Article

Experiments and Crystal Plasticity Simulations on Plastic Anisotropy of Naturally Aged and Annealed Al–Mg–Si Alloy Sheets

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Abstract: The influence of the heat treatment on the plastic anisotropy of an Al–Mg–Si sheet was investigated by experiments and crystal plasticity simulations. Uniaxial tension tests were conducted for the naturally aged (T4 temper) and annealed (O temper) Al–Mg–Si sheets. Solute atoms Mg and Si form clusters in the T4 temper sheet, while they bind to form precipitates in the O temper sheet. It is found that the in-plane variation of the *R* value, texture, and grain size are almost identical for both sheets. By contrast, the anisotropy of the flow stress is clearly dissimilar; the flow stress is the highest in the diagonal direction for the O temper sheet, whereas the flow stress in that direction is nearly lowest for the T4 temper sheet. Thus, the heat treatment alters the anisotropy of the flow stress. The plastic behaviors of the specimens were simulated using the dislocation density-based crystal plasticity model. The influence of the dislocation interaction matrix on the plastic anisotropy was examined. The orientation dependence of the flow stress is found to be sensitive to the interaction matrix. The flow stresses predicted by the interaction matrix determined based on the dislocation dynamic simulation agree with the experimental results for the O temper sheet. Whereas this interaction matrix does not reproduce the flow stress anisotropy for the T4 temper sheet. When the interactions among the dislocations are set to equivalent—i.e., the interaction matrix is filled with unity—the crystal plasticity simulation results in the flow stress anisotropy that is similar to the experimental trend of the T4 temper sheet. In contrast to the flow stress, the *R* value is insensitive to the interaction matrix, and the predicted *R* values agree with the experimental results for both specimens.

Keywords: Al–Mg–Si alloy sheet; crystal plasticity; dislocation interaction matrix; anisotropy

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1. Introduction

The 6xxx series (Al–Mg–Si) heat-treatable aluminum alloy sheets are widely used for automobile body panels because of their desirable combination of characteristics, such as light weight and high strength. For automotive applications, AA6xxx sheets are heat treated in T4 temper via solution treatment, quenching, and natural ageing. During natural ageing, solute atoms Mg and Si form clusters. The clusters improve strength of sheet because they act as barriers to dislocation motion [1]. Stamped sheet panels are further strengthened in the paint bake cycle, where the clusters grow to fine needle-shaped β'' precipitates. As bake hardening controls the strength of a final product, the property of the artificial age hardening of AA6xxx is actively studied (e.g., [2–4]). By contrast, the present investigation focuses on the plastic anisotropy of the AA6xxx sheet. Plastic anisotropy plays an important role in the sheet-forming simulation, and an accurate anisotropic constitutive model is necessary for predicting failure, wrinkling, and springback.

The anisotropy of the flow stress and plastic deformation of AA6xxx sheets under several heat treatments were investigated. Khadyko et al. [5] investigated the microstructure and anisotropy of AA6063 extruded material in T4, T7, and O tempers. Furthermore, they found that the grain size, texture, and R value were almost the same irrespective of the difference in the heat treatment. In a subsequent study, Khadyko et al. [6] measured stress–strain curves and microstructures of AA6063 sheets in T1, T6, T7, and O tempers. The T6 temper exhibited the highest strength because of the formation of the β'' phases. However, the O temper yielded the lowest strength as the clusters bound to each other, thereby reducing the barriers to dislocation motion. Furthermore, it was reported that the heat treatment varied not only the strength of the specimen but also the flow stress anisotropy. Kuwabara et al. [7] measured the plastic behavior of A6016-T4 and -O sheets, which possess cube-oriented texture. The in-plane variation of the R value was nearly identical for the T4 and O temper sheets. The flow stress in the diagonal direction (DD) was lower than that for the rolling and transverse directions (RD and TD, respectively) for the T4 temper sheet, whereas it was the highest for the O temper sheet. Thus, the flow stress anisotropy of A6016 sheet depended on the heat treatment. The plastic anisotropy of AA6063-O reported by Khadyko et al. [6] was similar to that of A6016-O reported by Kuwabara et al. [7]. Furthermore, these AA6xxx-O sheets exhibited the same anisotropy as pure aluminums AA1050-O and AA1100-O [8–10]. For the T4 temper sheets, the similar type of flow stress anisotropy was observed for AA6016-T4 in [7,11,12] and AA6111-T4 [13]. Thus, in these experiments, the orientation dependence of the flow stress was opposite for AA6xxx-T4 and AA6xxx-O (and pure aluminum).

The mechanical interaction between the precipitate and matrix can be solved by adopting a matrix–inclusion type mean-field model [14–16]. This approach is effective for the precipitation hardened alloys. For the AA6xxx-T4 sheet, solute atoms and their clusters are dispersed. The clusters comprise 2 to about 100 atoms and are shearable [2,3]. Hence, the matrix–inclusion type approach does not fit to the T4 temper sheet, and a conventional crystal plasticity model is frequently used to predict the plastic behavior (e.g., [17–21]). Khadyko et al. [18] investigated the influence of the interaction matrix that provides the strength of the dislocation reaction on the plastic behavior of AA6060-T4. Different interaction matrices lead to noticeable differences in the evolution of flow stress anisotropy. They found that a simple latent hardening model was better than a sophisticated complex interaction matrix. Zecevic and Knezevic [19] reported that the simple latent hardening model with the experimentally determined parameter predicted the anisotropy in the stress–strain curve of AA6022-T4 sheet. Xie et al. [20] simulated the plastic behavior of AA6016-T4 and found that the predicted flow stress was sensitive to the interaction matrix. However, the adjustment of the components of the interaction matrix modestly improved the prediction accuracy. The aforementioned works showed that incorporation of the latent hardening improves the prediction accuracy of the anisotropy. These works focused on the plastic behavior of AA6xxx-T4 sheets, and the influence of the interaction matrix on the flow stress anisotropy of AA6xxx-O sheet was not examined. Moreover, it has not been clarified whether an adjustment of the interaction matrix is able to distinguish the difference in the flow stress anisotropy for the T4 and O temper sheets.

In this study, we investigated the plastic anisotropy of Al–Mg–Si alloy sheets by experiments and crystal plasticity simulations. For the Al–Mg–Si sheets in the T4 and O tempers, uniaxial tension tests were conducted in various material directions, and the in-plane plastic anisotropies in the flow stress and R value were measured. A dislocation density-based crystal plasticity model was used to predict the plastic behavior of the specimens. The role of the dislocation interaction matrix on the predicted plastic anisotropy was investigated in detail.

2. Uniaxial Tension Tests for Al–Mg–Si Alloy Sheets in T4 and O Temper

2.1. Material

The sheet metal used in the present investigation was a 1-mm-thick Al–Mg–Si alloy sheet produced by UACJ Corporation (UACJ Corp., Tokyo, Japan). The chemical composition is listed in Table 1. The sheet was solution treated and quenched; it was then stored at room temperature (T4 temper) for nine years before conducting the present experiment. To obtain the sheet in the O temper, the sheet in the T4 temper was annealed such that it was heated at a rate of 50 K/h, maintained at 673 K for 3 h, and then cooled to 300 K at a rate of 30 K/h. Hereafter, the sheets in T4 and O tempers are referred to as the T4 and O sheet/sample/specimen.

Table 1. Chemical composition of Al–Mg–Si sheet (mass %).

Si	Fe	Cu	Mn	Mg	Cr	Zn	Ti	Al
0.9	0.17	0.01	0.08	0.48	<0.01	0.23	0.03	Bal.

The textures of the T4 and O sheets were measured using the X-ray diffraction method. To measure the through-thickness-averaged texture, 40 sheet samples were stacked, and the pole densities of the {111}, {200}, {110}, and {311} planes was measured on the RD–ND plane. Here, ND refers to normal direction. From the measured pole densities, the orientation distribution function (ODF) was analyzed using LaboTex 3.0 (LaboSoft, Krakow, Poland). The ODF and the {111} pole figure are shown in Figure 1. The textures of the T4 and O samples were similar and developed around the cube orientation. The maximum intensity of the {111} pole figure was 5.8 and 4.6 for the T4 and O samples, respectively. Thus, the annealing slightly weakened the maximum intensity of the texture.

Figure 1. ODF and {111} pole figure for (a) T4 and (b) O temper sheets.

Grain size was determined using the line intercept method. For the T4 and O samples, equiaxed grains were observed on the RD–TD plane; the mean grain size was approximately 30 μm . The T4 and O specimens had almost identical grain morphologies.

In general, for T4 temper Al–Mg–Si alloys, 2 to about 100 of Mg and Si atoms form clusters, which are very small (<5 nm). The spatial arrangement of clusters can be observed by using 3D atom probe tomography [3]. During annealing these clusters bind and form large precipitates (1–2 μm), which are sparsely distributed [22].

2.2. Procedure for Uniaxial Tension Test

A dog-bone shaped specimen was machined from the O and T4 sheets for the uniaxial tension test. The angle between the longitudinal axis of the specimen and the RD was set as $\theta = 0^\circ, 15^\circ, 30^\circ, 45^\circ, 60^\circ, 75^\circ$, and 90° . The length and width of the parallel section were 75 mm and 12.5 mm, respectively. The uniaxial tension was performed at a cross-head speed of 6 mm/min, which resulted in a strain rate of $1 \times 10^{-3} \text{ s}^{-1}$. The speckle pattern was painted on the specimen surface, and the deformation was measured by the digital image correlation method (Aramis 6.3). The deformation gradient was determined and the logarithmic strain was calculated as $\ln U$, where U denotes the right stretch tensor. A representative logarithmic strain was defined as the mean value of the logarithmic strain in a 50 mm $\times$ 12.5 mm area at the center of the specimen; ε_l and ε_w denote the representative logarithmic strain in the longitudinal and width directions, respectively. True stress was calculated as $\sigma = (F/A_0) \exp \varepsilon_l$, where F denotes the tensile load and A_0 denotes the initial cross-sectional area. The plastic strain was determined by subtracting the elastic strain as $\varepsilon_l^p = \varepsilon_l - \sigma/E$ and $\varepsilon_w^p = \varepsilon_w + \nu(\sigma/E)$, where E and ν are the Young's modulus and Poisson's ratio, respectively. The R value, which is the ratio of the width to thickness plastic strains, was determined under the assumption of incompressibility as $R = \varepsilon_w^p / (-\varepsilon_l^p - \varepsilon_w^p)$.

2.3. Results of Uniaxial Tension Test

For the T4 specimen, the uniaxial tension tests were conducted for two duplicate specimens. The difference in the flow stresses was less than 1%, and the reproducibility of the experiment was satisfactory in capturing the anisotropy of the specimen. Figure 2a shows one of the duplicate true stress–logarithmic strain curves of the T4 specimen. The flow stress was the highest at $\theta = 0^\circ$ and the lowest at $\theta = 60^\circ$. The flow stress at $\varepsilon_l^p = 0.002, 0.05, 0.1, 0.15$, and 0.2 was determined and normalized by that for $\theta = 0^\circ$. The normalized flow stress is shown in Figure 2b. Here, the mean values of the two duplicate results are plotted. The normalized flow stress was unity at $\theta = 0^\circ$, it decreased to the lowest value of approximately 0.94–0.95 at $\theta = 60^\circ$, and increased to approximately 0.96 at $\theta = 90^\circ$. The normalized flow stress was concave upward, and this trend was retained irrespective of the amount of applied strain. Figure 2c shows the R values at $\varepsilon_l^p = 0.05, 0.1, 0.15$, and 0.2 . The mean value of the two duplicate experiments was plotted, and the difference in R for the duplicate experiments was 0.02 at most. R was approximately 0.8, 0.3, and 0.7 at $\theta = 0^\circ, 45^\circ$ and 90° , respectively. The lowest R in $\theta = 45^\circ$ is a typical feature of a cube textured sheet [23,24]. The R value increased slightly as the plastic strain increased.

Figure 2. Results of uniaxial tension for T4 temper sheet. (a) True stress–logarithmic strain curve; (b) Normalized flow stress; and (c) R value.

Figure 3 shows the results of the uniaxial tension tests for the O specimen. Figure 3a shows the true stress–logarithmic strain curve. The flow stress was the highest at $\theta = 45^\circ$ and the lowest at $\theta = 90^\circ$. The normalized flow stress is shown in Figure 3b. At $\epsilon_l^p = 0.002$, the in-plane variation of the flow stress was relatively small. Subsequently, as the plastic strain increased, the normalized flow stress increased at $\theta = 45^\circ$ and decreased at $\theta = 90^\circ$. The variation of the flow stress in the form of the concave downward curve was opposite to that for the T4 specimen. In addition, the normalized flow stress continuously evolved for the O specimen, which was in contrast to the T4 specimen. Figure 3c shows the R values. The R values were approximately 0.8, 0.35, and 0.7 for $\theta = 0^\circ$, 45° , and 90° , respectively, and they increased slightly with an increase in the plastic strain. The in-plane variation of the R value was almost the same for the O and T4 specimens. At $\theta = 45^\circ$, the R value was slightly higher for the O specimen than that for the T4 specimen. This result was attributable to the reduction of the cube texture component by annealing.

Figure 3. Results of uniaxial tension for O temper sheet. (a) True stress–logarithmic strain curve; (b) Normalized flow stress; and (c) R value.

In the experiment, the overall trend of the variation of R was almost the same for the T4 and O specimens. This agreement was consistent with the textures of these specimens, which were nearly identical as shown in Figure 1. The lowest R at $\theta = 45^\circ$ for both specimens was caused by the strong cube texture component. The polycrystal plasticity simulation can reproduce such a variation in the R value for the cube textured sheet [23,24].

Contrary to the R value, the in-plane variation of the normalized flow stress was considerably dissimilar for these specimens. It was concave upward and downward for the T4 and O specimens, respectively. The in-plane flow stress varied in the opposite direction. Furthermore, the variation of normalized flow stress varied with the plastic strain for only the O specimen. The annealing of the specimen altered the orientation dependence of the flow stress. The texture and grain morphology of the T4 and O specimens were the same, and they cannot explain these discrepancies in the flow stress anisotropy.

3. Crystal Plasticity Simulations

3.1. Dislocation-Density Based Crystal Plasticity Model

Face-centered cubic (fcc) crystals with 12 $\{111\} \langle 110 \rangle$ slip systems were considered. $\mathbf{s}^{(\alpha)}$ and $\mathbf{m}^{(\alpha)}$ denote unit vectors representing the slip direction and the normal to the slip plane, respectively. The resolved shear stress on the α th slip system, $\tau^{(\alpha)}$, is obtained by $\tau^{(\alpha)} = \mathbf{s}^{(\alpha)} \cdot \boldsymbol{\sigma} \cdot \mathbf{m}^{(\alpha)}$, where $\boldsymbol{\sigma}$ denotes the Cauchy stress. The slip rate of the α th slip system, $\dot{\gamma}^{(\alpha)}$, is given by

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \text{sgn}(\tau^{(\alpha)}) \left| \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right|^{1/m} \quad (1)$$

where $\dot{\gamma}_0$ is the reference slip rate, m is the strain-rate sensitivity exponent, and $g^{(\alpha)}$ is the resistance to slip.

The slip resistance is given by

$$g^{(\alpha)} = \tau_0 + \bar{\alpha}\mu b \sqrt{\sum_{\beta} A^{\alpha\beta} \rho^{(\beta)}} \quad (2)$$

where τ_0 is the intrinsic friction to slip, μ is the shear elastic modulus, b is the magnitude of the Burgers vector, $\rho^{(\alpha)}$ is the dislocation density associated with the α th slip system, and $A^{\alpha\beta}$ is a matrix representing the strength of dislocation interaction. For the fcc crystal, $A^{\alpha\beta}$ is constructed using six parameters [25,26]: A_{self} for self-interaction, A_{cp} for coplanar interaction, A_{cl} for colinear interaction, A_{gl} for glissile junction, A_{LC} for Lomer–Cottrell lock, and A_{H} for Hirth lock.

For the evolution of dislocation density, the Kocks–Mecking type model [27,28] was adopted as

$$\dot{\rho}^{(\alpha)} = \frac{1}{b} \left(\frac{\sqrt{\sum_{\beta} B^{\alpha\beta} \rho^{(\beta)}}}{k_1} - k_2 \rho^{(\alpha)} \right) |\dot{\gamma}^{(\alpha)}| \quad (3)$$

where k_1 and k_2 are material parameters, and $B^{\alpha\beta}$ is an interaction matrix constructed by six parameters: B_{self} , B_{cp} , B_{cl} , B_{gl} , B_{LC} , and B_{H} . The subscript distinguishes the type of interaction.

3.2. Procedure for Simulation of Polycrystalline Sheet

In the simulation, a polycrystal model consisted of 1728 ($=12 \times 12 \times 12$) elements as shown in Figure 4. An eight-node element with selective reduced integration was used. One crystal orientation was assigned to one element, and the polycrystal model possesses totally 1728 crystal orientations. The 1728 crystal orientations were generated from the experimental ODF. A procedure to obtain the 1728 discrete crystal orientations from ODF is described in Appendix A.

Figure 4. Polycrystal aggregate model consisting of 1728 elements. One element represents one grain.

For the simulation of polycrystals, we used the homogenization method described in Yoshida and Okada [29], which follows the procedure developed by Wu and Ohno [30], and Ohno et al. [31]. A periodic boundary condition was imposed. For the elastic–viscoplastic material, one can obtain the macroscopic (homogenized) constitutive relationship in the form of

$$\dot{\bar{\sigma}} = \bar{\mathbf{C}} : \bar{\mathbf{D}} - \bar{\mathbf{P}} \quad (4)$$

where macroscopic quantities are denoted by bars, $\overline{(\bullet)}$. Namely, $\bar{\sigma}$, $\bar{\mathbf{C}}$, $\bar{\mathbf{D}}$, and $\bar{\mathbf{P}}$ are the macroscopic quantities of the Jaumann rate of Cauchy stress, elastic moduli, stretching, and viscoplasticity-associated term, respectively. From Equation (4) and $\dot{\bar{\sigma}} = \dot{\bar{\sigma}} - \bar{\mathbf{W}} \cdot \bar{\sigma} + \bar{\sigma} \cdot \bar{\mathbf{W}}$,

one can obtain the relationship between the Cauchy stress rate, $\dot{\bar{\sigma}}$, and the velocity gradient, $\dot{\mathbf{L}}$. The fifteen components of $\mathbf{L}$ and $\dot{\bar{\sigma}}$ are unknown. To simulate the uniaxial tension test, nine components were specified as

$$\bar{L}_{11} = \dot{\epsilon}, \bar{L}_{21} = \bar{L}_{32} = \bar{L}_{31} = 0, \text{ and } \dot{\bar{\sigma}}_{22} = \dot{\bar{\sigma}}_{33} = \dot{\bar{\sigma}}_{12} = \dot{\bar{\sigma}}_{23} = \dot{\bar{\sigma}}_{31} = 0 \quad (5)$$

where $\dot{\epsilon}$ was determined such that $\sqrt{(2/3)\mathbf{D} : \mathbf{D}}$ became 10^{-3} s^{-1} . The constitutive equation determines the remaining six unknown components.

4. Results

4.1. O Temper Sheet

For all simulations of the O sheet, material parameters were set as $\tau_0 = 9.5 \text{ MPa}$, $\bar{\alpha} = 0.35$, $\mu = 27 \text{ GPa}$, $b = 2.86 \times 10^{-10} \text{ m}$, $\rho^{(\alpha)} = 10^{-10} \text{ m}^{-2}$ (initial value), $\dot{\gamma}_0 = 0.002$, and $m = 0.002$. Material parameters k_1 and k_2 were identified such that the predicted true stress–logarithmic strain curve for $\theta = 0^\circ$ agreed with the experimental curve. Uniaxial tension for the O sheet was performed with five sets of the interaction matrix denoted by O-1 to O-5, listed in Table 2. For model O-1, the components of the interaction matrix were taken as $A^{\alpha\beta} = 1$ for all interactions, $B^{\alpha\beta} = 0$ for the self and coplanar interactions, and $B^{\alpha\beta} = 1$ for the other interactions. The predicted flow stress and R value are shown in Figure 5a. The normalized flow stress was less than unity in most of the loading directions, except for those at $\epsilon_l^p = 0.002$. These predictions were considerably different from the experimental results (Figure 3b). The predicted R value is shown in Figure 5b. The R value was the lowest at $\theta = 45^\circ$, and it increased with the plastic strain. Thus, the predicted R value was similar to the experimental observations. Closer examination reveals that the predicted R values at $\theta = 0^\circ$ and 90° are higher than the experimental results, and those at $\theta = 45^\circ$ are lower. The difference is approximately 0.1 at most.

The influence of the interaction matrices, $A^{\alpha\beta}$ and $B^{\alpha\beta}$, was examined. For model O-2, we referred to the interaction coefficients determined based on the discrete dislocation dynamic simulation [25]. The reported interaction coefficients were normalized by the coefficient for self-interaction A_{self} . Multiplication of the interaction coefficients for the model O-2 by 0.122 recovers the coefficients reported in [25]. The predicted flow stress is shown in Figure 6a. The flow stress was the highest at $\theta = 45^\circ$, and it increased with the plastic deformation. These predictions agreed with the experimentally observed flow stress variation (Figure 3b). For model O-3, the $A^{\alpha\beta}$ for the self and coplanar interactions were set to unity and those for the other latent interactions were taken to be 1.4. As shown in Figure 6b, the predicted flow stress was the highest between $\theta = 30^\circ$ and 45° , and the general trend was similar to that in the experiment. However, the anisotropic hardening was not predicted; the variation of normalized flow stress did not evolve even when the plastic strain increased. From these simulations, it was found that the flow stress is sensitive to the interaction matrix $A^{\alpha\beta}$, and $A^{\alpha\beta}$ determined from the discrete dislocation dynamics simulation provides a better agreement with the experimental results for the O temper sheet.

Table 2. Material parameters in crystal plasticity simulation for the O sheet.

Notation	k_1	$k_2 \text{ (m)}$	$A^{\alpha\beta}$	$B^{\alpha\beta}$
O-1	6.90	6.35×10^{-8}	1.0 for all	
O-2	6.42	6.68×10^{-8}	$A_{\text{self}} = A_{\text{cp}} = A_{\text{LC}} = 1, A_{\text{c1}} = 5.12, A_{\text{H}} = 0.57,$ $A_{\text{gl}} = 1.12$	$B_{\text{self}} = B_{\text{cp}} = 0; 1.0 \text{ for others}$
O-3	6.83	6.12×10^{-8}	$A_{\text{self}} = A_{\text{cp}} = 1; 1.4 \text{ for others}$	
O-4	8.95	5.81×10^{-8}	1.0 for all	1.0 for all
O-5	10.52	5.87×10^{-8}		$B_{\text{self}} = B_{\text{cp}} = B_{\text{LC}} = 1, B_{\text{c1}} = 5.12, B_{\text{H}} = 0.57,$ and $B_{\text{gl}} = 1.12$

Figure 5. Crystal plasticity prediction with model O-1. (a) Normalized flow stress and (b) R value.

Figure 6. Crystal plasticity prediction of normalized flow stress for (a) model O-2, (b) model O-3, (c) model O-4, and (d) model O-5.

For model O-4, all interaction matrices are set to $A^{\alpha\beta} = 1$ and $B^{\alpha\beta} = 1$ to examine the influence of $B^{\alpha\beta}$. The predicted flow stresses are shown in Figure 6c. The predicted flow stresses were similar to the prediction with the model O-1 and were dissimilar to the experimental results. The influence of $B^{\alpha\beta}$ was further examined by adopting the model O-5, in which $B^{\alpha\beta}$ determined based on the discrete dislocation dynamic simulation were

used and $A^{\alpha\beta}$ was set as unity. As shown in Figure 6d, the predicted flow stress was almost the same as that for the model O-1 and O-4. Thus, the interaction matrix $B^{\alpha\beta}$ has less influence on the anisotropy of the flow stress.

So far, the influence of $A^{\alpha\beta}$ and $B^{\alpha\beta}$ on the orientation dependence of the flow stress has been examined. Their effects on the R value are shown in Figure 7. The R values at $\varepsilon_l^p = 0.1$ are plotted. The R values predicted with the models O-1 to O-5 were closely plotted. The largest scatter was as small as 0.04 at $\theta = 75^\circ$. Thus, the R value was almost insensitive to the interaction matrix $A^{\alpha\beta}$ and $B^{\alpha\beta}$, and the texture is the most influential parameter.

Figure 7. R values predicted with model O-1, O-2, O-3, O-4, and O-5 are compared with the experimental results of the O temper sheet. R value is evaluated at $\varepsilon_l^p = 0.1$.

4.2. T4 Temper Sheet

The uniaxial tension for the T4 specimen was simulated. For the simulations, $\tau_0 = 65.4$ MPa, $B^{\alpha\beta} = 0$ for the self and coplanar interactions, and $B^{\alpha\beta} = 1$ for the other interactions. The parameters $\bar{\alpha}$, μ , b , $\dot{\gamma}_0$, m , and initial dislocation density were the same as those used for the simulations of the O specimen. Here, we only investigated the influence of $A^{\alpha\beta}$ on the plastic behavior of the T4 specimen as the interaction matrix $B^{\alpha\beta}$ had little effect as shown in Section 4.1. Simulation was performed with four sets of material parameters shown in Table 3.

Table 3. Material parameters in crystal plasticity simulation for the T4 sheet.

Notation	k_1	k_2 (m)	$A^{\alpha\beta}$	$B^{\alpha\beta}$
T4-1	10.7	1.57×10^{-8}	1.0 for all	$B_{\text{self}} = B_{\text{cp}} = 0$; 1.0 for others
T4-2	11.1	1.45×10^{-8}	$A_{\text{self}} = A_{\text{cp}} = A_{\text{LC}} = 1$, $A_{\text{cl}} = 5.12$, $A_{\text{H}} = 0.57$, $A_{\text{gl}} = 1.12$	
T4-3	10.7	1.56×10^{-8}	$A_{\text{self}} = A_{\text{cp}} = 1$; 1.4 for others	
T4-4	8.17	1.72×10^{-8}	$A_{\text{self}} = A_{\text{cp}} = 1$; 0.5 for others	

Figure 8a shows the predicted normalized flow stress for model T4-1, for which all the interaction coefficients are set to unity, i.e., $A^{\alpha\beta} = 1$. The predicted variation of the flow stress was similar to that for the model O-1, for which $A^{\alpha\beta} = 1$ for all interactions. The flow stress around $\theta = 45^\circ$ was initially higher than unity and subsequently became lower than unity. For the strain range of $\varepsilon_l^p \geq 0.1$, the predicted normalized flow stress was similar to the experimental results, though the flow stresses around $\theta = 45^\circ$ and 60° were much lower in the experiment. Contrary to the O sheet, the interaction matrix of $A^{\alpha\beta} = 1$ predicts the experimental trend of the variation of flow stress for the T4 sheet.

Figure 8. Crystal plasticity predictions of normalized flow stress with (a) model T4-1, (b) model T4-2, (c) model T4-3, and (d) model T4-4.

$A^{\alpha\beta}$ determined from the discrete dislocation dynamics simulations were adopted for model T4-2, and the predicted flow stress is shown in Figure 8b. The flow stress was the highest between $\theta = 30^\circ$ and 45° regardless of the applied plastic strain. This orientation dependence is similar to the predictions for the model O-2. The concave downward shape of the predicted normalized flow stress was opposite to the experimental results. The interaction matrix determined based on the discrete dislocation dynamics simulation did not predict the experimental trend of the T4 sheet, although it predicted the experimental trend of the O sheet. For model T4-3, the interaction matrix was set as $A^{\alpha\beta} = 1$ for the self- and coplanar interactions and $A^{\alpha\beta} = 1.4$ for the other latent interactions. The results are shown in Figure 8c. The normalized flow stress was the highest between $\theta = 30^\circ$ and 60° . This behavior was the same as the predictions with the model O-3 and was dissimilar to the experimental results. Thus, the increase in the latent hardening parameter did not improve the prediction accuracy for the T4 sheet.

For model T4-4, the latent interaction coefficients were set to $A^{\alpha\beta} = 0.5$, while the interaction coefficients remain $A^{\alpha\beta} = 1$ for the self- and coplanar interactions. The predicted flow stresses are shown in Figure 8d. The predictions for the model T4-4 were close to those for the model T4-3, although the predicted normalized flow stress around $\theta = 45^\circ$ was slightly reduced for the model T4-4. The latent interaction was 1.0, 1.4, and 0.5 for the models T4-1, T4-3, and T4-4, respectively, and the model T4-1 predicted the lowest normalized flow stress around $\theta = 45^\circ$. Thus, neither increase nor decrease in the latent hardening coefficient improves the predictions.

The predicted R values for the models T4-1 to T4-4 are shown in Figure 9. Contrary to the flow stress, the variation in the R value was not affected by the interaction matrix $A^{\alpha\beta}$. This result is consistent with those for the O specimen.

Figure 9. R values predicted with model T4-1, T4-2, T4-3, and T4-4 at $\varepsilon_l^p = 0.1$ are compared with the experimental results.

In this section, we found that the influences of interaction matrix on the orientation dependence of flow stress was almost identical for the T4 and O specimens. Thus, the interaction matrix $A^{\alpha\beta}$ is one of the most influential factors that govern orientation dependence of flow stress. For the T4 specimen, the interaction matrix filled with unity, i.e., $A^{\alpha\beta} = 1$ for all the interactions, resulted in the variation of flow stress similar to the experimental results for large strain range, while it did not predict the experimental trend for the O sheet. The interaction matrix determined from the dislocation dynamics simulations, which reproduced the flow stress anisotropy of the O sheet, did not predict the experimental trend of the T4 sheet. Thus, there is no unique interaction matrix that can predict the flow stress anisotropy of the O and T4 sheets. The interaction matrix has to be adjusted for a given material, if one utilizes the present form of crystal plasticity model that does not explicitly include the influence of the cluster and/or the precipitates.

5. Discussion

It is demonstrated that the flow stress anisotropy of the O sheet in the present experiments is higher at $\theta = 45^\circ$ than those at $\theta = 0^\circ$ and 90° . This orientation dependence of flow stress was similar to that of AA1100-O and AA1050-O [8–10]. This result can be explained in terms of their microstructures. During the annealing of the specimen, the solute atoms bind and sparsely distributed precipitates (Mg_2Si) are created (e.g., [22]). Hence, the obstacles to dislocation motion are reduced in the annealed O temper sheet. Since there are fewer dispersed solute atoms, the O sheet is akin to pure aluminum. In addition, the cube orientation is the main texture component for both the O sheet and pure aluminum. These microstructural features could yield the same orientation dependence of the flow stress.

Crystal plasticity simulations for the O sheet showed that the interaction coefficients determined based on the discrete dislocation dynamics simulation (model O-2) results in the predictions in agreement with the experimental results. This result can be interpreted as follows. Since there are few dispersed solute atoms and sparsely distributed precipitates for the O sheet, the obstacle to dislocation motion is primarily the dislocation. In the discrete dislocation dynamic simulation, neither the solute atoms nor the precipitates are considered, hence interaction among dislocations is solely mechanism of work hardening. Thus, the major mechanism of the work hardening is identical for both the O sheet and the discrete dislocation dynamic simulation.

The present experiments show that the flow stress anisotropy of the T4 sheet is significantly different from that of the O sheet. In the T4 sheet, the solute atoms are dispersed and form clusters, which are the main microstructural differences from the O sheet. It is reported that the dislocation walls with dense dislocation density is observed for a pure aluminum alloy [32]. Whereas the dislocation walls are weak or are not formed in AA6xxx-T4, as the solute atoms and clusters act as barriers to the formation of dislocation cells [33]. Regarding these facts, in addition to the interaction among dislocations, the interactions of solute atom–dislocation and cluster–dislocation and their influence on the anisotropy have to be considered. This could explain the reason why the interaction matrix determined by discrete dynamic simulation does not predict the anisotropy of flow stress of the T4 sheet. However, the reason that the interaction matrix of $A^{\alpha\beta} = 1$ provides a variation of flow stress similar to the experimental results is not clear now. Moreover, the interaction matrix of $A^{\alpha\beta} = 1$ failed to predict the anisotropy flow stress right after the plastic yielding. To solve these issues, further investigations are necessary on the influences of solute atoms and clusters on the dislocation motion and resulting plastic anisotropy.

The interaction between the Guinier and Preston (GP) zone and screw dislocation in the Al–Cu alloy was examined using atomistic simulations [34]. The occurrence of cross slip significantly reduced the shear strength. When the GP zone was less than 3 nm, the dislocation cross-slipped far from the GP zone and overcame the GP zone on the cross-slip plane. Clusters in AA6xxx-T4 were reported to be smaller than 3 nm [3]. From these data, we expect that some amount of screw dislocations cross-slipped in front of the clusters in the T4 sheet. According to the Friedel–Escaig type cross-slip model, a part of dissociated dislocation on the glide plane has to constrict once. Subsequently, it dissociates and glides on the cross-slip plane. In this process, not only the Schmid stress on the glide plane—but also the Escaig stress on the glide plane and the Escaig and Schmid stresses on the cross-slip plane—affect the cross-slip activation. The incorporation of the cross-slip process, which includes the orientation-dependent Schmid and Escaig stresses, might be one of the possible extensions of the current crystal plasticity model. The investigation along this line of thought is beyond the scope of this work and will be our future work.

The present study shows that the interaction matrix affects the flow stress anisotropy, and this result is consistent with the conclusions in the literature [18,19]. However, the present results disclaim the possibility that the latent hardening improves the prediction accuracy of the flow stress anisotropy for the T4 sheet. Khadyko et al. [18] successfully predicted the general trend of flow stress anisotropy of AA6060-T4 with various interaction matrixes. The flow stress anisotropy of their specimen, which is machined from an extruded plate, is much larger than the present experimental data, and their R value that ranges between nearly zero and 1.8 shows severe anisotropy. The influence of texture seems to be strong for their material, hence various interaction matrixes could capture the experimental trend. Zecevic and Knezevic [19] simulation showed that the latent hardening improves the prediction accuracy of flow stress. They assessed the anisotropy in the normalized flow stress only at a tensile strain of 0.18. In the present work, the interaction matrix of $A^{\alpha\beta} = 1$ predicted the flow stress anisotropy close to the experimental results in a large strain range. At this point, these results are consistent. However, in a small strain range, the predictions were dissimilar to the experimental results in the present work. Namely, the interaction matrix of $A^{\alpha\beta} = 1$ induced the anisotropic work hardening, and this is also a topic to be investigated.

6. Conclusions

In the present investigation, uniaxial tension tests were conducted for Al–Mg–Si sheets in T4 and O tempers, and the plastic anisotropy was evaluated. The experiments clearly disclose the difference in the anisotropy of flow stress for the T4 and O temper sheets. For the O temper sheet, the normalized flow stress is the highest in the diagonal direction, and the work hardening is anisotropic. For the T4 specimen, the normalized flow stress in the diagonal direction is close to the lowest, and the anisotropic work hardening is

not exhibited. Thus, the present experiment demonstrates that the annealing alters the orientation dependence of the flow stress in opposite direction. By contrast, the in-plane variation of the R value is almost identical for these sheets.

The dislocation density-based crystal plasticity model was used to predict the plastic behavior of the specimens. The dislocation interaction matrix has a remarkable impact on the flow stress anisotropy, while it does not have an influence on the prediction of R value. The crystal plasticity model with an interaction matrix determined based on the discrete dislocation dynamic simulation can accurately predict the flow stress anisotropy of the specimen in the O sheet, whereas this interaction matrix cannot predict the anisotropy of flow stress for the T4 sheet. The interaction matrix filled with unity reproduce the variation of flow stress similar to the experimental results of the T4 sheet for the large strain range. Thus, there is no unique interaction matrix that can predict the flow stress anisotropy of the O and T4 sheets. The interaction matrix has to be carefully determined for a given material for the accurate simulation of the flow stress anisotropy.

No interaction matrix investigated in the present work accurately predicts the flow stress anisotropy in small strain range of the T4 sheet. Further investigation is needed on this point. It has to be investigated how solute atoms and clusters contribute to the resistance to the plastic glide and alter the resulting plastic anisotropy. The authors continue the investigation along this line.

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Appendix A

Discretization of ODF

Polycrystal model used in the present study consists of 1728 ($= 12^3$) equi-volume grains. A total of 1728 orientations were generated from the experimental ODF. A procedure similar to the STAT proposed by Toth and Van Houtte [35] was developed.

The ODF is constructed by the intensities at N_{grid} grid points (or boxes). The Euler angles associated with the i th grid point are denoted by $\varphi_1(i)$, $\phi(i)$, and $\varphi_2(i)$. From the intensity and Euler angles, the volume fraction of the i th box $V_f(i)$ can be calculated. The cumulative function $F(i)$ can be obtained by integrating the volume fractions.

$$F(i) = \sum_{j=1}^i V_f(j) \text{ for } i = 1, \dots, N_{\text{grid}} \quad (\text{A1})$$

Here, the cumulative function is $F(0) = 0$ and $F(N_{\text{grid}}) = 1$.

We now consider a procedure to select N_L sets of Euler angles. Introducing an integer k , we find j that satisfies

$$F(j-1) < \frac{k}{N_L} \leq F(j), \text{ for } k = 1, \dots, N_L \quad (\text{A2})$$

Since k ranges from 1 to N_L , N_L sets of Euler angles are selected with a constant interval of volume fraction. To satisfy orthotropy rigorously, three orientations are added for each set.

$$(\varphi_1, \phi, \varphi_2) \rightarrow (\pi - \varphi_1, \phi, -\varphi_2), (\pi + \varphi_1, \phi, \varphi_2), (-\varphi_1, \phi, -\varphi_2) \quad (\text{A3})$$

Finally, $n_L = 4N_L$ orientations are obtained. If n_L is sufficiently large, n_L equi-volume grains can accurately represent the statistical property of the ODF. In the present work, $n_L = 10^6$ was considered. The Euler angles determined here are used as a reference texture for the following processes.

Next, $N (\ll N_L)$ sets of Euler angles are selected. Using random numbers S ranging from 0 to 1, we find j that satisfies

$$F(j-1) < \frac{k+S-1}{N} \leq F(j), \text{ for } k = 1, \dots, N, \text{ with } 0 \leq S \leq 1 \quad (\text{A4})$$

Since k ranges from 1 to N , N sets of Euler angles are selected. To satisfy the orthotropy, three equivalent orientations are added (Equation (A3)). Finally, one obtains $n = 4N$ orientations. The variable interval of the volume fraction is used in Equation (A4) instead of the constant interval, which works well only if one selects a large number of orientations. Because the selected Euler angles depend on random numbers, one can produce a number of different sets of Euler angles. The aforementioned procedure is repeated M times with different random numbers. In the present work, we took $n = 1728$ and $M = 1000$.

So far, one has obtained the reference Euler angles consisting of n_L orientations and M sets of Euler angles consisting of n orientations. Using these discrete orientations in conjunction with the Taylor model, the uniaxial tension is simulated at every 15° between RD and TD, and the ratio of the width strain to the thickness strain is determined. In addition, the in-plane strain ratio under balanced biaxial tension is determined. These eight strain ratios for the reference texture are denoted by $\beta_{\text{ref}}(i)$ for $i = 1-8$. The eight strain ratios for M sets of Euler angles are denoted by $\beta(i, j)$ for $i = 1-8$ and $j = 1-M$. The error is assessed by

$$\text{error}(j) = \sum_{i=1}^8 \frac{|\beta(i, j) - \beta_{\text{ref}}(i)|}{\beta_{\text{ref}}(i)} \text{ for } j = 1-M \quad (\text{A5})$$

After assessing the error for all M sets of Euler angles, the set of Euler angles that provides the least error can be identified. Such a set of Euler angles captures the statistical property of ODF well. This set of Euler angles was used for the simulations in the present work.

The use of the Taylor model facilitates the uniaxial tension simulations for a large number of orientations n_L and for a number of sets of orientations. In this procedure, the strain ratio β is calculated because the anisotropy of the strain ratio is more sensitive to the texture than that of the flow stress. The Taylor model is used to assess the statistical property of discretized orientations, and its prediction accuracy against experimental data is not critical in this procedure.

References

1. Ringer, S.P.; Polmear, I.J.; Hono, K.; Sakurai, T. Cluster hardening in an aged Al-Cu-Mg alloy. *Scr. Mater.* **1997**, *36*, 517–521. [\[CrossRef\]](#)
2. Marceau, R.K.; de Vaucorbeil, A.; Sha, G.; Ringer, S.P.; Poole, W.J. Analysis of strengthening in AA6111 during the early stages of aging: Atom probe tomography and yield stress modelling. *Acta Mater.* **2013**, *61*, 7285–7303. [\[CrossRef\]](#)
3. Aruga, Y.; Kozuka, M.; Takaki, Y.; Sato, T. Formation and reversion of clusters during natural aging and subsequent artificial aging in an Al-Mg-Si alloy. *Mater. Sci. Eng. A* **2015**, *631*, 86–96. [\[CrossRef\]](#)
4. Engler, O.; Schäfer, C.; Myhr, O.R. Effect of natural ageing and pre-straining on strength and anisotropy in aluminium alloy AA6016. *Mater. Sci. Eng. A* **2015**, *639*, 65–74. [\[CrossRef\]](#)

5. Khadyko, M.; Dumoulin, S.; Hopperstad, O.S. Texture gradients and strain localisation in extruded aluminium profile. *Int. J. Solids Struct.* **2016**, *97*, 239–255. [\[CrossRef\]](#)
6. Khadyko, M.; Myhr, O.R.; Hopperstad, O.S. Work hardening and plastic anisotropy of naturally and artificially aged aluminium alloy AA6063. *Mech. Mater.* **2019**, *136*, 103069. [\[CrossRef\]](#)
7. Kuwabara, T.; Mori, T.; Asano, M.; Hakoyama, T.; Barlat, F. Material modeling of 6016-O and 6016-T4 aluminum alloy sheets and application to hole expansion forming simulation. *Int. J. Plast.* **2017**, *93*, 164–186. [\[CrossRef\]](#)
8. Li, F.; Bate, P.S. Strain path change effects in cube textured aluminium sheet. *Acta Metal. Mater.* **1991**, *39*, 2639–2650. [\[CrossRef\]](#)
9. Lopes, A.B.; Barlat, F.; Gracio, J.J.; Duarte, J.F.; Rauch, E.F. Effect of texture and microstructure on strain hardening anisotropy for aluminum deformed in uniaxial tension and simple shear. *Int. J. Plast.* **2003**, *19*, 1–22. [\[CrossRef\]](#)
10. Zhang, K.; Holmedal, B.; Hopperstad, O.S.; Dumoulin, S.; Gawad, J.; Van Bael, A.; Van Houtte, P. Multi-level modelling of mechanical anisotropy of commercial pure aluminium plate: Crystal plasticity models, advanced yield functions and parameter identification. *Int. J. Plast.* **2015**, *66*, 3–30. [\[CrossRef\]](#)
11. Lademo, O.G.; Engler, O.; Keller, S.; Berstad, T.; Pedersen, K.O.; Hopperstad, O.S. Identification and validation of constitutive model and fracture criterion for Al-Mg-Si alloy with application to sheet forming. *Mater. Des.* **2009**, *30*, 3005–3019. [\[CrossRef\]](#)
12. Kami, A.; Dariani, B.M.; Vanini, A.S.; Comsa, D.S.; Banabic, D. Numerical determination of the forming limit curves of anisotropic sheet metals using GTN damage model. *J. Mater. Process. Technol.* **2015**, *216*, 472–483. [\[CrossRef\]](#)
13. Lee, M.G.; Kim, D.; Kim, C.; Wenner, M.L.; Wagoner, R.H.; Chung, K. Spring-back evaluation of automotive sheets based on isotropic-kinematic hardening laws and non-quadratic anisotropic yield functions Part II: Characterization of material properties. *Int. J. Plast.* **2005**, *21*, 883–914.
14. Bate, P.; Roberts, W.T.; Wilson, D.V. The plastic anisotropy of two-phase aluminum alloys—I. Anisotropy in unidirectional deformation. *Acta Metall.* **1981**, *29*, 1797–1814. [\[CrossRef\]](#)
15. Han, C.S.; Wagoner, R.H.; Barlat, F. On precipitate induced hardening in crystal plasticity: Theory. *Int. J. Plast.* **2004**, *20*, 477–494. [\[CrossRef\]](#)
16. Li, Y.L.; Kohar, C.P.; Mishra, R.K.; Inal, K. A new crystal plasticity constitutive model for simulating precipitation-hardenable aluminum alloys. *Int. J. Plast.* **2020**, *132*, 102759. [\[CrossRef\]](#)
17. Wu, P.D.; Lloyd, D.J. Analysis of surface roughening in AA6111 automotive sheet. *Acta Mater.* **2004**, *52*, 1785–1798. [\[CrossRef\]](#)
18. Khadyko, M.; Dumoulin, S.; Cailletaud, G.; Hopperstad, O.S. Latent hardening and plastic anisotropy evolution in AA6060 aluminium alloy. *Int. J. Plast.* **2016**, *76*, 51–74. [\[CrossRef\]](#)
19. Zecevic, M.; Knezevic, M. Latent hardening within the elasto-plastic self-consistent polycrystal homogenization to enable the prediction of anisotropy of AA6022-T4 sheets. *Int. J. Plast.* **2018**, *105*, 141–163. [\[CrossRef\]](#)
20. Xie, Q.; Van Bael, A.; An, Y.G.; Lian, J.; Sidor, J.J. Effects of the isotropic and anisotropic hardening within each grain on the evolution of the flow stress, the r-value and the deformation texture of tensile tests for AA6016 sheets. *Mater. Sci. Eng. A* **2018**, *721*, 154–164. [\[CrossRef\]](#)
21. Hama, T.; Yagi, S.; Maeda, Y.; Maeda, Y.; Takuda, H. Evolution of plastic deformation behavior upon strain-path changes in an A6022-T4 Al alloy sheet. *Int. J. Plast.* **2021**, *137*, 102913. [\[CrossRef\]](#)
22. Khadyko, M.; Marioara, C.D.; Dumoulin, S.; Børvik, T.; Hopperstad, O.S. Effects of heat-treatment on the plastic anisotropy of extruded aluminium alloy AA6063. *Mater. Sci. Eng. A* **2017**, *708*, 208–221. [\[CrossRef\]](#)
23. Barlat, F.; Richmond, O. Prediction of tricomponent plane stress yield surfaces and associated flow and failure behavior of strongly textured fcc polycrystalline sheets. *Mater. Sci. Eng.* **1987**, *95*, 15–29. [\[CrossRef\]](#)
24. Kuroda, M.; Ikawa, S. Texture optimization of rolled aluminum alloy sheets using a genetic algorithm. *Mater. Sci. Eng. A* **2004**, *385*, 235–244. [\[CrossRef\]](#)
25. Kubin, L.; Devincere, B.; Hoc, T. Modeling dislocation storage rates and mean free paths in face-centered cubic crystals. *Acta Mater.* **2008**, *56*, 6040–6049. [\[CrossRef\]](#)
26. Yoshida, K.; Ishii, A.; Tadano, Y. Work-hardening behavior of polycrystalline aluminum alloy under multiaxial stress paths. *Int. J. Plast.* **2014**, *53*, 17–39. [\[CrossRef\]](#)
27. Kocks, U.F.; Mecking, H. Physics and phenomenology of strain hardening: The FCC case. *Progress Mater. Sci.* **2003**, *48*, 171–273. [\[CrossRef\]](#)
28. Teodosiu, C. Dislocation Modelling of Crystalline Plasticity. In *Large Plastic Deformation of Crystalline Aggregates*; Teodosiu, C., Ed.; Springer: Vienna, Austria, 1997; pp. 21–80.
29. Yoshida, K.; Okada, N. Plastic flow behavior of fcc polycrystal subjected to nonlinear loadings over large strain range. *Int. J. Plast.* **2020**, *127*, 102639. [\[CrossRef\]](#)
30. Wu, X.; Ohno, N. A homogenization theory for time-dependent nonlinear composites with periodic internal structures. *Int. J. Solids Struct.* **1999**, *36*, 4991–5012. [\[CrossRef\]](#)
31. Ohno, N.; Okumura, D.; Noguchi, H. Microscopic symmetric bifurcation condition of cellular solids based on a homogenization theory of finite deformation. *J. Mech. Phys. Solids* **2002**, *50*, 1125–1153. [\[CrossRef\]](#)
32. Liu, Q.; Juul Jensen, D.; Hansen, N. Effect of grain orientation on deformation structure in cold-rolled polycrystalline aluminium. *Acta Mater.* **1998**, *46*, 5819–5838. [\[CrossRef\]](#)
33. Rauch, E.F.; Gracio, J.J.; Barlat, F.; Lopes, A.B.; Duarte, J.F. Hardening behavior and structural evolution upon strain reversal of aluminum alloys. *Scr. Mater.* **2002**, *46*, 881–886. [\[CrossRef\]](#)

-
34. Singh, C.V.; Mateos, A.J.; Warner, D.H. Atomistic simulations of dislocation–precipitate interactions emphasize importance of cross-slip. *Scr. Mater.* **2011**, *64*, 398–401. [[CrossRef](#)]
 35. Toth, L.S.; Van Houtte, P. Discretization techniques for orientation distribution functions. *Textures Microstruct.* **1992**, *19*, 229–244. [[CrossRef](#)]