Modeling continuous dynamic recrystallization of lightweight alloys by coupling polycrystal plasticity approach

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Abstract. In the thermo-mechanical process of lightweight alloys, such as aluminum alloys, complex microstructure evolutions are inevitably involved via the continuous dynamic recrystallization (CDRX) featured with extensive formation of subgrains followed by progressive transition into new grains. In this study, a novel fully integrated CDRX-VPSC (visco-plastic self-consistent) model is established. First, numerical formulations for formation and rotation of subgrains are addressed by reasonably tackling the grain boundary characteristics, and also the concept of generation for CDRX grains is newly introduced. By considering these two aspects, the grain population is updated according to the complex grain boundary evolutions. In the VPSC module of the integrated modeling, the shear strain rate, dislocation density, and orientation are calculated to update the grain populations and grain sizes in the CDRX module. The validation of the proposed model is conducted by simulating the hot compression of extruded AA7075 sheet, in which the DRX mechanism is controlled by the subgrain related dynamic recovery (DRV) and CDRX. The simulated flow stresses, microstructural evolutions (grains size and DRX fractions), and texture features agree well with reported experimental observations.

1. Introduction
High strength aluminium (Al) alloys, such as AA 7075 alloy (or Al-Zn-Mg-Cu alloy), has been widely used for manufacturing structural components for aircrafts and automobiles in recent years [1]. For AA7075 alloy with an inferior formability at ambient temperature, thermal-mechanical processes, including forging, extrusion and stamping, are widely applied. During hot forming process, the material usually undergoes complex microstructure evolution via dynamic restoration, e.g., dynamic recovery (DRV) and dynamic recrystallization (DRX) [2].

In past decades, intensive experimental studies on AA7075 alloy have been conducted [3-6]. Sun et al. [3,7] investigated the dynamic restoration behavior of an extruded AA7075 alloy during compressions at a wide temperature and strain rate range (250 ~ 450 °C and 0.01 ~ 10 s⁻¹). The results indicate that DRX behavior under investigated conditions is mainly governed by continuous DRX (CDRX), during which new recrystallized grains (e.g., CDRX grains) are formed via the formation and rotation of sub-boundaries (e.g., subgrains). Yang et al. [4] suggested that the cold rolled AA7075 alloy (> 0.4 strain) could exhibit superplasticity during sequent hot tension at low strain rate (< 2.9×10⁻³), in
which CDRX occurs with the assistance of grain boundary sliding (GBS). Besides, the CDRX behavior of AA 7075 alloy is also closely related to the initial grain size [5].

Based on these results aforementioned, it reveals that the CDRX is a complicated process involving formation of subgrains identified with low angle boundaries (LAGBs) and gradual evolution to CDRX grains bounded with high angle boundaries (HAGBs). Thus, modeling the microstructural evolution during CDRX is of great essential to optimize the parameters for hot forming processing. However, differentiating with the wide existence of DDRX modeling, few CDRX model are available because of its physical complexity [2,8]. Gourdet and Montheillet [9] proposed a simple internal-state-variable (ISV) model, which show the capability to capture the stress-strain curve, crystallite size, and misorientation distribution of LAGBs. Recently, Sun et al. [7] modified this ISV model and applied it for the extruded AA7075 alloy. Although great efforts were paid in their works [7,9], it still lacks modeling implementation of CDRX grain generation, that is, the DRX fraction and DRX grain size can’t be predicted. Moreover, the grain orientation, as an important feature of grain, is also hardly captured by ISV method. In addition, the ISV method treats all the grain with same deformation behavior, e.g., the grain level heterogeneity deformation is totally ignored.

In this study, we establish fully coupled VPSC-CDRX model, which implements the key formulations of CDRX grain generation and constrained grain growth into the well-known VPSC model. The current paper realizes the coupled computation of mechanical response, microstructural evolution (sub- and CDRX grain), crystallographic texture and deformation modes. In section 2, the summary of theoretical model is described, but whole derivation and detailed discussion can be referred to the authors other paper [10].

2. Fully coupled VPSC-CDRX model

2.1. Dislocation density based hardening law for VPSC model

In VPSC model, the plastic deformation of each grain is coordinated by slipping (or twinning). The shear rate $\dot{\gamma}^s$ of slip (or twinning) system $s$ can be expressed by a power law [11]:

$$\dot{\gamma}^s = \dot{\gamma}_0 \frac{\sigma : p^t}{\tau_c^s} \text{sgn}(\sigma : p^t) \tag{1}$$

where the $\dot{\gamma}_0$ is reference shear strain rate and $m = 20$. $\tau_c^s$ is the critical shear resolved shear stress, $\sigma$ is the applied stress, and $p^t$ is the Schmid tensor dependent on grain’s orientation.

As well known, the slip resistance ($\tau_c^s$ in Eq. (1)) is mainly decided by the dislocation interactions [12]. In this work, a modified Kocks and Mecking (K-M) equation is proposed to consider the influence of the formation and rotation on the dislocation density evolution, which can be expressed as [13]:

$$\dot{\rho}^s = k_b \sqrt{\rho^s} \dot{\gamma}^s - k_1^s(T,\dot{\gamma}^s)\rho^s \dot{\gamma}^s - k_2^s(T,\dot{\gamma}^s)\rho^s \dot{\gamma}^s \tag{2}$$

where the $\dot{\gamma}^s = \sum_{s\in c}\dot{\gamma}^s_{1,2} |$ which is the sum of absolute shear strain rate of slip (or twinning) system $s$ belonging to the certain slip (or twinning) mode $\alpha$. The first term indicates the dislocation accumulation; second and third terms are the dislocation annihilation term (denoted as $\dot{\rho}^{\alpha+}$) and particular dislocation term related to subgrain formation and rotation (denoted as $\dot{\rho}^{\alpha-}$), respectively.

As suggested by Beyerlein and Tomé [14], the slip resistance can be calculated as:

$$\tau_c^s = \tau_0^s + \chi_1 \mu(T) b^s \sqrt{\rho^s} + \chi_2 \mu(T) \frac{b^s}{\delta_{sub}} \tag{3}$$

where $\chi_1$ and $\chi_2$ are material constants, $b^s$ is the length of Burgers vector of mode $\alpha$. $\mu(T)$ is the temperature dependent shear modulus. In Eq. (3), $\tau_0^s$ is the initial resistance. The second and third increased items origin from the barrier effects of forest dislocation and grain boundaries.
2.2. Physically based CDRX model

2.2.1. Formation and rotation of subgrain boundary. Given the wide discussions, the dislocation density (or its stored energy) serves as an effective tool for bridging the plastic deformation and microstructural changes. For LAGB with its miorientation \( \theta \) being less than a critical \( \theta_c \) (usually taken as 15\(^\circ\)), a simple and classical relationship \( \theta = b / D \) can be estimated, where \( D \) assumed to be \( 1/\sqrt{\rho} \) is the spacing distance between two neighbouring dislocations [15]. Considering the contribution of different slip modes, \( \rho^2 = \sum_i \rho_i^2 \), the formation rate of the new LAGB area per volume with a low initial misorientation \( \theta_0 \) (set to be 1\(^\circ\)) can be formulated as [9]:

\[
\dot{S}_{\text{sub}} = c_1 \left( \frac{b}{\theta_0} \right) \rho^2.
\]  
(4)

After the LAGB formation, its misorientaiton \( \theta \) increases with the successively absorbing the dislocations into the boundary. The rotation rate of the LAGB (e.g., subgrain boundary) is manly affected by fraction of HAGBs, dislocation density, strain rate, grain boundary energy, and grain size. In addition, a discrete approach is used, which is inspired by the wide application of EBSD measurements where the misorientation angle of grain boundary can be statistically quantified. Thus, the rotation rate of LAGB with a discrete angle \( \theta_i \) can be established as:

\[
\dot{\theta}_i = c_2 (1-f_{HAGB}) f_{\text{sub},i} b \left[ (1-c_1) \rho^2 \right]^{3/2} \frac{E_i}{d_p} \left( \frac{d_0}{d_n} \right)^{1/3}.
\]  
(5)

where \( c_2, \xi_1 \), and \( \xi_2 \) are fitting constants, and \( f_{HAGB} \) is the area fraction of HAGBs. \( f_{\text{sub},i} \) and \( E_i \) are the area fraction and energy of LAGB with a misorientation \( \theta_i \). \( d_0 \) and \( d_n \) are the reference and initial grain sizes used.

2.2.2. Evolution of subgrain boundary. During hot forming, the area of subgrain boundaries increases with the formation of new LAGBs, as indicated in Eq. (1). When the misorientation angle of LAGB is increased the critical \( \theta_c \), it evolves to be HAGBs. Besides, the subgrain boundaries may also be swept by the migration of recrystallized grain boundary, which in turn reduces the sub-boundary area. And therefore, the area of subgrain boundary can be updated by a rate as:

\[
\dot{S}_{\text{sub}} = c_3 \left( \frac{b}{\theta_0} \right) \rho^2 - f_{\text{sub},N} S_{\text{sub}} \dot{\theta}_N - c_3 S_{\text{sub}} S_{\text{rec},m} S_{\text{rec},n}^{1/2} v
\]  
(6)

where \( c_3 \) is a material constant. \( f_{\text{sub},N} \) is the area fraction of subgrain boundaries with the maximum misorientation \( \theta_0 \). \( S_{\text{sub}} \) is the total area of subgrain boundary. In accordance with the changes in subgrain boundary, \( S_{\text{rec}} = f_{\text{sub},N} S_{\text{sub}} \dot{\theta}_N \) is increase rate of the area of new recrystallized boundary with. In addition, \( S_{\text{rec}}^+ \) and \( S_{\text{rec},m} \) are the total area and mobile area of recrystallized grain boundary. \( v \) is the migration speed of recrystallized grain boundary. The term \( (S_{\text{rec},m} / S_{\text{rec}})^{1/2} \) is introduced to integrate the constrained grain growth. For the detail discussion of immobilization process of recrystallized grain boundary, it is referred to [10].

2.2.3. Generation of CDRX grains and CDRX fraction. With the continuous formation of HAGBs, new CDRX grains are induced. By taking advantage of reasonable tracking of formation of new HAGBs, we propose a generation criteria for new CDRX grains in a physical perspective. With the assumption of spherically shaped grains, this generation rate can be calculated as

\[
\dot{\rho} = c_4 (1-f) \frac{d_0^3}{2 \delta_n^2} S_{\text{rec}}^+.
\]  
(7)
where $c_3$ is a material constant.

In general, the increase of the CDRX fraction is contributed by two aspects: (i) generation of new CDRX grains with the initial size of $r_0$, which is set to be same with the temporal subgrain size when it is formed; (ii) growth of existing CDRX grains [10].

2.3. Model application to AA7075 alloy

The coupled VPSC-CDRX model is applied to simulate the uniaxial hot compressions of an extruded AA7075, reported by Sun et al. [3,7]. For Al alloy, only 12 {111}<110> slip systems are considered during all the simulation. The parameters of VPSC-CDRX model can be classified into two types: (i) hardening parameters of matrix and DRX grains. The hardening parameters of matrix are fitted to flow stress curves before peak stresses. For CDRX grains, the hardening parameters are determined by fitting the softening curves (after the peak stresses). (ii) parameters for the evolution of subgrain and recrystallized grain boundary areas, as well as for DRX grain formation and growth. The DRX parameters are determined from the softening behavior and microstructural characteristics. The exact values of initial and fitting parameters used for the coupled VPSC-CDRX simulation is not presented here for simplification, and there can be found in [10].

3. Results and discussions

3.1. Flow stress

Fig. 1 compares the predicted stress–strain curves (lines) by the VPSC-CDRX model and their comparisons with experimental results (symbols). As can be seen, good agreement between experiment and prediction is attained, which evidences that the proposed VPSC-CDRX model can capture the mechanical responses during hot deformation.

At initial straining, all the curves show rapid strain hardening. Moreover, the flow stress becomes higher under lower temperatures and higher strain rates. Under strain rates of 0.01 s$^{-1}$ (Fig. 1(a)), the single peak stresses are observed at small plastic strains (< 0.05). After this, the stresses gradually soften and saturate with further straining. Whereas, for the strain rate of 10 s$^{-1}$ in Fig. 1(b), the flow stress is almost constant after early hardening, that is, no obvious peak stress exists. These unique features of mechanical responses are well reproduced by the proposed VPSC-CDRX model. At low temperature and high strain rate(623 K and 10 s$^{-1}$), deviation between experiment and simulation appears at small plastic strain mainly, which mainly comes from the somewhat quick multiplication of dislocation (density).

![Fig. 1. Comparison of predicted with measured flow stress at: (a) 0.01 s$^{-1}$, and (b) 10 s$^{-1}$ [10].](image)

3.2. Evolution of DRX volume fraction

Fig. 2 shows the evolution of calculated DRX fractions under different temperatures and strain rates as well as experimental results at 0.7 strain. It suggests a reasonable capture of the experimental DRX
behavior via the proposed VPSC-CDRX model.

From the results in Fig. 2, two evolution tendencies for DRX fraction can be summarized as follows: (i) at constant temperature, the DRX fraction decreases dramatically with the strain rate increasing. This indicates that the major dynamic restoration mechanism changes from DRX to DRV under increased strain rates, which is consistent with the experimental observations [3,6,16]; (ii) under a constant strain rate, the DRX fraction increases with temperature rising, and the differences among various temperatures become larger with the deformation proceeding. At 10 s$^{-1}$, the DRX fractions for 623 K and 673 K are almost the same.

For all deformation cases, the accumulation of the DRX fraction begins at small strain ($< 0.05$), which explains the early appearance of peak stress, as shown in Fig. 2. From Eq. (3), the hardening effect contributed by subgrain boundaries is close related to size of subgrain (i.e., the third term in Eq. (3)). At 10 s$^{-1}$, the sizes of subgrain are less than 1.5 μm. Thus, a relatively obvious hardening effect is introduced, which can exceed the limited flow softening from the very low DRX fractions ($f_{\text{DRX}} < 0.05$ till 0.8 strain). Because of this, there is no obvious peak stress in the flow stress of Fig. 1(d).

Fig. 2. Evolution of DRX volume fractions (lines) with different temperatures and strain rates and experimental results (symbols) at strain of 0.7 exacted from EBSD and OM images in Sun’s work by Image-Pro Plus 6 software [10].

3.3. Evolution of subgrain and DRX grain size

Fig. 3 compares the predicted and measured average subgrain and DRX grain sizes at 0.7 strain as well as the subgrain size at 1.2 strain. As shown in Fig. 3(a), the DRX grain size is larger than that of subgrains under the same deformation condition. However, this size differences in sub- and DRX grain size is limited, where the maximum size difference is still less than 1 μm because of the constrained grain growth. This prediction is well supported by the comparison of experimental subgrain and DRX grain sizes (symbols in Fig. 3(a)). Moreover, the DRX grain size increases as the temperature increases under a constant strain rate. With the strain increasing to 1.2, the experimental subgrain sizes are well predicted by the VPSC-CDRX model, again. These agreements prove the capability of VPSC-CDRX model to depict the evolution of microstructural features.
Conclusions

In this paper, a novel VPSC-CDRX model is proposed for the first time. Given as the formulations and agreements between the predicted and experimental data, the following results can be summarized:

1. Based on the widely experimental observations, a new CDRX model was proposed. In this new model, several key issues are stressed, including the reasonable reformulations of the formation and rotation of subgrain boundaries, “generation” rate of CDRX grains, and the constrained grain growth caused by immobilization process.

2. The framework of the VPSC-CDRX is well established by integrating the proposed CDRX model into the well-developed VPSC crystal plasticity model.

3. The mechanical responses and evolution of subgrain size for extruded AA7075 alloy could be reasonably predicted under various temperatures and strain rates. Furthermore, the predicted evolution of the DRX grain size and DRX fraction agreed with the experimentally reported results.

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