Original Article

Deformation behavior and anisotropic response of 2060 Al-Cu-Li alloy: experimental investigation and computational homogenization-based crystal plasticity modeling

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ABSTRACT

Since AA2060-T8 was launched the past few years, it was crucial to understand the deformation behavior and to establish a multi-scale model that can link the microstructural state of this alloy with its mechanical behavior. Thus, a computational homogenization-based crystal plasticity modeling was proposed to predict the deformation behavior and capture the anisotropic response of AA2060-T8 at different deformation conditions. Uniaxial tensile tests were accomplished at room temperature and strain rates of 0.001 and 0.1s⁻¹ using samples with different fiber orientations to experimentally investigate the deformation behavior and anisotropic response of AA2060-T8. Thereafter, to clarify the details of the in-grain deformation features, a representative volume element was established to describe the real microstructure of AA2060-T8 in which each grain was discretized using many finite elements. Afterwards, a dislocation density-based crystal plasticity model was developed to describe the behavior of grains and simulate the plastic deformation of AA2060-T8. The material parameters utilized in the crystal plasticity model was determined from the stress–strain curves of the samples tested at loading direction of 30° with respect to rolling direction and strain rate of 0.001s⁻¹. Additionally, a periodic boundary condition was modified to consider both geometrical and deformation induced anisotropy. The achieved results from the proposed computational homogenization method are in remarkable agreement with that obtained from experimental work. This means that the proposed computational homogenization method is able to predict the deformation behavior and capture the anisotropic response of AA2060-T8 at various deformation conditions.

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1. **Introduction**

Currently, the family of third generation Al-Li alloy is a promising nominee for the components used in aerospace, aircraft, and military applications due to its outstanding mechanical properties such as, low density, high specific stiffness and strength, and good corrosion resistance [1,2]. These remarkable properties are mainly attributed to the addition of Li to the Al matrix. For instance, adding 1 wt.% of Li increases the elastic modulus and reduces the density of alloys approximately 6% and 3%, respectively [2,3].

In 2011, Alcoa Company introduced AA2060-T8 as a new 3rd generation Al-Li alloys to supersede AA7075-T6 and AA2024-T3 for fuselage, lower and upper wings structures [2]. Although AA2060-T8 alloy displays outstanding properties, it exhibits poor formability at room temperature, which impedes its broad applications [2]. Since AA2060-T8 was introduced few years ago, few records have been accomplished to investigate the relation between the mechanical response and the texture of this alloy. For instance, Abd El-Aty et al. [4] investigated the tensile properties of AA1420, AA8090 and AA2060-T8 sheets under different loading directions and wide range of strain rates. They stated that the tensile properties of AA2060-T8 do not show constant trend with increasing the strain rate. Additionally, they reported that the high-speed forming can be considered as an effective method to improve the formability of AA2060-T8 at room temperature. Gao et al. [5] studied the feasibility of manufacturing aircraft component from AA2060-T8 sheet using hot forming in-die quenching process. They found that the optimum strain rate and temperature to manufacture this component from AA2060-T8 are 2 s^−1 and 470 °C respectively. Ou et al. [6] investigated the hot deformation behavior of AA2060-T8 and they found that dynamic recovery is the main dynamic softening mechanism of AA2060-T8. Furthermore, they found that optimum hot forming conditions are between strain rate and temperature range of 0.01–3 s^−1 and 380–500 °C, respectively. Jin et al. [7] studied the development of the texture and mechanical properties of AA2060-T8 during bending and observed that the mechanical strength of AA2060-T8 was increased in three directions with decreasing the bending radius. Thereafter, Jin et al. [8] investigated the dislocation boundary structures of the AA2060-T8 during bending, and found three types of microstructures were formed during bending. The first one was observed in grains with Cube orientation, which consists of large dislocation cells; the second was detected in grains with Goss, brass and, copper orientations; whereas the third was noticed in grains with S orientation. Later, Jin et al. [9] analyzed the damage mechanism and the microstructure evolution of AA2060-T8 during bending. They reported that the strain localization in the free surface of the bent samples actuated damage to the microstructure. At the beginning of bending, the crack initiation lied on the free surface with maximum strain and the shear crack was propagated along the macro-shear band.

From the above-mentioned literature, it is obvious that factors controlling the deformation behavior and anisotropic response of AA2060-T8 notably at room temperature and different fiber orientations are rarely investigated. Therefore, it is crucial to investigate the deformation behavior and anisotropic response of AA2060-T8 at room temperature and various strain rates and fiber orientation to correlate the microstructural state of this alloy with the mechanical response. Hence, it is necessitated to establish a multi-scale model that can predict the deformation behavior and capture the anisotropic response of AA2060-T8 at different strain rates and room temperature, and adjoin the microstructural state of this alloy with its mechanical behavior. Within this realm, computational homogenization-based crystal plasticity finite element method (CH-CPFEM) is noticeably effective technique to predict the deformation behavior of materials, capture the anisotropic response and provide the macroscopic response with respect to microstructure parameters (grain shape, size, shape, and order distribution).

CPFEM is one of the attractive methods applied to investigate the deformation behavior of single crystals since it can observe the heterogeneous deformation arising from the effect of initial crystallographic orientations and the collective motions of dislocations [10]. Additionally, several mean-field methods such as viscoplastic self-consistent (VPSC) model has been developed numerically and analytically to investigate the texture evolution and predict the deformation behavior of polycrystals during deformation [11]. VPSC model has shown its capability to predict the flow stress and texture evolution of polycrystals, in turn used to construct macroscopic continuum constitutive models within the scheme of multiscale modeling [12]. However, the local stress and strain fields developed in a single grain cannot be evaluated by VPSC model. This may lead to a huge variations on the local level for strongly anisotropic crystals. Besides, the statistical analysis of the microstructures not permitting the investigation of the influence of the real grain shape and the details of the grain spatial distributions [10]. Thus, more advanced homogenization methods are necessary to effectively relate the global responses and microstructural state of the materials.

In this context, a CH-CPFEM was proposed to predict the tensile deformation behavior and capture the anisotropic response of a novel 3rd generation Al-Li alloy AA2060-T8 at room temperature, strain rate of 0.001 and 0.1 s^−1, and different sample orientation (i.e. 0°, 30°, 45°, 60°, and 90° w.r.t. RD). The representative volume element (RVE), which represents the real microstructure of the AA2060-T8 (where each grain is discretized with many finite elements) was used in homogenization procedure to consider the in-grain deformation behavior. Additionally, a general periodic boundary condition (PBC) was modified to consider both the geometrical anisotropy and deformation induced anisotropy. The initial microstructures and the micro-textures of the AA2060-T8 (which detected by EBSD measurements) were used to build up the RVE model. Thereafter, some of the material parameters were determined from the stress–strain curves of sample cut in 30° with reference to rolling direction (RD) and at strain rate of 0.001 s^−1. The predictability of the proposed CH-CPFEM to predict the tensile deformation of AA2060-T8 was validated via comparing the predicted results with the results acquired from experiments. Further validations were accomplished through calculating statistical parameters, such as correlation coefficient (R), average absolute
relative error (AARE), root mean square error (RMSE), and normalized mean bias error (NMSE) to quantitatively measure the reliability and evaluate the predictability of the proposed strategy.

2. Experimental material and procedures

The material used in current investigation is a novel 3rd generation Al-Li alloy 2060-T8 sheet (2 mm thickness). The chemical compositions (wt.%) of as-received AA2060-T8 sheet are as follows: Al – balance, Li – 0.75, Cu – 3.95, Mg – 0.85, Zn – 0.7, Mn – 0.3, Ag – 0.25, and Zr – 0.11. Optical microscopy (OM) was used to detect the microstructure of as-received AA2060-T8 sheet as shown in Fig. 1. The specimens used for microstructure characterization were cut at RD, ground by silicon carbides papers, mechanically polished by diamond pastes, and finally etched by Keller’s reagent solution (6% HCl, 6% HNO3 and 85% H2O). Furthermore, the texture and grain size of the AA2060-T8 sheet were characterized by HKL Channel 5 EBSD analysis system. The texture components, such as S, Cube, Goss, Copper, and Brass were determined within 15° of the nearest ideal component. The quasi-static tensile tests were carried out using a 100 kN Instron machine at room temperature and strain rates of 0.001, 0.01, and 0.1 s⁻¹, where, every testing condition was repeated at least for three specimens. In order to investigate the anisotropic response of AA2060-T8 sheet, the specimens used in quasi-static tensile testing were machined at various angles (i.e. 0°, 30°, 45°, 60°, 90° w.r.t. RD). The details of sample specifications and the machine used in this study are depicted in Fig. 2. Finally, the fracture morphologies of the

Fig. 1 – Microstructure of as-received AA2060-T8 sheet characterized by OM.

Fig. 2 – (a) The geometrical characteristics of the specimens used in the quasi-static tensile test (all dimensions in mm). (b) The samples machined in different directions (0°, 30°, 45°, 60°, and 90°) w.r.t. RD. (c) The details of Instron machine used in quasi-static tensile testing.
3. Experimental results

3.1. Effect of strain rate and fiber orientation on tensile properties and anisotropic behavior

The data of stress–strain were obtained by the testing system and by fitting; the stress–strain curves of AA2060 at various fiber orientations and strain rate of 0.001 and 0.1 s⁻¹ are presented in Fig. 3a and b, respectively. Each stress–strain curve of the curves depicted in Fig. 3 can be divided into elastic, yield and hardening zones. The first zone is elastic zone, where, a linear relationship existed between the stress and strain. The Young’s modulus of AA2060-T8 sheet obtained from the test results is 75 GPa. The second zone is the yield zone, where, the strain-rate has an obvious effect on the yield strength, in which by increasing the strain rate, the yield strength was increased from 470 to 495 MPa. The third and last zone is hardening zone, where the AA2060-T8 sheet exhibits work hardening behavior, and the work hardening rate of these curves were changed with respect to loading direction and strain rate

As depicted in Figs. 3 and 4, under the same working conditions (room temperature and loading direction), the yield and flow stresses were increased by increasing strain rates from 0.001 s⁻¹ to 0.1 s⁻¹. Meanwhile, the elongation to fracture decreased by increasing the strain rate, notably for the samples at RD and 90° w.r.t. RD, which implies that the fiber orientation or loading direction has a significant influence on the tensile properties (i.e. yield strength, ultimate tensile strength, and elongation to fracture). The effect of fiber orientation or loading direction on the yield and ultimate tensile strengths is depicted in Fig. 4a, meanwhile, the influence of the loading direction on the elongation to fracture is presented in Fig. 4b. Under the same working conditions (room temperature and strain rate), the change in sample orientation from 0° to 60° w.r.t. RD resulted in decreasing the yield and ultimate tensile strengths, with sharp increase in elongation to fracture in particular for the samples at 45° to 60° w.r.t. RD; for the sample orientations beyond 60° the yield and ultimate tensile strengths were increased, while the elongation to fracture was decreased.

From the aforementioned discussion, it is obvious that the mechanical behavior of AA2060-T8 is clearly depending on the fiber orientations, and its tensile properties are varying w.r.t. the fiber orientation. This signifies that tensile properties of AA2060-T8 sheet exhibit a serious degree of in-plane anisotropy. The observed differences in yield and ultimate tensile strengths in AA2060-T8 were caused by the synergistic and independent interactive influences of the changes in the degree and nature of crystallographic texture, and the intrinsic variations in the volume fraction of the main strengthening
precipitates [2,4]. Furthermore, the anisotropy in elongation to fracture was attributed to shearing of the Al-Li precipitates and the resultant flow localization orientation w.r.t. the current stress states; the distribution and density of the intermediate and coarse grain size of the intermetallic particles; the type, distribution and morphology of the main precipitates; recrystallization degree, type and history of deformation process before artificial aging; strength of grain boundaries; the width of precipitate-free zones, and fracture modes [2–4]. Thus, the fracture morphologies of the tested samples were observed using SEM to investigate the fracture modes under different loading directions and strain rates. In general, the orientation dependence of tensile properties of AA2060-T8 sheet is not amenable to any forthcoming analysis because it is affected by many test conditions and parameters.

3.2. Fracture surface morphology

Since the fracture morphology is a reflective for the ductility and strength of the tensile samples, SEM was used to figure out the fracture modes and describe the microscopic fracture features of the tensile samples tested at various loading directions and strain rates. The fracture modes of Al-Li alloys are relying on various microstructural features as summarized in Fig. 5. These features are controlled by alloy processing, composition, and heat treatment procedures [3,13]. The common modes of fracture and the features associated with them in Al-Li alloys are brittle intergranular fractures, cleavage of large constituent particles, “ductile” intergranular fractures, localized, transgranular shear fractures and dimpled transgranular fractures [3,13,14]. The stresses needed for these fracture modes vary from small for brittle intergranular fracture and cleavage of constituent particles to huge for transgranular fractures with deep dimples [13–15].

Fig. 6 presents the typical fracture morphologies of the tensile samples tested at different tensile conditions. As presented in Fig. 6, the fracture morphologies of AA2060-T8 displayed various characteristics varying with the loading direction and strain rates as summarized in Fig. 7. The fracture morphologies of the samples tested at loading directions of 45° and 60° w.r.t. RD and strain rate of 0.001 s⁻¹ exhibit ductile fracture characterized by sizable dimples as depicted in Fig. 6g and j. The volume fraction of the dimples in the fracture surfaces of the aforementioned samples (i.e. 45° and 60° w.r.t. RD) are notably high as compared to the fracture surfaces of the other samples tested at strain rate of 0.001 s⁻¹ and loading direction of 30° w.r.t. RD (which shows mixed ductile and brittle fracture as shown in Fig. 6d) and samples tested at loading directions of 0° and 90° w.r.t. RD (which show brittle mode of fracture as depicted in Fig. 6a and m respectively and summarized in Fig. 7). On the other hand, with increasing the strain rate to 0.01 and 0.1 s⁻¹, the fracture modes appeared to be mixed ductile and brittle fracture at loading directions of 45° and 60° w.r.t. RD as depicted in Fig. 6b, i, k, as well as l and brittle fracture for the samples tested at loading directions of 0°, 30° and 90° w.r.t. RD as shown in Fig. 6b, c, e, f, n and o. The aforementioned discussion is in good agreement with the tensile properties determined for these samples and substantiates the superior values of the elongation obtained for the samples tested at loading directions of 45° and 60° w.r.t. RD as shown in Fig. 4b.

4. Computational homogenization using crystal plasticity finite element modeling

In order to predict the tensile deformation behavior of AA2060-T8 sheet in terms of microstructure parameters (grain size, shape and order distribution) by CH-CPFEM, three vital features are required. These features are: (1) a constitutive model that describes the grains behavior to reveal the actual deformation mechanisms; (2) realistic and representative description of the microstructure via RVE model; and (3) material parameters to precisely describe the behavior of grains. In the following section the details of each feature used in current investigation will be discussed. The required steps to predict the deformation behavior and capture the anisotropic response of AA2060-T8 sheet through a proposed CH-CPFEM are summarized in the flowchart as shown in Fig. 8. In this investigation, a single crystal plasticity model was used as a constitutive model of AA2060-T8 grains, hence, in the next section the details of this model will be discussed.

4.1. Crystal plasticity model

An implicit implementation of a single crystal plasticity model was accomplished in ABAQUS/FE code as a UMAT subroutine. The details of the dislocation density-based crystal plasticity model, which was introduced firstly by Cheong et al. [16] will be introduced in this section.

As reported by Asaro [17], in rate-dependent crystal plasticity constitutive model, the deformation gradient F was decomposed into a plastic FP and elastic parts FE, as written in Eq. (1). FP maps the material point in the reference
Fig. 6 – Fracture morphologies of the tensile samples tested at different loading conditions and strain rates characterized by SEM: (a) $0^\circ/\dot{\varepsilon} = 0.001\,\text{s}^{-1}$, (b) $0^\circ/\dot{\varepsilon} = 0.01\,\text{s}^{-1}$, (c) $0^\circ/\dot{\varepsilon} = 0.1\,\text{s}^{-1}$, (d) $30^\circ$ w.r.t. RD/\dot{\varepsilon} = 0.001\,\text{s}^{-1}$, (e) $30^\circ$ w.r.t. RD/\dot{\varepsilon} = 0.1\,\text{s}^{-1}$, (f) $30^\circ$ w.r.t., (g) $45^\circ$ w.r.t. RD/\dot{\varepsilon} = 0.001\,\text{s}^{-1}$, (h) $45^\circ$ w.r.t. RD/\dot{\varepsilon} = 0.1\,\text{s}^{-1}$, (i) $45^\circ$ w.r.t. RD/\dot{\varepsilon} = 0.01\,\text{s}^{-1}$, (j) $60^\circ$ w.r.t. RD/\dot{\varepsilon} = 0.001\,\text{s}^{-1}$, (k) $60^\circ$ w.r.t. RD/\dot{\varepsilon} = 0.01\,\text{s}^{-1}$, (l) $60^\circ$ w.r.t. RD/\dot{\varepsilon} = 0.1\,\text{s}^{-1}$, (m) $90^\circ$ w.r.t. RD/\dot{\varepsilon} = 0.001\,\text{s}^{-1}$, (n) $90^\circ$ w.r.t. RD/\dot{\varepsilon} = 0.01\,\text{s}^{-1}$, and (o) $90^\circ$ w.r.t. RD/\dot{\varepsilon} = 0.1\,\text{s}^{-1}$.
configuration w.r.t. the intermediate configuration \( \tilde{\beta} \), while \( F^e \) describes the rotation and stretch of the slip systems from \( \tilde{\beta} \) to the present configuration.

\[
F = F^s F^p
\]  
\(^1\)

Usually, \( F^p \) and \( F^s \) are not consistent, however, the constitutive description of \( F^p \) introduces a unique description of intermediate configuration \( \tilde{\beta} \). Asaro \(^17\) assumed that \( \text{det} F^p = 1 \), and \( \text{det} F^e > 0 \), thus, \( F^p \) and \( F^e \) are invertible, furthermore, \( F^p \) follows the isochoric deformation.

The spatial velocity gradient tensor (L) can be decomposed to plastic and elastic components as:

\[
L = L^e + L^p \tag{2}
\]

\[
L = F F^{-1} \tag{3}
\]

Therefore,

\[
L^p = F^s L^p F^e^{-1} \tag{4}
\]

\[
L^e = F^s F^e^{-1} \tag{5}
\]
where \( \mathbf{L}^p \) is a spatial velocity gradient described in intermediate configuration, which is defined by Eq. (6)

\[
\mathbf{L}^p = \mathbf{F}^p \mathbf{F}^p : \mathbf{F}^p \mathbf{F}^p^{-1}
\]

(6)

Thus (L) can be described as:

\[
\mathbf{L} = \mathbf{F}^e \mathbf{F}^e : \mathbf{F}^e \mathbf{F}^e^{-1}
\]

(7)

The evolution of the plastic flow is presented as:

\[
\mathbf{L}^p = \sum_{a=1}^{n} j^a S^a
\]

(8)

\( j^a \) is the shearing rate on the \( \alpha \)-slip system and \( S^a \) is the orientation tensor which characterize the slip systems with slip direction and slip-plane normal \( (n^a_0) \) \([17,18]\), so \( S^a \) is defined as:

\[
(S^a = m^a_0 \otimes n^a_0)
\]

(9)

For F.C.C. crystal structures, the crystallographic slip is assumed to occur on the \{111\} \{110\} slip systems. The slip direction \( (m^a_0) \) in the present configuration was described to its form in intermediate configuration \( \beta \) as:

\[
m^a_0 = \mathbf{F}^e m^a_0
\]

(10)

Besides, the equivalent slip plane normal \( (n^a_0) \) was defined as:

\[
n^a_0 = n^a_0 \mathbf{F}^e \mathbf{F}^e^{-1}
\]

(11)

where it is supposed that \( m^a_0 \) and \( n^a_0 \) are orthogonal to each other.

The mechanical response of single crystals was defined using a hyper-elastic constitutive equation, so, the stress–strain relationship can be defined via the Helmholtz free energy per unit volume \( (\psi) \). Mostly, the elastic deformation in crystalline materials is infinitesimal compared with the plastic deformation. Accordingly, it is supposed that the functional form of \( (\psi) \) as a quadratic form of the elastic Green–Lagrange strain on \( \beta, \mathbf{E}^e \) \([17–21]\).

Thus, we have

\[
\psi(\mathbf{E}^e) = \frac{1}{2} \mathbf{E}^e : \mathbf{C} : \mathbf{E}^e
\]

(12)

where

\[
\mathbf{E}^e = \frac{1}{2} (\mathbf{C}^e - \mathbf{I})
\]

(13)

\[
\mathbf{C}^e = \mathbf{F}^e \mathbf{T}^e \mathbf{F}^e
\]

(14)

\( \mathbf{C} \) is the fourth-order anisotropic elastic tensor and \( \mathbf{I} \) is the identity tensor. Therefore, the constitutive equation of the stress response was defined through \( (\mathbf{T}^e = \frac{3}{2} \mathbf{F}^e) \), so,

\[
\mathbf{T}^e = \mathbf{C} : \mathbf{E}^e
\]

(15)

where \( \mathbf{T}^e \) is the second Piola–Kirchhoff stress tensor in \( \beta \), which is the work-conjugate to the elastic Green–Lagrange strain tensor \( \mathbf{E}^e \) and is related to the Cauchy stress tensor \( (\sigma) \) as introduced in Eq. (16).

\[
\mathbf{T}^e = \mathbf{F}^e \mathbf{E}^e \mathbf{F}^e^{-1}
\]

(16)

and

\[
\mathbf{J}^e = \det \mathbf{F}^e
\]

(17)

The stress power per unit volume in \( \beta \) is described by

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

(18)

The flow rule associated with the slip shearing rates on the arbitrary slipping systems with the resolved shear stresses was defined by \([22]\) as:

\[
\dot{\gamma}^a = \dot{\gamma}_0 \exp \left[ \frac{F_0}{k_B \theta} \left( 1 - \left( \frac{\mathbf{J}^e - 1}{\tau_0 / \mu_0} \right)^p \right) \right] \text{sgn}(\dot{\gamma}^a)
\]

(19)

where \( \dot{\gamma}_0 \) is reference slip rate, \( k_B \) is Boltzmann constant, \( \theta \) is absolute temperature, and \( \tau_0 \) is the lattice friction at 0 K. In addition, \( F_0 \) is the Helmholtz free energy of activation, \( \mu_0 \) and \( \mu \) are the shear moduli at 0 and \( \theta \) K, respectively. In order to identify the shape of the energy-barrier profile associated with the interactions between dislocations and obstacles, \( p \) as well as \( q \) were considered to be present in the range of \( 0 \leq p \leq 1 \) and \( 1 \leq q \leq 2 \), respectively \([23]\).

The resolved shear stress tensor \( (\mathbf{T}^e) \) can be defined by

\[
\omega^p = \sum_a \tau^a \dot{\gamma}^a
\]

(20)

where

\[
\omega^p = (\mathbf{C}^e \mathbf{T}^e) \mathbf{G}^p
\]

(21)

Thus,

\[
\tau^a = (\mathbf{C}^e \mathbf{T}^e) : S^a
\]

(22)

According to generalized Taylor law, the total athermal slip resistance parameter \( S_T^a \) was evaluated by \([16,21]\) as:

\[
S_T^a = \lambda \mu b \sqrt{\sum_{\rho=1}^{N} h^{\rho \beta} \rho^{\beta}_{\rho}}
\]

(23)

where \( \lambda \) is the statistical coefficient that explains the deviation from the regular spatial arrangement of the dislocation densities. Additionally, \( \mu \) is the shear modulus, \( b \) is the magnitude of the Burgers vector, and \( h^{\rho \beta} \) is the dislocation interaction matrix that clarify the increasing rate of the slip resistance on the \( \alpha \)-slip system by the reason of shearing on the \( \beta \)-slip system. Many studies have been accomplished and proposed different equations based on the back-extrapolation of latent hardening experiments \([24,25]\), or discrete dislocation dynamics \([26–28]\). However, in this investigation, for simplicity \( h^{\rho \beta} \) can be introduced as:

\[
h^{\rho \beta} = \omega_1 + (1 - \omega_2) \delta^{\rho \beta}
\]

(24)
where \( \omega_1 \) and \( \omega_2 \) are the interaction coefficients and \( \delta^{ij} \) is the Kronecker delta.

In order to display their different mobility, the total statistically stored dislocation density was decomposed as:

\[
\rho' = \rho_{\text{edge}} \sqrt{\sum_{\beta=1}^{N} \rho_{\text{edge}}^\beta - 2d_e \rho_{\text{edge}}^\beta} \bigg| \gamma^a \bigg|
\]

\( \rho_{\text{edge}}^\beta \) is the pure edge dislocation components.

\( \rho_{\text{edge}} \) is the pure edge dislocation components.

(25)

A new evolution formulations were proposed by Cheong et al. [16] for the components of screw and edge dislocation density by formulating the balance laws between dislocation generation and annihilation as:

\[
\dot{\rho}_{\text{screw}}^\beta = \frac{C_s}{b} K_s \sqrt{\sum_{\beta=1}^{N} \rho_{\text{screw}}^\beta - \rho_{\text{edge}}^\beta} \bigg| \gamma^a \bigg|
\]

(26)

\[
\dot{\rho}_{\text{edge}}^\beta = \frac{C_e}{b} K_e \sqrt{\sum_{\beta=1}^{N} \rho_{\text{edge}}^\beta - \rho_{\text{edge}}^\beta} \bigg| \gamma^a \bigg|
\]

(27)

\( C_s \) and \( C_e \) represent for the fraction of the total slip rate contribution via edge and screw segments respectively. \( K_s \) and \( K_e \) are dimensionless proportionality constants controlling the mobility of the dislocations. \( d_e \) and \( d_s \) are vital for the recovery processes that give the maximum distances for mutual annihilation between the antiparallel edge and screw and edge dislocations to happen, respectively.

4.2. Computational homogenization framework

Computational homogenization technique is basically relying upon the characteristics and finite element simulation of the RVE models which represent the real state of the microstructure. Generally, there are three types of RVE models used in computational homogenization of polycrystalline materials. These models are voxel or cuboidal model, truncated octahedron based model, and grain-based RVE model. The voxel models consisted of brick-shaped finite elements, where, every cubic element describes a single grain as depicted in Fig. 9a. Although voxel models have been extensively utilized to predict the deformation behavior of polycrystalline materials, it cannot determine the heterogeneous in-grains deformation developed in their grains [10]. Thence, truncated octahedron model, and grain-based RVE model are recently used to address the issues of voxel models, because of their ability to assess the heterogeneous intra-granular deformation fields through discretizing each grain by many elements. In the truncated octahedron model, the shape of grains were idealized as a truncated octahedron because it can fill the space without any gap or overlap. Thus, this RVE model can describe the microstructure of the polycrystalline materials more accurate than the voxel and grain-based RVE models. Nevertheless, the time consumed for simulating polyhedron RVE model is very high and the improvement of the accuracy of the results obtained from simulation is not equivalent to the time consumed during FE simulation. Thence, in this investigation, a grain-based RVE model was used to address the issues of aforementioned RVE models. In grain-based model, each grain was represented by many cubic elements, thus, it may contain more information about the distribution of grain sizes and shapes of polycrystalline materials. In this study, it was assumed that grain-based RVE model has an equiaxed grains and the RVE model was discretized 100 × 100 × 100 C3D8R elements. The grain-based RVE model used in this study is depicted in Fig. 9b, where, this RVE model consisted of 50 grains, and different colors describe different grains. The description of the initial texture of the as-received materials is a critical issue during creating the grain-based RVE model, since many researchers assumed an initially isotropic state (the initial texture could be represented by a random set of crystallographic orientations) [29–31]. On the other hand, most of as-received polycrystalline materials exhibit the initially anisotropic textures. Therefore, in current investigation, to assign the initial texture to an RVE model, the initial crystallographic data obtained from the EBSD measurement reduced by the coarsening technique that remove the pixel every two pixels and reduces the number of points in a dataset by a factor of four. This technique was repeated to obtain 50 crystallographic orientations, which approximate the initial texture of

Fig. 9 – (a) Voxel RVE model with 1000 cubic element, where each grain was represented by one cubic element and different colors represent different grains. (b) Grain-based RVE model which contains 50 grains, where each grain was described by many cubic elements.
the AA2060-T8 sample. The texture distribution and grain size may influence the macroscopic response of the RVE model, but the results of surface measurement obtained from EBSD could not accurately reflect the sub-surface distribution of the grain in the real materials. Nevertheless, as shown in the following results, the macroscopic stress-strain curves may be determined precisely if the number of elements in RVE model is adequate. The initial texture of AA2060-T8 sheet represented by (1 1 1) pole figure with 50 grains is depicted in Fig. 10.

The mechanical behavior of the proposed grain-based RVE model was determined via finite element simulation, where, the RVE model was directly utilized as finite element meshes (one voxel represents one cubic finite element). Thereafter, suitable boundary condition should be considered to apply them on the faces of every cubic element. Huet et al. [29], Hazanov et al. [30] and Segurado et al. [31] reported that the mechanical behavior of polycrystalline materials acquired by implementing periodic boundary conditions (PBC) on the faces of the cubic elements is closer to the real behavior than those obtained from other boundary conditions as depicted in Fig. 11a. Generally, for most boundary conditions, the better estimation of the effective properties is depending on size of RVE, where, increasing the size of RVE caused better estimation of the effective properties [32]. However, for certain RVE size, PBC displays a remarkable estimation than other boundary conditions as depicted in Fig. 11a. PBC supposed that the RVE deformed as jigsaw puzzles, so that all space may be filled with a periodic translation of RVE along the Cartesian axes as presented in Fig. 11b, c, and d. Furthermore, PBC can maintain the compatibility between adjacent boundaries of the RVEs before and after deformation, in particular, for the polycrystalline materials which exhibit anisotropic behavior, where, the deformation of RVE can be non-uniform even if the macroscopic external loading is uniform. Thence, in this investigation, PBC was used to consider the deformation-induced anisotropy due to the evolution of the textures and geometrical anisotropy due to the initial textures of AA2060-T8 sheet.

As shown in Fig. 12, the deformation of the RVE attached to a material point X is related to the local deformation map of the homogenized macro-continuum as

\[ x = \bar{F}X + \bar{w} \]  \hspace{1cm} (28)

or

\[ F = \bar{F} + \tilde{F} \] \hspace{1cm} (29)

where \( \bar{w} \) is the fluctuation field due to heterogeneous microstructure.

By similarly, the microscopic displacement field can be decomposed into macroscopic fluctuation and homogeneous parts as:

\[ u = u + \tilde{u} = [F(X, t) - 1]y + \tilde{u} \] \hspace{1cm} (30)

The macroscopic deformation gradient \( F \) at a material point \( X \) is the volume average of the microscopic deformation \( F \) of RVE, so,

\[ \bar{F} = \frac{1}{V} \int_B F \ dV \] \hspace{1cm} (31)

so,

\[ \tilde{F} = \frac{1}{V} \int_{\partial B} x \otimes N \ dA \] \hspace{1cm} (32)

In Eq. (29), the divergence theorem was used to express the deformation gradient in terms of the spatial position and surface normal of the boundary. Therefore, by referring Fig. 12,
In polycrystalline description, strain was supposed to be the same. Furthermore, the initial slip resistance was set to be higher than that of the pure aluminum single crystals because of the precipitation hardening. The determined material parameters used in this investigation are listed in Table 1. Furthermore, all the material constants used in current study were determined from the stress-strain curve of the test-sample machined at 30° w.r.t. RD and strain rate of 0.001 s⁻¹. These material constants reproduced well the results obtained from experimentation for the other fiber orientations and strain rates.

### Table 1 - Material parameters and constants of as-received AA2060-T8 sheet.

<table>
<thead>
<tr>
<th>Material parameters</th>
<th>Cᵣ</th>
<th>Cᵢ</th>
<th>Kᵣ</th>
<th>Kᵢ</th>
<th>dᵣ</th>
<th>dᵢ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>0.5</td>
<td>0.5</td>
<td>24.2 × 10⁻³</td>
<td>48.5 × 10⁻³</td>
<td>7.0 nm</td>
<td>35.0 nm</td>
</tr>
</tbody>
</table>

Therefore, dislocation density-based crystal plasticity finite element method was used to describe the behavior of grains of AA2050-T8 sheet. The undeformed and deformed grain-based RVE model after 10% uniaxial straining is depicted in Fig. 13. The heterogeneous deformation happened in a single grain as depicted in Fig. 13b, because of the interaction effects between adjacent grains. The efficiency of the proposed CH-CPFEM to predict the tensile deformation behavior and capture anisotropic response of AA2060-T8 were verified through correlating the stress-strain curves obtained from experimentation with those predicted from FEM simulation. The comparison between the predicted and experimental results is presented as shown in Fig. 14.

For the alloys with random textures, the anisotropic behavior is caused by the development of the deformation-induced texture. However, for the alloys possessing an initial texture, the anisotropic behavior is attributed to both initial microstructure and deformation-induced textures. Hence, texture evolution of as-received AA2060-T8 sheet was also predicted to investigate the ability of CH-CPFEM to capture the anisotropic response of metallic materials. The comparison between the (111) pole figure obtained from simulation and experimentation of as-received AA2060-T8 (which displays a typical rolling texture with the β-fiber extending from Brass to Copper texture components) is presented in Fig. 15.

![Image](image.png)

**Fig. 12** - The deformation x of cube shaped microstructure was driven via the local deformation of the macrostructure, where x decomposed into homogeneous (Fx) and nonhomogeneous parts (w).

The deformation behavior and anisotropic response of AA2060-T8 sheet was determined using FE simulation of the RVE model, where dislocation density-based crystal plasticity finite element method was used to describe the behavior of grains of AA2050-T8 sheet. The undeformed and deformed grain-based RVE model after 10% uniaxial straining is depicted in Fig. 13. The heterogeneous deformation happened in a single grain as depicted in Fig. 13b, because of the interaction effects between adjacent grains. The efficiency of the proposed CH-CPFEM to predict the tensile deformation behavior and capture anisotropic response of AA2060-T8 were verified through correlating the stress-strain curves obtained from experimentation with those predicted from FEM simulation. The comparison between the predicted and experimental results is presented as shown in Fig. 14.

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\[
\frac{1}{v} \int F \, dV = \frac{1}{v} \int w \otimes N \, dA = \frac{1}{v} \left[ \int_{\partial B^+} \dot{w}^+ \otimes N^+ \, dA 
+ \int_{\partial B^-} \dot{w}^- \otimes N^- \, dA \right] \tag{33}
\]

where (+) and (−) denote the surface normal of opposite sides. The periodic boundary conditions, \(w^+ = w^-\), satisfies Eq. (13).

In order to apply the kinematic constraint, the difference of the displacement fields of two opposite surfaces can be described as

\[
\dot{u}^+ - \dot{u}^- = \left[ \ddot{F}(x, t) - I \right] \left( y^+ - y^- \right) = u(x) \tag{34}
\]

In current investigation, we wrote a python script to detect the corresponding nodes on the opposite two surfaces and to constrain their degrees of freedom according to aforementioned description, and \(u(x)\) stands for the displacement of the master node.

The final crucial feature necessitated to determine the mechanical response of AA2060-T8 sheet using CH-CPFEM is the material parameters which are essential to describe the grains behavior accurately. These material parameters (which used in the dislocation density-based CP model) were divided into two categories. The first category was for the flow rule, and the second category for hardening related to the dislocation annihilation and multiplication. The set of material parameters in the former was acquired from the calibration results for polycrystalline Al alloys. From these parameters \((C_r, C_i, K_r, K_i, d_r, d_i)\), only \(K_r\) and \(d_r\) were adjustable to approximate the stress-strain behavior. In addition, the set of material parameters of pure aluminum single crystals was adopted as baseline. It is believed that the precipitation due to Li particles fit the hardening rate of AA2060 alloys. On the other hand, the slip resistance of different slip systems in the grains of polycrystalline aggregate can be dissimilar due to the different hardening in the previous deformation. Thus, for simplicity, it was supposed that the dislocations are evenly distributed and therefore the initial slip resistance of each slip system was assumed to be the same. Furthermore, the initial slip resistance was set to be higher than that of the pure aluminum single crystals because of the precipitation hardening. The determined material parameters used in this investigation are listed in Table 1. Furthermore, all the material constants used in current study were determined from the stress-strain curve of the test-sample machined at 30° w.r.t. RD and strain rate of 0.001 s⁻¹. These material constants reproduced well the results obtained from experimentation for the other fiber orientations and strain rates.

### Verification of the proposed CH-CPFEM

The deformation behavior and anisotropic response of AA2060-T8 sheet was determined using FE simulation of the RVE model, where dislocation density-based crystal plasticity finite element method was used to describe the behavior of grains of AA2050-T8 sheet. The undeformed and deformed grain-based RVE model after 10% uniaxial straining is depicted in Fig. 13. The heterogeneous deformation happened in a single grain as depicted in Fig. 13b, because of the interaction effects between adjacent grains. The efficiency of the proposed CH-CPFEM to predict the tensile deformation behavior and capture anisotropic response of AA2060-T8 were verified through correlating the stress-strain curves obtained from experimentation with those predicted from FE simulation. The comparison between the predicted and experimental results is presented as shown in Fig. 14.

For the alloys with random textures, the anisotropic behavior is caused by the development of the deformation-induced texture. However, for the alloys possessing an initial texture, the anisotropic behavior is attributed to both initial microstructure and deformation-induced textures. Hence, texture evolution of as-received AA2060-T8 sheet was also predicted to investigate the ability of CH-CPFEM to capture the anisotropic response of metallic materials. The comparison between the (111) pole figure obtained from simulation and experimentation of as-received AA2060-T8 (which displays a typical rolling texture with the β-fiber extending from Brass to Copper texture components) is presented in Fig. 15.
A remarkable agreement between the results acquired from CH-CFFEM and experimentation in all examined conditions as shown in Figs. 14 and 15 signifies that the proposed CH-CFFEM strategy can predict the tensile deformation behavior and capture the anisotropic response of AA2060-T8 under various strain rates and fiber orientation. These superb agreements are caused by combining the physical mechanisms of the plastic deformation and the crucial details of the microstructure of AA2060-T8 sheet in the computational model.
Further validation was carried out to quantitatively measure the reliability and evaluate the predictability of the proposed CH-CFEM via calculating standard statistical parameters \([33–38]\) such as correlation coefficient \((R)\), average absolute relative error \((\text{AARE})\), root mean square error \((\text{RMSE})\), and normalized mean bias error \((\text{NMBE})\). \(R\) is a crucial parameter used to measure the strength of linear relationship between experimental and predicted results \([33]\), where if \(R\) is close to 1, this implies that the predictability of the proposed strategy is significant. Eq. \((35)\) was used to calculate \(R\) as:

\[
R = \frac{\sum_{i=1}^{N}(E^i - \bar{E})(P^i - \bar{P})}{\sqrt{\sum_{i=1}^{N}(E^i - \bar{E})^2 \sum_{i=1}^{N}(P^i - \bar{P})^2}} \tag{35}
\]

where \(E^i, \bar{E}, P^i, \bar{P}\) and \(N\) are experimental stress, mean value of experimental stresses, stresses predicted through simulation, mean value of predicted stresses and total number of points used in this investigation respectively.

\(\text{AARE}\) and \(\text{RMSE}\) are unbiased parameters used to quantify the ability of CH-CFEM to predict the deformation behavior exactly \([34–37]\). \(\text{AARE}\) and \(\text{RMSE}\) were calculated by Eqs. \((36)\) and \((37)\), where the small amount of \(\text{AARE}\) means that the reliability of the CH-CFEM strategy is remarkable and vice versa \([37]\).

\[
\text{AARE} \ (%) = \frac{1}{N} \sum_{i=1}^{N} \frac{|E^i - P^i|}{E^i} \times 100 \tag{36}
\]

\[
\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (E^i - P^i)^2} \tag{37}
\]

The last statistical parameter is \(\text{NMBE}\), which was used to quantify the mean bias in the predictions from CH-CFEM strategy, where the negative and positive values of \(\text{NMBE}\) indicate underprediction and overprediction respectively \([38]\). \(\text{NMBE}\) was calculated by Eq. \((38)\) as:

\[
\text{NMBE} \ (%) = \left(\frac{1}{N} \sum_{i=1}^{N} (E^i - P^i)\right) \times 100 \tag{38}
\]

The correlations between the results predicted by CH-CFEM and those obtained from experimentation at different fiber orientation and strain rate range of 0.001–0.1 s\(^{-1}\) are presented in Fig. 16. Furthermore, the values of \(R\), \(\text{AARE}\), \(\text{RMSE}\), and \(\text{NMBE}\) are listed in Table 2, which verify that the proposed CH-CFEM can predict the tensile deformation behavior of AA2060-T8 exactly at room temperature and different strain rates and fiber orientation.

### Table 2 – The values of \(R\), \(\text{AARE}\), \(\text{RMSE}\), and \(\text{NMBE}\) at \(\dot{\varepsilon} = 0.001–0.1\) s\(^{-1}\).

<table>
<thead>
<tr>
<th>Value</th>
<th>(\dot{\varepsilon})</th>
<th>(R)</th>
<th>(\text{AARE}) (%)</th>
<th>(\text{RMSE}) (MPa)</th>
<th>(\text{NMBE}) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.001</td>
<td>0.001 s(^{-1})</td>
<td>0.994703</td>
<td>2.72</td>
<td>5.51</td>
<td>0.153</td>
</tr>
<tr>
<td>0.01</td>
<td>0.01 s(^{-1})</td>
<td>0.99484</td>
<td>2.57</td>
<td>4.45</td>
<td>−0.108</td>
</tr>
<tr>
<td>0.1</td>
<td>0.1 s(^{-1})</td>
<td>0.996161</td>
<td>3.475938</td>
<td>6.85117</td>
<td>0.238212</td>
</tr>
</tbody>
</table>

6. Conclusions

In this study, a novel third-generation Al-Li alloy AA2060-T8 sheet was characterized to understand tensile deformation behavior and anisotropic response of this alloy under different strain rates and fiber orientations. Furthermore, in order to adjoin the microstructural state of AA2060-T8 with its mechanical behavior, CH-CFEM was proposed to capture the anisotropic behavior and predict the macroscopic response of this alloy with respect to microstructure parameters. Based on the achieved results from current investigating, the main conclusions can be deduced as follows:

- The yield and flow stresses increased and elongation was decreased with increasing strain rates. Meanwhile, the tensile deformation behavior of AA2060-T8 was clearly dependent upon the fiber orientations, which signifies that tensile properties of AA2060-T8 sheet exhibit a serious degree of in-plane anisotropy.
- The fracture modes of AA2060-T8 are varying from ductile to brittle fracture with respect to fiber orientations and strain rates, which is in line with the results obtained from experimental work.
- The dislocation density-based crystal plasticity model was developed to represent the constitutive equation of each
grain and simulate the plastic deformation of AA2060-T8. Then, this model was implemented as a user-subroutine UMAT of the ABAQUS finite element code. Afterwards, the grain-based RVE model was established to represent the real microstructure of AA2060-T8, and by FE simulation of this RVE model, the deformation behavior and anisotropic response of AA2060-T8 sheet was determined. Thereafter, a periodically boundary condition was modified to consider both deformation induced and the geometrical anisotropy since AA2060 sheet exhibit in-plane anisotropy in its tensile properties.

- A remarkable agreement between the results is acquired from CH-CPFEM and experimentation under all examined conditions. This implies that the proposed CH-CPFEM strategy can predict the deformation behavior and capture the anisotropic response of AA2060-T8 under various forming conditions. These superb agreements were caused by conjoining the physical mechanisms of the plastic deformation and the crucial details of the microstructural AA2060-T8 sheet in the computational model.

**Conflicts of interest**

The authors declare no conflicts of interest.

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