Prediction of tensile deformation behavior of Al-Li alloy 2060-T8 by computational homogenization-based crystal plasticity finite element method

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Abstract. In current study, a computational homogenization-based crystal plasticity (CP) modelling was presented to determine the deformation behavior of a novel third-generation Al-Li alloy 2060-T8 at room temperature, strain rate of 0.01 s\(^{-1}\) and various loading directions. The computational homogenization strategy used a representative volume element (RVE) which describes the real microstructure of AA2060-T8 sheet to consider the in-grains deformation behavior. Besides, a periodically boundary condition was modified to consider both deformation induced anisotropy and the geometrical anisotropy. The initial microstructures and micro-textures of the AA2060-T8 sheet were determined by EBSD measurements, as well as used to build up the RVE model. The material parameters used in CP modelling was determined from the stress-strain curve obtained from the tensile test at strain rate of 0.001 s\(^{-1}\) and loading direction of 30° with reference to rolling direction. The results obtained from computational homogenisation strategy keep a remarkable agreement with the results determined from experimentation. In conclusion, the computational homogenization based CPFEM is able to predict the deformation behavior and capture the anisotropic response of AA2060-T8 sheet at various deformation conditions.

1. Introduction

Recently, the 3rd generation Al-Li alloys is attractive for military and aerospace applications because their properties are superior compared to those of conventional Al alloys. In 2011, Alcoa Company introduced AA2060-T8 as a new 3rd generation Al-Li alloys to supersede AA2024-T3 and AA7075-T6 for fuselage, upper and lower wings structures [1]. Despite AA2060-T8 alloy displays superior mechanical and physical properties, it exhibits poor formability at room temperature, which impedes its broad applications. The existence of crystallographic texture leads the AA2060-T8 to exhibit anisotropic mechanical properties during deformation [2]. Because of AA2060-T8 alloy was introduced since few years, few studies were accomplished to figure out the relation between the mechanical response and crystallographic texture of this alloy. Accordingly, it is crucial to investigate the deformation behavior, and govern the factors which influence the anisotropic response and formability of AA2060-T8 at different deformation conditions to associate the mechanical response of this alloy with the microstructural state.
Therefore, in current investigation, a computational homogenization framework based on crystal plasticity finite element modelling is proposed to predict the deformation behavior of AA2060-T8 at room temperature and strain rate of 0.01 s\(^{-1}\). The predictability of the proposed strategy to determine the macroscopic response of AA2060-T8 is validated by comparing the experimental results with those obtained from simulation. Further verification was accomplished by calculating important statistical parameters such as R (correlation coefficient), AARE (average absolute relative error), RMSE (root mean square error), as well as NMBE (normalized mean bias error) to quantitatively measure the predictability of the proposed method.

2. Experimentation

2.1. Material description

The chemical composition and the microstructure of as-received AA2060-T8 sheet is shown in Table 1 and figure 1, respectively.

**Table 1.** The chemical composition of the AA2060-T8 observed through OES

| Li  | Cu  | Mg  | Ag  | Zr  | Mn  | Zn  | Al  |
|-----|-----|-----|-----|-----|-----|-----|-----|
| 0.75| 3.95| 0.85| 0.25| 0.11| 0.3 | 0.4 | Balance |

2.2. Uniaxial tensile tests

The tensile tests were carried out using A 100 kN Instron m/c at room temperature and strain rate of 0.01 s\(^{-1}\). The samples used in tensile tests were machined in various angles (i.e. 0°, 30°, 45°, 60°, 90°) to the rolling direction (RD). The stress-strain curves of AA2060-T8 at strain rate of 0.01 s\(^{-1}\) and various loading directions are shown in figure 2.

As depicted in figure 2, AA2060-T8 is displaying an obvious anisotropic behavior, which signifies that the tensile deformation behavior of this alloy is obviously relying upon the loading directions.

3. Computational homogenization-based crystal plasticity modelling

In order to predict the tensile deformation behavior of polycrystalline materials by computational homogenization-based crystal plasticity modelling, three vital features are required. These features are a constitutive model that describe the behavior of grains; realistic description of the microstructure via RVE model; and set of material parameters. The following section will discuss briefly the details of each feature used in current investigation.

3.1. Crystal plasticity model

A dislocation density-based single crystal plasticity model has developed and implemented as a UMAT subroutine in ABAQUS finite element code. Some details about the constitutive model is described
below. The model assumes a multiplicative decomposition of the deformation gradient into the elastic and plastic components [3, 4] as:

\[ F = F^e F^p \]  

(1)

where, \( F^e \) depicts the stretch and rotation of the slip systems from \( \tilde{F} \) to the present configuration. On the other hand, \( F^p \) defines the material point in the reference configuration with respect to the intermediate configuration \( \tilde{F} \), keeping the structure of lattice unaltered.

The spatial velocity gradient tensor (\( L \)) can be additively decomposed also into its elastic and plastic parts as \( L = L^e + L^p \) and \( L = F F^{-1} \), so, \( L^e = \tilde{F} F^e F^{-1} \) and \( L^p = F^e \tilde{F} F^p F^{-1} \), therefore

\[ L = F^e F^{-1} + F^e \tilde{F} F^p F^{-1} \]  

(2)

where, the spatial velocity gradient described in \( \tilde{F} \) is \( \tilde{L}^p (= F^p F^p^{-1}) \). The evolution of the plastic flow, which is the sum of the shear rates on overall slip systems, can be introduced as:

\[ \dot{\Gamma}^p = \sum_{\alpha=1}^{n} \dot{\gamma}^\alpha \mathbb{S}^\alpha, \quad \mathbb{S}^\alpha = m_0^\alpha \otimes n_0^\alpha \]  

(3)

where, \( \dot{\gamma}^\alpha \) is the shearing rate on the \( \alpha \)-slip systems, besides, orientation tensor \( \mathbb{S}^\alpha \) describes the slip systems with slip direction \( m_0^\alpha \) and slip-plane normal \( n_0^\alpha \) [3, 4]. For F.C.C crystals, the crystallographic slip is supposed to take place on twelve \( \{111\} \{110\} \) slip systems. The slip direction (\( m^\alpha \)) in the current configuration and the equivalent slip plane normal (\( n^\alpha \)) are defined as:

\[ m^\alpha = F^e m_0^\alpha, \quad n^\alpha = n_0^\alpha F^{-1} \]  

(4)

where, we assumed that \( m_0^\alpha \) and \( n_0^\alpha \) are orthogonal to each other. A hyper-elastic constitutive model is used to describe the mechanical behavior of single crystals, so, the stress-strain relationship was defined by the Helmholtz free energy per unit volume, \( \psi \). In most crystalline alloys, the elastic deformation is infinitesimal compared to the plastic deformation, thus we assume the functional form of the Helmholtz free energy as a quadratic form of the elastic Green-Lagrange strain on \( \tilde{F}, E^e \). Thus,

\[ \psi(C^e) = \frac{1}{2} E^e : \mathbb{C} : E^e, \quad \text{with} \quad E^e = \frac{1}{2} (C^e - I) \quad \text{and} \quad C^e = F^e T F^e \]  

(5)

where, \( \mathbb{C} \) is the fourth-order anisotropic elasticity tensor and \( I \) are the identity tensor respectively. Thus, the constitutive equations for the stress response, by the relationship \( T^e = \frac{\partial \psi}{\partial E^e} \), thus, the stress power per unit volume in \( \tilde{F} \) is introduced by

\[ \omega^p = (C^e T^e) \tilde{L}^p \]  

(6)

The flow rule which relates the slip shearing rates on the arbitrary slip systems with the resolved shear stresses can be defined as [3, 4]:

\[ \dot{\gamma}^\alpha = \gamma_0 \exp \left[ \frac{F_0}{k_B \theta} \left( 1 - \frac{|\tau^\alpha - S_{\alpha}^S|}{\tau_0 n^\alpha / \mu_0} \right) \right] \text{sgn}(\tau^\alpha) \]  

(7)

where, \( \gamma_0 \) is a reference slip rate, \( k_B \) is Boltzmann constant, \( \theta \) is absolute temperature and \( F_0 \) is the lattice friction at 0 K. Besides, \( F_0 \) is the Helmholtz free energy of activation, as well as \( \mu_0 \) and \( \mu \) are the shear moduli at 0 and 0 K respectively. Finally, the resolved shear stress tensor (\( \tau^\alpha \)) is illustrated by:

\[ \omega^p = \sum_{\alpha} \tau^\alpha \gamma^\alpha, \quad \text{so,} \quad \tau^\alpha = (C^e T^e) \mathbb{S}^\alpha \]  

(8)

The total athermal slip resistance parameters \( S_{\alpha}^T \) were taken to evolve through the generalized Taylor law [4] as:

\[ S_{\alpha}^T = \frac{\lambda \mu b}{\sum_{\beta=1}^{N} h_{\alpha \beta} \rho_T^\beta} \]  

(9)

where, \( \lambda, \mu, b, h_{\alpha \beta} \) are the statistical coefficient clarifying the deviation from the regular spatial arrangement of the dislocation densities, the shear modulus, the magnitude of the Burgers vector, and the dislocation interaction matrix respectively.
In order to reflect their different mobility, the total statistically stored dislocation density can be additively decomposed into edge and screw types as:

\[ \rho^a_T = \rho^e_T + \rho^s_T \]  \hspace{1cm} (10)

where \( \rho^a_T \) is the pure edge dislocation density and \( \rho^s_T \) is the screw dislocation density. Cheong et al. [4] proposed evolution models for the components of both screw and edge dislocation density through formulating the balance laws between the dislocation generation and annihilation:

\[ \dot{\rho}^e_T = \frac{C_e}{b} \left[ K_e \left( \sum_{b=1}^{N} \rho^b_T \right)^2 - 2d_e \rho^e_T \right] \left| \gamma^a \right| \]  \hspace{1cm} (11)

\[ \rho^s_T = \frac{C_s}{b} \left[ K_s \left( \sum_{b=1}^{N} \rho^b_T \right)^2 - \rho^e_T \left( K_s \pi d^2_s \sum_{b=1}^{N} \rho^b_T - 2d_s \right) \right] \left| \gamma^a \right| \]  \hspace{1cm} (12)

where, \( C_e \) and \( C_s \) are the fraction of the total slip rate contribution by edge and screw segments, respectively. Besides, \( K_e \) and \( K_s \) are dimensionless proportionality constants controlling the mobility of the dislocations, also, recovery processes are associated with the terms, \( d_e \) and \( d_s \), which give the maximum distances for mutual annihilation between antiparallel edge and screw dislocations to take place, respectively.

3.2. Computational homogenization framework

Computational homogenization method is basically relying upon the characteristics and finite element simulation of the RVE model of the microstructure. In this study, grain-based RVE model was used since it determine the in-grain heterogeneous deformation produced in the grains via discretizing each grain to many sub-grains by many finite elements. Thence, it can efficiently contains more details about the distribution of the grain sizes and shapes in polycrystalline metals. In recent investigation, it’s assumed that the polycrystalline RVE has an equiaxed grain shapes. The grain-based RVE model was generated by the neper software, which can generate a polycrystal RVE model. The RVE model was discretized \( 100 \times 100 \times 100 \) C3D8R elements as shown in figure 3 (a). The mechanical behavior of the proposed RVE model was determined obtained by the finite element modelling. The proposed RVE model was directly used as a finite element meshes (each voxel corresponding to one cubic finite element). The periodic boundary condition (PBC) was applied on the cubic cell faces because the homogenized polycrystal behavior obtained under these conditions is usually closer to the exact solution than those derived with imposed displacement or forces. Additionally, PBC is also considering both the deformation induced anisotropy due to the evolution of the textures and geometrical anisotropy due to the initial textures of AA2060 sheet. Besides, it consider the compatibility between adjacent boundaries of the RVEs after and before deformation [5]. Finally, the third crucial feature mandatory to successfully determine the mechanical behavior of AA2060 sheet by computational homogenization-based crystal plasticity modelling is a set of material parameters which is vital to characterize the grains behavior correctly. This set of parameters (used in the dislocation density-based CP model) was divided into two types. The first and second types are for the flow rule and hardening related to the dislocation multiplication and annihilation. These parameters are \( C_s \), \( C_e \), \( K_e \), \( K_s \), \( d_e \), and \( d_s \), where, \( C_s \) and \( C_e \) stand for the fraction of the total slip rate contribution by screw and edge segments, respectively. \( K_e \) and \( K_s \) are constants governing the dislocations mobility, furthermore, \( d_e \) and \( d_s \) are the maximum distances for mutual annihilation between the antiparallel edge and screw dislocations to occur, respectively. \( C_e \) and \( C_s \) are set to be 0.5 to reflect the assumption that the slip contribution from edge and screw dislocations was the same. The parameters \( K_s \) is set to be twice of \( K_e \), and \( d_s = 5d_e \) according to Ha et al. [3] and Cheong et al. [4]. Thus, \( K_s \) and \( d_s \) were adjusted to fit the stress-strain curve of samples cut at 30° with respect to RD and strain rate of 0.001 s\(^{-1}\). Table 2 lists the determined material parameters used in current study. The parameters which obtained from stress-strain curve was determined from the stress-strain curve of samples cut at 30° with respect RD and strain rate of 0.001 s\(^{-1}\).

**Table 2.** A set of material parameters of AA2060-T8 sheet

| Material parameters | Ce  | Cs  | Ke  | Ks  | de  | ds  |
|---------------------|-----|-----|-----|-----|-----|-----|
| values              | 0.5 | 0.5 | 24.2X10\(^{-3}\) | 48.5X10\(^{-3}\) | 7.0 nm | 35.0 nm |
4. Verification of the proposed computational homogenization strategy

The mechanical response of AA2060-T8 sheet was determined by finite element simulation of the RVE model in which a dislocation density single crystal plasticity model was used as a constitutive equation to model each grain. Figure 3 (b) depicted deformed grain-based RVE model after 10 % uniaxial straining. As shown in this figure, a heterogeneous deformation occurred in a single grain because of the effects of the interaction between adjacent grains.

Figure 3. Grain-based RVE model (a) before deformation, and (b) after 10 % uniaxial deformation. The RVE model used in current investigation was consisted of 50 grains, where different colours stand for different grains

In order to validate the predictability of the proposed computational homogenization strategy, the experimental results (stress-strain curves) was compared with those obtained from finite element simulation as depicted in figure 4. The agreements between the predicted and experimental results are remarkable in all examined conditions as shown in figure 4. Further validation was carried out by calculating R, AARE, RMSE, and NMBE [6] to evaluate the reliability and quantitatively measure the predictability of the proposed computational homogenization strategy. These statistical parameters were calculated by:

\[ R = \frac{\sum_{i=1}^{N}(\sigma_{exp_i} - \sigma_{predicted_i})^2}{\sum_{i=1}^{N}(\sigma_{exp_i} - \sigma_{predicted_i})^2} \times 100 \]  

\[ AARE \, (\%) = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{\sigma_{exp_i} - \sigma_{predicted_i}}{\sigma_{exp_i}} \right) \times 100 \]  

\[ RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N}(\sigma_{exp_i} - \sigma_{predicted_i})^2} \]  

\[ NMBE \, (\%) = \frac{(1/N)\sum_{i=1}^{N}(\sigma_{exp_i} - \sigma_{predicted_i})}{(1/N)\sum_{i=1}^{N}\sigma_{exp_i}} \times 100 \]

where, \( N \) is the total number of points used in this study, \( \sigma_{exp_i} \) and \( \sigma_{predicted_i} \) are the experimental stress and predicted stress obtained from simulation. Besides, \( \sigma_{exp} \) is the mean value of experimental stresses and \( \sigma_{predicted} \) is the mean value of the predicted stresses. The values of R, ARRE %, RMSE and NMBE are summarized in table 3.
Figure 4. Correlation between experimental and predicted stress-strain curves for AA2060-T8 at strain rate of 0.01 s\(^{-1}\) and loading directions of (a) 0°, (b) 30°, (c) 45°, (d) 60°, and (e) 90° w.r.t RD.

Table 3. The values of R, ARRE%, RMSE, and NMBE% at strain rate of 0.01 s\(^{-1}\)

| Value | R     | ARRE% | RMSE (MPa) | NMBE% |
|-------|-------|-------|------------|-------|
|       | 0.99484 | 2.57 | 4.45 | -0.108 |

5. Conclusion

Computational homogenization-based crystal plasticity finite element modelling was proposed to predict the tensile deformation behavior of AA2060-T8 sheet at room temperature, various loading directions and strain rates of 0.01 s\(^{-1}\). A dislocation density-based single crystal plasticity constitutive model was developed to describe the behavior of grains in order to reflect the real deformation mechanisms of the crystal. Afterwards, the developed model was implemented as a user-subroutine UMAT of the ABAQUS FE code. The computational homogenization strategy is basically depended on the finite element simulation of RVE which represents the real microstructure of AA2060-T8 where each grain is discretized with many finite elements to consider the in-grain deformation behaviors. A PBC is developed to consider both the geometrical anisotropy due to the initial textures and deformation induced anisotropy due to the evolution of the textures. The agreements between the experimental and the predicted results are remarkable in all examined conditions. These remarkable agreements are attributed to incorporating the physical mechanisms of the plastic deformation and the crucial microstructural details in the computational model. This means that the proposed computational homogenization strategy can predict the tensile deformation behavior of AA2060-T8 (polycrystalline materials) accurately at room temperature and different strain rates and loading directions.

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