Quantitative Phase Field Simulation of α Particle Dissolution in Ti–6Al–4V Alloys Below β Transus Temperature

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Abstract A quantitative phase field method of multi-component diffusion-controlled phase transformations coupled with the Kim–Kim–Suzuki model was applied to study the effect of initial particle size distribution (PSD) in 3D and space distribution in 2D on dissolution of α particles in Ti–6Al–4V alloy below β transus temperature in real time and length scale. The thermodynamic and mobility data were obtained from Thermo-Calc and DICTRA softwares, respectively. The results show that the volume fractions of α particles decay with time as: $f = f_{eq} + (f_0 - f_{eq}) \exp(-Kt^n)$ for four cases of PSD. The sequence of dissolution kinetics from fast to slow is: uniform PSD, normal PSD, lognormal PSD and bimodal PSD. The space distribution is found to be a major factor affecting the dissolution kinetics and the microstructures. When the distance of the particles is less than critical value, the dissolution rates reduce with the decrease in distance. The Al and V concentration fields around the particles appear more obvious soft impingement.

KEY WORDS: Dissolution; Phase field model; Ti–6Al–4V; Initial PSD; Space distribution

1 Introduction

Titanium alloys are widely used in aerospace, medical and chemical industries due to their high strength/weight ratio, low modulus and good corrosion resistance, etc. The performances of titanium alloys depend strongly on their microstructure which is relevant to different

thermomechanical treatments, including smelting, solution treatment, multi-forging and rolling. The α phase in duplex microstructure will be dissolved during deformation at high temperature [1]. The deep understanding of dissolution kinetics will help to control the dissolution time exactly which avoids long holding time at high temperature resulting in abnormal grains and to gain better mechanical properties further. Some experiments [2–5] and simulations [6, 7] have been done to study the α phase dissolution behavior in titanium alloys. Li et al. [2] have researched the effects of heat treatments on the microstructure of Ti–8V–1.5Mo–2Fe–3Al alloy. The shape of α_p transformed from globular to strip while extending solution time from 1 to 4 h at 780 °C. The shape transformation was facilitated by the stored deformation energy in the hot working process. Semiatin et al. [3] studied the dissolution kinetics of lamellar branches in an α – β titanium alloy with a colony α microstructure at 900 and 955 °C. The branch recession rate was about 4 and 10 $\mu\text{m/h}$, respectively. Jones et al. [4] explored the effects of heat-treatment temperature and time on the microstructure of Ti–5Al–5Mo–5V–3Cr. The system approximately approached nominal

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equilibrium when the alloy was heated at 810 °C for 920 s. However, a significant reduction occurred when the solution time extended to 24 h, the α volume fraction dropping from 4.5 to 0.6%. The similar reduction in α volume fraction was observed with the sample held at 835 °C. The microstructure morphology was determined by the solution treatment temperature. Fan et al. [5] found that Ti–7Mo–3Nb–3Cr–3Al alloy possesses slower α to β dissolution rate compared with Ti–5Al–5Mo–5V–3Cr. The low dissolution rate of α phase can be attributed to the increase in the large Mo atoms.

With the development of phase field method as the power tool of modeling the microstructure, a quantitative phase field modeling has been constructed [6] to study the growth and dissolution of a single circular α precipitate in 2D in Ti–Al–V. The chemical mobility in the interface region gave a positive deviation from the simple linear interpolation. The 1D results were fitting well with results in DICTRA. Benoit et al. [7] studied the dissolution behavior of complicated duplex microstructure composed of globular precipitates and intragranular plates during continuous heat treatment in near- β titanium alloys by the same method. The results showed the intragranular plates dissolved faster than the large precipitates due to Gibbs–Thomson effect. Besides the phase field model, there are some other methods dealing with dissolutions of other alloys [8–18]. In the Ref [18], impingement of the diffusion fields from adjacent precipitates is not considered. But the soft impingement can affect the kinetics of diffusion-controlled dissolution. Meanwhile, these methods were limited to single-particle system or multi-particle system where the uniform and lognormal PSD had been considered. However, there were few works about the dissolution under complicated initial PSD and space distribution for titanium alloys. Therefore the quantitative phase field method is applied to study the dissolution of α particles below β transus temperature with complicated PSD in 3D and space distribution in 2D, respectively, in experimentally relevant length and time scales in this work. The thermodynamic data and mobility data are obtained from the Thermo-Calc and DICTRA softwares, respectively. The types of common PSD in alloy include as follows. The typical grain size distribution was lognormal in a polycrystalline [19]. The Normal was actual PSD which was observed on Ti–6Al–4V samples that had been water quenched after soaking for long times at typical alpha/beta heat-treatment temperature [20]. The homogeneous grain-refinement microstructure formed by severe plastic deformation of accumulative roll-bonding (ARB) processed Ti during annealing increased yield strength [21]. The bimodal grain size distribution by sintering mechanically milled powders achieved the good tensile ductility [22]. The dissolution kinetics of multi-particles with previous four cases of initial PSD (uniform PSD, normal PSD,

lognormal PSD, bimodal PSD) and with four types of space distributions are investigated in detail.

2 Phase Field Method

The phase field method was used to describe phase transformations in an n -component system. $n - 1$ concentration fields and a set of order parameter fields are needed. The local free energy of the system as a function of the concentration and order parameter fields can be obtained directly from the CALPHAD technique [6, 23–27]. In the paper, order parameter $\eta = 1$ describes the α phase and $\eta = 0$ describes the β phase.

The total Gibbs free energy of the system can be written:

$$G = \frac{1}{V_m} \int_v \left(G_m + \frac{k}{2} \sum_i |\nabla \eta_i|^2 \right) dV, \quad (1)$$

where V_m is the molar volume, k is the gradient energy coefficient, and G_m is the local molar free energy which can be written as a function of temperature (T), composition X and order parameter $\eta(r, t)$:

$$G_m = p(\eta)G_m^\alpha(X, T) + (1 - p(\eta))G_m^\beta(X, T) + q(\eta), \quad (2)$$

where $p(\eta) = \eta^3(10 - 15\eta + 6\eta^2)$, and $q(\eta) = \omega\eta^2(1 - \eta)^2$. And ω is the height of the imposed double-well hump. $G_m^\alpha(X, T)$ and $G_m^\beta(X, T)$ are the molar free energy of α phase and β phase, respectively, which can be obtained from the Thermo-Calc software. The temporal evolutions of the field parameters are governed by the time-dependent Ginzburg–Landau equation [28] and the generalized Cahn–Hilliard diffusion equations [29] on the basis of the phenomenological Fick–Onsager equation [30]:

$$\frac{\partial \eta}{\partial t} = -L \left(\frac{\partial G_m}{\partial \eta} - k \nabla^2 \eta \right), \quad (3)$$

$$\frac{1}{V_m^2} \frac{\partial X_k}{\partial t} = \nabla \cdot \left(\sum_{i=1}^{n-1} M_{ki}(T, X, \eta) \nabla \frac{\partial G}{\partial X_i} \right), \quad (4)$$

where L is the kinetics coefficient characterizing the evolution of order parameter, $M_{ki}(T, X, \eta)$ is the chemical mobility in the fixed-volume frame of reference. In a single phase p ($p = \alpha, \beta$), according to the Andersson and Agren [31], the chemical mobilities M_{ki}^p are related to the atomic mobilities M_l^p ($l = 1 \dots n$), which can be obtained from the DICTRA mobility database.

$$M_{ki}^p = \frac{1}{V_m} \sum_{l=1}^n (\delta_{il} - X_i)(\delta_{lk} - X_k) X_l M_l^p, \quad (5)$$

where δ_{il} and δ_{lk} are the Kronecker delta.

In a structurally and compositionally non-uniform system, the chemical mobility is assumed to be [32]:

$$M_{ki} = \eta M_{ki}^{\alpha} + (1 - \eta) M_{ki}^{\beta}. \quad (6)$$

In order to overcome the interface thickness limit in the traditional phase field model, the KKS model [33] is applied in the method. In the interface, the following relationship must be kept:

$$X_i = (1 - p(\eta))X_i^{\beta} + p(\eta)X_i^{\alpha}. \quad (7)$$

$$\frac{\partial G_i^{\alpha}}{\partial X_i} = \frac{\partial G_i^{\beta}}{\partial X_i} = G'_i. \quad (8)$$

On the base of the equations above, the new evolution equations can be obtained:

$$\frac{\partial X_k}{\partial t} = V_m \nabla \cdot \left(\sum_{i=1}^{n-1} M_{ki}(T, X, \nabla G'_i) \right), \quad (9)$$

$$\frac{\partial \eta}{\partial t} = -\frac{L}{V_m} \left\{ p' \left[(G_m^{\alpha} - G_m^{\beta}) - G'_{A1} (X_{A1}^{\alpha} - X_{A1}^{\beta}) \right. \right. \\ \left. \left. - G'_v (X_v^{\alpha} - X_v^{\beta}) \right] + \omega q' - k \nabla^2 \eta \right\}, \quad (10)$$

$$\text{where} \quad p' = \frac{dp}{d\eta} = 30\eta^2(1 - \eta)^2 \quad \text{and} \\ q' = \frac{dq(\eta)}{d\eta} = 2\omega\eta(1 - \eta)(1 - 2\eta).$$

Then the dimensionless governing equations are:

$$\frac{\partial X_k}{\partial \tau} = \tilde{\nabla} \cdot \left(\sum_{i=1}^{n-1} \tilde{M} \tilde{\nabla} \tilde{G}'_i \right), \quad (11)$$

$$\frac{\partial \eta}{\partial \tau} = -\tilde{L} \left\{ p' \left[(\tilde{G}_m^{\alpha} - \tilde{G}_m^{\beta}) - \tilde{G}'_{A1} (X_{A1}^{\alpha} - X_{A1}^{\beta}) \right. \right. \\ \left. \left. - \tilde{G}'_v (X_v^{\alpha} - X_v^{\beta}) \right] + 2\tilde{\omega}\eta(1 - \eta)(1 - 2\eta) - \tilde{k} \tilde{\nabla}^2 \eta \right\}, \quad (12)$$

where, $\tilde{G}_m^{\alpha} = G_m^{\alpha}/G_0$, $\tilde{G}_m^{\beta} = G_m^{\beta}/G_0$, $\tilde{L} = l_0^2 L/(V_m M_0)$, $\tilde{M} = V_m M_{ki}/M_0$, $\tilde{\omega} = \omega/G_0 = 4V_m \sigma/(G_0 \lambda)$, $\tilde{k} = k/(G_0 l_0^2) = 8V_m \sigma \lambda/(\pi^2 G_0 l_0^2)$, $\tilde{\nabla} = l_0 \nabla$, $\tau = M_0 G_0 t/l_0^2$.

The periodic boundary conditions are set [27]. The real interface layer width between α and β phases is on the nanometer scale. For an actual system of $45 \mu\text{m} \times 45 \mu\text{m} \times 45 \mu\text{m}$, the simulation is difficult. The reason is that the computation is extensive due to 4.5×10^4 meshes along all dimensions. As the KKS model removes the dependence of the interface energy on the interface thickness, the phase transformation kinetics can be simulated correctly even if the thickness is much larger than the real width [33]. So the larger mesh size $0.2236 \mu\text{m}$ is adopted. The interface thickness is $\lambda = 7 l_0$.

Because of the incoherent phase interface, the interfacial energy $\sigma = 0.5 \text{ J/m}^2$, $\tilde{\omega} = 2.56 \times 10^{-4}$, $\tilde{k} = 2.54 \times 10^{-3}$, $V_m = 10^{-5} \text{ m}^3/\text{mol}$, the normalizing quantities $\Delta G_m = 50 \text{ kJ/mol}$, $M_0 = 10^{-18} \text{ mol} \cdot \text{m}^2/\text{s/J}$, time step $dt = 0.1 \text{ s}$, spatial step dx (dy, dz) $= l_0 = 0.2236 \mu\text{m}$ and the kinetic coefficient $\tilde{L} = 80$, which is determined in such

a way as to ensure a diffusion-controlled dissolution process. The isothermal aging at $T = 1213 \text{ K}$ is considered. The interfacial energy and kinetic coefficient are assumed to be isotropic in the paper. The reliability of the quantitative phase field calculation of particle dissolution would be given in Sect. 3.1.

3 Results and Discussion

3.1 The Verification of Quantitative Phase Field Model

In order to verify the phase field model of alpha dissolution in titanium alloy in Sect. 2, a system of 200 meshes is chosen ($45 \mu\text{m}$). The system is in equilibrium initially at 1173 K where α volume fraction is about 45%, the compositions of Al (molar fraction) in matrix and α phase are 0.093, 0.113, respectively, and the composition of V (molar fraction) in matrix and α phase is 0.052 and 0.016, respectively. The system is heated to 1213 K (two-phase zone) subsequently.

The results from the phase field method are compared with the sharp interface simulation results in DICTRA in Fig. 1. The dissolution kinetics of alpha phase (Fig. 1a), the evolution of concentration field V (Fig. 1b) and Al (Fig. 1c) are given. Although the formulation of chemical mobility is different with that in the Ref. [6], excellent agreements in both PFM and DICTRA have been obtained. There is a little difference in interface (Fig. 1b, c). The main reason is that the type of interface in DICTRA is sharp, but it is diffusive in phase field method.

3.2 3D Simulation of the Effects of Initial PSD on α Particle Dissolution

In order to obtain equiaxed microstructure which has good performances (plasticity, stability thermal and fatigue strength), the titanium alloy usually is heated in two-phase zone where the dissolution of α particles occurs [1]. In the present paper, $200 \times 200 \times 200$ meshes are chosen and the length is about $45 \mu\text{m}$ along each dimension. The spatial distributions of spherical α particles in β matrix are in random state. The volume fraction of α particles is about 19%. In matrix and α phase, the concentration of Al (molar fraction) is 0.098, 0.118, respectively, and the concentration of V (molar fraction) is 0.041, 0.013, respectively. Assume that Ti–6Al–4V alloy is in equilibrium initially at 1200 K and the alloy is heated to 1213 K (two-phase zone) subsequently.

Figure 2 shows four types of initial PSD (uniform, normal, lognormal and bimodal) and corresponding microstructure evolution. The clear dissolution processes

Fig. 1 Dissolution of α phase in PFM and DICTRA. **a** The dissolution kinetics, **b** evolution of concentration V, **c** evolution of concentration Al

Fig. 2 Initial PSD and microstructural evolution in the process of solution treatment with corresponding initial PSD in Ti-6Al-4V alloy: **a, e, i** uniform; **b, f, j** normal; **c, g, k** lognormal; **d, h, l** bimodal; initial PSD **a–d**; microstructure at 0 s **e–h**; microstructure at 1000 s **i–l**

are exhibited in the four cases. The smaller particles dissolve quickly and disappear finally. The bigger particles diminish gradually. Jones *et al.* [4] had observed the similar dissolution process below β transus temperature during the thermomechanical processing of Ti-5Al-5Mo-5V-3Cr. For the four cases, the phenomena that the shapes of some particles evolve from sphere to ellipse and evolve from smaller particles to bigger particles are observed at 1000 s,

which is more obvious for the case of uniform PSD. The microstructure evolution of particles is different with the previous results [27, 34]. All particles had the same size initially and dissolved at the same rate [27]. In this paper, although every particle radius of uniform PSD is $2.24 \mu\text{m}$ ($10 l_0$), the radii of the particles are different in the later stage of dissolution. The shape transformations of the particles are more obvious at 1213 K in the study than that

Fig. 3 Evolution of concentration field Al **a–d** and V **e–h** in the middle cross section with initial lognormal PSD in Ti–6Al–4V alloy: **a, e** 0 s; **b, f** 500 s; **c, g** 1000 s; **d, h** 2000 s

at 1223 K in case of uniform PSD with the same initial configuration [34].

The evolutions of Al and V concentration fields in the middle cross section in case of initial lognormal PSD are shown in Fig. 3. Some shapes of particles change from initial circular to elliptical in the section. The reason is that the distributions of Al and V concentrations around the particles are non-uniform. The Al and V concentrations are high in matrix along L1 and L2 in Fig. 3, which result in the slower dissolution of the particles. The elliptical particles appear as the result of soft impingement which is different from the reason in the Ref. [2]. The phase model can deal with the soft impingement in the process of precipitate dissolution, and it is more rational than the numerical method [18].

The temporal evolution of volume fraction of α particles with four different PSD is given in Fig. 4. The solid lines represent the exponential fitting to simulation data by the following function:

$$f = f_{eq} + (f_0 - f_{eq}) \exp(-Kt^n), \quad (13)$$

where f_{eq} is the final equilibrium volume fraction of α particles at $T = 1213$ K, f is the volume fraction of α particles with time t , f_0 is the initial volume fraction of α particles, K and n are constants. The results from phase field method are in good agreement with the function (13), namely the volume fractions of α particles decay exponentially with time in four cases of PSD. The values of K and n are different in four cases of PSD (Table 1), which represent the different rates of dissolution. The dissolution rates of particles from fast to slow are: uniform PSD, normal PSD, lognormal PSD and bimodal PSD. The

Fig. 4 Temporal evolution of volume fraction of α particles with four initial PSD

Table 1 Values of K and n with different initial PSD

PSD	K	n
Uniform	0.0656	0.5617
Normal	0.0681	0.5195
Lognormal	0.0684	0.5120
Bimodal	0.0591	0.5046

controlling mechanism for the different dissolution kinetics resulting from different particle distributions should be the solute diffusion. The different dissolution rates are due to different radii of the largest particles in the four cases of PSD. The radius of the largest particles for the case with bimodal PSD is $5.81 \mu\text{m}$ ($26 l_0$), but radii for the case with the uniform, normal and lognormal are $2.24 \mu\text{m}$ ($10 l_0$),

4.02 μm ($18 l_0$) and 5.37 μm ($24 l_0$), respectively. The rate of dissolution decreases with increase in the largest particle radius [23]. While the uniform distribution leads to the fast diffusion of solute in the whole domain and thus quickens the dissolution process. The other main reason is that all particles have same initial radii, limiting the Gibbs–Thompson effect to the lower. The slowest dissolution rate for bimodal PSD is affected by both particle coarsening and soft impingement. In case of bimodal PSD, the more small particles feed the growth of large ones because of the Gibbs–Thompson effect, which slows down the dissolution of the large particles, as was observed in the Ref. [7]. But the soft impingement is not main factor because the number of small particles ($r < 10l_0$) is 3.3 times more than big ones ($r > 10l_0$) in Fig. 2d. At about 200 s, a large number of small particles vanish (Fig. 5), resulting in the larger distance of neighboring particles in bimodal PSD. From the Fig. 2, we can see the soft impingement is not most obvious. During the later stage of dissolution, the dissolution rates of α particles are slower. In case of uniform PSD, there is a sharp reduction in volume fraction of particles from the 18.92% at 0 s to 4.45% at 300 s. Holding for 1000 s at 1213 K, the volume fraction has a slight reduction to 1.78%. At 2000 s, it reaches to stable value. The similar evolution of dissolution kinetics was observed in Ref. [4]. The dissolution of α particles is faster at the beginning of solution treatment. However, it becomes to a slower process at the later. The reason is the gradient of solute is greater which has advantage of diffusion at the beginning. So the dissolution kinetics is fast. With the dissolution going on, a lot of solute piles up. The solute concentration in matrix is increased which has disadvantage of diffusion, and the kinetics of dissolution is slower.

The temporal evolution of the average particle radius with four types of initial PSD is different (Fig. 5). In case of bimodal PSD, the average radius of particles decreases,

Fig. 5 Temporal evolution of the average particle radius with four initial PSD

then increases and after that decreases monotonically with time. The average radius of particles decreases monotonically with time for the others PSD.

During the dissolution of α particles, the evolution of particles accompanied by the vanishing of smaller particles which results in the less number of particles and the average particle radius increasing and by the diminishing of bigger particles which leads the average particle radius decreasing. The evolution of average particle radius is relevant to the ratio of particle diminishing rate over particle vanishing rate. When the particle dissolution begins, all particles begin to diminish when the particle diminishing rate is dominant, the average particle radius decreases. At the later of dissolution, the smaller particles vanish quickly when the particle vanishing rate is dominant, the average particle radius begins to increase. Therefore, the phenomenon that the curve decreases after the beginning and increases after that is observed in case of bimodal PSD. For the cases with uniform PSD, normal PSD and lognormal PSD, the particle vanishing rate is dominant, and the average radius of particles decreases monotonously.

3.3 2D Simulation of the Effect of Space Distribution on α Particle Dissolution

The effect of space distribution on dissolution of α particles was examined. The simple with 200×200 meshes is chosen. The length is about 45 μm along each dimension. The systems with two circular α particles in the β matrix are equilibrated at 1200 K initially. The dissolution of α particles would occur instantly when the heat-treatment temperature raise up 1213 K. Here, the space distribution refers to the distance of two α particles (D), that is, the distance of point P_1 and point P_2 (Fig. 6a). In this section, four types of space distributions are considered. The boundary conditions are set mirror boundary. The other parameters are set as Sect. 3.2.

The microstructure evolution and dissolution kinetics of two circular α particles in four cases of space distribution are different at the later process of dissolution in Figs. 6 and 7. When the distance of the particles is 13.42 μm , the particles dissolve at the same rate and the shapes of α particles still keep the circular (Fig. 6e). In the other three cases, two circular α particles become elliptical (Fig. 6f, g) and are combined to form one particle, respectively (Fig. 6h). The shape transformations of particles appear more obvious with the decrease in distance of neighboring particles. The reason is the critical distance without soft impingement between the particles is almost 5.63 μm ($25l_0$) at 1213 K. When the distance of particles is over critical value, the particles dissolve at the same rate and the shapes of α particles still keep the circular which are

Fig. 6 Microstructure of two circular α particles in four cases of space distribution in the dissolution process: **a, e** 13.42 μm ; **b, f** 4.48 μm ; **c, g** 2.24 μm ; **d, h** 0 μm ; **a–d** 0 s; **e–h** 1500 s

Fig. 7 Dissolution kinetic of two circular α particles in four cases of space distribution

consistent with the hypothesis in Ref. [27]. From the Fig. 7, we can see the dissolution rates reduce with the decrease in distance of neighboring particles. The dissolution rate is the fastest when the distance is 13.42 μm . It is the slowest under the condition of tangent particles. At the initial condition, the distance of neighboring particles is smaller and the soft impingement is more obvious, resulting in the more rapid increasement of solute concentration around particles which has disadvantage of solute diffusion. Therefore, the kinetics of dissolution is slower and the shape transformations of particles appear more obvious. Although the 3D simulation of space distribution would give more convincing results, the consequences of 2D simulation can explain the effect qualitatively.

The soft impingement is the most obvious in the process of dissolution in case of uniform PSD in Sect. 3.2 (Fig. 2i) because there is the largest number of particles, resulting in the smallest distance of particles. However, the soft impingement has been weakened at 1223 K in case of uniform PSD [34]. The atomic diffusivity increases with the elevation of solution temperature. The faster diffusivities of atoms make solutes diffuse away very easily at 1223 K. Therefore, the critical distance without soft impingement is less than that at 1213 K.

4 Conclusion

A quantitative phase field method of multi-component diffusion-controlled phase transformations coupled with KKS model was applied to study the effects of initial PSD in 3D and space distribution in 2D on dissolution of α particles, respectively, below β transus temperature in Ti–6Al–4V alloy in real time and length scale. The volume fractions of α particles decay with time as: $f = f_{\text{eq}} + (f_0 - f_{\text{eq}}) \exp(-Kt^n)$. The sequence of 3D dissolution kinetics for different PSD from fast to slow is: uniform PSD, normal PSD, lognormal PSD and bimodal PSD. The temporal evolution trends of average radius under uniform, normal and lognormal PSD are similar in the process of dissolution. But, for the bimodal PSD, it decreases firstly, then increases and after that decreases with time gradually. The shapes of some particles evolve from sphere to ellipse and

evolve from smaller particles to bigger particles at the later stage of dissolution in case of uniform PSD as the result of soft impingement. The space distribution of the particles is a main factor which affects the dissolution kinetics and microstructure. When the distance of the particles is over critical value, the α particles dissolve at same rate. Otherwise, the dissolution kinetics of the particles is reduced with the decrease in distance and the soft impingement phenomenon is more obvious.

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