Microstructure-based crystal plasticity modeling of AA2024-T3 aluminum alloy defined as the $\alpha$-Al, $\theta$-Al$_2$Cu, and S-Al$_2$CuMg phases based on real metallographic image

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Keywords: microstructural modeling, crystal plasticity, AA2024-T3 aluminum alloy, $\alpha$-Al; $\theta$-Al$_2$Cu; S-Al$_2$CuMg

Abstract
The increase in the strength of the Al–Cu–Mg alloys is to a large extent due to the formation and distribution of submicroscopic $\theta$-Al$_2$Cu and S-Al$_2$CuMg phases in the aluminum ($\alpha$-Al) matrix, which causes these alloys to have unique properties such as high initial hardening rate. This paper aimed to examine the anisotropic plasticity and flow behavior of the AA2024-T3 aluminum alloy by measuring the distinctive properties of each of the $\theta$-Al$_2$Cu, S-Al$_2$CuMg, and $\alpha$-Al phases at the micro-level and using a microstructure-based crystal plasticity model during single-strand tensile strength. The real microstructure of AA2024-T3 aluminum alloy obtained from scanning electron microscopy (SEM) was utilized in the calculations using the polycrystalline image processing method of the phases as a Representative Volume Element (RVE). Each phase’s crystal orientations and texture were randomly generated, given the lattice parameters and their crystal structure. The computational results were compared with the experimental data of the AA2024-T3 aluminum alloy tensile test, the data of the crystal plasticity model without considering the microstructure, and the Johnson-Cook model. Given the heterogeneity of the microstructure and crystal orientations of the grains, it was shown that the maximum internal stress under tensile loading occurred along with local hardening in the $\alpha$-Al phase adjacent to the grains of the $\theta$-Al$_2$Cu and S-Al$_2$CuMg phases, which was about 43300 MPa.

1. Introduction
Although most metals are alloyed with aluminum, relatively few have sufficient solid solubility to act as the main additive element in alloys. Out of common elements, only copper, magnesium, zinc, and silicon have significant solubility. 2000 Series aluminum alloys are heat-treatable alloys that are obtained from the solid copper in aluminum solution. Due to their very high fracture toughness and acceptable tensile strength, these alloys are usually used as a plate in wing reinforcement of passenger aircraft, automotive industries, etc [1].

Al–Cu–Mg alloy systems, such as the AA2024-T3 alloy, are age or precipitation hardening processes whose mechanical properties are controlled. The soluble constituents formed due to eutectic freezing are the main microstructural properties that influence the mechanical properties of these alloy systems [1]. The elastic and plastic anisotropy of the phases in the metal deformation process indicates the heterogeneity of the deformation of materials at the micro-scale. Therefore, polycrystalline materials behave very differently at the micro-scale compared to the macro scale. Thus, local stresses and strains within phases will be non-uniform and discontinuous. Stresses and strains will depend not only on the grain orientation of the phases but also on the constraints created by the grains of adjacent phases. Hence, the macroscopic mechanical properties of the dual-phase and multi-phase alloys are dependent on several variables, including grain crystal orientation, chemical composition, distribution, and morphology of each of the constituent phases of each alloy. Also, each of these
phases affected the anisotropy resulting from the crystallographic slip at a microscopic scale, which is a requirement for plastic deformation at the macroscopic scale [2].

Several experimental and numerical studies have recently reported on the constituent phases of the AA2024-T3 alloy, the mechanical properties and chemical composition of each of those phases, and their effect on the mechanical properties of this alloy. According to a study by Huges et al. (2010), $\theta$-Al$_2$Cu and S-Al$_2$CuMg phases are the main constituents in the AA2024-T3 alloy, accounting for up to 39% of the entire alloy [3]. Huges et al. (2013) also reported that the composition of the intermetallic compounds was constant in ten different batches of AA2024-T3 aluminum alloy [4]. Okayasu et al. (2012) produced the Al-33%Cu eutectic alloy using the Ohno continuous casting (OCC) technique to express the importance of investigating the effect of the $\theta$-Al$_2$Cu phase on the tensile properties and fatigue of Al-Cu alloys. They also researched the hardness of the $\theta$ phase. In this study, they stated that the hardness of the $\theta$ phase is 2.8 times that of the $\alpha$-Al phase [5]. Zhang et al. (2012) used the first-principles calculations based on the density functional theory (DFT) to investigate the structural, elastic, and electronic properties of Al$_2$Cu ($\theta$) and Al$_2$CuMg (S) phases in the Al–Cu–Mg series. They suggested that the $\theta$ and S phases represented the characteristic of ductility and brittleness, respectively. Comparatively, they determined that the $\theta$ phase had better isotropy in compression, while the S phase had higher isotropy in shear strength and stiffness [6]. Li et al. (2014) and García-Hernández et al. (2019) specified that the heat treatment and the copper to magnesium rate (Cu/Mg) determined the effect of each of the S-Al$_2$CuMg and $\theta$-Al$_2$Cu phases on the AA2024 alloy. Their findings could be summarized in three parts. Firstly, when the ratio of copper to magnesium was more than 8, the strengthening of Al–Cu–Mg alloys was done by $\theta$ phase. Secondly, for ratios between 4 to 8, both phases S and $\theta$ were responsible for strengthening Al–Cu–Mg alloys. Finally, for ratios between 1.5 to 4, phase S was the most effective phase for strengthening Al–Cu–Mg alloys [7, 8]. Liu et al. (2019) developed a crystal plasticity model based on the confined layer slip mechanism by taking into account the nanoscale Al–Al$_2$Cu alloy to study the buckling behavior of nanolaminates. Using their proposed computational model, they showed that the critical compression strain associated with buckling increased with the thickness of the layer lowered. This result was consistent with micro-pillar tests [9]. Liu et al. (2019) used atomistic simulation to investigate the mechanical properties and structure of plastic deformation of plates (111)$\alpha||$(110)$\theta$. The

![Figure 1. Scanning electron micrographs of AA2024-T3 alloy, indicating the cluster of S-phase and $\theta$-phase particles: (a) BSE image and EDX spectra of the particles; (b) SE image.](image)
unexpected shear strain created in the Al$_2$Cu phase was attributed to the continued slip on the Al-Al$_2$Cu interface plane and the dislocations on the Al-Al$_2$Cu interface plane [10]. Based on previous studies, implementing the effects of the microstructure on mechanical behaviors was not possible with a homogenized plasticity model [11]. Therefore, these models could be applied on larger scales than microstructures, because of which the mechanical behavior for each material with different microstructures had to be calibrated. Thus, to overcome such limitations, Al-Abbasi et al. (2003) developed a micro-mechanical model for two-phase steels consisting of dispersed martensite phases in a ferrite field [12]. Qin et al. (2018) used macroscopic testing and micromechanics simulations to investigate multiaxial plasticity behavior of Dual Phase (DP) 600 steel based on a real metallographic image. They reported that the micromechanics modeling allowed for the detection of local stress state variations in the material and deformation localization [13]. Basu et al. (2018) used the RVE based micromechanical model to address the effect of micro-structural inhomogeneity in Macro-mechanical response of 20MnMoNi55 steel. They proved that the strain partitioning between constituent phases gives rise to plastic strain localization in softer matrix [14]. Jia et al. (2021) performed microstructure-based numerical modeling of the deformation heterogeneity and ferrite recrystallization in a dual-phase (DP) steel by using the crystal plasticity finite element method (CPFEM). They found that the CPFEM method could well reveal various scenarios of strain localizations occur in the deformation of two-phase microstructures [15].

In this paper, by modeling the α-Al, θ-Al$_2$Cu, and S-Al$_2$CuMg phases as RVE models, the Stress-Strain response of AA2024-T3 alloy has been examined by measuring the distinctive properties of each of the θ-Al$_2$Cu, S-Al$_2$CuMg, and α-Al phases. Besides, the effect of the crystal orientation of the grains of the phases on the macroscopic behavior of AA2024-T3 alloy has also been investigated using a microstructure-based crystal plasticity model during uniaxial tensile loading on a microscopic scale. The results were then generalized to the entire AA2024-T3 alloy. Sensitivity of the results of the proposed model was studied as well by examining the experimentally obtained data, including the results of the AA2024-T3 aluminum alloy tensile test [16], the

Figure 2. Distribution of the (a) grains of (b) θ-phase and S-phase inside α-Al matrix.

Figure 3. Grain size histogram of the phases: (a) θ-phase; (b) S-phase.
The microstructure of AA2024-T3 aluminum alloy was measured using a scanning electron microscope (SEM) with dimensions of 25 μm × 17 μm as an aluminum base (α-Al) with S-Al2CuMg and θ-Al2Cu phases. Figure 1 showed SEM images using (a) secondary electrons (SE), (b) backscattered electrons (BSE), (c) in-lens detector, and (d)–(f) energy-dispersive X-ray (EDX) spectroscopy of phase particles in the different positions of the AA2024-T3 aluminum microstructure. Figure 2 illustrated the distribution of S-Al2CuMg and θ-Al2Cu phases and grains in the α-Al field. The area fraction of the α-Al, θ-Al2Cu, and S-Al2CuMg phases were 77.2%, 9.4%, and 13.4%, respectively. These values were calculated using the ImageJ metallographic image analysis software [20]. The number of grains of each of the θ and S phases in the aluminum field was 14, shown in figure 3. A Histogram, i.e., an illustrative method for displaying the relative frequency of the grain size, was used to examine the grain size of the θ and S phases. The ImageJ metallographic image analysis software was employed to define the metallographic image scale in the software in terms of image pixel spacing. Moreover, the ASTM-E112-based planimetric procedure was utilized to compute the mean grain size for each phase (figures 3(a), (b)). The grain size on the x-axis was illustrated so that the grain size would increase from left to right. The weight values of the grains or their weight percentages, also known as frequency, were located on the y-axis. By examining the grain size histogram, it could be inferred that the mean grain sizes for the θ and S phases were 0.85 μm and 1 μm, respectively.

The elastic properties of the said phases were calculated based on the second-order elastic constants and determined using the fitting of the linear Stress-Strain curve [9, 21]. In terms of elastic properties, α-Al was defined as cubic, and the θ-Al2Cu and S-Al2CuMg phases were defined as orthotropic (table 1). Figure 4 showed the proposed multiscale method, which presented different longitudinal scales and the related simulation tools results of the crystal plasticity model without considering microstructures [17], and the results of Johnson–Cook model [18, 19] in terms of YS and UTS.

### 2. Materials and methods

The microstructure of AA2024-T3 aluminum alloy was measured using a scanning electron microscope (SEM) with dimensions of 25 μm × 17 μm as an aluminum base (α-Al) with S-Al2CuMg and θ-Al2Cu phases. Figure 1 showed SEM images using (a) secondary electrons (SE), (b) backscattered electrons (BSE), (c) in-lens detector, and (d)–(f) energy-dispersive X-ray (EDX) spectroscopy of phase particles in the different positions of the AA2024-T3 aluminum microstructure. Figure 2 illustrated the distribution of S-Al2CuMg and θ-Al2Cu phases and grains in the α-Al field. The area fraction of the α-Al, θ-Al2Cu, and S-Al2CuMg phases were 77.2%, 9.4%, and 13.4%, respectively. These values were calculated using the ImageJ metallographic image analysis software [20]. The number of grains of each of the θ and S phases in the aluminum field was 14, shown in figure 3. A Histogram, i.e., an illustrative method for displaying the relative frequency of the grain size, was used to examine the grain size of the θ and S phases. The ImageJ metallographic image analysis software was employed to define the metallographic image scale in the software in terms of image pixel spacing. Moreover, the ASTM-E112-based planimetric procedure was utilized to compute the mean grain size for each phase (figures 3(a), (b)). The grain size on the x-axis was illustrated so that the grain size would increase from left to right. The weight values of the grains or their weight percentages, also known as frequency, were located on the y-axis. By examining the grain size histogram, it could be inferred that the mean grain sizes for the θ and S phases were 0.85 μm and 1 μm, respectively.

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### Table 1. Material parameters of α-Al, θ-Al2Cu, and S-Al2CuMg phase used in the simulations [16, 23].

| Parameters | α-Al | θ-Al2Cu | S-Al2CuMg |
|------------|------|---------|-----------|
| Elastic Moduli (MPa) | \( C_{11} = 205600 \) | \( C_{11} = 115900 \) | \( C_{11} = 90800 \) |
| | \( C_{12} = 25500 \) | \( C_{12} = 33500 \) | \( C_{12} = 38700 \) |
| | \( C_{22} = 205600 \) | \( C_{22} = 174100 \) | \( C_{22} = 35000 \) |
| | \( C_{13} = 106750 \) | \( C_{13} = 46800 \) | \( C_{13} = 30000 \) |
| | \( C_{23} = 60410 \) | \( C_{23} = 38700 \) | \( C_{23} = 26600 \) |
| | \( C_{44} = 28340 \) | \( C_{44} = 153100 \) | \( C_{44} = 70200 \) |

| Reference slip rate \( \dot{\gamma}_{\text{ref}} \) (S⁻¹) | 0.0018 | 0.0006 | 0.0006 |
| Rate sensitivity \( n \) | 12 | 5 | 5 |
| Self-hardening \( h_0 \) | 75 | 1000 | 1000 |
| \( \tau_s \) | 65 | 680 | 680 |
| Latent hardening \( \tau_0 \) | 63 | 160 | 160 |
| \( \theta \) | 1 | 1 | 1 |
Figure 5. True tensile stress-strain response of $\theta\text{-Al}_2\text{Cu}$ along [001] direction.

Table 2. Slip directions $s^\alpha$ and planes $m^\alpha$ of the slip systems of the phases $\alpha$ in Miller indices notation.

| Phases | $\alpha\text{-Al}$ | $\theta\text{-Al}_2\text{Cu}$ | S-$\text{Al}_2\text{CuMg}$ |
|--------|--------------------|-----------------|-----------------|
|        | $m^\alpha$ | $s^\alpha$ | $m^\alpha$ | $s^\alpha$ | $m^\alpha$ | $s^\alpha$ |
| 1 | (111) | [0 1 1] | (011) | [1 1 1] | (100) | [0 1 2] |
| 2 | (111) | [1 0 1] | (011) | [1 1 1] | (100) | [0 1 2] |
| 3 | (111) | [1 0 1] | (101) | [1 1 1] | (100) | [0 2 1] |
| 4 | (1 1 1) | [1 0 1] | (101) | [1 1 1] | (100) | [0 2 1] |
| 5 | (1 1 1) | [1 1 0] | (110) | [1 1 1] | (010) | [2 0 1] |
| 6 | (1 1 1) | [0 1 1] | (110) | [1 1 1] | (010) | [2 0 1] |
| 7 | (11 1) | [0 1 1] | (0 1 1) | [1 1 1] | (010) | [1 1 0] |
| 8 | (1 1 1) | [1 1 0] | (0 1 1) | [1 1 1] | (010) | [1 1 0] |
| 9 | (1 1 1) | [1 1 0] | (1 0 1) | [1 1 1] | (010) | [1 1 0] |
| 10 | (1 1 1) | [1 1 0] | (1 0 1) | [1 1 1] | (010) | [1 1 0] |
| 11 | (1 1 1) | [1 1 0] | (1 1 0) | [1 1 1] | (010) | [1 1 0] |
| 12 | (1 1 1) | [1 1 0] | (1 1 0) | [1 1 1] | (010) | [1 1 0] |

Figure 6. Inverse pole figures (IPF) for the (a) $\alpha\text{-Al}$ phase, (b) $\theta\text{-Al}_2\text{Cu}$ phase, and (c) S-$\text{Al}_2\text{CuMg}$ phase random texture utilized in this work.
for the relationship between the respective scale and predicting the crystal’s mechanical response at a macro scale. Five material parameters were required for developing a numerical model of the Stress-Strain behavior of materials at the level of crystal plasticity calculations. The two parameters of the flow law could be estimated from other reports and research published in this field. The three other parameters in the hardening law were $h_0$, initial hardening modulus, $\tau_0$, initial YS, and $\tau_s$, stress at the I stage. These three parameters could be applied directly using molecular dynamic simulations (atomistic simulation) and discrete dislocations. They can then be transferred hierarchically at the level of crystal plasticity calculations [22].

In this study, the parameters of self-hardening, latent hardening, strain rate sensitivity, slip system strength, and hardening law parameters, i.e., $h_0$, $\tau_0$, and $\tau_s$, have been adapted from the studies by Eisenlohr et al [24] and Liu et al [9]. As shown in figure 5, the $\theta$-Al$_2$Cu phase constituent material parameters were calibrated with the Stress-Strain diagram of the atomistic simulation along [001] $\theta$ [10]. The mechanical properties of the S-Al$_2$CuMg phase were calculated from the elastic parameters at small strains [23, 25].

Experimental and theoretical research results showed the Burgers vectors $[110], [100], [1/2][111], and [001]$ and slip planes (100), (110), (112), and (011) for the $\theta$-Al$_2$Cu phase [9, 26]. The S-Al$_2$CuMg phase was stretched along [100]$_{\text{Al}}$ on the (210)$_{\text{Al}}$ [27]. Aluminum crystals were represented by twelve slip systems, displayed by a combination of four slip planes (111) and three slip plane orientations [110] for each plane. Table 2 showed the phase slip systems used in numerical calculations.

The crystal orientations of the phase grains were randomly in the ATEX software considering the parameters of the crystal lattice and their crystalline structures (table 3) [28]. They were then assigned to numerical microstructures. Figure 2 displayed the grains with different crystal orientations with different colors. Figure 6 showed the investigated crystal orientations of the phases in the AA2024-T3 aluminum alloy sample and their corresponding positions in the Inverse Polar figure (IPF).

| Phases      | Method  | $\alpha$-Al | $\theta$-Al$_2$Cu | S-Al$_2$CuMg |
|-------------|---------|--------------|-------------------|---------------|
| Cryst. sys. | —       | Cubic        | Orthorhombic      | Tetragonal    |
| a(Å)       | Experiments | 4.050 [29]  | 4.28 [30]         | 4.0119 [31]  |
| Calculations | 4.050 [32]  | 4.121 [21]  | 4.050 [21]     |
| b(Å)       | Experiments | —          | 4.28 [30]         | 9.2652 [31]  |
| Calculations | —          | 4.121 [21]  | 9.279 [21]     |
| c(Å)       | Experiments | —          | 2.405 [30]        | 7.124 [31]   |
| Calculations | —          | 2.898 [21]  | 7.206 [21]     |
| $\alpha(\degree)$ | —     | 90          | 90                | 90           |
| $\beta(\degree)$ | —     | 90          | 90                | 90           |
| $\gamma(\degree)$ | —     | 90          | 90                | 90           |

| Figure 7. Mesh and boundary conditions on the RVE microstructure of AA2024-T3 alloy. |
3. Microstructural modeling

3.1. Microstructure extraction

The OOF2 program was used for two-dimensional modeling of the microstructure of AA2024-T3 aluminum alloy based on what was displayed in the real metallographic image of the sample. The distribution and form of the S-Al\(_2\)CuMg and θ-Al\(_2\)Cu phases in the α-Al field were modeled as the RVE by separating the phase pixels with different colors created in the graphic software on the SEM image (figure 1). The type of meshing in this kind of modeling was Skeleton meshing. It should be noted that Skeleton meshing cannot be considered as a finite element meshing type as it does not contain any information concerning finite element interpolation functions. This type of meshing can recognize the positions and shapes of the elements, which are the phases in metallographic photography. According to the generated mesh, there were 24009, 4895, and 6997 elements in the α-Al, θ-Al\(_2\)Cu, and S-Al\(_2\)CuMg phases, respectively. The size of each element was between 0.04–0.12 \(\mu\)m, and the elements were of the CPS3 and CPS4 types.

3.2. Boundary conditions

The finite element software used to simulate the proposed model was ABAQUS 6.14 software. After meshing, the RVE model was put in the ABAQUS software environment, and the tensile test simulation process was performed by taking into account the boundary conditions specified in figure 7. Tensile test simulation was applied in the proposed model with a strain rate of 0.001 S\(^{-1}\).

3.3. Numerical procedure

The framework is based on the theory of elasto-viscoplastic deformation widely used along slip planes, which rivets to the work of Rice [33], Peirce \textit{et al} [34], and Asaro [35]. In this framework, the Schmid tensor, representing the elementary deformation structures, is projected onto individual slip planes. A visco-plastic power law provides a constitutional formulation for the strain rate \(g\) of the system α [34]:

\[
\dot{g}^{(\alpha)} = \frac{\tau^{(\alpha)}}{h^{(\alpha)}} \left( \frac{\tau^{(\alpha)}}{\tau_s} \right)^n \text{sgn} \left( \frac{\tau^{(\alpha)}}{\tau_s} \right)
\]

(1)

Where \(\dot{g}^{(\alpha)}\), \(\tau^{(\alpha)}\), \(\tau_s\), \(h^{(\alpha)}\) and \(n\) are the slip rate, reference strain rate, resolved shear stress, the current strength of \(\alpha\) slip system, and the strain rate sensitivity parameter, respectively. The determination of \(\dot{g}^{(\alpha)}\) is then obtained by:

\[
\dot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha\beta} \dot{g}^{(\beta)}
\]

(2)

Where \(h_{\alpha\beta}\) is the module of hardening, for self-hardening \((\alpha = \beta)\) and \((\alpha \neq \beta)\) for latent hardening is used herein. This paper uses the hardening law of Peirce \textit{et al} [36], which proposes both self-hardening and latent hardening of the slip systems approach to identify the hardening effect in crystalline materials.

\[
h_{\alpha\alpha} = h(\gamma) = h_0 \text{sech}^2 \left( \frac{h_0 \gamma}{\tau_i - \tau_0} \right)
\]

(3)

Where \(h_0\) represents for the initial hardening module, \(\tau_0\) the initial yield stress, \(\tau_i\) the saturation stress, \(\gamma\) Taylor’s accumulated shear strain on all slip systems which obtained by:

\[
\gamma = \sum_{\alpha = \beta} \int_0^t |\dot{g}^{(\alpha)}| \, dt
\]

(4)

The latent hardening modulus is defined by:

\[
h_{\alpha\beta} = qh(\gamma)(\alpha \neq \beta)
\]

(5)

This model was applied as a user material subroutine (UMAT) by Huang [37] in the finite element ABAQUS software. This subroutine is suitable for FCC and BCC materials. It can be utilized for the small deformation, finite-strain, and finite-rotation theory. The simulation results can therefore be regarded as independent of the rate. For each family of slip \(\alpha\), the cumulative shear strain is calculated as the integral of over time equation (1). To calculate the deformation system’s contributions to the total deformation, the cumulative slip activity is characterized according to the strain rate of each system to the entire strain. In an attempt to assess each contribution to deformation as a whole, the cumulative slip activity is computed by the strain rate of the system to the overall strain.
4. Results and discussion

In this research, the $\alpha$-Al, $\theta$-Al$_2$Cu, and S-Al$_2$CuMg phases were modeled as the RVE, the plastic behavior of all phases ($\alpha$, S, $\theta$) of the AA2024-T3 aluminum alloy sheet. Furthermore, the plastic behavior of the entire AA2024-T3 sheet was investigated according to the different plastic behaviors of each phase using a...
microstructure-based crystal plasticity model during uniaxial tensile loading. The effect of the crystal orientation of the phases on the macroscopic behavior of the alloy was also included in the calculations.

Figure 8 showed the real Stress-Strain distribution of AA2024-T3 aluminum alloy related to the crystal plasticity model based on the proposed real microstructure. In this study, the results of the plasticity model based on real microstructure presented in the paper were compared with the results of experimental data of tensile test of AA2024-T3 aluminum alloy [16], the results of crystal plasticity model without considering microstructure [17], and the results of Johnson-Cook model [18, 19]. According to the findings, there was a good agreement between the results of the crystal plasticity model based on real microstructure and the results of experimental data compared to other models.

The proposed numerical approach was significantly capable of estimating YS and UTS. This approach was more reliable than the data obtained from the crystal plasticity model without considering microstructure and Johnson-Cook model. For instance, the UTS calculated by the crystal plasticity model based on the microstructure was 520 MPa, which was quite close to the UTS obtained from the experimental results (522 MPa). The UTSs calculated for the crystal plasticity model without considering microstructure and Johnson-Cook were 405 MPa and 562 MPa, respectively.

Figure 9 showed the stress distribution of the AA2024-T3 aluminum alloy in three stages of deformation (1, 3, and 5 μm). As can be seen, the colors of the areas with θ-Al₂Cu and S-Al₂CuMg phase geometry were much brighter than those with α-Al phase geometry. By this argument, no significant stress has evolved due to the 1 μm deformation in the α-Al phase. However, the stress has increased significantly in the θ-Al₂Cu and S-Al₂CuMg phases by 1 μm. As shown in figure 10, when 1 μm deformation was applied, the shear lines began to develop in the α-Al phase and expand until the 5 μm deformation, so there was apparent strain heterogeneity.

Based on figure 9, the properties of the α-Al phase have changed due to variation of distance from the grains of θ-Al₂Cu and S-Al₂CuMg phases. Also, it could be seen that with the emergence of local hardening phenomenon in the α-Al phase adjacent to grains of θ-Al₂Cu and S-Al₂CuMg phases, internal tensile stress has increased dramatically to 43300 MPa. This phenomenon was because of the heterogeneity of the microstructure and the crystal orientations of the grains in the plasticity modeling based on the real microstructure of the
AA2024-T3 aluminum alloy. Thus, using the effects of this heterogeneity has not only led to a more precise calculation of macro stress of the material, but it has also made the stress distribution and stress focal points more visible and caused better modeling of the start of the shear line as well.

Figure 11 disclosed the plastic behavior of each $\alpha$-Al, S, or $\theta$ phases of the AA2024-T3 aluminum alloy sheet. As can be seen, the S-Al$_2$CuMg phase had the highest stress with 910 MPa, and the $\alpha$-Al phase had the highest strain with 0.18 mm mm$^{-1}$.

Figure 12(a) showed the stress distribution curve for the path in figure 12(b); figure 12(c) showed the strain distribution curve for the path in figure 12(d). According to figure 12, there was a difference between the stress and strain distributions in the $\alpha$-Al, $\theta$-Al$_2$Cu, and S-Al$_2$CuMg phases. This result indicated that the mechanical response was dependent on the microstructure. In other words, it disclosed the difference in the performance of each of the phases.

The sensitivity of the results related to the studied parameters was investigated by comparing the experimental data with the microstructure-based crystal plasticity model results in terms of YS and UTS of the material. The microstructure-based crystal plasticity model results were consistent with the experimental data with 98% confidence. The error in the experimental data could be due to the lack of independent control over the microstructural parameters in the experimental microstructures. For example, experimental samples had different volume fractions of different phases and grain sizes. In addition, the grain orientation distribution could not be compared properly due to the lack of respective experimental data. Therefore, in this study, random orientation was considered for the microstructure.

5. Conclusions

In this paper, the $\alpha$-Al, $\theta$-Al$_2$Cu, and S-Al$_2$CuMg phases were modeled as RVE to examine the Stress-Strain behavior of AA2024-T3 aluminum alloy by taking into account the distinctive properties of each of the phases, i.e., $\theta$-Al$_2$Cu, S-Al$_2$CuMg, and $\alpha$-Al. The present study also aimed to investigate the use of a microstructure-based crystal plasticity model during uniaxial tensile loading. In the proposed model, microstructure heterogeneity and change of grain crystal orientations played essential roles in determining the behavior of crystals and matter. Since the phases must be considered crystalline in the theory of crystal plasticity, the crystal orientations of the grains of different phases were randomly attributed to numerical microstructures according to the parameters of the crystal lattice and their structures in ATEX software [28]. Anisotropic plastic deformations in the $\alpha$-Al, $\theta$-Al$_2$Cu, and S-Al$_2$CuMg phases were considered by moving dislocations on twelve slip systems (111) [110], (110) [111], and (100) [210], respectively. The crystal plasticity parameters of the introduced constituent material were adapted from the studies of Eisenlohr et al [24] and Liu et al [9].

By comparing the results of the microstructure-based crystal plasticity model presented in the paper with the results of the experimental data [16], it was concluded that there was a clear consistency between the results of the microstructure-based crystal plasticity model with the experimentally obtained data. This finding is indicative of the ability of the modeling framework utilized in this study in modeling the respective alloy and its phases. The proposed numerical approach was also significantly capable of estimating YS and UTS. This finding disclosed that the numerical approach was more reliable than the data attained from the crystal plasticity model.
without considering microstructure and Johnson-Cook model. For example, the UTS calculated using the crystal plasticity model was based on the 520 MPa microstructure, which was rather close to the UTS obtained from the experimental results (522 MPa).

During the simulation process, a clear pattern of the shear line was formed for the values of low strains (in the 1 μm deformation stage), which indicated the ability of the proposed model to predict the behavior of matter at
low strains. It was also concluded that the maximum internal stress under tensile load occurred due to the phenomenon of local hardening in the α-Al phase adjacent to the grains of the θ-Al2Cu and S-Al2CuMg phases (approx. 43300 MPa).

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Conflict of the interest

None.

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