Crystal plasticity and continuum mechanics-based modelling of deformation and recrystallization textures in aluminum alloys

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Abstract. This contribution provides a brief overview on modeling the deformation textures by combining both crystal plasticity approaches and models based on principles of continuum mechanics, dealing with a flow of a material during deformation. The behavior of Al alloys during deformation is analyzed by means of well-established crystal plasticity theories such as full constraints Taylor, advanced Lamel, visco-plastic self-consistent and Cluster V model. As a first approximation, the deformation flow in rolling is approximated by plane strain compression, however, it is shown that an improvement in texture prediction is reached by considering strain heterogeneities, evolved across the thickness of a rolled sheet. The effective modeling strategies employed in texture simulations are discussed in the current contribution. It is analyzed how microstructural heterogeneities might influence the evolution of recrystallization texture and plastic strain ratio in aluminum alloys.

Keywords: texture, Al alloys, deformation, recrystallization, crystal plasticity, continuum mechanics.

1. Introduction
Thermo-mechanical processing of flat aluminum products involves both deformation and recrystallization processes, which cause specific texture evolution. The crystallographic texture, evolved during thermo-mechanical processing, is mainly affected by technological parameters such as the degree of deformation, strain mode, recrystallization temperature e.t.c. The influence of technological parameters on microstructure and texture evolution can be revealed by means of numerical approaches, dealing with (i) strain distribution in deformed material, (ii) strain partitioning in polycrystalline aggregate and (iii) stress relaxation in a given crystal subjected to internal or external influence. Over the past several decades, extensive research endeavors in the field of plasticity, micro- and nano-mechanics have led to the development of various models enabling understanding of material’s behavior during plastic deformation on different length scales. The so-called engineering scale, dealing with macroscopic properties of a material such as stress, strain and hardening parameters, considers each material as a continuum and therefore the crystallographic aspects of microstructure evolution during deformation are neglected. Various aspects of continuum mechanics (CM) are incorporated for instance in finite element (FEM) or flow-line (FLM) models. Contrarily, Taylor-type crystal plasticity (CP) homogenization models [1-5], dealing with partitioning of macroscopic load in a polycrystalline aggregate, are not capable of explaining the effect of various
technological parameters on the deformation flow. Basic principles of both continuum mechanics and crystal plasticity theories extend our understanding on deformation process and enable explaining mesoscopic scale’s phenomena involved in recrystallization (RX).

Controlling the evolution of crystallographic texture during thermo-mechanical processing is of crucial importance since the texture is one of the main sources of plastic anisotropy. The main sources of anisotropy in polycrystalline systems are discussed in detail elsewhere [6]. Employing Taylor-type homogenization approaches enables modeling the anisotropy of plastic strain ratio, which in turn provides information on material’s behavior during deep drawing operation. This aspect of mesoscopic performance is of importance particularly in deep-drawing qualities of Al alloys used for instance in the automotive industry. Although many efforts have been made to model the texture development during processing chain, but there are many aspects of crystallographic texture evolution, which are still not explained by existing models. In this view, the current contribution provides a brief overview on modeling the deformation textures by combining both CP and CM approaches and employing various boundary conditions. The influence of grain interaction phenomena, incorporated in particular CP model, on the quality of deformation texture prediction is analyzed and the effective strategies employed in texture simulations are presented. It is evaluated how microstructural heterogeneities might influence the evolution of recrystallization and plastic strain ratio in aluminum alloys.

2. Experimental and Computational Procedure

Al-Mg-Si aluminum alloy from 6016 series was investigated in the current study. In order to ensure a high degree of rolling reduction in one pass, the investigated material was subjected to heat treatment at 550°C prior to cold rolling. The annealed material with fully recrystallized microstructure and the initial thickness of 1.125 mm was cold rolled to a final thickness in one pass with 47% reduction. The roll diameter of 129 mm ensured a high contact length to mean thickness ratio \((l/h = 5.86)\).

The through-thickness pre-rolling, cold rolling and recrystallization textures were measured by means of electron back scattering diffraction (EBSD) detector attached to scanning electron microscope. EBSD data were collected with Hikari type detector. The orientation contrast scans were collected and analyzed by the commercial OIM-TSL-6® software. In the case of recrystallized microstructures, the acceleration voltage of SEM was kept at 20kV, while acquisition of EBSD patterns in the deformed sample was realized at a lower acceleration voltage of 15kV in order to avoid overlapping of acquired pattern with those originating from deeper layers. The investigated samples were 70° tilted with respect to the EBSD detector, whereas the data were acquired on a hexagonal scan grid. The EBSD measurements were carried out in the plane perpendicular to the sample transverse direction (TD-plane) extending over the entire thickness of the investigated sample. The EBSD dataset of the deformed sample consists of \(\approx 5.6 \times 10^5\) indexed points and the total number of grains measured is \(\approx 5000\), whereas the number of grains sampled prior to rolling is \(\approx 8000\) with \(\approx 4.5 \times 10^5\) indexed points.

Samples for EBSD examination were prepared by mechanical grinding and polishing according to the typical procedure, finishing with 1 μm diamond paste. The final preparation step was electrolytic polishing for \(\approx 1\) min at a voltage of 18V with A2 Struers® electrolyte, cooled to temperatures ranging between -5 and 0°C.

Both measured orientation data and simulated ones were post-processed with the MTM-FHM software, developed by Van Houtte [7], to the purpose of meaningful comparison. The discrete sets of orientations obtained both from the experimental measurements and texture simulations were converted to continuous ODFs by superimposing a Gaussian peak for each individual orientation with a spread of 7° around the exact orientation. The ODFs are presented in the \(\varphi_2=\text{const}\) sections.

The texture evolution during cold rolling was predicted by taking into account only the \((111)<110>\) octahedral slip systems with the following crystal plasticity (CP) approaches: the full constraints Taylor model (FCT) [1, 2], the visco-plastic self-consistent (VPSC) model [4], the Alamel model [2, 3] and Cluster-V model [5]. For modeling purposes, the experimentally measured textures
were converted to continuous ODFs and subsequently discretized according to a method proposed by Tóth and Van Houtte [8]. According to this procedure, the total number of experimentally measured points is reduced to a set of 8000 equally weighted orientations. As a first approximation, the rolling was approximated by plane strain compression (PSC). However, in order to obtain more accurate displacement fields across the thickness of rolled materials, two-dimensional finite element calculations and flow-line modeling [9] were performed. In the FEM calculations, the isotropic material’s plastic behavior is described with the stress-strain curve fitted by piecewise linear segments, whereas the rolls were considered as fully rigid objects. The following material parameters were used in simulations for isotropic aluminum matrix: Young’s Modulus $E = 68.9$ GPa, Poisson’s ratio $\nu = 0.33$ and the yield strength $\sigma_y = 80$ MPa. In the case of FEM and FLM simulations, the displacement fields were extracted from the surface, 1/10th, 1/5th, 3/10th, 2/5th of the half thickness and mid-thickness plane. The extracted outputs were fed to the CP codes for calculation of through-thickness textures. Results obtained by FEM-CP and FLM-CP simulations were compared with the textures computed by assuming homogeneous plane strain deformation across the entire thickness in rolled materials.

3. Brief description of crystal plasticity models

Simulation of crystallographic texture evolution in a polycrystalline aggregate, subjected to an arbitrary strain mode, is generally completed by means of crystal plasticity approaches. These theories enable explaining how the macroscopic strain is translated to the mesoscopic level. Crystal plasticity models employed in the current investigation (FC Taylor [1], Alamel [2, 3], VPSC [4] and Cluster V [5]) employ diverse interaction phenomena on the grain level while considering each grain as a perfect crystal. In the full constraints approach, each grain behaves individually independently of neighbors, while the macroscopic strain velocity field $L_{ij}$ and the microscopic counterpart of individual crystal $l_{ij}$ are identical. In contrast to the FC Taylor theory, the behavior of a number of neighbors is accounted for in the grain interaction CP models [2-5]. A short-range Alamel, an intermediate-range Cluster V and a long-range VPSC models were employed for calculation the texture evolution during rolling. In the grain interaction approach such as Alamel, the polycrystalline aggregate is subdivided into a number of pairs. The equilibrium of stresses and the strain compatibility are fulfilled in the considered pair of crystals. Additionally, the interaction between grains is conditioned by the orientation of grain boundary, which is defined via grain boundary segment orientation distribution function. In the visco-plastic self-consistent model one particular grain, approximated by an ellipsoidal visco-plastic inclusion, interacts with its surroundings represented by a hypothetical homogeneous effective medium (HEM). The homogeneous effective medium represents an averaged constitutive behavior of polycrystalline aggregate surrounding a given crystal. In the self-consistent approach, the stress applied to the outer boundary of the HEM gives rise to local deviations of strain rates in its vicinity. In the constitutive law, the degree of interaction is expressed by means of so-called interaction parameter $n_{eff}$, which represents the deviation of the strain rate in particular grain with respect to the macroscopic average one. Assumption of $n_{eff}=0$ assures identical strain-rate state in each grain of a polycrystalline aggregate and this is known as full constraints Taylor or upper-bound approximation. Self-evidently, the secant formulation with $n_{eff}=1$ is fairly stiff and resembles many features of the full constraints model. By way of contrast to linearization schemes with a low value of $n_{eff}$, the tangent approximation with $n_{eff}=20$ assumes relatively uniform stress state in the polycrystalline material. As soon as $n_{eff} \to \infty$ a stress deviation diminishes to zero (Sachs model) and therefore a lower-bound approximation is maintained. Obviously, the choice of linearization scheme has a great impact on the results of texture simulation. In the current calculations, $n_{eff}$ is considered to be 10, corresponding to an intermediate grain interaction level. In the cluster V model, the polycrystalline aggregate is subdivided into a number of clusters consisting of five grains, however, each particular grain assembly is exposed to the Taylor type interaction. The grain interaction inside individual clusters is approximated by the VPSC linearization scheme with $n_{eff} = 10$. 
4. Modeling the material’s flow by continuum mechanics-based approaches

4.1 Geometrical Approaches

Plane strain compression (PSC) is the simplest geometrical approach, which is often used in approximating the rolling process. This approach primarily accounts for a change of material’s shape and enables the estimation of an important technological parameter such as strain $e$. This strain mode is justified to a large extent due to the fact that the ratio between the compressive strains ($e_{33} = -e_{11}$) and other components of strain tensor $e_{ij}$ ($i \neq j$) is large. Assuming a linear dependence of elongation change with time, the deformation gradient tensors ($F$) gains the following form:

$$F = \begin{bmatrix} \frac{h_f}{h_i} + 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{h_f}{\Delta h + h_f} \end{bmatrix}$$

where $h_i$ is the initial sheet thickness, $h_f$ is the final sheet thickness, $t$ is time ($t$ is normalized between 0 and 1) and $\Delta h = (h_i - h_f)$.

Knowing the deformation gradient tensor enables calculating the strain velocity gradient tensor $L$, which is used in crystal plasticity calculations.

$$L = \dot{F} F^{-1} = \begin{bmatrix} \frac{\Delta h}{\Delta h + h_f} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\Delta h}{\Delta h + h_f} \end{bmatrix}$$

It should be underlined that this approximation excludes both the effect of roll gap geometry and strain heterogeneity across the thickness of a sheet. In this analysis, the components of $L$ tensor might be approximated by a formula, used for the estimation of a true strain ($L_{11} = -L_{33} \approx \ln(h_i/h_f)$).

Shear strain $e_{13}$ evolving due to the roll gap geometry during rolling can be calculated by [10]:

$$e_{13} = \frac{\Delta h}{R(h_i - (\Delta h/2)^2/5)^2}$$

where $R$ is a roll radius.

Since for small strain increments $\dot{e}_{13} = 0.5(L_{13} + L_{31})$, and in this analysis $L_{31} = 0$, consequently $L_{13} = 2e_{13}$. Taking into consideration that $e_{13}$ strain is mainly concentrated within a thin sub-surface layer, it is reasonable to assume an exponential character of the shear strain distribution:

$$e_{13}^s = e_{13} \exp \left( \frac{s-1}{s} \right)$$

here, the superscript $s$ indicates the position of a given layer with respect to the surface of a sheet. In the equation $s$ might change between 0 and 1: $s=1$ for the surface while $s=0$ for the mid-thickness plane.

Combining equations 2-4 enables calculation of strain velocity gradient tensor $L^s$ for various thickness layers $s$:

$$L^s = \begin{bmatrix} \frac{\Delta h}{\Delta h + h_f} & 0 & 0 \\ 0 & 0 & 2e_{13}^s(h_f + h_f) \\ 0 & 0 & \frac{\Delta h}{\Delta h + h_f} \end{bmatrix}$$

4.2 Finite element modeling

In order to account for the effect of various rolling parameters such as the reduction level, the initial sheet thickness, the friction conditions, the circumferential velocity of the rolls, and their diameter on the deformation flow, finite element simulations were performed. The behavior of anisotropic material was studied. It is important to note that the FEM outputs depend on the choice of friction condition. Inasmuch as the rolling was performed on well-lubricated surfaces of both sheet and rolling cylinders, the deformation with a constant Coulomb friction coefficient $\mu$, slightly exceeding the minimum value necessary for rolling ($\mu = 1.1 \cdot \mu_{\text{min}}$), was assumed in this study. The value of $\mu_{\text{min}}$ was approximated by the following formula [11]:
4.3 Flow line modeling

Flow line model is an analytical solution of continuum mechanics-based equations, describing the material’s flow in rolling under predefined boundary conditions. In the FLM, developed by Decroos et al [9], a kinematically admissible displacement velocity field fulfills the following boundary conditions: (i) material’s velocity is uniform across the thickness at the entrance and the exit of the rolling process, (ii) the incompressibility condition is fulfilled at all points of the rolled material, (iii) material strictly follows the prescribed streamlines in the middle and surface of the plate, while some deviation from the predefined stream-lines is allowed for other layers, (iv) at the surface, the velocity field is prescribed by means of model parameter $\alpha$ that is linked to the friction conditions between the rolls and the plate ($\alpha$ ensures a difference between velocities of surface and mid-thickness layers), (v) the variation of the velocity across the thickness is conditioned by the $n$-th power law. The comprehensive mathematical description of this approach is described by Decroos et al [9]. In the current contribution the model parameters $\alpha$ and $n$ are set as to resemble the deformation patterns, calculated by FEM.

5. Rolling texture simulation

Prior to cold rolling, annealing process has ensured a strong recrystallization texture (Fig.1), which tends to transform to the $\beta$ fiber described analytically by [12]:

$$\{h, 1, h+1\} \left( \frac{2h(h+1)}{3/4-h}, \frac{2h(h+1)}{1/2-h}, \frac{h}{h-3/4}, \frac{2h}{h-1/2} \right)$$

(7)

Fig. 2 reveals the distribution of $L_{ij}$ components calculated by equations 2 and 5. It is obvious from Fig. 2 that the shear component $L_{13}$ drastically diminishes from the surface toward the mid-thickness independently of the model used. The shear components $L_{13}$, calculated by formula 5, are significantly smaller compared to ones computed either by FEM or FLM. Fig. 3 shows results of texture simulations with various both CP and continuum mechanics-based approaches.

The quality of texture simulation is assessed by means of texture index difference ($TID \equiv \int \left( f_{exp}(g) - f_{sim}(g) \right)^2 dg$), which rises with the increase of differences between the compared ODFs. The CP models are capable of reproducing individual texture components along the $\beta$-fiber as well as the retained RX orientation with various degree of accuracy. A short-range grain interaction of the Alamel model accounts for the most accurate texture prediction, independently of strain mode approximation. Both, the intermediate and long-range grain interaction schemes, incorporated in the Cluster V and VPSC models respectively, provide the second most successful and at the same time very comparable and texture prediction. Regarding CM approaches, both FEM and FLM are superior over the geometrical approximations. It seems that computationally less heavy flow line model is capable of providing texture prediction comparable to one simulated with the $L_{ij}$ obtained from the finite element model, independently of CP approach employed.
Fig. 2. Strain velocity gradient components $L_{ij}$ calculated for various boundary conditions: a) PSC, equation 2; b) PSC+$e_{ij}$, equation 5; (c-e) FEM; (f-h) FLM. For a meaningful comparison, time $t$ is normalized between 0 and 1.
6. Modeling the influence of recrystallization texture on plastic strain ratio

Many of the principles and concepts addressed by the above-discussed CP models also apply to RX phenomena. Various RX modeling approaches [13-16] are based on orientation selection or determination of nucleation spectra, considering the diversity in dissipation of plastic power in different crystal orientations. This is of particular importance while investigating the effect of microstructural heterogeneities on the evolution of recrystallization texture. The evolution of nucleation spectra in the bulk of a material as well as at micro shear bands or in the particle affected deformation zone might be explained by RX models considering both basic principles of micromechanics and crystal plasticity approaches [15-18].

Accounting for strain path heterogeneities in the vicinity

Fig.3. Simulated textures with different both crystal plasticity and continuum mechanics-based approaches. The TID number for a given pair of CP and CM models is indicated on the corresponding ODF section.

Fig.4. Simulated $r$-value profiles with the Alamel model.
of non-deformable inclusions allows explaining the appearance of the P \(\{111\}<233>\), \(\{100\}<130>\) or weak \(\gamma\)-fibre \(\langle111\rangle//\text{ND}\) orientations, which typically evolve in particle containing Al alloys [15, 16]. Likewise, considering strain path deviations inside the copper-type shear bands from the macroscopic one sheds light on the evolution of P, Goss \(\{011\}<100>\) and Q \(\{013\}<231>\) orientations [17, 19]. The evolution of mentioned texture components has a decisive influence on anisotropy of plastic strain ratio, which measured in tension at various angles with respect to rolling direction (RD). The conventional measure of plastic anisotropy (Lankford value or \(r\)-value) can be modelled by means of CP approaches with reasonable accuracy [18]. The normal anisotropy \(\bar{r}\) is calculated from the ratio of a true strain in the sheet transverse direction to the logarithmic strain in the sheet normal direction at various angles to RD and averaged by a trapezoidal rule, while the degree of planar anisotropy \(\Delta r\) is assessed based on the \(r\)-value profile in the plane of a rolled sheet. Fig. 4 reveals the effect of various hypothetical RX textures on the plastic strain ratio. First, the \(r\)-value profile of a material, characterized by a strong Cube \(\{001\}<100>\) mixed with weaker Goss texture, is examined (Fig.4, texture A). This type of texture often dominates in Al-alloys [18,19, 20] after recrystallization and tends to produce a V-shaped \(r\)-profile with a local minimum at \(-45^\circ\) with respect to RD (Fig.4, Lankford profile A). The estimated normal anisotropy for the A-type texture (\(\bar{r}=0.72\)) might ensure a minimum level of deep drawability, however, the high value of in-plane anisotropy (\(\Delta r=1.29\)) makes this material inappropriate for deep drawing applications. In ideal case, the in-plane anisotropy should be minimized to zero and this can be accomplished by texture randomization. Taking into consideration that it is almost impossible to produce an isotropic material with a random texture, it is assumed here that the strongly textured material A is randomized, and, as a result a B-type texture is evolved, consisting of a weakly developed Cube and Goss components (Fig.4, texture B). The A and B-type textures are qualitatively identical, while the quantitative diversity accounts for significant changes in Lankford profiles. Even if the normal anisotropy of B-type texture (\(\bar{r}=0.8\)) did not improve drastically as compared to A-type counterpart, the planar anisotropy (\(\Delta r=0.47\)) reveals considerable improvement. It is evident that even after severe texture randomisation the \(r\)-value is still anisotropic, i.e. dependent on the direction of the tensile sample axis. It should be mentioned, that during thermo-mechanical processing, the evolution of particular texture component occurs at the expense of other orientations. For instance, the evolution of Cube-oriented grains, which dominate in Al alloys after recrystallization, can be suppressed by activating nucleation at microstructural heterogeneities (shear bands) or via particle stimulated nucleation (PSN) mechanism. Each nucleation phenomenon produces characteristic orientation spectrum, as noted previously. Since texture weakening caused either by PSN or via nucleation at shear bands is not of random nature, it is assumed that the A-type texture is randomized by the P, Q, weak \(\gamma\)-fibre and components scattered around these orientations. The resulting C-type texture (Fig.4) serve to produce a V-shaped \(r\)-profile with \(\bar{r}=0.75\) and \(\Delta r=0.32\). Even though the normal anisotropy remains far below the desired value of \(\bar{r}=1\), the planar anisotropy seems to be acceptable for deep drawing.

Fig. 4 clearly demonstrates that the presence of orientations, originating from microstructural heterogeneities (P and Q) which evolve at the expense of components evolved in the bulk of a material, leads to decrease in planar anisotropy while the value of normal anisotropy does not improve significantly. In summary, application of CP models enables explaining the evolution of crystallographic textures and related properties in materials with various crystal structures [18, 21-23].

7. Conclusions
Analyzing the quality of texture simulation indicates that grain interaction phenomena, incorporated in CP calculations, play far more important role than CM-based approximation of deformation. Approximation of strain path by either FEM or FLM is superior over the geometrical approximations. Analytical flow line model combined with a given CP approach is capable of providing texture prediction as accurate as one simulated with the strain path obtained from the FEM.
The improvement of texture prediction by the Alamel model justifies the importance of short-range grain interactions in CP modeling. It seems that the intermediate grain interaction, incorporated in the Cluster V model, is the second most important homogenization scheme, occurring during deformation. Since the quality of simulation by the VPSC model is comparable to the Cluster V approach, this suggests that long-range grain interactions cannot be neglected while modeling the texture evolution. Modeling the plastic strain ratio with CP models indicates that presence of texture components, originating from microstructural heterogeneities, tends to decrease the planar anisotropy and, thus, enhances the forming characteristics of a material.

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