Modeling of the Retrogression Microstructure Behavior of 7075 Aluminum Alloy

Baohua Nie¹, Peiying Liu¹, Tietao Zhou¹, Zheng Zhang¹, Zhiwei Du²

¹Department of Materials Science and Engineering, Beihang University, Xueyuan Road 37, Haidian District, Beijing, China
²General Research Institute for Nonferrous Metals, Xinjiekouwai Street 2, Haidian District, Beijing, China

In this paper, a numerical model, coupled with the dissolution, growth and coarsening of precipitates, is developed to describe the microstructure evolution during retrogression treatment of 7075 alloy, an ultra-high strength toughness aerospace aluminum alloy. The prediction of microstructure parameters, such as precipitates radius, volume fraction, density, are performed for both interior grain and grain boundary. An idealized grain boundary affected zone is established to predict the microstructure evolution of grain boundary precipitates, the morphology of which has strong influence on SCC resistance of this alloy. The model explores the effect of retrogression temperature on the microstructure of retrogression for 7075 alloy and provides foundation for the optimization of RRA heat treatment to the ultra-high strength 7000 series aluminum alloys. The model is generally in good agreement with the experimental data performed by J.K.Park[3] and can be used to understand clearly the process of retrogression treatment of 7000 series aluminum alloys.

Keywords: retrogression treatment; 7075 Aluminum Alloy; modeling; grain boundary precipitate

1 Introduction

Retrogression and re-aging treatment (RRA) has the effect on enhancing the stress corrosion cracking (SCC) resistance of 7075 aluminum alloy, while retaining the strength of it in T6 condition [1]. Most researchers have focused on the influence of retrogression and re-aging parameters on microstructures and properties of alloys [2,3] and modified RRA treatment for thick section components by using lower retrogression temperatures [4-6]. However, the evolution of microstructure and properties during the process is not clearly understood, and there are still some disagreements with the influence of retrogression treatment on microstructure and properties. The alloy retrogressed for short time corresponding to the minimum hardness was supposed to obtain the best combination of strength and resistance to SCC [1], whereas Wallace et al[4] demonstrated that the minimum was not necessary for an optimum time for the retrogression treatment.

It is valuable for a microstructure model to predict the microstructure changes during retrogression treatment, which is crucial to the mechanical and SCC properties. Many models, based on Kampmann and Wangner numerical (KWN) framework, were developed to predict the evolution of microstructure and properties for isothermal [7] and non-isothermal treatments [8,9], but less attention has been paid on retrogression treatment.

The aim of the present work is to develop a model based on KWN framework to quantitatively describe microstructure evolution in retrogression process of 7075 aluminum alloy and provide foundation for the optimization of RRA heat treatment to the ultra-high strength aluminum alloys.
2 Microstructure model

The model is based on the KWN model and classic growth theory is used to calculate the dissolution, growth and coarsening of precipitates during retrogression. The microstructure parameters, such as mean particles radius, volume fraction, density, matrix concentration, were calculated. The model considers the precipitates with spherical morphology and stoichiometric equilibrium composition of η phase (MgZn₂). Nucleation and phase transformation from the η' to the η phase have not been taken into account during retrogression [8]. The dissolution, growth and coarsening of MgZn₂ precipitates is controlled by Mg atom diffusion.

2.1 Microstructure model within grain

2.1.1 Growth/dissolution kinetics

The dissolution or growth of the precipitates with radius r and solute mole fraction X_p depends on whether the particle/matrix interface mole fraction X_i exceeds the mean mole fraction X_m or not. The growth or dissolution rate can be expressed[10]:

\[
\frac{dr}{dt} = D \frac{X_m - X_i}{r} \frac{X_p - X_i}{X} \frac{dX}{dt}
\]

(1)

And a new research shows a proper formulation for intermetallic precipitates [11]:

\[X_i = X_e \exp \left( \frac{2\sigma_{eq}}{X_e r^{eq}} \right)\]

(2)

where X_e is equilibrium mole fraction at the matrix, \(\sigma\) is the particle/matrix interfacial energy (J m⁻²) and \(V_m\) is the molar volume of the precipitate MgZn₂ (m³mol⁻¹). The critical radius \(r^*\) of a precipitate that neither will grow nor dissolve can be evaluated by the modified Gibbs-Thomson equation as [12]:

\[
r^* = \frac{4\sigma_{eq} V_m}{X_e r^{eq}} \left[ \ln \left( \frac{X_m}{X_e} \right) \right]^{-1}
\]

(3)

2.1.2 Growth and coarsening kinetics

The precipitates will be pure coarse if the mean radius and the critical radius are equal [7]. The coarse rate can be evaluated by [13]:

\[
\frac{dr}{dt}_{coars} = \frac{4}{27} \frac{X_p}{\alpha^2 X_p - X_i} \frac{R_0 D}{r^*}
\]

(4)

where \(R_0 = 2\sigma V_m/(RT)\), \(\alpha = V_{at}^M/V_{at}^P\)

The rate of variation of the density of precipitates in pure coarsening is given as [13]

\[
\frac{dN}{dt}_{coars} = \frac{4}{27} \frac{X_p}{\alpha^2 X_p - X_i} \frac{R_0 D}{r^*} \left[ \frac{R X_p}{r^* X_p - X_i} \left( \frac{3}{4\sigma^2} + N \right) \right]^{-3N}
\]

(5)

The evolution of the mean radius and the density, coupled with the growth and coarsening of precipitate, can be described as [7]

\[
\frac{dr}{dt} = \left(1 - f_{coars} \right) \frac{dr}{dt}_{growth} + f_{coars} \frac{dr}{dt}_{coars}
\]

(6)

\[
\frac{dN}{dt} = f_{coars} \frac{dN}{dt}_{coars}
\]

(7)

where \(f_{coars}\) is coarsening fraction and expressed as:
2.2 Microstructure model at grain boundary

The growth of precipitates at grain boundaries was introduced to describe the coarsening of grain boundary precipitates, and the grain boundary precipitates growth rate is expressed as[14, 15]:

\[
\frac{dR}{dt} = \frac{A_v \sqrt{Dt}}{2\pi^{3/2} R^2} \left( X_m - X_i \right)
\]

Where \( A_v \) is the collector plate area defined for a circular area around the precipitates as: \( A_v = 4\pi D_{GB} \Delta t \). \( D_{GB} \) is diffusion coefficient along a grain boundary.

However, the grain boundary precipitates will coarsen when the mole fraction around grain boundary \( X_m \) approaches the particle/matrix interface mole fraction \( X_i \). In that case, we assume the grain boundary precipitates are embedded into a grain boundary affected zone (GBAZ), which is isolated from the matrix. That is because the matrix atoms, such as Mg, Zn, can not promptly diffuse into grain boundary affected zone if the dramatically growth of grain boundary precipitates at high retrogression temperature have been considered. The microstructure evolution of grain boundary precipitates, similar to the within grain precipitates, involving simultaneous growth and coarsening can be described by Eq(2)~Eq(8). whereas, the growth rate of grain boundary precipitates is properly evaluated by Eq(9) and the diffusion coefficient \( D \) during the process of coarsening is considered as diffusion coefficient along a grain boundary \( D_{gb} \).

2.3 Choice of input data

The object of study is commercial 7075 aluminum alloy (Al5.5Zn2.5Mg1.6Cu0.28Cr0.3Mn). The average radius of matrix precipitates in the initial temper (T6) was found to be about 3.8nm, and the total volume of precipitates is 2.9% [2]. The radius of matrix precipitates size distribution is supposed to obey a Gaussian law with width scale as \( \Delta = R/4 \)[7]. The initial population of grain boundary precipitates have an average radius of approximately 13.4nm[3]. According to the reference[14], the volume of grain boundary precipitates is estimated to 0.058%. The mole fractions of precipitates calculated by Thermo-calc software are shown in Table 1. The input data used in the microstructure models to simulate the sequence of microstructure changes occurring during retrogression of 7075 aluminum alloy are summarized in Table 2. The particle/matrix interfacial energy is assumed constant through out the calculations.

<table>
<thead>
<tr>
<th>Table 1 the mole fraction of precipitates</th>
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<tr>
<td>( X_p )</td>
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<td>value(at.%)</td>
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<th>Table 2 Summary of input data used in the microstructure model</th>
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<tr>
<td>( D_{0Mg} )(m^2s^{-1})</td>
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<tr>
<td>value</td>
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4 Results and Discussion

4.1 Microstructure evolution within grain

Fig. 1 shows the evolution of matrix microstructure during retrogression at different temperatures. The precipitates below critical radius will gradually dissolve into matrix, and the ones above that are supposed to undergo the growth and coarsening, as is illustrated in Fig.1a. The precipitates with radius close to 1 nm, will dramatically dissolve into matrix, owing to the Gibbs-Thomson interfacial effect. Correspondingly, it will reduce the volume fraction and increase the Mg concentration in the matrix (Fig.1b, d).

As the retrogression temperature is elevated from 200°C to 240°C, more precipitates dissolve into the matrix, leading to a more decrease in the volume fraction of precipitates and a more increase in corresponding Mg concentration, the corresponding retrogression time decrease. It is interested that the lowest volume fraction of precipitates retrogressed at 200°C is higher than the initial stage due to the dissolution of small volume fraction. Fig.1c reveals that the growth and coarsening of indissoluble precipitates is more significant at higher retrogression temperature. Compared to the gradual growth of precipitates at retrogression temperature of 200°C, the precipitates growth at retrogression temperature of 220°C and 240°C can be divided three region: the precipitates radius increase gradually during the first and the final region, similar to the behavior of retrogression at 200°C; while a rapid increase in precipitates radius occurs in the second region,

![Image of Fig. 1](image-url)
which is promoted by the increase in Mg concentration in the matrix. Furthermore, the growth and coarsening of matrix precipitates during retrogression predicted by the model is in good quantitative agreement with experimental observations of J.K. Park[3], although the experimental radius is slightly larger than the predicted results, which is one consequence of re-aging treatment[2].

4.2 Microstructure evolution at grain boundary

The evolution of microstructure at grain boundary during retrogression is shown in Fig.2. Significant coarsening has occurred in the initial retrogression stage, because the mean radius is close to the critical radius. Correspondingly, there are an increase in precipitates radius and a distinct decrease in precipitates density. At the same time, the coarsening of grain boundary precipitates causes solute depletion around the grain boundary, which is in agreement with the conclusions of N. Kamp et al [14]. Fig.2d also reveals that the Mg concentration around grain boundary is much lower than that of the matrix, forming the precipitate-free zones (PFZ). Furthermore, the model predictions for the radius of grain boundary precipitates is verified by the TEM experiments of J.K. Park[3], because the experimental radius, corresponding to retrogression and re-aging treatments, is close to the radius retrogression precipitates due to little increase in grain boundary precipitates radius after re-aging treatment, as is shown in Fig.2a.

Fig.2 Evolution of microstructure parameters in the grain boundary during retrogression. (a) precipitates radius and critical radius for dissolution at retrogression temperature of 240°C; (b) The radius of indissoluble precipitates (c) precipitates density; (d) matrix and GBAZ solute concentration
The coarsening of precipitates is more remarkable with the elevation of retrogression temperature. According to Fig.2a and Fig.2c, the unchanged density of grain boundary precipitates retrogressed at 200°C indicated that the pure growth of grain boundary precipitates may occur during first minute retrogression, while the grain boundary precipitates retrogressed at 240°C will experience pure coarsening stage in the initial of retrogression, improving the resistance to SCC. W.Wallace [17] considered that the grain boundary precipitates with size greater 20nm is a hydrogen-bubble nucleation, leading to enhancing the better stress corrosion cracking (SCC). Thus, as is predicted by the present model, the alloy will producing the better SCC property if it is retrogressed at 240°C for 24 seconds, 220°C for 126 seconds and 200°C for 433 seconds, respectively.

5 Conclusions

A numerical analytical model based on the KWN model has been developed to predict microstructure evolution in 7075 aluminum alloy during retrogression. The model considers the combination of dissolution, growth and coarsening of precipitates. An idealized grain boundary affected zone is established to predict the microstructure evolution at grain boundary. Predicted changes in precipitates radius show good qualitative agreement with experimental results performed by J.K. Park [3]. The prediction by the present model shows 7075 aluminum alloy will produce a better SCC property if it is retrogressed at 240°C for 24 seconds, 220°C for 126 seconds and 200°C for 433 seconds, respectively.

Reference