Modelling the Competitive Growth of Primary, Allotriomorphic, and Secondary Alpha in Ti-6Al-4V

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The competitive formation of allotriomorphic $\alpha$ along the prior $\beta$ grain boundaries, secondary $\alpha$-phase and the growth of globular primary $\alpha$ is described for the Ti-6Al-4V alloy during continuous cooling. The formation kinetics of the different morphologies of the $\alpha$-phase is related to the nucleation rate of allotriomorphic $\alpha$ and secondary $\alpha$ as well as with the V supersaturation at the $\beta$ matrix. A mesoscale physical model is developed for the allotriomorphic $\alpha$ and secondary $\alpha$ based on classical nucleation and growth of platelets. The growth of the primary $\alpha$ is modelled as the growth of a spherical particle embedded in a supersaturated $\beta$ matrix. Continuous cooling tests at two different holding temperatures in the $\alpha+\beta$ field, 930 °C and 960 °C, and five different cooling rates, 10, 30, 40, 100 and 300 °C/minutes, are conducted. Additionally, interrupted tests are conducted at different temperatures to determine the progress of growth of primary $\alpha$ and formation of allotriomorphic and secondary $\alpha$-phases during cooling. The size of primary $\alpha$ increases, while its circularity decreases with decreasing cooling rate. The area fractions of primary $\alpha$ decrease with increasing cooling rate and increasing holding temperature. Moreover, the lower the cooling rate, the thicker the plates of allotriomorphic $\alpha$ and secondary $\alpha$. The growth of primary $\alpha$, as well as the formation of allotriomorphic $\alpha$ plates is observed at the beginning of the cooling stage. The formation of secondary $\alpha$ occurs at last and is nearly negligible for very low cooling rates. The model is able to accurately predict the different $\alpha$-phase formation behaviours and the obtained results show good agreement with the experimental ones.

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I. INTRODUCTION

The mechanical properties of Ti-6Al-4V, especially fatigue resistance, toughness and ductility, are strictly correlated with its microstructure formed during the industrial thermomechanical treatments. Different microstructures can be achieved, i.e. martensitic, lamellar, equiaxed or bimodal, and they are related to the cooling rates after the thermomechanical treatment. A bimodal microstructure consisting of lamellar $\alpha$ and globular primary $\alpha$ ($\alpha_p$) is usually desired because of the combination of high ductility and high toughness. The globular $\alpha_p$ phase grows during cooling, while lamellar or secondary $\alpha$ ($\alpha_{SEC}$) nucleates and grows at the prior $\beta$ grain boundary or from the primary alpha. Moreover, a third morphology of $\alpha$-phase, named allotriomorphic $\alpha$ ($\alpha_{GB}$), also forms along the grain boundaries during cooling.

The growth of $\alpha_p$ phase is diffusion-controlled. For very slow cooling rates, the $\beta$-phase transforms mainly into $\alpha_p$. Thus, the resulting microstructure consists of almost only large equiaxed $\alpha_p$ with small amounts of retained $\beta$-phase. The amount of $\alpha_p$ decreases for increasing cooling rates and other morphologies of $\alpha$-phase are formed. Semiadi et al. observed that $\alpha_p$ exhibits epitaxial growth for Ti-6Al-4V controlled by the diffusion of V in the $\beta$-phase. The slower the cooling the larger the range in which the growth of $\alpha_p$ is pronounced. The retardation and finally the end of $\alpha_p$ growth with decreasing temperature during cooling can be attributed to two simultaneous effects related to the formation of $\alpha_{SEC}$ and $\alpha_{GB}$: (1) a geometric restriction for growth (pinning effect), and (2) a decrement of the supersaturation of elements in the $\beta$ matrix. The matrix supersaturation is the driving force for the growth of $\alpha_p$ as well as for the formation of $\alpha$ and $\alpha_{GB}$. In this way,
the growth of $z_p$ competes with the formation of $z_a$ and $z_{GB}$ for intermediate cooling rates (between 5 and 300 °C/minutes).\[^5\]

The presence of a rim-like region of $\alpha$-phase surrounding the $z_p$ was observed in a near-$\alpha$ Ti60 alloy during cooling.\[^4\] The rim-$\alpha$ phase had the same crystallographic orientation as the interior of the $z_p$ particle, thus evidencing the epitaxial growth of the primary $\alpha$-phase. Further analysis showed that the growth of $z_p$ particles was mainly controlled by diffusion of aluminium and molybdenum for the Ti60 alloy. The nucleation rate and growth of $z_{GB}$ depends on the available energy and time for growth.\[^4\]

Furthermore, extensions from $z_p$ with same crystallographic orientation were observed preferentially along the $\beta/\beta$ boundary suggesting formation of $z_{GB}$ along $\beta/\beta$ grain boundary from $z_p$.\[^3\] Sun et al.\[^6\] observed for a near-$\alpha$ alloy TA15 (Ti-6Al-2Zr-1Mo-IV) cooled from the $\beta$-phase field preferential nucleation of $z_{GB}$ at triple junctions of the $\beta$ grains, and then grew to one side of the grain boundary forming a flat plate. The $z_{GB}$ can also nucleate from the middle of one $\beta/\beta$ grain boundary due to high levels of local supersaturation forming an unconnected layer of $z_{GB}$. The formation of $z_{GB}$ depends on the available energy and time for growth. Therefore, different morphologies of $z_{GB}$ were observed: flat, zig-zag, and a mix of both.

Different modelling approaches were proposed for the $\beta\rightarrow\alpha$-phase transformation.\[^7-15\] Classical Kolmogorov–Johnson–Mehl–Avrami (KJMA) equation was applied to predict the phase transformation kinetics in Ti-6Al-4V.\[^7\] The growth of $z_{GB}$ was modelled using the diffusion solution for the growth of plate-like particles,\[^8\] ellipsoid particles,\[^8,9\] and ledge growth\[^8,10,11\]. A cellular automation model based on diffusion, mixed and interface phase transformation was proposed by Song et al.\[^12\] for phase transformation in titanium alloys. Phase field models were also developed\[^13-15\] and showed notably accuracy to predict the growth of particles in case of complex supersaturation fields in the particle growth front.\[^14\]

Semiatin et al.\[^4\] proposed a model for the growth of $z_a$ using the exact solutions of diffusion equations with the following considerations: (a) the diffusion coefficients were corrected with a thermodynamic factor for the specific composition of the material, and (b) the supersaturation degree reached during cooling is the driving force for the diffusion process.\[^8\] Meng et al.\[^16\] complemented the model proposed by Semiatin et al.\[^4\] by considering the effect of thermal history on the diffusion field around the $z_a$ and the overlap of diffusion fields of growing phases.\[^17\]

Extensive modelling of the formation of $z_{SEC}$ was performed by Katzarov et al.\[^18\] The morphology, distribution, and geometry of the $z_{SEC}$ was simulated using finite element modelling implemented to solve the diffusion equation on the domain occupied by the $\beta$-phase. A random nucleation model as a function of the supersaturation of V in the matrix was implemented for 1-D and 2-D simulations of the formation of $z_{SEC}$. It was observed that lower cooling rates lead to faster transformation of $\beta\rightarrow z_{SEC}$, considering the same temperature. Additionally, the thickness dependency of the $z_{SEC}$ on temperature during isothermal treatment was also measured and simulated. Despite the broad capability of prediction of the model proposed by Katzarov et al.,\[^18\] the model was developed only for $\beta\rightarrow\alpha$ transformation from the $\beta$ field and not from the $\alpha + \beta$ field. Using a similar approach, the precipitation of $z_{SEC}$ in competition with the epitaxial growth of $z_p$ was modelled and simulated for a TA15 alloy.\[^5\] In this case, the diffusion of Mo in $\beta$-phase was the controlling mechanisms for $\beta\rightarrow\alpha$ transformation. The growth of $z_{SEC}$ was proposed to be a competition between direct interference from interface stability, where no misorientation is observed between the nucleating plate and the substrate, and sympathetic nucleation, where low-angle boundaries exist between the nucleating plate and the pre-existing substrate.

Robust, accurate and computational simple models to simulate the $\beta\rightarrow\alpha$ transformation are necessary to predict and control the evolution of the microstructure in components with complex shapes produced by thermomechanical processing. Here we propose a simple model that is able to couple the competitive growth of primary $\alpha$ and formation of allotriomorphic $\alpha$ as well as secondary $\alpha$-phases. The results are compared with systematic measured data acquired for different continuous cooling experiments below the $\beta$-transus temperature.

II. EXPERIMENTAL PROCEDURES

A. Material

A cobbled Ti-6Al-4V in the $\beta$ and $\alpha + \beta$ fields with further annealing at 730 °C for 1 hour followed by air cooling was used for this investigation. The $\beta$-transus calculated using JMatPro\(^\text{®} v.10\) is ~995 °C and the chemical composition is listed in Table I.\[^19\] Cylindrical samples with a diameter of 5.5 mm and a length 10 mm were heat treated in a dilatometer.

B. Heat Treatments

A dilatometer DIL 805A/D (TA Instruments, Hüllhorst, Germany) was used to perform continuous cooling heat treatments. The tests were carried out in a protective atmosphere of argon. After heating with a rate of 30 °C/minutes, the samples were held for 1 hour at two different holding temperatures in the $\alpha + \beta$ field, 930 °C and 960 °C, and then continuously cooled up to room temperature. The cooling was conducted using five different cooling rates: 10, 30, 40, 100 and 300 °C/minutes. Interrupted continuous cooling heat treatments were carried out to elucidate the mechanism/s governing the $\beta\rightarrow\alpha$ transformation during cooling. After heating with 30 °C/minutes, the samples were held for 1 hour at a constant temperature of 960 °C. The subsequent cooling was performed with 10 and 100 °C/minutes. The samples were quenched using argon flow for four different temperatures, 900, 875, 850 and 800 °C.
C. Metallography and Microstructure Investigation

The samples were polished using OP-S (oxide polishing suspension) after a conventional grinding procedure from grit 500 up to 2000. The samples were etched with the Kroll’s reagent: 91 ml water, 6 ml HNO₃ (69 vol Pct) and 3 ml HF (40 vol Pct). The prepared samples were investigated using light optical (LOM) and scanning electron (SEM) microscopy. A minimum of five representative LOM micrographs were analysed for each cooling rate and holding temperature for quantification of the globular αₚ. The thickness of α_GB as well as of α_SEC were measured following the stereology procedures for quantification described by Tiley et al.[20] For comparison, the interspace distance between the lamellas of α_SEC and the thickness of α_GB were manually measured to obtain a thickness distribution. For each micrograph, the particles of α_p were manually marked using software GIMP (GNU Image Manipulation Program)[21] and analysed using ImageJ software.[22] The SEM analyses were conducted using a Tescan Mira3 microscope equipped with a Hikari EBSD camera. SE images were acquired using an acceleration voltage of 10 kV and a working distance of 12 mm. A minimum of five representative SE micrographs were acquired to measure the thickness of α_GB and α_SEC. An acceleration voltage of 25 kV and a working distance of 15 mm were used for the EBSD measurements. An area of 200 µm x 200 µm was measured using a step size of 0.2 µm. The data treatment was performed using the OIM DataAnalysis® software. A confidence index standardization was performed considering a minimum grain size of ten points and minimum boundary misorientation angle of 12 deg. Finally, the neighbour confidence index correlation was used to re-index the data-points with confidence index lower than 0.75.

D. Modelling Strategy

In the proposed model, the formation of α_SEC, α_GB and α_p is computed simultaneously. The implementation is detailed and are separated mainly on nucleation kinetics (does not apply for the α_p) and growth kinetics. The growth of α_p during cooling in heat treatments conducted below the β-transus temperature was modelled based on Reference 4. The growth of α_GB and α_SEC were modelled based on the classical model of nucleation and diffusion equation for the growth of a platelet.[5] The microstructure is modelled as consisted of three major morphologies of α-phase: α_p, α_SEC and α_GB, all embedded in a β-phase matrix, as schematically shown in Figure 1.

1. Growth of primary alpha (α_p)

Semiatin et al.[4] showed that for Ti-6Al-4V the growth of globular α_p phase during cooling is limited only by V diffusion due to supersaturation. The inter-diffusion coefficient of V in β titanium D_V as a function of temperature T is calculated from Reference 23 and also adopted in the model of Semiatin et al.[4] as well as Villa et al.[24] Eq. [1].

\[D(\mu m^2/s) = 1 \times 10^8 \exp \left( - \frac{17460}{T} \right)\]  

[1]

The growth of a spherical particle embedded in an infinite matrix of composition C_M is given according to Eq. [2].

\[D(\mu m^2/s) = 1 \times 10^8 \exp \left( - \frac{17460}{T} \right)\]  

[2]
\[
d\frac{R}{dr} = 2\lambda^2 \frac{D}{R}
\]
where \( R \) is the radius of the particle, \( D \) is the diffusion coefficient and \( \lambda \) is a growth rate parameter denoting the interface \( \alpha_p/\beta \) and is calculated according to Eq. [3].

\[
\left\{ \lambda^2 e^{\Omega} \right\} \left[ e^{-\Omega} + \lambda \pi/2 \text{erfc}(\lambda) \right] = \frac{1}{2}
\]

The parameter \( \Omega \) denotes supersaturation and is calculated according to Eq. [4].

\[
\Omega = \frac{(C_M - C_1)}{(C_p - C_1)}
\]

where \( C_1 \) is the composition of the matrix-\( \alpha_p \) interface and \( C_p \) is the composition of the \( \alpha_p \) phase. \( C_1 \) is considered as the equilibrium phase composition obtained from the phase diagram of the alloy at the calculated temperature considering a diffusion-controlled reaction. \( C_p \) is considered as the equilibrium phase composition of the \( \alpha \)-phase obtained from the phase diagram. It is considered a constant value with respect to temperature and equivalent to the \( V \) content of the phase diagram. It is considered a constant value with respect to temperature and equivalent to the \( V \) concentration in \( \alpha \)-phase. Following this assumption, all \( \alpha \) morphologies have same \( C_p \). The compositions are given in wt.Pct.

The supersaturation is the driving force for the growth of \( \alpha_p \). The \( \alpha \)-phase fraction at equilibrium as well as the chemical composition \( C_1 \) was calculated using the software JMatPro® v.10 in wt.Pct and are shown in Figures 2(a) and (b), respectively. To account for the soft impingement on the “far-field” matrix composition, \( C_M \) is calculated using a usual mass balance between the total fraction of \( \alpha \) \( (f_{\alpha}) \) phase, as given in Eq. [5].

\[
C_M = \frac{(C_0 - f_{\alpha} - C_x)}{(1 - f_{\alpha})}
\]

\( C_0 \) is the nominal concentration of \( V \) in the material.

2. Formation of allotriomorphic alpha (\( \alpha_{GB} \))

Similar to the growth of \( \alpha_p \), the partial enrichment of \( V \) along the formed \( \beta/\beta \) phase boundary is observed. Due to high anisotropy in interfacial energy a plate-like morphology of the \( \alpha \)-phase is observed to form along the \( \beta/\beta \) grain boundaries. In the present model, the lengthening is considered notably higher in comparison to the thickening as also suggested by phase field simulation. Therefore, the increase in the volume fraction of \( \alpha_{SEC} \) or \( \alpha_{GB} \) originates mainly from increase in number density and their thickness. The nucleation, growth and overall transformation kinetics of grain boundary allotriomorphic platelets were proposed for steels and titanium alloys. Following a similar approach, when the nucleation time is neglected, the nucleation rate of precipitates is given according to Eq. [6].

\[
d\frac{dN_{GB}}{dt} = N_{0GB}(1 - f_{\alpha_p} - f_{\alpha_{GB}} - f_{\alpha_{SEC}}) \exp \left( \frac{Q}{RT} \right) \exp \left( -\frac{\Delta G^*_{NucGB}}{RT} \right)
\]

where \( N_{0GB} \) is a pre-exponent term corresponding to the number of incubation sites multiplied by a constant and fitted according to an empirical power law to account for the effect of the initial prior beta grain size, Eq. [7]. \( Q \) is the activation energy for atomic migration across the interface and assumed to be half of the activation energy for diffusion. \( \Delta G^*_{NucGB} \) is the energy barrier for heterogeneous nucleation, \( R \) the molar gas constant and \( T \) the temperature. \( f_{\alpha_p}, f_{\alpha_{GB}} \) and \( f_{\alpha_{SEC}} \) are the calculated volume fraction of \( \alpha_p, \alpha_{GB} \) and \( \alpha_{SEC} \), respectively, and their sum is the total fraction of alpha phase \( (f_{\alpha}) \).

\[
N_{0GB} = 6.9 \times 10^4 \left( \frac{GS_0}{GS} \right)^{0.5}
\]

where \( GS_0 \) is a reference grain size and considered as 35 \( \mu \text{m} \) in the current model and \( GS \) is the prior beta grain size. The energy barrier for heterogeneous nucleation of \( \alpha_{GB} \) is calculated according to Eq. [8].

\[
\Delta G^*_{NucGB} = - \frac{(A_{GB})^3}{(RT)^2 \ln \left( \frac{C_M}{C_0} \right)}
\]

where \( A_{GB} \) is a parameter obtained according to the nucleation at grain boundary \( (A_{gb}) \), or sympathetic nucleation \( (A_{SYM}) \), or a sum of contributions of both (adopted in the current model), Eq. [9].

\[
A_{GB} = 0.12A_{SYM} + 0.88A_{gb}
\]

where

\[
A_{SYM} = \left( 4\pi N_A \gamma_{xgb} \gamma_{xzx}\gamma_{m} \right)^{1/3}
\]

\[
A_{gb} = \left( \frac{16\pi N_A ^{3/2} S(\theta) \gamma_{m}}{3} \right)^{1/3}
\]

where \( N_A \) is the Avogadro constant \( (N_A = 6.02214076 \times 10^{23} \text{mol}^{-1}) \), \( \gamma_{gb} \) is the interface energy between \( \beta/\beta \)-phases and considered \( \gamma_{gb} = 0.10 \text{ J/ m}^2 \), \( \gamma_{xzx} \) is the interface energy of \( \alpha/\alpha \)-phase and...
\( \gamma_{xx} = 0.30 \text{ J/m}^2 \) \cite{5}. \( V_m \) is the atomic volume of Ti \((V_m = 1.0896 \times 10^{-5} \text{ m}^3\text{mol}^{-1}) \) and \( S(\theta) \) is a shape factor given as a function of the wetting angle of the optimum embryo shape. \cite{18} \( \gamma_{gb} (S(\theta))^{1/3} = 0.012 \text{ Jm}^{-2} \) \cite{18} A small variation in the interface energies \( (\gamma_{gb} \text{ or } \gamma_{xx}) \) notably impacts the nucleation rate. In the case of the sympathetic nucleation, \( A_{SYM} \) is a function of both, \( \gamma_{gb} \) (second order) and \( \gamma_{xx} \) (first order). On the other hand, for nucleation at grain boundary, \( A_{gb} \) is a function of only \( \gamma_{gb} \) (third order). Thus, a small increase or decrease in \( \gamma_{gb} \) and \( \gamma_{xx} \) would affect notably \( A_{SYM} \) and/or \( A_{gb} \), increasing or decreasing the nucleation rate significantly, respectively. Finally, the model is adjusted with respect to the measured data as shown in Eq. \[9\] where a weighted sum of both \( A_{SYM} \) and \( A_{gb} \) is considered. The critical thickness \( \left( B_{GBCrit} \right) \) for a disc-like \( \alpha_{GB} \) to nucleate is calculated according to Eq. \[12\].

\[
B_{GBCrit} = - \frac{4\gamma_{gb}}{D_{GVBG}} \tag{12}
\]

where \( D_{GVBG} \) is the chemical free energy of phase transformation obtained using Eq. \[13\] \cite{3}.

\[
\Delta G_{VBG} = \frac{C_1 - C_p^{GBP}}{1 - C_1} \left( \frac{RT}{1 + \frac{\partial C_1}{\partial C_M}} \right) \ln \left( \frac{C_1}{C_M} \right) \tag{13}
\]

\( C_p^{GBP} \) is the concentration of \( V \) in the \( \alpha_{GB} \) assumed equal to the \( V \) concentration in the \( \alpha_p \) (\( C_p^{GBP} = C_p \)).

If the misfit strain energy is ignored, the nucleus of \( \alpha_{GB} \) grows by diffusion process by thickening of a planar disordered boundary via ledge growth mechanism. The lengthening of a platelet is significantly faster than the thickening due to high anisotropy in interfacial energy. Therefore, the evolution in the volume fraction of \( \alpha_{GB} \) is only dependent on the variation of the number density of \( \alpha_{GB} \) and its thickness. The variation in number density is related to the number of nuclei and calculated according to Eq. \[6\]. The thickening of the \( \alpha_{GB} \) is modelled according to Eq. \[14\].

\[
\frac{dB_{GB}}{dt} = \frac{2m_{GB}^2 \lambda_{GB}^2 D_{GB}}{B_{GB}} \tag{14}
\]

where \( B_{GB} \) is the thickness of the \( \alpha_{GB} \), \( m_{GB} \) is a ledge coefficient to account for the planar disordered growth \cite{10} and fitted as 5 for the investigated alloy, \( D \) is the diffusivity of \( V \) in the \( \beta \) matrix and \( \lambda_{GB} \) is a growth rate parameter denoting the interface \( \alpha_{SEC} / \beta \) and is calculated according to Eq. \[15\].

\[
\pi^{1/2} \exp \left( \frac{\lambda_{GB}^2}{2} \right) \text{erfc} (\lambda_{GB}) = \Omega_{\alpha_{GB}} \tag{15}
\]

where \( \Omega_{\alpha_{GB}} = (C_1 - C_M) / (C_1 - C_p^{GBP}) \) is a dimensionless supersaturation parameter, and considered equal to \( \Omega \) because \( C_p^{GBP} = C_p \). Similar to the growth of precipitates, the mean thickness of the platelets is calculated according to Eq. \[16\]. \cite{25}

\[
\frac{d\bar{B}_{GB}}{dt} = \frac{dB_{GB}}{dt} + \frac{1}{N_{GB}} \frac{dN_{GB}}{dt} (B_{GBcrit} - \bar{B}_{GB}) \tag{16}
\]

The first term corresponds to the growth of the existing platelets of \( \alpha_{GB} \), while the second one represents the contribution of new nuclei of critical size calculated according to Eq. \[12\]. The overall fraction of \( \alpha_{GB} \) is calculating according to Eq. \[17\].

\[
f_{\alpha_{GB}} = N_{GB} \bar{B}_{GB} \tag{17}
\]

The parameters used for the simulation of the formation of \( \alpha_{GB} \) are listed Table A1.

3. Formation of secondary alpha (\( \alpha_{SEC} \))

The formation of \( \alpha_{SEC} \) is modelled similar to the formation of \( \alpha_{GB} \), i.e. nucleation of disc platelets and growth. The colony size is not modelled, but only the thickness of the formed \( \alpha_{SEC} \) platelets and its number density (interpreted as the total number of formed nuclei of \( \alpha_{SEC} \)). The lengthening is considered notably faster in comparison to the thickening of the \( \alpha_{SEC} \), thus neglected. Due to high anisotropy in interfacial energy, platelet-like \( \alpha_{SEC} \) is formed. Differently from the growth of \( \alpha_{GB} \) that is along the \( \beta / \beta \) grain boundaries, the growth of \( \alpha_{SEC} \) occurs from the grain boundary towards the centre of the prior \( \beta \) grain as well as sympathetic growth from the \( \alpha_p \). Not considering any nucleation time, the rate of nucleation of \( \alpha_{SEC} \) is given according to Eq. \[18\].

\[
\frac{dN_{SEC}}{dt} = N_{SEC} \left( 1 - f_{\alpha_p} - f_{SEC} - f_{SEC} \right) \exp \left( - \frac{Q}{RT} \right) \exp \left( - \frac{\Delta G_{NuSEC}^{*}}{RT} \right) \tag{18}
\]

where \( N_{SEC} \) is a pre-exponent term similar to \( N_{GB} \) and fitted as \( 6 \times 10^7 \times \Delta G_{NuSEC}^{*} \) is the energy barrier for heterogeneous nucleation of the \( \alpha_{SEC} \) and calculated according to Eq. \[19\].

\[
\Delta G_{NuSEC}^{*} = \frac{(A_{SEC}^*)^3}{(RT)^2 \left( \ln \left( \frac{C_M}{C_M} \right) \right)^2} \tag{19}
\]

where \( A_{SEC}^* \) is fitted and calculated according to Eq. \[20\].

\[
A_{SEC}^* = 0.56 A_{SYM} + 0.44 A_{gb} \tag{20}
\]

The critical thickness \( B_{SEC} \) for a disc-like \( \alpha_{SEC} \) to nucleate is calculated according to Eq. \[21\].

\[
B_{SEC} = \frac{4\gamma_{gb}}{D_{GSEC}} \tag{21}
\]

where \( \gamma_{gb} \) is the interface energy between \( \alpha \) and \( \beta \)-phases, \( D_{GSEC} \) is the chemical free energy of phase transformation of \( \alpha_{SEC} \) obtained using Eq. \[22\]. \cite{3}.

\[
\Delta G_{SEC}^{*} = \frac{C_1 - C_p^{SEC}}{1 - C_1} \frac{RT}{1 + \frac{\partial C_1}{\partial C_M}} \ln \left( \frac{C_1}{C_M} \right) \tag{22}
\]
$C_P^{SEC}$ is the concentration of V in the $z_{SEC}$, considered to be equal to the V concentration in the $z_P$ and $z_{GB}$ ($C_P^{SEC} = C_P^{z_P} = C_P$).

The growth of the thickness of $z_{SEC}$ is modelled as the growth of $z_{GB}$. The thickening of the $z_{SEC}$ is given according to Eq. [23].

$$\frac{dB_{SEC}}{dt} = \frac{2m_{SEC}\lambda_{SEC}^2}{B_{SEC}} D$$  \hspace{1cm} [23]

where $B_{SEC}$ is the thickness of the $z_{SEC}$, $m_{SEC}$ is a ledge coefficient and fitted as 3 for the investigated alloy, $D$ is the diffusivity of V in the $\beta$ matrix and $\lambda_{SEC}$ is a parameter denoting the interface $z_{SEC}/\beta$ that is calculated according to Eq. [24].

$$\pi^{1/2} \exp(\lambda_{SEC}^2) \text{erfc}(\lambda_{SEC}) = \Omega_{SEC}$$  \hspace{1cm} [24]

where $\Omega_{SEC} = (C_1 - C_M)/(C_1 - C_P^{SEC})$ is a dimensionless supersaturation parameter. The mean thickness of the $z_{SEC}$ is calculated according to Eq. [25].[30]

$$\frac{dB_{SEC}}{dt} = \frac{1}{N_{SEC}} \frac{dN_{SEC}}{dt} (B_{SEC \text{crit}} - B_{SEC})$$  \hspace{1cm} [25]

The first term corresponds to the growth of the existing platelets of $z_{SEC}$, while the second represents the contribution of new nuclei of critical size calculated according to Eq. [21]. The overall fraction of $z_{SEC}$ is calculating according to Eq. [26].

$$f_{SEC} = N_{SEC}B_{SEC}$$  \hspace{1cm} [26]

The parameters used for the simulation of the formation of $z_{SEC}$ are listed Table A1.

### III. RESULTS AND DISCUSSION

Figures 3(a) and (b) show representative microstructures of the Ti-6Al-4V argon quenched after holding at 930 °C and 960 °C for 1 hour, respectively. The measured area fractions of $z_P$ are 38.6 ± 2.8 and 18.2 ± 3.3 Pct for the heat treatment at 930 °C and 960 °C, respectively. Sparsely and nearly separated $z_P$ particles are found in a matrix of martensite ($z'$), originally a matrix of $\beta$-phase. The partial agglomeration of $z_P$ is higher for the heat treatment at 930 °C, Figure 3(a). No trace of $z_{SEC}$ is observed. However, the $z_P$ particles slightly deviates from an ideal spherical shape particle.

#### A. Experimental Observations

1. Influence of the Cooling Rate

Representative micrographs of the continuously cooled microstructure after holding for 1 hour at 930 °C and 960 °C are shown in Figure 4. The cooling rate of 10 °C/minutes leads to a nearly fully equiaxed microstructure in both cases. The shape of the $z_P$ exhibits higher irregularities in the case of 960 °C, decreasing its circularity. It is difficult to distinguish the lamellas of $z_{SEC}$ or $z_{GB}$ from the globular $z_P$ for samples cooled down at 10 °C/minutes. The growth of $z_P$ is also observed for the cooling rate of 30 °C/minutes. The increase in cooling rate leads to a clear formation of $z_{SEC}$, as well as of $z_{GB}$ phase. For 30 °C/minutes, $z_{GB}$ exhibits bulges, as well as the $z_P$ phase. Higher cooling rates lead to less pronounced growth of $z_P$.

A detailed analysis of the microstructure after continuous cooling from 930 °C and 960 °C is seen in the SE micrographs of Figure 5. The $z_{GB}$ and $z_{SEC}$ are highlighted in dashed red and green lines, respectively. For the cooling rate of 300 °C/minutes, the presence of very fine acicular-like martensite ($z'$) is marked in yellow and in its vicinity plate-like $z_{SEC}$ is also observed. The morphology of $z_{SEC}$ deviates slightly from an ideal flat plate-like morphology. Serrations and discontinuous interlamellar $\beta$-phase are observed, especially for the cooling rate of 30 °C/minutes. Moreover, the above-mentioned irregularities of the shape of $z_P$ and $z_{GB}$ are observed. The serrations at the interfaces of $z_P$ are related to the surface instability due to competitive growth of $z_{GB}$, $z_{SEC}$ and $z_P$. When the $z_{SEC}$ or $z_{GB}$ are formed in the vicinity of an $z_P$ particle, it either hinders the local movement of the interface of the $z_P$ and/or changes the supersaturation for its growth. Comparably, if $z_{SEC}$ nucleates from $z_{GB}$ it also changes its interface movement kinetics and supersaturation field.

![Fig. 3—Representative BSE micrographs of the investigated Ti-6Al-4V after 1 h at (a) 930 °C followed by argon quenching; (b) 960 °C followed by argon quenching.](image-url)
for growth. Since the time for diffusion is higher the slower the cooling rate, the serrations are more pronounced for the 30°C/minute compared to 300°C/minute. A nearly flat plate-like $\alpha_{GB}$ is observed for the cooling rate of 300°C/minute.

Figure 6 illustrates the effect of the cooling rate on the distributions of the diameter of $\alpha_{P}$ (Figure 6(a)), the circularity of $\alpha_{P}$ (Figure 6(b)), and the thicknesses of $\alpha_{GB}$ (Figure 6(c)) and $\alpha_{SEC}$ (Figure 6(d)). The distributions were normalized and fitted using a lognormal distribution and only the fitted data are shown in Figure 6. An increase in diameter of $\alpha_{P}$ with decrease in cooling rate is observed. The circularity of $\alpha_{P}$ decreases with decreasing cooling rate due to the interface serrations for lower cooling rates. The thickness of $\alpha_{GB}$ or $\alpha_{SEC}$ is smaller with narrower distribution for
higher cooling rate. The distributions for the cooling rate of 10 °C/minutes are not shown due to the difficulty to distinguish $\alpha_P$ from $\alpha_{GB}$ or $\alpha_{SEC}$.

2. Sequence of Phase Formation
To clarify the sequence of formation of the different morphologies of $\alpha$-phase, Figure 7 exhibits the typical micrographs after interrupted heat treatments. The $\alpha_P$,
\( \alpha_{GB} \) and \( \alpha_{SEC} \) are highlighted in blue dashed line, red dashed line and green dashed line, respectively. The formation of \( \alpha_{GB} \) initiates from the globular \( \alpha_p \), as well as from triple points of the \( \beta \) grains. The fraction of the grain boundary that is occupied by \( \alpha_{GB} \) is very low for 900 °C. At 850 °C the grain boundaries are nearly completely decorated with \( \alpha_{GB} \). Irregular growth of \( \alpha_{GB} \) seems to occur at 800 °C and is more pronounced for 10 °C/minutes. Nucleation and growth of \( \alpha_{GB} \) do not seem to be significant at temperatures higher than 900 °C for the two investigated cooling rates, leading to comparable evolution behaviour of the \( \alpha_{GB} \) after holding at temperatures of 930 °C and 960 °C. Formation of \( \alpha_{SEC} \) is not pronounced up to 850 °C. Although Figure 7 shows the presence of \( \alpha_{SEC} \) for 10 °C/minutes, its area fraction is notably smaller in comparison to cooling at 100 °C/minutes.

To investigate the growth of the \( \alpha_{GB} \) along the \( \beta \) grain boundaries from the \( \alpha_p \), Figure 8 shows the inverse pole figure maps (IPF) of the EBSD measurements for four interrupted heat treatments. The presence of \( \alpha_{GB} \) formed from the \( \alpha_p \) is highlighted by a dashed white circle. In this case, none or very small (below 2 deg) misorientation angle is observed between the \( \alpha_p \) and the formed \( \alpha_{GB} \). The presence of high-angle grain boundaries (boundary misorientation angle higher than 15 deg) is highlighted in white lines. Two nucleation sites were identified for \( \alpha_{GB} \) (a) at \( \alpha_p \) boundaries as a consequence of a morphological instability due to the presence of an existing \( \beta-\beta \) grain boundary, and (b) at \( \beta \) triple points and flat grain boundaries. There is no clear crystallographic relationship between the formed \( \alpha_{GB} \) from the \( \alpha_p \) and the particle of \( \alpha_p \) or at the ones formed at \( \beta \) triple points. It seems that the local supersaturation and surface energy play an important role in the determination of the different nucleation sites. At \( \beta \) triple points, the high surface energy can promote the nucleation of \( \alpha_{GB} \), while the nucleation of \( \alpha_{GB} \) at the flat \( \beta \) grain boundaries without \( \alpha_p \) is promoted by a high local supersaturation due to large interspacing between the \( \alpha_p \).

B. Model Performance

The simulated area fraction of \( \alpha_p \), mean \( \alpha_p \) diameter, mean thickness of \( \alpha_{GB} \) and mean thickness of \( \alpha_{SEC} \) are in good agreement with respect to the experimental results. The fitting parameters are in the same range as reported in other investigations.\(^{[5,18]} \) The results corroborate with the work of Semiatin et al.\(^{[4]} \) and Meng et al.\(^{[5]} \) This work adds the competitive growth of \( \alpha_p \), \( \alpha_{GB} \) and \( \alpha_{SEC} \). The nucleation of \( \alpha_{GB} \) and \( \alpha_{SEC} \) were modelled separately and different free energies for nucleation were considered. Despite of not considering the thermo-historical information included in the model proposed by Meng et al.\(^{[5]} \) and despite of not accounting for complex supersaturation fields that are possible to predict when using phase field models,\(^{[14]} \) the adoption of a ledge constant to the exact solution showed to be sufficient to achieve notably accuracy in a simple coupled model. The differences between measured and simulated data are dependent on both measurement limitations and model assumptions. The stereological procedures adopted for phase quantification have an inherent error. For instance, the assumption that all \( \alpha_{SEC} \) are platelets neglects the amount of \( \alpha_{SEC} \) that can exhibit a disc shape or more irregular morphology. Furthermore, the assumption of \( \alpha_p \) as isolated spherical particles impacts directly the prediction of the \( \alpha_p \) growth. The \( \alpha_p \) particles are observed to be partially agglomerated as well as slightly elongated due to initial cobbled microstructure. Those differences can explain the deviations and relatively high standard deviation observed in Figure 9.

1. Influence of the Cooling Rate

The cooling rate plays an important role in the formation of the different morphologies of \( \alpha \)-phase. The following statements can be inferred:

- During continuous cooling, the fraction of \( \alpha_p \) increases rapidly until 800 °C (Figures 9(a) and 11(d)). The area fraction of \( \alpha_p \) increases for decreasing cooling rate. The model describes accurately the area fraction evolution apart from 30 and 40 °C/minutes for the holding temperature of 960 °C (Figure 9(b)).
- The diameter of \( \alpha_p \) increases with decreasing cooling rate (Figures 9(c) and 11(a)).
- The calculated and measured thickness of the \( \alpha_{GB} \) are in the range of 1–4 \( \mu \m) and it increases with decreasing cooling rate (Figures 10(a) and (b)). Slightly thicker \( \alpha_{GB} \) is observed for the holding temperature of 960 °C. The higher supersaturation
grade of the matrix at 960 °C, in addition to the faster growth after nucleation during the initial stages at high temperatures, can explain this difference with respect to the sample cooled from 930 °C.

- The thickness of $\alpha_{\text{SEC}}$ was in the range of 0.5 to 2 µm and it increases with decreasing cooling rate (Figures 10(b) and (c)). Since the $\alpha_{\text{SEC}}$ is formed at temperatures slightly lower than for the $\alpha_{\text{GB}}$, its
formation is less influenced by the different holding temperatures.

2. Evolution of Microstructural Features

The developed model predicts also the evolution of the microstructural features: mean diameter and area fraction of $\alpha_P$, mean thickness and area fraction of $\alpha_{GB}$, and mean thickness and area fraction of $\alpha_{SEC}$ and they are plotted in Figure 11 for the holding temperature of 960°C. The growth of the $\alpha$-phase morphologies for temperatures lower than 600°C is negligible. The formation of $\alpha_{GB}$ starts close to 920°C. Figures 11(b) and (e) show a high growth rate for $\alpha_{GB}$ at around 900°C, while the growth for temperatures lower than 800°C is not significant. These evolutions are in good agreement with the experimental observations depicted in Figure 7. The $\alpha_{SEC}$ formation starts at 875°C, with a significant growth until 700°C, explaining the micrographs in Figure 7. Figure 11(f) shows that the fraction of $\alpha_{SEC}$ abruptly decreases when the cooling rate increases from 100 to 300°C/minutes. The low nucleation rate and low time for diffusion explain this behaviour and are confirmed by the presence of martensite in the microstructure after cooling down at 300°C/minutes. Rae 31 proposed a time-temperature-transformation diagram for Ti-6Al-4V where the martensitic starting temperature is $\sim$850°C [32] and martensite is formed if this temperature is achieved within $\sim$5 s. To obtain a fully martensitic microstructure, the temperature of $\sim$700°C should be achieved within $\sim$1 s from the holding temperature. [31] It deviates slightly from the results observed for cooling at 300°C/minutes, where $\alpha_{SEC}$ is still observed. Although the formation of martensite is not included in the model, the lower formation of $\alpha_{SEC}$ is used as an indication for it.

3. Additional Physical Features

Figure 12 shows the nucleation rate of $\alpha_{GB}$ (Figure 12(a)) and $\alpha_{SEC}$ (Figure 12(b)) for the holding temperature of 960°C. The supersaturation of V within the $\beta$-phase matrix is shown in Figure 12(c). The predicted nucleation rate of $\alpha_{GB}$ is significantly smaller compared to $\alpha_{SEC}$ because only the grain boundaries are considered sites for nucleation and formation of $\alpha_{GB}$. The estimated prior $\beta$ grain size is 35 μm. Therefore, the density number of platelets of $\alpha_{GB}$ is notably smaller compared to $\alpha_{SEC}$.

A summary with the temperature for the beginning of nucleation and for the maximum nucleation rate is shown in Table II. The $\alpha_{GB}$ nucleates first compared to $\alpha_{SEC}$. The temperature for the beginning of nucleation tends to increase with decrease cooling rate. An exception is calculated for the 10°C/minutes cooling rate. In this case, the predominant growth of $\alpha_P$ leaves no supersaturation to activate earlier nucleation of $\alpha_{GB}$. Similar tendency is observed for the $\alpha_{SEC}$. The slightly lower temperatures for nucleation in the case of 10°C/minutes is more pronounced, as expected due to the higher free energy for nucleation (Eq. [9] in comparison to Eq. [20]). The dependency on the cooling rate in the case of the nucleation rate follows similar behaviour compared to the beginning of nucleation. The temperatures for maximum nucleation rate are 40°C lower compared to the temperature for the beginning of nucleation for the $\alpha_{GB}$. In the case of the $\alpha_{SEC}$, this difference varies between 80 and 100°C.
interrupted heat treatments (Figure 7) showed that \( \alpha_{SEC} \) forms at lower temperatures compared to \( \alpha_{GB} \). Similar trend is exhibited by the simulated nucleation rates of \( \alpha_{SEC} \). The incomplete formation of \( \alpha_{SEC} \) for high cooling rates (Figures 5 and 11) is also predicted in the current model, since the temperature for maximum nucleation rate of \( \alpha_{SEC} \) lies close to 800°C. Furthermore, the notable low amount of \( \alpha_{SEC} \) formed during low cooling rates is also observed (Figure 4) and agrees with the model prediction.

The formation of the different morphologies is driven by the degree of supersaturation of the V in the \( \beta \)-phase, and its evolution during cooling is shown in Figure 12(c). It raises rapidly up to 810°C, temperature slightly lower compared to the maximum nucleation rate of \( \alpha_{SEC} \) (Table II). Moreover, an intensive formation of \( \alpha_{SEC} \) is observed between 850 and 800°C (Figure 7). Higher supersaturation promotes nucleation of \( \alpha_{GB} \) and \( \alpha_{SEC} \) as well as growth of \( \alpha \). The simulation and the microstructure analysis show that the growth of \( \alpha \) is favourable for lower cooling rates, while formation of \( \alpha_{SEC} \) is promoted for higher cooling rates. The lower time for diffusion at high cooling rates increases the supersaturation of V of the \( \beta \) matrix, thus promoting the formation of \( \alpha_{SEC} \). The long time for diffusion for low cooling rates promotes the growth of \( \alpha \).

### Table II. Approximate Simulated Nucleation Temperatures for the Cooling Rates of 10, 30, 40, 100 and 300°C/min at Isothermal Treatments at 930°C and 960°C

| Cooling Rate [°C/minutes] | Temperature for the Beginning of Nucleation [°C] | Temperature for Maximum Nucleation Rate [°C] |
|---------------------------|-------------------------------------------------|-----------------------------------------------|
|                           | \( \alpha_{GB} \) | \( \alpha_{SEC} \) | \( \alpha_{GB} \) | \( \alpha_{SEC} \) | \( \alpha_{GB} \) | \( \alpha_{SEC} \) |
| 10                        | 917               | 945               | 877               | 908               | 883               | 908               | 794               | 846               |
| 30                        | 916               | 944               | 888               | 912               | 880               | 904               | 819               | 851               |
| 40                        | 916               | 944               | 888               | 912               | 879               | 903               | 816               | 847               |
| 100                       | 915               | 942               | 888               | 913               | 877               | 900               | 800               | 829               |
| 300                       | 912               | 940               | 887               | 912               | 876               | 889               | 787               | 811               |

**IV. SUMMARY AND CONCLUSIONS**

The sequence of formation and growth of the different morphologies of \( \alpha \)-phase (primary, secondary and allotriomorphic) in Ti-6Al-4V were investigated during cooling from isothermal treatments below the \( \beta \)-transus temperature. A mesoscale physical model to account for the competitive growth of the different morphologies was developed. Nucleation and growth of \( \alpha_{GB} \) as well as of \( \alpha_{SEC} \) are modelled based on the nucleation and growth of platelets. The growth of \( \alpha \) is modelled as the growth of a spherical particle. The simulated results are in agreement with the obtained results and the following conclusions are inferred:

- Growth of \( \alpha \) is more pronounced for low cooling rates and occurs more notable up to 800°C
- Regular (planar) interface shape of \( \alpha_{GB} \) is observed decorating the prior \( \beta \) grain boundaries for high cooling rates. For low cooling rates, irregular shapes are observed
- \( \alpha_{GB} \) nucleates preferentially from existing \( \alpha_{P} \) phase. For higher cooling rates nuclei in triple points of the \( \beta \) grains and other regions of the prior \( \beta /\beta \) grain boundary are observed. The higher nucleation rate for those cooling rates can explain the different behaviour
Formation of $\alpha_{SEC}$ occurs at a lower temperature for the same cooling rate compared to the formation of $\alpha_{GB}$. The predicted temperature for maximum nucleation rate of $\alpha_{GB}$ is $\sim 80^\circ C$ higher compared to the one for the maximum nucleation rate of $\alpha_{SEC}$.

- $\alpha_{SEC}$ nucleates from the already existing $\alpha_{GB}$ as well as at the interface with the $\beta$.
- The variation of nucleation rate with respect to the cooling rate is notably more pronounced for the $\alpha_{SEC}$ compared to $\alpha_{GB}$.
- A sharp increase of $V$ supersaturation in the $\beta$ matrix is observed up to $850^\circ C$, which is attributed to contributing to the formation of $\alpha_{SEC}$, especially for cooling rates higher than $10^\circ C$/minutes.

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**APPENDIX**

A Matlab® routine was developed to implement the model to couple the growth of the $\alpha_p$ and the formation and growth of $\alpha_{GB}$ and $\alpha_{SEC}$. The used parameters are listed in Table A1.

| Table A1. List of the Parameters Used for the Modelling of the Growth of $\alpha_p$ and Formation and Growth of $\alpha_{GB}$ and $\alpha_{SEC}$ |
|----------------------------------------------------------|
| Description                                             | Parameter         | Value         | Reference                  |
| V Concentration in the Alloy                            | $C_0$             | 4.21          | chemical composition measurement |
| V Concentration in $\alpha_p$ Phase                     | $C_p$, $C_p^{GB}$, $C_p^{SEC}$ | 2.0           | [6]                   |
| V Concentration at the $\alpha$/ $\beta$ Interface      | $C_1$             | function of temperature | calculated with JMatPro® v.10 |
| Pre-exponent Nucleation Parameter for $\alpha_{GB}$     | $N_0^{GB}$        | function of prior $\beta$ grain size: $6.9 \times 10^4 (G_{S0})^{0.5}$ | empirical from this work |
| Reference Grain Size for the Nucleation of $\alpha_{GB}$| $G_{S0}$          | 35 $\mu$m     | fitting parameter. this work |
| Pre-exponent Nucleation Parameter for $\alpha_{SEC}$    | $N_0^{SEC}$       | $6 \times 10^7$ | fitting parameter. this work |
| Parameter for Activation Energy of Nucleation for $\alpha_{GB}$ | $A_{GB}^*$       | $2.79 \times 10^3$ | fitting parameter. this work |
| Parameter for Activation Energy of Nucleation for $\alpha_{SEC}$ | $A_{SEC}^*$      | $8.35 \times 10^3$ | fitting parameter. this work |
| Parameter for Activation Energy of Nucleation for Sympathetic Growth | $A_{SYM}$        | $1.39 \times 10^4$ | [5]               |
| Parameter for Activation Energy for Nucleation at $\alpha$/ $\beta$ Interface | $A_{\alpha\beta}$ | $1.27 \times 10^3$ | [20]            |
| $\alpha$/ $\beta$ Interface Energy                     | $\gamma_{\alpha\beta}$ | 0.10 J/m$^2$ | [20]               |

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Table A1. continued

| Description | Parameter | Value | Reference |
|-------------|-----------|-------|-----------|
| Interface Energy | $\gamma_{12}$ | 0.30 J/m$^2$ | [5] |
| Ti atomic Volume | $V_m$ | 1.0896x10$^{-5}$ | [5] |
| Shape Factor | $S(\theta)$ | 0.001728 | [20] |
| Activation Energy for Diffusion | $Q$ | 145.17 kJ/mol | [6] |
| Activity Coefficient | $\frac{\partial V}{\partial C_i}$ | 0.9 | [6] |
| Ledge Coefficient for $a_{GB}$ Growth | $m_{GB}$ | 5 | fitting parameter, this work |
| Ledge Coefficient for $a_{SEC}$ Growth | $m_{SEC}$ | 3 | fitting parameter, this work |

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