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Multi-scale modeling of the effect of crystallographic texture

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Abstract. Among processes involving plastic deformation, sheet metal forming requires a most accurate description of plastic anisotropy. One of the main sources of mechanical anisotropy is crystallographic texture, which induces directionality in the macroscopic plastic properties of the polycrystalline metallic alloy sheets (e.g. anisotropy in yield stresses, Lankford coefficients). Recently, we develop a single-crystal yield criterion that satisfies the intrinsic symmetries of the constituent crystals and the condition of insensitivity to hydrostatic pressure [1]. Moreover, this single-crystal criterion is defined for any 3-D stress state. It was shown that the use of this single-crystal criterion for the description of the plastic behavior of the constituent crystals in conjunction with appropriate homogenization procedures leads to an improved prediction of the plastic anisotropy in macroscopic properties under uniaxial loading for polycrystalline aluminum alloys. In this paper, using this polycrystalline model, we simulate the deformation response of sheets of various crystallographic textures. Examples demonstrate the predictive capabilities of the model to describe the influence of the crystallographic texture on the macroscopic behavior and on the final shape of parts obtained using deep-drawing.

Introduction

Elastic/plastic constitutive models based on macroscopic orthotropic yield criteria are usually used to describe the mechanical behavior of metallic materials and leads to accurate predictions when applied to sheet forming operations (e.g. see [2]). Another approach is to use multi-scale models which explicitly account for the plastic response of the constituent at the grain scale as well as a statistical description of the texture of the material. Usually the grain-level behavior is modeled using a viscoplastic approach based on a power-type law or a rate-independent model based on the Schmid law or a regularized form of Schmid law (e.g. see [3–6]).

Recently, Cazacu, Revil, and Chandola [1] developed an analytical yield criterion for single-crystals. For any 3-D stress state, this yield function is continuous and differentiable and satisfies the symmetries requirements associated with the cubic lattice. Consequently, this yield criterion accounts for the specificities of the plastic flow of the crystal. For general loadings, four anisotropy coefficients are involved in this yield criterion. It was shown that the use of this single-crystal criterion for the description of the plastic behavior of the constituent crystals in conjunction with appropriate homogenization procedures leads to an improved prediction of the plastic anisotropy in macroscopic properties under uniaxial loading for polycrystalline aluminum alloys (see [7,8]).

While one ingredient of a multi-scale model is the constitutive model at the crystal scale level, another ingredient is the texture of the material. For aluminum alloys, the texture plays an important role and induce specific effects on forming properties, resulting in the formation of specific earing profile during cup deep drawing [9]. Depending on the rolling reduction and rolling temperature, the textures of rolled aluminum vary between the typical cube recrystallization texture and the typical rolled Aluminum texture. For a same aluminum alloy, changing the texture induce a change in the earing profile [10]. In this paper, using our polycrystalline model, we simulate the deformation response of sheets of various crystallographic textures.

Polycrystalline model based on Cazacu et al. [1] single-crystal law

In our model, the polycrystalline material is represented by a finite set of grains characterized by orientation and volume fraction to reproduce the material texture. Elastic deformations are modeled using Hooke's law for the type of symmetry shown by cubic crystals. The crystal plastic behavior is modeled using the Cazacu et al. single-crystal criterion [1], normality rule, and isotropic hardening described by a Swift-type law. The effective stress of the single-crystal is expressed in terms of cubic stress-invariants and relative to the Cartesian coordinate system $Ox_1x_2x_3$ associated with the crystal axes is given by:

$$\bar{\sigma}_{grain} = \frac{3}{\left(27-4cn_1^2\right)^{1/6}} \left\{ \begin{array}{l} \left[\frac{1}{2}m_1\left(\sigma_{11}'^2+\sigma_{22}'^2+\sigma_{33}'^2\right)+m_2\left(\sigma_{12}'^2+\sigma_{13}'^2+\sigma_{23}'^2\right)\right]^3 \\ -c\left[n_1\sigma_{11}'\sigma_{22}'\sigma_{33}'-n_3\left(\sigma_{33}'\sigma_{12}'^2+\sigma_{11}'\sigma_{23}'^2+\sigma_{22}'\sigma_{13}'^2\right)+2n_4\sigma_{12}'\sigma_{13}'\sigma_{23}'\right]^2 \end{array} \right\}^{1/6} \tag{1}$$

where $\boldsymbol{\sigma}'$ denotes the Cauchy stress deviator, m_1, m_2, n_1, n_3, n_4 are anisotropy coefficients and c is a parameter that describes the relative importance of the second-order and third-order cubic stress-invariants on yielding. The plastic strain-rate of each crystal $\mathbf{d}^{\mathrm{p}}_{grain}$ is uniquely defined for any stress state and can be easily calculated as:

$$\mathbf{d}^{\mathbf{P}} = \dot{\lambda}\frac{\partial \bar{\sigma}_{grain}}{\partial \boldsymbol{\sigma}} \tag{2}$$

where $\dot{\lambda}$ is the plastic multiplier, and $\bar{\sigma}$ is given by Eq.1.

The multi-scale model using the single-crystal law (1) was implemented in a finite-element (FE) framework. In the FE calculations, the polycrystal behavior is obtained by considering 250 grains per element. It is considered that the total strain-rate of each grain belonging to a given element is equal to the overall strain-rate $\mathbf{D}$. At the time increment *(n)*, the stress in each grain is computed by solving the governing equations, namely:

$$\begin{aligned} &\mathbf{D}^{(\mathrm{n})}_{grain} = \left(\mathbf{R}^{(\mathrm{n})}\right)^T \mathbf{D}^{(\mathrm{n})}\mathbf{R}^{(\mathrm{n})} \\ &\mathbf{D}^{(\mathrm{n})}_{grain} = \mathbf{D}^{\mathrm{e(n)}}_{grain} + \mathbf{D}^{\mathrm{p(n)}}_{grain} \\ &\boldsymbol{\sigma}^{(n)}_{grain} = \boldsymbol{\sigma}^{(n-1)}_{grain} + \left(\mathrm{C}^{el}:\mathbf{D}^{\mathrm{e(n)}}_{grain}\right)\mathrm{dt} \\ &\bar{\sigma}^{(n)}_{grain} - Y\left(\bar{\varepsilon}^{p\,(\mathrm{n})}_{grain}\right) \le 0 \\ &\mathbf{D}^{\mathrm{p(n)}}_{grain} = \dot{\lambda}_{grain}\frac{\partial \bar{\sigma}^{(n)}_{grain}}{\partial \boldsymbol{\sigma}} \end{aligned} \tag{3}$$

where $\mathbf{D}^{(\mathrm{n})}_{grain}$, $\mathbf{D}^{\mathrm{p(n)}}_{grain}$ and $\mathbf{D}^{\mathrm{e(n)}}_{grain}$ are respectively the crystal's total strain-rate, the plastic and elastic strain-rate with C^{el} being the fourth-order elasticity tensor , $\boldsymbol{\sigma}^{(n-1)}_{grain}$ and $\boldsymbol{\sigma}^{(n)}_{grain}$ are the stress tensors at the beginning and end of the increment, respectively, while $\bar{\varepsilon}^{p\,(\mathrm{n})}_{grain}$ is the equivalent plastic strain in the given grain, $Y\left(\bar{\varepsilon}^{p\,(\mathrm{n})}_{grain}\right)$ is the hardening law, and $\dot{\lambda}_{grain}$ the plastic multiplier. The stress of the polycrystal at the end of the increment is given by:

$$\boldsymbol{\sigma}^{(n)} = \left(\sum_{\mathrm{i}} w_{\mathrm{i}}\mathbf{R}^{(\mathrm{n})}_{\mathrm{i}}\left(\boldsymbol{\sigma}^{(n)}_{grain}\right)_{\mathrm{i}}\left(\mathbf{R}^{(\mathrm{n})}_{\mathrm{i}}\right)^T\right) \Big/ \left(\sum_{\mathrm{i}} w_{\mathrm{i}}\right) \tag{4}$$

where $\left(\boldsymbol{\sigma}_{grain}^{(n)}\right)_{i}$ is the stress tensor of grain *i*, and $\mathbf{R}_{i}^{(n)}$ is the transformation matrix for passage from the crystal axes of grain *i* to the loading frame axes, while w_i is the weight of the grain *i*. To describe the macroscopic response of FCC polycrystals, the model given by Eq. 1-4 was implemented in the commercial FE solver Abaqus Standard (implicit solver, see Abaqus (2014)). A polycrystalline aggregate composed of N crystals was associated with each FE integration point. The set of governing equations are solved for each of the constituent crystals using a fully-implicit backward Euler method.

Influence of the Initial Texture of the Material on The Earing Profile for Aluminum Alloy

Hirsch [10] has shown that for an Al-Mg-Mn alloys, it is possible by changing the rolling reduction and rolling temperature to change the texture of the material from a typical cube recrystallization texture to a ß-fiber rolling texture. This change in texture components leads to a change in the earing profile during cup deep-drawing. For a typical recrystallized aluminum alloy, a four ear profile with a minimum height at 45° to the rolling direction (RD) is observed, while for a ß-fiber rolling texture, a four ear profile with maximum height at 45° to RD is obtained (see [9]).

The polycrystalline model described in the previous section was used to assess it capability to accurately describe the influence of the initial texture of the material on the earing profile. For this purpose, the coefficients involved in the yield criterion [1] are kept fixed (i.e. $m_1 = 0.36$, $m_2 = 0.18$, $n_1 = 0.21$, $n_1 = 0.11$ $n_4 = 0.08$ and $c = 1.227$) and only the initial texture of the material is changed to reflect different rolling conditions. Two generic textures were generated using the software MTex [11] and the experimental observations reported in [10]. The main components and their weights are summarized in Table 1.

Table 1. Texture components and their weights.

Cube recrystallized Texture					Rolling Texture				
Texture component	Euler Angles			weight	Texture component	Euler Angles			weight
	ϕ_1	ψ	ϕ_2			ϕ_1	ψ	ϕ_2	
Cube	0	0	0	55%	C	90	35	45	20%
R	63	31	60	25%	S	63	31	60	20%
Goss	70	45	0	10%	B	35	45	0	60%
P	45	15	10	5%					
Q	0	45	0	5%					

For the cube recrystallized texture material, the pole figures as well as the anisotropy in uniaxial yield stresses and r-values obtained with the polycrystalline model with the given set of parameters are plotted in Fig. 1. It is to be noted that the polycrsytalline model predicts a minimum r-value of 0.6 along the direction 45° from RD and two maxima which are located along RD and TD. Concerning the yield stresses, the maximum is predicted at 45° from RD at minima are along RD and TD.

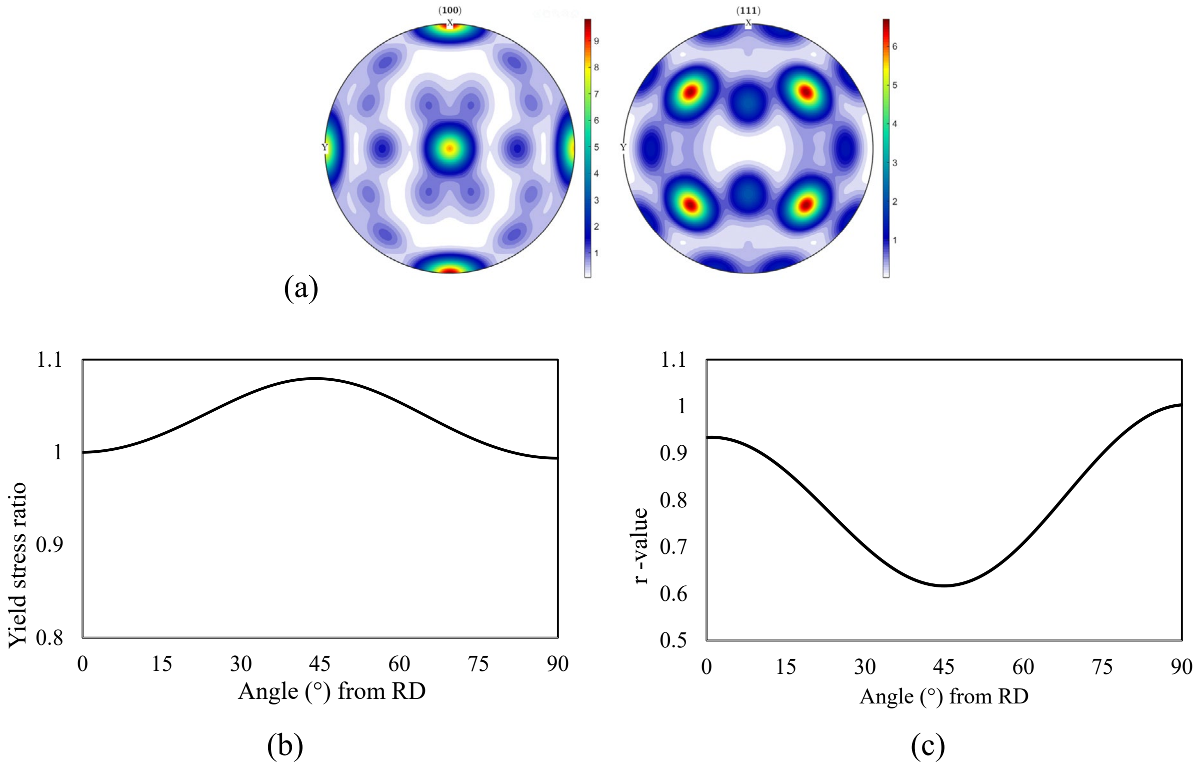

Fig. 1. Cube recrystallized material: (a) (100) and (111) pole figure; predictions of the anisotropy using the polycrystalline model based on the single-crystal law [1]: b) Uniaxial tensile flow stresses; (c) Lankford coefficients (r-values).

For the rolling texture material, the pole figures as well as the anisotropy in uniaxial yield stresses and r-values obtained with the polycrystalline model are shown in Fig. 2. Note that for a rolling texture, the polycrsytalline model predicts a maximum r-value along the direction ~ 45° from RD (r = 1.51), while the two minima are located along RD and TD.

Comparisons between the anisotropy predictions obtained with the polycrystalline model based on the single crystal yield criterion [1] with the same single crystal anisotropy coefficients show the influence of the initial texture of the material on its mechanical response. While for typical cube texture, it is predicted that the minimum r-value is obtained for a tensile test at an angle of 45 ° from RD, for a typical rolling texture, a maximum r-value is obtained for the same orientation. It is also worth noting that the amplitude of the r-value variation predicted also depends on the initial texture.

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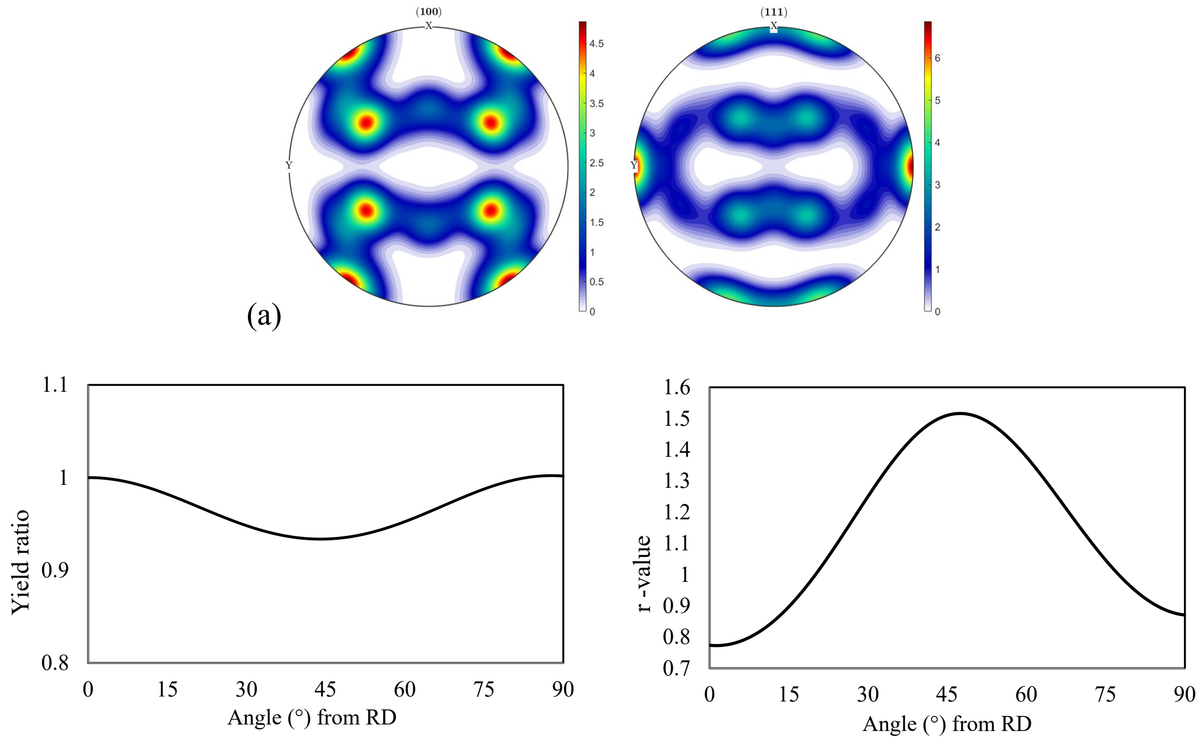
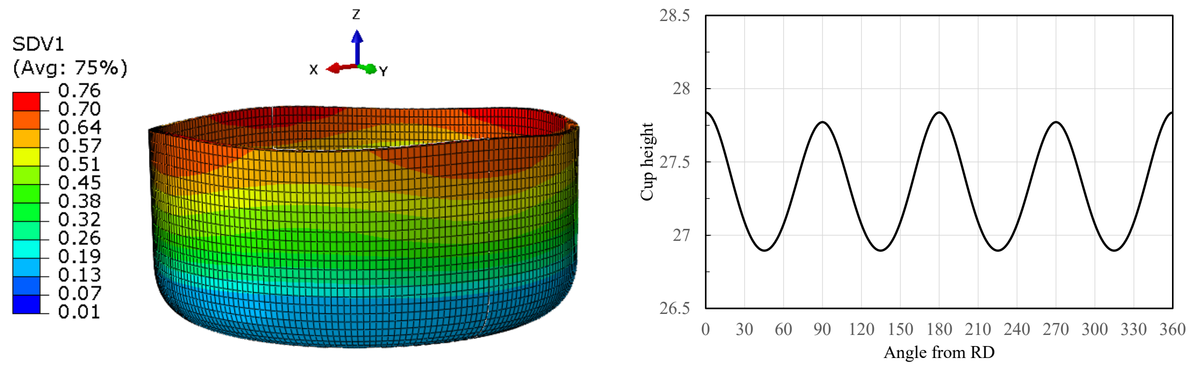


(b) (c)

Fig. 2. Rolling texture material : (a) (100) and (111) pole figure; predictions of the anisotropy using the polycrystalline model based on the single-crystal law [1]: (b) Uniaxial tensile flow stresses; (c) Lankford coefficients (r-values).

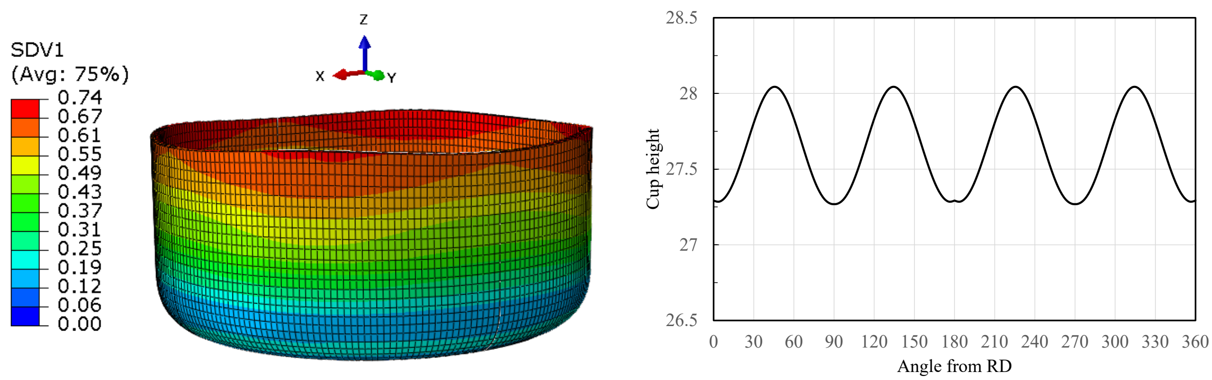
The polycrystalline model based on the Cazacu et al. [1] single crystal criterion (see Eq.(1)) was applied to study the influence of the initial texture of the material on the forming of a cylindrical cup. A blank of thickness 1 mm and radius of 50 mm was drawn by a punch of radius 30 mm into a die of opening radius of 31.2 mm. The blank-holder force was of 40 kN. In all the FE simulations presented hereafter, a polycrystalline aggregate composed of 250 orientations representative of the overall texture of the material is associated with each FE integration point. In the FE simulations of the circular cup, a total of 10900 reduced integration elements (Abaqus C3D8R) was used to mesh a quarter of the blank, resulting in the consideration of 2 725 000 grains in the FE simulation. In terms of computational time, one simulation of the cup drawing process performed using 6 cores takes about 3h40 on a desktop computer (Intel Core i7-4770 / 16GB RAM).

For the cube recrystallized texture material, the predicted isocontours of the equivalent plastic strain of the fully drawn cup using the polycrystalline model is shown in Fig.3 along with the predicted earing profile. For this initial texture, it is predicted a 4 ears profile with the maximum height being obtained for RD and the minimum height being obtained at 45° from RD. For the rolling texture material, using the same anisotropy coefficients (i.e. $m_1 = 0.36$, $m_2 = 0.18$, $n_1 = 0.21$, $n_1 = 0.11$ $n_4 = 0.08$ and $c = 1.227$), the polycrystalline model based on the single crystal criterion [1] also predicts a four ears profile, but with the maximum height obtained for the 45° from RD direction and the minimum height obtained at RD and TD.



(a) (b)

Fig. 3. FE results obtained with the polycrystalline model based on the Cazacu et al. [1] single crystal criterion (with m_1 = 0.36, m_2 = 0.18, n_1 = 0.21, n_1 = 0.11 n_4 = 0.08 and c = 1.227) for an aluminium alloy with a cube recrystallized texture : (a) Isocontours of the equivalent plastic strain; (b) earing profile.



(a) (b)

Fig. 4. FE results obtained with the polycrystalline model based on the Cazacu et al. [1] single crystal criterion (with m_1 = 0.36, m_2 = 0.18, n_1 = 0.21, n_1 = 0.11 n_4 = 0.08 and c = 1.227) for an aluminium alloy with a rolling texture: (a) Isocontours of the equivalent plastic strain; (b) earing profile.

To further compare the predictions of the polycrystalline model for the two different materials, in Fig 5 are superposed the predictions of the earing profile and the punch load. It is worth recalling that in the simulations, only the initial texture was different, the material parameters and deep drawing process parameters (friction, type of elements, blankholder forces) being the same. It is to be noted that the polycrystalline model is able to capture the influence of the initial texture on the mechanical response of the material and furthermore on the earing profile obtained during cup deep-drawing. Furthermore, the trends seen experimentally in a Al-Mg-Mn alloy by [9] are also accurately predicted by the polycrystalline model, that is for a typical recrystallized aluminum alloy, a four ear profile with a minimum height at 45° to RD is predicted, while for a rolling texture, a four ear profile with the maximum height at 45° to RD is predicted, which is similar to experimental observations. Furthermore, the polycrystalline model predicts an slightly higher punch force for the material with a rolling texture than for the material with a cube recrystallized texture.

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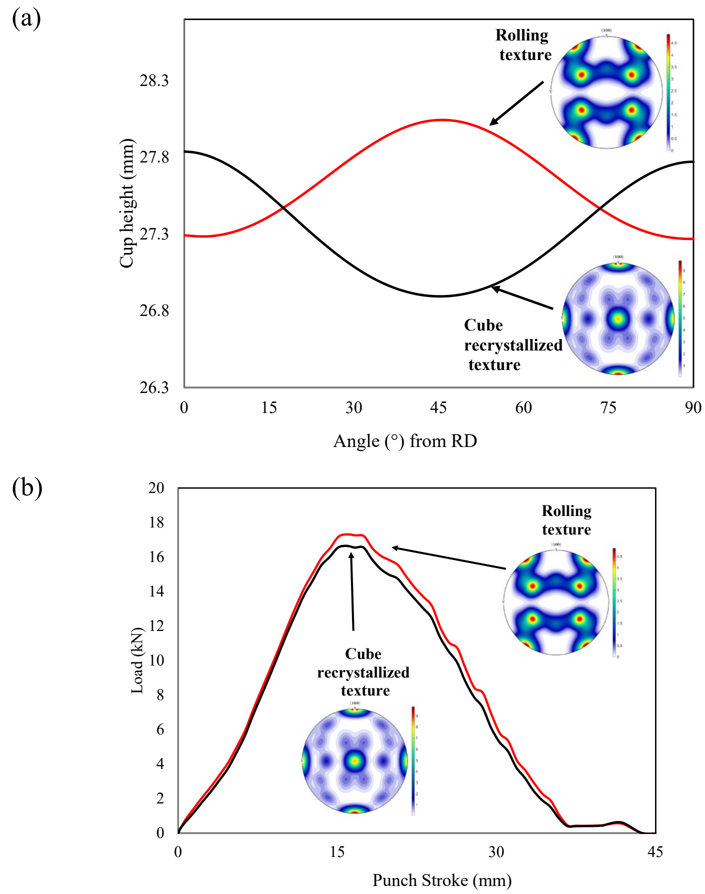

Fig. 5. Comparison of the predictions obtained with the polycrystalline model based on the Cazacu et al. [1] single crystal criterion (with $m_1 = 0.36$, $m_2 = 0.18$, $n_1 = 0.21$, $n_1 = 0.11$ $n_4 = 0.08$ and $c = 1.227$) for aluminium alloys with a cube recrystallized texture and a rolling texture, respectively: (a) earing profile; (b) forming force vs. punch stroke.

Summary

In this paper, we further illustrated the capabilities of the polycrystalline model [7] to predict the mechanical response of aluminum alloys in forming operations. Key in the formulation of this polycrystalline model is the use for the description of the plastic behavior at the crystal scale, the recent single-crystal yield criterion [1]. This cubic single-crystal yield criterion is defined for any stress state and involves the correct number of anisotropy coefficients required to satisfy the intrinsic symmetries of the cubic lattice and the condition of yielding insensitivity to hydrostatic pressure.

Using this polycrystalline model, simulation of the cup drawing process have been simulated for two aluminum alloy with different initial textures in order to investigate the influence of the initial texture on the shape of the formed part. The first material considered is characterized by a cube recrystallized texture. For this material, the polycrystalline model predicts a minimum r-value at 45° orientation and the maximum for TD. This in turn results in a predicted four ears profile with a minimum height at 45° to RD. Using the same set of material parameters, but changing the initial texture to a typical rolling texture, the polycrystalline model predict a completely different anisotropy for the material. For a rolling texture, it is predicted a minimum r-value for RD and TD while the maximum r-value is predicted for the 45° direction. Similarly, the polycrystalline model is also able to account for the influence of the initial texture on the final shape of the cup. For a rolling texture, a four ear profile with the maximum height at 45° to RD is predicted. These predictions are in agreement with experimental observations on Al alloys, i.e. the transition from a cube recrystallized texture to a rolling texture induce a transition between an ear profile with the minimum height at 45° to an earing profile with the maximum height at 45°. Furthermore, the polycrystalline model predict a slightly higher punch force for the material with a rolling texture than a material with a cube recrystallized texture.

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