
Figure 8: $\Sigma_{11}$ vs. $\epsilon_{11}^{\text{mean}}/\epsilon_{11}^{\text{median}}$ and $\Sigma_{22}$ vs. $\epsilon_{22}^{\text{mean}}/\epsilon_{22}^{\text{median}}$ for different orientation distributions: (a) random, (b) cube, (c) Goss, (d) copper, (e) brass, and (f) S. For each orientation distribution, the results from the mesh $20 \times 20 \times 5$ are shown at the top row, and $40 \times 40 \times 5$ are at the bottom row. Each line corresponds to an orientation distribution instance. $\rho$ represents the strain path that $\epsilon_{\text{minor}} = \rho \epsilon_{\text{major}}$ (see Eq. (20)). Note $\Sigma_{11}$ and $\Sigma_{22}$ are obtained by averaging over integration points.
Figure 8 (continued)
If the strain hardening effect is too strong due to the texture effect, the strain hardening capacity would be exhausted on slip system basis very quickly. Thus, the above observation is not in conflict with the fact that a stronger strain hardening favors a better formability.

iii. Calculated formability limit diagrams

By collecting the \( \epsilon_{\text{major}} \) where the maximum stress occurs in Fig. 9, the calculated FLDs are shown in Fig. 10. The mean and extrema values of different orientation distribution instances are shown in Fig. 11.

Though from a statistically point of view, all the orientation distribution instances for a given orientation distribution are the same (see Figs. 4 and B.1), the calculated FLDs still exhibit a certain scatter shown in Figs. 10 and 11. Yet, all the orientation distribution instances still follow the same FLD trend for a given orientation distribution. The scatter introduced by using different distribution instances is not entirely surprising, as the localized deformation is a local event which probably highly depends on the local spatial orientation distribution.

Fig. 11 also shows the calculated FLDs by using mesh \( 40 \times 40 \times 5 \) are slightly lower than those by \( 20 \times 20 \times 5 \). A possible reason is the application of PBC. If a localized deformation band is to be formed, the orientation or the shape of the band should fulfill the applied PBC. Thus, PBC may impose certain restriction to the localized deformation. In a larger unit cell, there is more freedom for the localized deformation band to adopt its orientation or shape which is less restricted by the imposed PBC.

The texture dependence revealed in Figs. 10 and 11 is that (i) cube has the best formability, and it is the only orientation distribution whose formability limit increases when \( \rho \) increases; (ii) random, copper, and S have comparable formability to each other, and all of them are better than Goss and brass; (iii) Goss has the poorest formability.

The calculated texture dependence in this study is actually in good agreement with Fig. 4(f) in Ref. [32]. This agreement is surprising for the main reason that the origin of the localized deformation in this study is the microstructural heterogeneity, while in Ref. [32] (MK-model in conjunction with Taylor model) it is a pre-defined geometrical imperfection. It seems the governing effect is only the texture.

This unexpected agreement can be perhaps rationalized as the follows. During the early stage of deformation, small grooves (similar to geometrical imperfection) on the surface develop due to the heterogeneous deformation at the grain scale. The geometrical orientations and the depths of these grooves can be random. Only some of them are able to grow eventually to a volume of localized deformation which carries the overall deformation. The above process has been observed in many studies [55, 56, 74] where full field CP-FEM is applied. Though in Ref. [32] a mean field model was applied, different groove orientations were tested and the one which gives the lowest formability was chosen.

Essentially, the major difference between this study and Ref. [32] is the selection process of the potentially growing grooves. Here, it is by numerically solving the mechanical equilibrium conditions, and in Ref. [32] it is by a brutal force search. MK-model ignores how a groove develops in the first place, but in a polycrystalline material, heterogeneous deformation always occurs, and the surface grooves could develop at very early stages of deformations (see Fig. 5, Fig. 6 and [55, 56, 74]). The above discussion offers a more reasonable physical picture of the MK-model than what has been being perceived that the postulate of a geometrical imperfection is arbitrary.

iv. Limitations of this study

The first limitation is FEM itself, as it requires considerable computational power. Though in this study DAMASK is implemented in such way that it is compatible with the share memory parallel version of LS-Dyna, and each simulation could be finished within a reasonable time frame, it still requires a lot of computational resources, e.g. multiple CPUs and a large amount of stack memory. An better alternative might be the spectral method based solver [75, 76], particularly given the recent demonstration of its capability of including free surface in the model [77].

The second limitation is the application of PBC. The main purpose of applying PBC is to model a very large sheet metal by a small unit cell where lower length scale microstructure information can be included. If a localized deformation band is to be formed, the orientation of the band should fulfill the applied PBC. This implies that PBC might restrict the orientation or shape of the localized deformation band, which would in turn potentially overestimate the formability. This restriction might be mitigated by using a larger simulation unit cell. This is because the restriction by PBC are mostly imposed on the boundaries of a simulation unit cell, and in a larger simulation unit cell, the fraction of elements that are less influenced by PBC would be higher.

IV. Summary

We demonstrate that it is feasible to apply full field crystal models to calculate the formability limit diagram without assuming any initial geometrical imperfection.
(a) random  (b) cube  (c) Goss  (d) copper  (e) brass  (f) S

Figure 9: $\Sigma_{11}$, $\Sigma_{22}$, and other $\Sigma_{ij}$ vs. $\varepsilon_{\text{major}}$ for different orientation distributions: (a) random, (b) cube, (c) Goss, (d) copper, (e) brass, and (f) S. Each line corresponds to an orientation distribution instance. $\rho$ represents the strain path that $\varepsilon_{\text{minor}}=\rho \varepsilon_{\text{major}}$ (see Eq. (20)). Note $\Sigma_{11}$ and $\Sigma_{22}$ are obtained by averaging over integration points. $\rho = 0.0$ and $\rho = 1.0$ are by both the meshes $20 \times 20 \times 5$ and $40 \times 40 \times 5$; $\rho = 0.2, 0.4, 0.6, 0.8$ are by the mesh $20 \times 20 \times 5$; and $\rho = 0.25, 0.5, 0.75$ are by the mesh $40 \times 40 \times 5$ (see Fig. 2). The solid circles mark the location of the maximum stress of $\Sigma_{11}$ or $\Sigma_{22}$ which is at a smaller $\varepsilon_{\text{major}}$ than the other.
Figure 10: Simulated right hand side of formability limit diagrams of the metal sheets with different orientation distributions. The results of the same orientation distribution instance are connected by lines.

Figure 11: Simulated right hand side of formability limit diagrams of the metal sheets with different orientation distributions. It only shows the mean and extrema values of different orientation distribution instances. All orientation distributions are shown in gray in each figure as a background.
The intrinsic microstructural heterogeneity in polycrystalline model is sufficient to trigger the localization event in the simulations.

In this study, the localized deformation is monitored by the statistical distributions of the strains. The observed localization is connected to the stress softening effect. Thus, the maximum stress appeared on the stress-strain curve is proposed as the criterion to identify the formability limit. By using this criterion, formability limit diagrams are constructed for different initial orientation distributions. It is observed that cube orientation exhibits the best formability; random, copper, and S are very comparable, but better than Goss and brass; and Goss has the poorest formability.

The texture dependence of the formability is surprisingly in good agreement with a previous study by using the MK-model where an initial geometrical imperfection is assumed. Though based on different physical origins or grooves induced by the early stage plastic deformation of polycrystalline materials could serve as the geometrical imperfection assumed in the MK-model. Thus, the crystallographic texture becomes the dominant effect on the resulting formability limit diagrams.

ACKNOWLEDGMENTS

The author would like to thank Dr. Martin Diehl and PD Dr. Franz Roters at Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany for the initial discussion on incorporating DAMASK and LS-Dyna. The author would also like to express his gratitude to Dr. Tobias Erhart at DYNAmore GmbH, Stuttgart, Germany for the discussion of user defined subroutines in LS-Dyna. This work has been supported by the European Regional Development Fund (EFRE) in the framework of the EU-program 'TWB Investition in Wachstum und Beschäftigung Österreich 2014-2020', and the federal state Upper Austria.

A. INFEASIBILITY OF APPLYING BIFURCATION THEORY TO RATE DEPENDENT CONSTITUTIVE LAWS

Here we show the reason that it is infeasible to apply the bifurcation theory to rate dependent constitutive laws. First, we briefly describe the bifurcation theory formulated by Rice and co-workers [78, 79, 80, 81]. Consider the quasi-static rate fields, $\dot{F}$ and $\dot{P}$ (deformation gradient rate and first Piola-Kirchhoff rate), in a homogeneous solid which is being homogeneously deformed, and in this solid a localized band is formed. $F$ inside and outside the band is expressed as

$$F^b = \dot{F} + \Delta F$$  \hspace{1cm} (A.1)

where the superscripts $b$ and $o$ represent the quantities inside the band and outside the band, and $\Delta F$ is only within the band. If the $F$ is still continuous at the interface of the band, according to Hadamard compatibility condition for a singular interface inside a solid, Eq. (A.1) is written as

$$\dot{F}^b = \dot{F}^o + g \otimes n^b$$  \hspace{1cm} (A.2)

where $n^b$ is the normal direction of band in the reference configuration, and $|n^b| = 1$. $g$ is a vector which is unknown at the moment. The equilibrium condition at the interface requires that

$$n^b \dot{p}^b = n^b \dot{p}^o$$  \hspace{1cm} (A.3)

To proceed further, the relation between $F$ and $P$ is required. Here, we derive their relation according to the constitutive formulation in Section i. We start with Eq. (14) that

$$P = F F_p^{-1} S F_p^{-T}$$  \hspace{1cm} (A.4)

Its partial derivative with respect to time, $t$, reads

$$\frac{\partial P}{\partial t} = \frac{\partial F}{\partial t} F P^{-1} S F_p^{-T} + F \frac{\partial (F_p^{-1})}{\partial t} F_p^{-T} + F F_p^{-1} S \frac{\partial (F_p^{-T})}{\partial t}$$  \hspace{1cm} (A.5)

The partial derivative in the second term in Eq. (A.5), $\frac{\partial (F_p^{-1})}{\partial t}$, is derived as,

$$\frac{\partial F}{\partial t} F P^{-1} + F_p \frac{\partial (F_p^{-1})}{\partial t} = 0$$  \hspace{1cm} (A.6)

$$\frac{\partial (F_p^{-1})}{\partial t} = - F_p^{-1} \frac{\partial F}{\partial t} F_p^{-1} = - F_p^{-1} L_p$$

Similarly, the partial derivative in the fourth term in Eq. (A.5), $\frac{\partial (F_p^{-T})}{\partial t}$, can be expressed as,

$$\frac{\partial (F_p^{-T})}{\partial t} = - L_p \dot{F}_p^{-T}$$  \hspace{1cm} (A.7)
The partial derivative in the third term in Eq. (A.5), $\frac{\partial S}{\partial t}$, can be expanded according to the chain rule,

$$\frac{\partial S}{\partial t} = \frac{\partial S}{\partial F_e} : \frac{\partial F_e}{\partial t}$$  \hspace{1cm} (A.8)

First, we derive the analytical expression of $\frac{\partial S}{\partial F_e}$ in Eq. (A.8). According to Eq. (12), the partial derivative of $S$ with respect to $F_e$ is

$$\frac{\partial S}{\partial F_e} = \frac{1}{2} \partial \left[ C : \left( F_e^T F_e - I \right) \right]$$

where $C$ is the single crystalline elastic stiffness tensor. Writing Eq. (A.9) in induce form,

$$\frac{\partial (S)_{ij}}{\partial (F_e)_{pq}} = \frac{\partial \left[ C_{ijkl} \left( F_e^T \right)_{km} (F_e)_{ml} \right]}{\partial (F_e)_{pq}}$$

$$= C_{ijkl} \left[ \frac{\partial \left( F_e^T \right)_{km} (F_e)_{ml}}{\partial (F_e)_{pq}} + \left( F_e^T \right)_{km} \frac{\partial (F_e)_{ml}}{\partial (F_e)_{pq}} \right]$$

$$= C_{ijkl} \left[ \frac{\partial F_e}{\partial lq} \delta_{kp} \delta_{lq} + \left( F_e^T \right)_{km} \delta_{mp} \delta_{lq} \right]$$

$\delta_{ij}$ is the Kronecker delta tensor. Thus in the above equation, $m = p$ when $\delta_{mp} = 1$, otherwise $\delta_{mp} = 0$, then the indices $m$ can be all replaced by $p$.

$$2 \frac{\partial (S)_{ij}}{\partial (F_e)_{pq}} = C_{ijkl} \left[ \delta_{kp} \left( F_e^T \right)_{pl} + (F_e)_{pk} \delta_{lq} \right]$$

$$= C_{ijkl} \left( \left( F_e^T \right)_{pl} + \left( F_e^T \right)_{kp} \delta_{lq} \right)$$

For the first term on the right hand side of the above equation, $\delta_{lq} = 1$ when $k = q$, otherwise $\delta_{lq} = 0$; and for the second term $\delta_{lq} = 1$ when $l = q$, otherwise $\delta_{lq} = 0$, then, it can be simplified further as

$$2 \frac{\partial (S)_{ij}}{\partial (F_e)_{pq}} = C_{ijkl} \left( F_e^T \right)_{pl} + C_{ijkq} \left( F_e^T \right)_{kp}$$

Considering the symmetry of the elastic stiffness tensor $C$ that $C_{ijkq} = C_{ijkq}$, and $(F_e)_{pl} = \left( F_e^T \right)_{lp}$, then

$$2 \frac{\partial (S)_{ij}}{\partial (F_e)_{pq}} = C_{ijkl} \left( F_e^T \right)_{lp} + C_{ijkq} \left( F_e^T \right)_{kp}$$

Since $l$ and $k$ are both dummy indices going through 1,2,3, the two terms on the right hand side of the above equation are essentially equivalent, then

$$2 \frac{\partial (S)_{ij}}{\partial (F_e)_{pq}} = 2 \cdot C_{ijkl} \left( F_e^T \right)_{lp}$$

Thus, in tensor form it is written as,

$$\frac{\partial S}{\partial F_e} = CF_e^T : T$$  \hspace{1cm} (A.10)

where $T_{ijkl} = \delta_{ik} \delta_{lj}$. The second term on the right hand side of Eq. (A.8) can be derived according to Eq. (7),

$$\frac{\partial F_e}{\partial F_e} = F_e = L_e F_e = \left( L - F_e L_e F_e^{-1} \right) F_e$$  \hspace{1cm} (A.11)

Substituting the respective terms in Eq. (A.8) by Eqs. (A.10) and (A.11), we arrive at

$$\frac{\partial S}{\partial l} = \left( CF_e^T : F_e - L_e F_e \right) : \dot{F} - \left( CF_e^T F_e : L_p^T \right)$$  \hspace{1cm} (A.12)

Putting Eqs. (A.6), (A.7) and (A.12) into Eq. (A.5), and writing $\frac{\partial S}{\partial t}$ into $A$, then we have

$$\dot{P} = \dot{F} F_p^{-1} S F_p^{-T} - F F_p^{-1} F_p S F_p^{-T} + F F_p^{-1} \left( \left( CF_e^T : T \right) F_p^{-T} : \dot{F} \right) F_p^{-T}$$  \hspace{1cm} (A.13)

Grouping some terms together, one obtains

$$\dot{P} = (H_1 + H_2) : \dot{F} - H_3$$  \hspace{1cm} (A.14a)

where

$$H_1 = IF_p^{-1} S F_p^{-T}$$  \hspace{1cm} (A.14b)

$$H_2 = \left( F_p^{-1} \left[ T : \left( F F_p^{-1} \left( \left( CF_e^T : T \right) F_p^{-T} \right) \right) \right) \right$$  \hspace{1cm} (A.14c)

$$H_3 = FF_p^{-1} \left[ L_p S + SL_p^T + \left( CF_e^T F_e : L_p^T \right) F_p^{-T} \right]$$  \hspace{1cm} (A.14d)
We now put Eq. (A.14a) together with Eq. (A.2) into Eq. (A.3). Then the equilibrium condition of Eq. (A.3) is written as

\[ n^b \left[ \left( H_1 + H_2^b \right) : \left( F^o + g \otimes n \right) - H_3^b \right] = n^b \left[ \left( H_1^b + H_2^b \right) : F^o - H_3^b \right] \] (A.15)

At the inception of the band formation, the solid is still homogenous, thus \( H_1^b = H_1^b, H_2^b = H_2^0, \) and \( H_3^b = H_3^0, \) then it becomes

\[ n^b \left( H_1 + H_2 \right) n^b = 0 \] (A.16)

In the above equation, if \( g \neq 0 \) when a band formation is possible, then \( n^b \left( H_1 + H_2 \right) n^b \) must be a singular matrix, meaning the determinant of it must be zero. The term \( H_1 + H_2 \) in Eq. (A.16) is dominated by \( H_2. \) It is for the reason that \( H_2 \) is close to the elastic stiffness tensor at the order of magnitude of 100 GPa, and \( H_1 \) is at 100 MPa. In reality, only when \( F_p \) becomes unrealistically large (see Eq. (A.14c)), \( n^b \left( H_1 + H_2 \right) n^b \) being a singular matrix becomes possible.

The general problem with rate dependent constitutive law is that the plastic deformation cannot be incorporated into the tangent moduli relating \( F \) and \( P, \) such as in Eq. (A.14a) that \( H_3 \) is the plastic deformation part which is not incorporated with \( F. \)

### B. Pole figures of all orientation distribution instances

In Fig. 4 of Section iii, we show the pole figures of some instances of the initial orientation distributions. Here we show all the pole figures of the orientation distribution instances used in this study in Fig. B.1.

**References**

[1] S. P. Keeler, “Circular grid system – a valuable aid for evaluating sheet metal formability,” SAE Technical Paper 680092, SAE International, Warrendale, PA, Feb. 1968. DOI: 10.4271/680092.

[2] G. M. Goodwin, “Application of strain analysis to sheet metal forming problems in the press shop,” SAE Technical Paper 680093, SAE International, Warrendale, PA, Feb. 1968. DOI: 10.4271/680093.

[3] W. F. Hosford and J. L. Duncan, “Sheet metal forming: A review,” JOM, vol. 51, pp. 39–44, Nov 1999.

[4] G. H. LeRoy and J. D. Embury, “Forming limit diagram for aluminum alloy 5154-o,” in *Formability: Analysis, Modeling and Experimentation* (A. K. Ghosh and H. L. Hecker, eds.), pp. 183–207, AIME, 1978.

[5] A. F. Graf and W. F. Hosford, “Calculations of forming limit for changing strain paths,” Metallurgical Transactions A, vol. 24, pp. 2497–2501, Nov 1993.

[6] T. B. Stoughton and X. Zhu, “Review of theoretical models of the strain-based FLD and their relevance to the stress-based FLD,” International Journal of Plasticity, vol. 20, pp. 1463–1486, Aug. 2004.

[7] K. Yoshida, T. Kuwabara, and M. Kuroda, “Path-dependence of the forming limit stresses in a sheet metal,” International Journal of Plasticity, vol. 23, pp. 361–384, Mar. 2007.

[8] T. B. Stoughton and J. W. Yoon, “Path independent forming limits in strain and stress spaces,” International Journal of Solids and Structures, vol. 49, pp. 3616–3625, Dec. 2012.

[9] D. Banabic, H.-J. Bunge, K. Pöhlandt, and A. E. Tekkaya, *Formability of Metallic Materials*. Engineering Materials, Berlin, Heidelberg: Springer Berlin Heidelberg, 2000.

[10] D. Banabic, F. Barlat, O. Cazacu, and T. Kuwabara, “Advances in anisotropy and formability,” International Journal of Material Forming, vol. 3, pp. 165–189, Sept. 2010. 00129.

[11] F. Abed-Meraim, T. Balan, and G. Altmeyer, “Investigation and comparative analysis of plastic instability criteria: application to forming limit diagrams,” The International Journal of Advanced Manufacturing Technology, vol. 71, pp. 1247–1262, Mar. 2014.

[12] D. Banabic, ed., *Multiscale Modelling in Sheet Metal Forming*. ESAFORM Bookseries on Material Forming, Cham: Springer International Publishing, 2016.

[13] M. Considère, “Mémoire sur l’emploi du fer et de l’acier dans les constructions,” Annales des ponts et chaussées. Mémoires et documents relatifs à l’art des constructions et au service de l’ingénieur, pp. 574–775, 1885.

[14] H. Swift, “Plastic instability under plane stress,” Journal of the Mechanics and Physics of Solids, vol. 1, no. 1, pp. 1 – 18, 1952.

[15] R. Hill, “On discontinuous plastic states, with special reference to localized necking in thin sheets,” Journal of the Mechanics and Physics of Solids, vol. 1, pp. 19–30, Oct. 1952. 01321.
Figure B.1: Pole figures of all orientation distribution instances used in this study. The leftmost pole figures in each subfigure are already shown in Fig. 4. The orientation generation was realized by using the method described in [68, 69, 70].
(g) copper for $20 \times 20 \times 5$ mesh

(h) copper for $40 \times 40 \times 5$ mesh

(i) brass for $20 \times 20 \times 5$ mesh

(j) brass for $40 \times 40 \times 5$ mesh

(k) S for $20 \times 20 \times 5$ mesh

(l) S for $40 \times 40 \times 5$ mesh

Figure B.1 (continued)
[16] P. Hora, L. Tong, and J. Reissner, “A prediction method for ductile sheet metal failure in FE-simulation,” in Numisheet’96, pp. 252–256, 1996.

[17] P. Hora, L. Tong, and B. Berisha, “Modified maximum force criterion, a model for the theoretical prediction of forming limit curves,” International Journal of Material Forming, vol. 6, pp. 267–279, June 2013.

[18] H. Aretz, “Numerical restrictions of the modified maximum force criterion for prediction of forming limits in sheet metal forming,” Modelling and Simulation in Materials Science and Engineering, vol. 12, no. 4, p. 677, 2004.

[19] N. Manopulo, P. Hora, P. Peters, M. Gorji, and F. Barlat, “An extended Modified Maximum Force Criterion for prediction of localized necking under non-proportional loading,” International Journal of Plasticity, vol. 75, pp. 189–203, Dec. 2015.

[20] Z. Marciniak and K. Kuczyński, “Limit strains in the processes of stretch-forming sheet metal,” International Journal of Mechanical Sciences, vol. 9, no. 9, pp. 609 – 620, 1967.

[21] D. Banabic, “A review on recent developments of marciniak-kuczynski model,” Computer Methods in Materials Science, vol. 10, pp. 225–237, 2010.

[22] D. Banabic, D.-S. Comsa, P. Eyckens, A. Kami, and M. Gologanu, Advanced Models for the Prediction of Forming Limit Curves, pp. 205–300. Cham: Springer International Publishing, 2016.

[23] J. Signorelli, M. Bertinetti, and P. Turner, “Predictions of forming limit diagrams using a rate-dependent polycrystal self-consistent plasticity model,” International Journal of Plasticity, vol. 25, pp. 1–25, Jan. 2009.

[24] S. Forest and E. Lorentz, “Localization phenomena and regularization methods,” Local approach to fracture, pp. 311–371, 2004.

[25] K. Yoshida and M. Kuroda, “Comparison of bifurcation and imperfection analyses of localized necking in rate-independent polycrystalline sheets,” International Journal of Solids and Structures, vol. 49, pp. 2073–2084, Aug. 2012.

[26] Y. Zhou and K. W. Neale, “Predictions of forming limit diagrams using a rate-sensitive crystal plasticity model,” International Journal of Mechanical Sciences, vol. 37, no. 1, pp. 1–20, 1995.

[27] P. D. Wu, K. W. Neale, and E. V. d. Giessen, “On crystal plasticity FLD analysis,” Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, vol. 453, pp. 1831–1848, Sept. 1997.

[28] J. Savoie, M. Jain, A. R. Carr, P. D. Wu, K. W. Neale, Y. Zhou, and J. J. Jonas, “Predictions of forming limit diagrams using crystal plasticity models,” Materials Science and Engineering: A, vol. 257, no. 1, pp. 128–133, 1998.

[29] P. D. Wu, K. W. Neale, E. Van der Giessen, M. Jain, S. R. MacEwen, and A. Makinde, “Crystal plasticity forming limit diagram analysis of rolled aluminum sheets,” Metallurgical and Materials transactions A, vol. 29, no. 2, pp. 527–535, 1998.

[30] P. Wu, S. MacEwen, D. Lloyd, and K. Neale, “Effect of cube texture on sheet metal formability,” Materials Science and Engineering: A, vol. 364, pp. 182–187, Jan. 2004.

[31] K. Inal, K. Neale, and A. Aboutajeddine, “Forming limit comparisons for FCC and BCC sheets,” International Journal of Plasticity, vol. 21, pp. 1255–1266, June 2005.

[32] K. Yoshida, T. Ishizaka, M. Kuroda, and S. Ikawa, “The effects of texture on formability of aluminum alloy sheets,” Acta Materialia, vol. 55, pp. 4499–4506, Aug. 2007.

[33] H. Wang, P. Wu, K. Boyle, and K. Neale, “On crystal plasticity formability analysis for magnesium alloy sheets,” International Journal of Solids and Structures, vol. 48, pp. 1000–1010, Mar. 2011.

[34] J. Signorelli and M. Bertinetti, “On the role of constitutive model in the forming limit of FCC sheet metal with cube orientations,” International Journal of Mechanical Sciences, vol. 51, pp. 473–480, June 2009.

[35] C. J. Neil and S. R. Agnew, “Crystal plasticity-based forming limit prediction for non-cubic metals: Application to mg alloy az31b,” International Journal of Plasticity, vol. 25, no. 3, pp. 379 – 398, 2009.

[36] M. Serenelli, M. Bertinetti, and J. Signorelli, “Investigation of the dislocation slip assumption on formability of BCC sheet metals,” International Journal of Mechanical Sciences, vol. 52, pp. 1723–1734, Dec. 2010.

[37] M. Yang, X. Dong, R. Zhou, and J. Cao, “Crystal plasticity-based forming limit prediction for FCC
materials under non-proportional strain-path,” Materials Science and Engineering: A, vol. 527, pp. 6607–6613, Sept. 2010.

[38] M. Serenelli, M. Bertinetti, and J. Signorelli, “Study of limit strains for FCC and BCC sheet metal using polycrystal plasticity,” International Journal of Solids and Structures, vol. 48, pp. 1109–1119, Apr. 2011.

[39] J. Signorelli, M. Serenelli, and M. Bertinetti, “Experimental and numerical study of the role of crystallographic texture on the formability of an electro-galvanized steel sheet,” Journal of Materials Processing Technology, vol. 212, pp. 1367–1376, June 2012.

[40] J. H. Kim, M.-G. Lee, D. Kim, and F. Barlat, “Crystal plasticity finite element analysis of ferritic stainless steel for sheet formability prediction,” International Journal of Plasticity, vol. 93, pp. 26–45, June 2017.

[41] M. A. Bertinetti, C. D. Schwindt, and J. W. Signorelli, “Effect of the cube orientation on formability for FCC materials: A detailed comparison between full-constraint and self-consistent predictions,” International Journal of Mechanical Sciences, vol. 87, pp. 200–217, Oct. 2014.

[42] G. Franz, F. Abed-Meraim, and M. Berveiller, “Strain localization analysis for single crystals and polycrystals: Towards microstructure-ductility linkage,” International Journal of Plasticity, vol. 48, pp. 1–33, Sept. 2013. 00039.

[43] C. Schwindt, F. Schlosser, M. Bertinetti, M. Stout, and J. Signorelli, “Experimental and Visco-Plastic Self-Consistent evaluation of forming limit diagrams for anisotropic sheet metals: An efficient and robust implementation of the M-K model,” International Journal of Plasticity, vol. 73, pp. 62–99, Oct. 2015.

[44] H. K. Akpama, M. Ben Bettaieb, and F. Abed-Meraim, “Localized necking predictions based on rate-independent self-consistent polycrystal plasticity: Bifurcation analysis versus imperfection approach,” International Journal of Plasticity, vol. 91, pp. 205–237, Apr. 2017.

[45] P. D. Wu, S. R. MacEwen, D. J. Lloyd, and K. W. Neale, “A mesoscopic approach for predicting sheet metal formability,” Modelling and Simulation in Materials Science and Engineering, vol. 12, no. 3, p. 511, 2004.

[46] E. Viatkina, W. Brekelmans, and M. Geers, “A crystal plasticity based estimate for forming limit diagrams from textural inhomogeneities,” Journal of Materials Processing Technology, vol. 168, pp. 211–218, Sept. 2005.

[47] T. Lloyd and M. W. Priddy, “Simulating strain localization in rolled magnesium,” Acta Materialia, vol. 129, pp. 149–158, May 2017.

[48] J. H. Kim, M.-G. Lee, J.-H. Kang, C.-S. Oh, and F. Barlat, “Crystal plasticity finite element analysis of ferritic stainless steel for sheet formability prediction,” International Journal of Plasticity, vol. 93, pp. 26–45, June 2017.

[49] B. Mohammed, T. Park, H. Kim, F. Pourboghrat, and R. Esmaeilpour, “The forming limit curve for multiphase advanced high strength steels based on crystal plasticity finite element modeling,” Materials Science and Engineering: A, vol. 725, pp. 250–266, 2018.

[50] F. Roters, P. Eisenlohr, L. Hantcherli, D. Tjahjanto, T. Bieler, and D. Raabe, “Overview of constitutive laws, kinematics, homogenization and multiscale methods in crystal plasticity finite-element modeling: Theory, experiments, applications,” Acta Materialia, vol. 58, pp. 1152–1211, Feb. 2010. 00599.

[51] K. Inal, P. D. Wu, and K. W. Neale, “Large strain behaviour of aluminium sheets subjected to in-plane simple shear,” Modelling and Simulation in Materials Science and Engineering, vol. 10, no. 2, p. 237, 2002.

[52] K. Inal, P. D. Wu, and K. W. Neale, “Instability and localized deformation in polycrystalline solids under plane-strain tension,” International Journal of Solids and Structures, vol. 39, no. 4, pp. 983–1002, 2002.

[53] K. Inal, P. D. Wu, and K. W. Neale, “Finite element analysis of localization in FCC polycrystalline sheets under plane stress tension,” International Journal of Solids and Structures, vol. 39, no. 13-14, pp. 3469–3486, 2002.

[54] K. W. Neale, K. Inal, and P. D. Wu, “Effects of texture gradients and strain paths on localization phenomena in polycrystals,” International Journal of Mechanical Sciences, vol. 45, pp. 1671–1686, Oct. 2003.

[55] P. D. Wu, D. J. Lloyd, M. Jain, K. W. Neale, and Y. Huang, “Effects of spatial grain orientation distribution and initial surface topography on sheet metal necking,” International Journal of Plasticity, vol. 23, pp. 1084–1104, June 2007.

[56] K. Yoshida, “Effects of grain-scale heterogeneity on surface roughness and sheet metal necking,”
REFERENCES

International Journal of Mechanical Sciences, vol. 83, pp. 48–56, June 2014.

[57] Y. Wu, Y. Shen, K. Chen, Y. Yu, G. He, and P. Wu, “Multi-scale crystal plasticity finite element method (CPFEM) simulations for shear band development in aluminum alloys,” Journal of Alloys and Compounds, vol. 711, pp. 495–505, July 2017.

[58] J.-B. Kim and J. W. Yoon, “Necking behavior of AA 6022-T4 based on the crystal plasticity and damage models,” International Journal of Plasticity, vol. 73, pp. 3–23, Oct. 2015.

[59] P. Hu, Y. Liu, Y. Zhu, and L. Ying, “Crystal plasticity extended models based on thermal mechanism and damage functions: Application to multiscale modeling of aluminum alloy tensile behavior,” International Journal of Plasticity, vol. 86, pp. 1–25, Nov. 2016.

[60] F. Roters, P. Eisenlohr, T. R. Bieler, and D. Raabe, Crystal plasticity finite element methods: in materials science and engineering. Weinheim: Wiley-VCH, 2010. OCLC: 699657776.

[61] D. Peirce, R. Asaro, and A. Needleman, “Material rate dependence and localized deformation in crystalline solids,” Acta Metallurgica, vol. 31, no. 12, pp. 1951 – 1976, 1983.

[62] https://damask.mpie.de/. DAMASK: the Düsseldorf Advanced MAterial Simulation Kit.

[63] F. Roters, P. Eisenlohr, C. Kords, D. Tjahjanto, M. Diehl, and D. Raabe, “DAMASK: the Düsseldorf Advanced MAterial Simulation Kit for studying crystal plasticity using an fe based or a spectral numerical solver,” vol. 3, pp. 3–10, 2012. IUTAM Symposium on Linking Scales in Computations: From Microstructure to Macro-scale Properties.

[64] F. Roters, M. Diehl, P. Shanthraj, P. Eisenlohr, C. Reuber, S. L. Wong, T. Maiti, A. Ebrahimi, T. Hoehrner, H. O. Fabritius, S. Nikolov, M. Friak, N. Fujita, N. Grilli, K. Janssens, N. Jia, P. Kok, D. Ma, F. Meier, E. Werner, M. Stricker, D. Weygand, and D. Raabe, “Damask - the Düsseldorf Advanced Material Simulation Kit for modeling multi-physics crystal plasticity, thermal, and damage phenomena from the single crystal up to the component scale,” Computational Materials Science, 2018. in press.

[65] http://www.lstc.com/products/ls-dyna. Livermore Software Technology Corporation.

[66] O. van der Sluis, P. Schreurs, W. Brekelmans, and H. Meijer, “Overall behaviour of heterogeneous elastoviscoplastic materials: effect of microstructural modelling,” Mechanics of Materials, vol. 32, no. 8, pp. 449 – 462, 2000.

[67] S. Li and A. Wongsto, “Unit cells for micromechanical analyses of particle-reinforced composites,” Mechanics of Materials, vol. 36, no. 7, pp. 543 – 572, 2004.

[68] K. Helming, “Texture approximations by model components,” Materials Science Forum, vol. 273-275, pp. 125–132, Feb. 1998.

[69] Z. Zhao, F. Roters, W. Mao, and D. Raabe, “Introduction of a texture component crystal plasticity finite element method for anisotropy simulations,” Advanced Engineering Materials, vol. 3, no. 12, pp. 984–990, 2001.

[70] D. Raabe and F. Roters, “Using texture components in crystal plasticity finite element simulations,” International Journal of Plasticity, vol. 20, no. 3, pp. 339–361, 2004. Owen Richmond Memorial Special Issue.

[71] H.-P. Gänser, E. Werner, and F. Fischer, “Forming limit diagrams: a micromechanical approach,” International Journal of Mechanical Sciences, vol. 42, no. 10, pp. 2041 – 2054, 2000.

[72] L. Zhang, W. Xu, C. Liu, X. Ma, and J. Long, “Quantitative analysis of surface roughness evolution in FCC polycrystalline metal during uniaxial tension,” Computational Materials Science, vol. 132, pp. 19–29, May 2017.

[73] P. Eisenlohr, M. Diehl, R. Lebensohn, and F. Roters, “A spectral method solution to crystal elastoviscoplasticity at finite strains,” International Journal of Plasticity, vol. 46, pp. 37 – 53, 2013. Microstructure-based Models of Plastic Deformation.

[74] http://www.lstc.com/products/ls-dyna. Livermore Software Technology Corporation.
[77] T. Maiti and P. Eisenlohr, “Fourier-based spectral method solution to finite strain crystal plasticity with free surfaces,” *Scripta Materialia*, vol. 145, pp. 37 – 40, 2018.

[78] J. W. Rudnicki and J. R. Rice, “Conditions for the localization of deformation in pressure-sensitive dilatant materials,” *Journal of the Mechanics and Physics of Solids*, vol. 23, no. 6, pp. 371–394, 1975.

[79] S. Stören and J. R. Rice, “Localized necking in thin sheets,” *Journal of the Mechanics and Physics of Solids*, vol. 23, no. 6, pp. 421–441, 1975.

[80] J. R. Rice, “The localization of plastic deformation,” in *Proceedings of the 14th International Congress on Theoretical and Applied Mechanics*, vol. 1, (Delft), pp. 207–220, North-Holland Publishing Co., 1976.

[81] J. Rice and J. Rudnicki, “A note on some features of the theory of localization of deformation,” *International Journal of Solids and Structures*, vol. 16, no. 7, pp. 597–605, 1980.