

# Characterization and modeling of forged Ti-6Al-4V Titanium alloy with microstructural considerations during quenching process

Renaud Julien, Vincent Velay, Vanessa Vidal, Yoann Dahan, Romain Forestier, Farhad Rezai-Aria

# ▶ To cite this version:

Renaud Julien, Vincent Velay, Vanessa Vidal, Yoann Dahan, Romain Forestier, et al.. Characterization and modeling of forged Ti-6Al-4V Titanium alloy with microstructural considerations during quenching process. International Journal of Mechanical Sciences, 2018, 142-143, pp.456-467. 10.1016/j.ijmecsci.2018.05.023. hal-01799489

# HAL Id: hal-01799489 https://imt-mines-albi.hal.science/hal-01799489

Submitted on 28 May 2018

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# Characterization and modeling of forged Ti-6Al-4V Titanium alloy with microstructural considerations during quenching process

R. Julien<sup>a</sup>, V. Velay<sup>a,\*</sup>, V. Vidal<sup>a</sup>, Y. Dahan<sup>b</sup>, R. Forestier<sup>b</sup>, F. Rézaï-Aria<sup>a</sup>

<sup>a</sup>Institut Clément Ader, Université de Toulouse; CNRS, Mines Albi, INSA, UPS, ISAE-SUPAERO, Campus Jarlard, 81013 Albi Cedex 09, France <sup>b</sup>Aubert et Duval, 75 Boulevard de la Libération, BP 173, 09102 Pamiers Cedex, France

### Abstract

The present investigation proposes an experimental device able to assess the thermomechanical behavior of Ti-6Al-4V Titanium alloy throughout the die-forging operation. Constitutive equations are developed to assess the influence of the process (die-forging temperature, cooling rate) and the microstructure parameters on the mechanical response of the alloy. For this purpose, a non-unified behavior model formulation is implemented, which defines two main mechanisms related to  $\alpha$  and  $\beta$ phases and allows the prediction of hardening, strain rate sensitivity and temperature, combined with the phase evolution that is dependent on the cooling conditions and which can greatly affect the mechanical behavior. This identification strategy is then applied for die-forging temperatures below the  $\beta$ -transus temperature, which requires microstructural information provided by SEM (Scanning Electron Microscopy) observations and image analysis. Finally, the approach is extended to die-forging temperatures above the  $\beta$ -transus temperature.

*Keywords:* Behavior modeling, Microstructural evolution, Heat treatment, Forged Titanium alloy

### <sup>1</sup> 1. Introduction

Titanium alloys are widely used in the aerospace industry for their well-known 2 high mechanical strength/weight ratio [1]. They can be used as forged semi-finished 3 products in many industrial applications. These products are transformed into final 4 parts by subsequent thermo-mechanical heat treatments and machining operations. 5 Depending on the temperature of the thermo-mechanical processing (TMP) and the 6 heat treatments (HT), various complex microstructures can be achieved. Titanium 7 alloys can be heat-treated above or below the  $\beta$ -transus temperature depending 8 upon the specific micro-structural aspects required in terms of grain size and morphology, as well as the existence of phases and mechanical strength requested by the 10 end-users. HT generally consists in an isothermal dwell for a certain period of time 11

<sup>\*</sup>Corresponding author

Email address: vincent.velay@mines-albi.fr (V. Velay)

following quenching. To fulfil the microstructural characteristics and mechanical 12 performance requirements and according to the size of the semi-finished products, 13 an appropriate quenching environment (e.g., air, oil, water, etc.) is selected. The 14 dimensions of the product and the quenching conditions can drastically influence 15 the spatial quenching rates, specifically the time-temperature history, in any points 16 in the product. In fact, quenching operations generate transient time-temperature 17 histories in a part, moving inwards from the surface to the bulk. One of the major 18 concerns, particularly for products with large dimensions, is to guarantee a homo-19 geneous microstructure through all regions of the product. Another major technical 20 concern is to avoid any excessive distortions during quenching and also hot tearing, 21 which result in internal defect initiation, such as micro- and/or mesoscopic crack-22 ing. While the post-quenching surface cracking can be eliminated by subsequent 23 machining, the undetectable internal cracking becomes a major parameter that can 24 drastically disqualify a semi-finished product for reasons of nonconformity. More-25 over, these operations induce important residual stresses in the part, which makes 26 the final milling stage difficult. Predicting the internal residual strains/stresses has 27 become mandatory in industrial practice. The relevant constitutive laws therefore 28 need to be developed. However, one important problem is that during HT and 29 quenching the microstructure and phases in titanium alloys evolve depending on the 30 kinetics of the phase evolutions, in that they are time-temperature rate dependent. 31 Furthermore, titanium alloys have a complex mechanical behavior, exhibiting strain 32 rate sensitivity effects [2, 3], which can be reproduced through viscosity laws [4–6]. 33 These effects becomes significant for temperatures greater than  $500^{\circ}C$  [7, 8]. De-34 pending on the test temperature, this phenomenon can be combined with hardening 35 effects induced by dislocation motions and resulting from a competition between 36 storage and annihilation terms [9, 10]. At very high temperatures, other mecha-37 nisms are induced, such as grain boundary sliding [11, 12]. Moreover, important 38 microstructural changes can occur, such as grain growth, or phase fraction evolu-39 tions, which themselves greatly influence the mechanical behavior, and therefore 40 need to be introduced in the model formulation [13–15]. Indeed, these evolutions 41 can involve strain hardening [5, 16] or softening due to dynamic recrystallization [17] 42 under large deformation conditions. Moreover, when the  $\beta$ -phase is predominant, 43 particular phenomena, caused by the pinning-depinning effect of the dislocation, 44 can affect the mechanical behavior (Yield point effect). This effect was investigated 45 at the scale of the single crystal [18, 19] then generalized at the scale of the poly-46 crystal [11, 20–22]. Hence, non-unified approaches can be implemented in order to 47 define several inelastic mechanisms associated with each phase evolution [14, 23–25]. 48 Such approaches can translate grain-boundary strengthening caused by a lamellar 49 microstructure [26–29]. 50

<sup>51</sup> The present study proposes a behavior model that is able to faithfully predict the <sup>52</sup> strain-stress response of the material during the quenching operation. Considering <sup>53</sup> all the aspects described above, a laboratory experiment testing facility has been <sup>54</sup> developed to conduct in-situ heat-treatment at temperatures beyond or lower than <sup>55</sup>  $\beta$ -transus temperature on a cylindrical specimen [30]. Then, tensile tests were com-<sup>56</sup> bined in order to assess the behavior of the alloy under transient thermo-mechanical <sup>57</sup> loadings. The microstructural evolutions are greatly influenced by the cooling rate

and can exhibit several phases (primary and secondary  $\alpha$  phase and  $\beta$  phase), the 58 proportions of which were assessed by SEM observations and image analysis. In such 59 complex conditions, the mechanical behavior was characterized for several temper-60 ature levels and cooling rates. From these experiments, non-unified constitutive 61 equations were implemented to define several mechanisms related to each phase. 62 They consider a rule of mixture between phases depending on the cooling condi-63 tions. This rule plays an important role on the activated mechanisms influencing 64 the mechanical behavior. The model formulation can take account of the strain rate 65 sensitivity and the hardening over a wide temperature range (from the die-forging 66 temperature to the ambient temperature) and several cooling rates connected to 67 various microstructural states. This behavior model was identified for die-forging 68 temperatures below the  $\beta$ -transus temperature. Finally, the approach was success-69 fully extended to die-forging temperatures above the  $\beta$ -transus temperature. 70

#### 71 2. Experimental procedures

#### 72 2.1. Material and device

Industrial thermo-mechanical heat treatment consists in 3 main operations, asshown in Fig. 1:

• forging at  $940^{\circ}C$ 

• die-forging at  $950^{\circ}C$ 

• tempering at  $730^{\circ}C$ .



Figure 1: Thermo-mechanical industrial process

The material studied in the present work was supplied by Aubert & Duval as 78 a billet of Ti-6Al-4V Titanium alloy after the forging operation. Cylindrical spec-79 imens were machined from this billet. At this stage, an equi-axed microstructure 80 was observed, which included  $\alpha$  primary nodules, decorated at grain boundaries 81 by the  $\beta$  phase, as shown in Fig. 2a. Depending on the microstructure needs 82 (equiaxed, duplex or lamellar morphology), the die-forging operation can be carried 83 out at different temperatures that are higher or lower than the  $\beta$ -transus tempera-84 ture  $(T_{\beta} = 1000^{\circ}C)$ . In the present case, the die-forging temperature considered is 85  $950^{\circ}C$  (i.e. below the  $\beta$ -transus temperature). During the cooling/quenching from 86

this temperature, the  $\beta$  phase transforms into a lamellar microstructure consisting of colonies of secondary  $\alpha$  in the  $\beta$  phase (labelled  $\beta_t$ ). At this die-forging temperature, the phase transformation is not entirely completed and a duplex microstructure is obtained, regardless of the cooling conditions (Fig. 2b at  $60^{\circ}C/min$ ).



Figure 2: Starting microstructure of Ti-6Al-4V : (a) after Forging, (b) after time-temperature heat treatment corresponding to the Die-Forging (cooling rate:  $60^{\circ}C/min$ ) [Kroll Reagent | SEM | × 2000]

The cooling rate greatly influences the induced microstructure. Indeed, the thick-91 ness of the secondary (lamellar)  $\alpha$ -phase diminishes as the cooling rate increases. In 92 order to characterize the mechanical behavior during the quenching operation af-93 ter die-forging, an experimental device was specially developed to reproduce the 94 industrial heat treatment. It is based on a Schenck hydropuls hydraulic tensile test 95 machine with a nominal force up to 250 kN. It allows an in-situ heat treatment 96 by using an induction coil, which ensures a homogeneous temperature at the center 97 of the sample. The specimens were heated by a 2 kW Celes generator. A cylin-98 drical specimen was first instrumented by 9 spot-welded thermocouples to control 99 the longitudinal and circumferential temperature gradients. In the gauge length, 100 thermal gradients were about  $1^{\circ}C/mm$  and  $1^{\circ}C/120^{\circ}$  angle respectively in longitu-101 dinal and circumferential directions. The strain was measured by high temperature 102 extension extension with ceramic rods and a 10 mm gauge length. The system allows fast 103 heating and cooling steps. During each test, the samples were heated up to  $950^{\circ}C$ 104 with a dwell time of 2 hours at this temperature (die-forging temperature). Then the 105 samples were cooled down to different temperatures (ranging from  $950^{\circ}C$  to room 106 temperature) before starting the mechanical loading. Thus, after only a few seconds 107 of dwell time, the tensile tests were performed in air atmosphere by maintaining the 108 temperature constant. The tensile test consisted in a first mechanical loading with 109 a constant strain rate and a maximal strain of 1%, followed by a tensile dwell time 110 of 10 min and a second loading to reach a total strain of 2%. At the end of the 111 mechanical test, air spraying was applied at the surface of the sample to prevent 112

an evolution of the microstructure (mainly the growth of the phases). A schematicview of the tests performed is shown in Fig. 3.



Figure 3: Test procedure (a) In-situ heat treatment; (b) Isothermal loading path

#### 115 2.2. Tensile tests

The test conditions (see Fig. 3) were selected in order to accurately reproduce the thermo-mechanical loadings induced in the billet during the die-forging step. This analysis led to three cooling conditions being considered ( $\dot{\theta} = \{5, 60, 200\}^{\circ}C/min$ ) and several strain rates ( $10^{-4}s^{-1} \leq \dot{\varepsilon} \leq 10^{-2}s^{-1}$ ). Moreover, three temperature domains were investigated:

- from  $950^{\circ}C$  to  $800^{\circ}C$
- from  $800^{\circ}C$  to  $500^{\circ}C$
- from  $500^{\circ}C$  to  $20^{\circ}C$

In the following section, the effects of the cooling rate, strain rate and test temperature on the stress-strain response are discussed. Interpretations are based on microstructural evolution analysis (fraction and size of  $\alpha_I$  nodules,  $\alpha_{II}$  lamellae or  $\beta$  phase).

#### 128 2.2.1. Influence of the cooling rate

As shown by many research works [6, 31] on the topic of microstructure evolution 129 during cooling from temperatures above 950°C, while the phase transformation ( $\beta \leftrightarrow$ 130  $\alpha$ ) mainly depends on the temperature, the cooling rate mainly affects the size of 131 the primary  $\alpha$  nodules as well as the initiation and growth of the  $\alpha_{II}$  phase, leading 132 to different sizes and morphologies. Five tensile tests at different temperature levels 133  $(\theta = \{950, 800, 700, 500, 300, 20\}^{\circ}C)$  were conducted with a constant strain rate 134 of  $10^{-2}s^{-1}$ . The present study shows that, during cooling, an important phase 135 transformation of  $\beta$  into  $\alpha_{II}$  occurs, mainly between 950°C and 900°C. This result 136 is confirmed by other research works [32, 33] and is illustrated in more detail in the 137

next section (section 2.2.2). Thus, for the tensile tests carried out at and above 138  $800^{\circ}C$ , it can be considered that the microstructure observed at room temperature 139 is the one generated at the test temperature, as shown by Fig. 4 for tests conducted 140 at  $20^{\circ}C$  and  $700^{\circ}C$  under various cooling conditions. For the rapid cooling rates 141  $(\theta = \{60, 200\} \circ C/min)$ , many thin  $\alpha_{II}$  lamellae can be observed in the transformed 142  $\beta$  grains. At a slower cooling rate ( $\dot{\theta} = 5^{\circ}C/min$ ), the nucleation of  $\alpha_{II}$  lamellae 143 takes a longer time to grow, leading to lamellar coarsening. Hence, the morphology 144 of these lamellae is quite similar to that of the  $\alpha_I$  nodules. 145



Figure 4: SEM observations for tensile tests performed at  $700^{\circ}C$  and  $20^{\circ}C$  for different cooling rates:  $5^{\circ}C/min$  (left),  $60^{\circ}C/min$  (center),  $200^{\circ}C/min$  (right) [Kroll Reagent | SEM |  $\times 2000$ ]

The corresponding tensile tests (see Fig. 5) show a significant hardening with 146 the increase in the cooling rate. This feature can be related to the decrease in 147 the  $\alpha_{II}$ -lamellar thickness with the cooling rate. This induces a higher number 148 of  $\alpha/\beta$  boundaries that can act as more obstacles to the dislocation movements. 149 This hardening is thus linked to the plasticity of the  $\alpha$  phase ( $\alpha_I$  nodules and  $\alpha_{II}$ ) 150 lamellae) as the evolution of the lamellar thickness can be related to the yield stress 151 [31, 34, 35] or to the hardness or the ductility of the material [27, 35]. Image analysis 152 was conducted to determine the  $\alpha_{II}$  lamellar thickness  $L \ (\theta = \{60, 200\} \circ C/min)$  and 153 the  $\alpha_I$  nodule size ( $\dot{\theta} = 5^{\circ}C/min$ ). Fig. 6 illustrates the evolution of  $\alpha_{II}$ -lamellae 154 thickness L for different cooling rates. As shown, this trend can be aligned to a power 155 law. By plotting the curve given by Eq. 1 in a bi-logarithmic diagram, parameter 156 B can be determined from the value of the slope. Regarding the  $\alpha_I$  nodules, the 157 observations do not exhibit a significant evolution, regardless of the test conditions. 158 The average size considered next is thus  $15\mu m$ . 159



Figure 5: Stress-Strain response for different cooling rates at  $20^{\circ}C(a)$ ; and  $700^{\circ}C(b)$  and a constant strain rate of  $10^{-2}s^{-1}$ 



Figure 6: Evolution of the  $\alpha_{II}$ -lamellae thickness with the cooling rate

$$L = B \times \dot{\theta}^{-1} \tag{1}$$

#### 160 2.2.2. Time effects: temperature and strain rate

As mentioned previously, the phase transformation, in terms of fraction of phase, no longer evolves below  $800^{\circ}C$ , as the transformation of  $\beta$  into mainly  $\alpha_{II}$  lamellae occurs between  $950^{\circ}C$  and  $800^{\circ}C$ , as shown in Fig. 7.

At 950°C, the  $\beta$  fraction can be deduced from the SEM images by analyzing the fraction of  $\beta$  matrix  $\beta_{HT}$  transformed through the fast cooling (air spraying) operated at the end of the mechanical test. At 900°C, the measurements are complex, as the cooling time (from 950°C to 900°C) is not long enough to clearly distinguish the transformed  $\beta$  phase induced by the controlled cooling rate and the fast cooling from 900°C to 20°C. Therefore, this temperature level will not be deeply investigated in



Figure 7: SEM observations for tensile tests performed at  $950^{\circ}C(a)$ ; and  $800^{\circ}C(b)$  for a cooling rate of  $60^{\circ}C/min$ [Kroll Reagent | SEM | × 2000]

the sequel. From these measurements, the evolution of the  $\beta$  fraction can be assessed (see Fig. 8).



Figure 8: Evolution of the  $\beta$ -phase fraction with the temperature

These results are very similar to those provided in the work of Elmer [32] showing, 172 in a Ti-6Al-4V alloy, the evolution with the temperature of the  $\beta$  phase amounts mea-173 sured by in situ X-ray diffraction techniques. As in our present study, it seems that 174 most of the  $\beta \leftrightarrow \alpha$  phase transformation occurs at a temperature in the  $800^{\circ}C - T_{\beta}$ 175 range. This therefore confirms that, during cooling, most of the  $\beta$  phase had com-176 pleted its transformation into  $\alpha_{II}$  phase around 800°C. Regarding the mechanical 177 behavior, as expected, the stress-strain curves show a decrease in the flow stress 178 with the temperature (see Fig. 9). Moreover, a significant stress relaxation occurs 179 during the tensile dwell time for the test temperature above  $500^{\circ}C$ , involving con-180 siderable viscous stress, whereas it is considerably reduced below this temperature. 181

Lastly, at  $950^{\circ}C$ , a yield point phenomenon is observed. It is probably due to a 182 pinning-depinning process of the dislocations in a *Cottrell atmosphere* [36, 37], as 183 observed in BCC metals. Indeed, in BCC metals (as the  $\beta$  phase), the dislocations 184 can be pinned by interstitials, in which case a higher force is required in order to 185 leave such dislocations away from their *Cottrel atmosphere*. Thus, during the first 186 loading at  $950^{\circ}C$ , this higher force is responsible for the upper yield point (stress 187 peak). After unpinning, the dislocations can move easily at a lower stress leading 188 to a slight stress softening. During the dwell time, the initial Cottrel atmosphere 189 is recovered (static recovery) involving a new stress peak after the second loading. 190 This phenomenon is predominant at 950°C where the mechanisms related to the  $\beta$ 191 phase play an important role, but vanishes at lower temperatures where the plastic 192 deformation is mainly governed by the  $\alpha$  phase. 193



Figure 9: Stress-Strain response for constant strain  $(10^{-2}s^{-1})$  and cooling  $(60^{\circ}C/min)$  rates at different temperatures  $\theta \leq 600^{\circ}C(a)$ ;  $\theta \geq 700^{\circ}C$  (b)

#### <sup>194</sup> 3. Behavior modeling

The previous analysis leads to the definition of 3 mechanisms acting on the mechanical behavior. The first one is related to the  $\beta$  phase, whereas the two others are related to the  $\alpha$  phase through the nodular part ( $\alpha_I$ ) and lamellar part ( $\alpha_{II}$ ).

#### 198 3.1. Non-unified Constitutive Equations

A homogeneous deformation (Eq. (2)) is assumed in each phase [14] and a strain partition of the total strain into elastic and plastic parts is considered (Eq. (3)).

$$\underline{\varepsilon^{t}} = \underline{\varepsilon^{t}_{\alpha_{I}}} = \underline{\varepsilon^{t}_{\alpha_{II}}} = \underline{\varepsilon^{t}_{\beta}}$$
(2)

$$\underline{\varepsilon_{\phi}^{t}} = \underline{\varepsilon_{\phi}^{e}} + \underline{\varepsilon_{\phi}^{p}} \quad \forall \phi = \alpha_{I}, \alpha_{II}, \beta$$
(3)

Hooke's law is given by Eq. 4 for each phase. And each strain component can be related to a phase ratio  $Z_{\Phi}$  (Eq. 5).

$$\underline{\sigma_{\phi}} = \underline{\underline{C_{\phi}}}(\underline{\varepsilon_{\phi}^{t}} - \underline{\varepsilon_{\phi}^{p}}) \quad \forall \phi$$
(4)

$$\underline{\varepsilon}^{e} = \sum_{\phi} Z_{\phi} \underline{\varepsilon}^{e}_{\underline{\phi}}; \qquad \underline{\varepsilon}^{p} = \sum_{\phi} Z_{\phi} \underline{\varepsilon}^{p}_{\underline{\phi}} \quad \text{with:} \qquad \sum_{\phi} Z_{\phi} = 1 \quad \forall \phi \tag{5}$$

<sup>203</sup> A von Mises yield surface is assumed for each phase, as shown by Eq. 6. Its <sup>204</sup> evolution is defined through an isotropic hardening variable  $R_{\phi}$ .

$$f_{\phi} = \sigma_{\phi}^{eq} - R_{\phi} - \sigma_{\phi}^{0} = 0 \quad \forall \phi \tag{6}$$

 $\sigma_{\phi}^{eq}$  and  $\sigma_{\phi}^{0}$ , are respectively the equivalent stress and the elasticity limit related to the phase  $\phi$ .

<sup>207</sup> This approach is in agreement with the thermodynamics of the irreversible pro-<sup>208</sup> cess defined by two potentials, the Helmotz free energy  $\psi$  and the dissipation po-<sup>209</sup> tential  $\Omega$ .

The free energy can be partitioned into elastic and inelastic parts  $\psi = \psi^e + \psi^{in}$ and, in the present study, formulated for each phase (Eq. 7).

$$\varrho\psi^e = \frac{1}{2}\sum_{\phi} Z^2_{\phi} \underline{\underline{C}}_{\phi} \underline{\underline{c}}_{\phi}^e : \underline{\underline{c}}_{\phi}^e; \quad \varrho\psi^{in} = \frac{1}{2}\sum_{\phi} Z^2_{\phi} b_{\phi} Q_{\phi} r_{\phi}^2 \quad \forall\phi$$
(7)

The state laws giving the Cauchy stress and the macroscopic isotropic hardening variable derive from this potential (Eq. 8).

$$\underline{\sigma} = \varrho \frac{\partial \psi^e}{\partial \underline{\varepsilon}^e} = \sum_{\phi} Z_{\phi} \underline{\sigma_{\phi}}; \qquad R = \varrho \frac{\partial \psi^{in}}{\partial r} = \sum_{\phi} Z_{\phi} R_{\phi} = \sum_{\phi} Z_{\phi} b_{\phi} Q_{\phi} r_{\phi} \tag{8}$$

with  $r_{\phi}$  the internal variable associated to the isotropic hardening.  $b_{\phi}$  and  $Q_{\phi}$ are temperature-dependent coefficients.

The dissipation potential  $\Omega$  allows definition of the evolution of the internal variables (Eq. 9). It includes, first, a static recovery part (Eq. 10) and a classical viscoplastic potential formulated in the form of a power law. However, its expression differs from one phase to another. Indeed, a similar form is used to describe the primary and secondary alpha phase (Eq. 11), whereas a particular form is considered for the  $\beta$  phase (Eq. 12) so as to reproduce the yield point phenomenon.

$$\Omega = \sum_{\phi} Z_{\phi}^{2} \left( \Omega_{\phi}^{p} + \Omega_{\phi}^{r} \right) \quad \forall \phi$$
(9)

$$\Omega^r_{\phi} = \frac{a_{\phi} R_{\phi}^2}{2 b_{\phi} Q_{\phi}} \quad \forall \phi \tag{10}$$

$$\Omega^p_{\alpha} = \frac{K_{\alpha}}{n_{\alpha} + 1} \left\langle \frac{f_{\alpha}}{K_{\alpha}} \right\rangle^{n_{\alpha} + 1} \quad \forall \alpha = \alpha_I, \alpha_{II} \tag{11}$$

$$\Omega_{\beta}^{p} = \frac{b_{\rho} \ \rho_{m}}{M} \frac{D}{n_{\beta} + 1} \left\langle \frac{f_{\beta}}{D} \right\rangle^{n_{\beta} + 1} \tag{12}$$

222

<sup>223</sup>  $K_{\alpha}$  and  $n_{\alpha}$  are temperature-dependent parameters of the phase  $\alpha = (\alpha_I, \alpha_{II})$ .  $a_{\phi}$ <sup>224</sup> defines the static recovery term in the hardening variables of each phase. Especially <sup>225</sup> for the  $\beta$ -phase, D is a material parameter,  $b_{\rho}$  is the Burgers vector,  $\rho_m$  the density <sup>226</sup> of mobile dislocations and M the Taylor factor.

<sup>227</sup> The viscoplastic flow derives from this potential (Eq. 13).

$$\underline{\dot{\varepsilon}^p} = \partial\Omega/\partial\underline{\sigma} = \sum_{\phi} Z_{\phi} \ \frac{3}{2} \ \frac{S_{\phi}}{\sigma_{\phi}^{eq}} \ \dot{p}_{\phi} = \sum_{\phi} Z_{\phi} \ \underline{\dot{\varepsilon}^p_{\phi}} \quad \forall\phi$$
(13)

where  $S_{\phi}$  is the deviatoric part of  $\sigma_{\phi}$ .

The cumulative plastic strain for each phase is given by Eq. 14 for the  $\alpha$  phase and Eq. 15 for the  $\beta$  phase.

$$\dot{p}_{\alpha} = \Omega_{\alpha}'(f_{\alpha}) = \left\langle \frac{f_{\alpha}}{K_{\alpha}} \right\rangle^{n_{\alpha}} \forall \alpha = \alpha_{I}, \alpha_{II}$$
(14)

231

$$\dot{p}_{\beta} = \Omega_{\beta}^{'}(f_{\beta}) = \frac{b_{\rho}\rho_{m}}{M} \left\langle \frac{f_{\beta}}{D} \right\rangle^{n_{\beta}}$$
(15)

Lastly, the evolution equation related to the isotropic hardening for each phase is determined from Eq. 16.

$$\dot{r} = -\partial\Omega/\partial R = \sum_{\phi} Z_{\phi} \dot{r}_{\phi} \quad \text{with:} \ \dot{r}_{\phi} = \dot{p}_{\phi} \left(1 - b_{\phi} r_{\phi}\right) - a_{\phi} r_{\phi} \quad \forall \phi \tag{16}$$

The positivity of intrinsic dissipation  $\mathcal{D}$  ensures good agreement of the model formulation with thermodynamic principles. It can be expressed by Eq. 17.

$$\mathcal{D} = \sum_{\phi} \underline{\sigma_{\phi}} : \underline{\dot{\varepsilon}_{\phi}}^{p} - \sum_{\phi} R_{\phi} \dot{r}_{\phi}$$
(17)

The positivity of  $\mathcal{D}$  can be proved by Eq. 18.

$$\mathcal{D} = \sum_{\phi} \left( f_{\phi} + R_{\phi} + \frac{R_{\phi}^2}{Q_{\phi}} \right) \dot{p}_{\phi} + \sum_{\phi} \frac{a_{\phi}}{b_{\phi}} \left( \frac{R_{\phi}}{Q_{\phi}} \right)^2 \ge 0$$
(18)

#### 237 3.2. Introduction of the microstructural parameters

The viscoplastic flows (Eq. 14 and 15) require the identification of material parameters for each phase, which were determined by using SEM observations and image analysis. Thus, the influence of the microstructural evolutions related to the cooling rate during the quenching stage can be introduced into the model formulation.

#### 243 3.2.1. $\alpha_I$ phase

The proposed model acts on the coefficient  $K_{\alpha_I}$  and establishes a relationship between this parameter and the average size of the primary  $\alpha$  nodules  $d_{\alpha_I}$ , as shown by Eq. 19 following the Hall-Petch law.

$$K_{\alpha_I} = K_1 \ d_{\alpha_I}^{-n_d} \tag{19}$$

with  $K_1$  a temperature-dependent material parameter and  $n_d$  the Hall-Petch coefficient,  $n_d = 0.5$ .

### 249 3.2.2. $\alpha_{II}$ phase

Similarly, the proposed law introduces a relationship, given by Eq. 20, between  $K_{\alpha_{II}}$  and the thickness of the  $\alpha_{II}$  lamellae L.

$$K_{\alpha_{II}} = K_2 L^{-n_L} \tag{20}$$

 $K_2$  and  $n_L$  are material parameters. L depends on the cooling rate  $\dot{\theta}$  (see Eq. 253 1).

#### 254 3.2.3. β phase

The mobile dislocations are at the root of the yield point phenomenon [24] and the density of these dislocations  $\rho_m$  is a part  $f_m$  of the density of the total dislocations  $\rho_t$  (Equation 21). Moreover, this part evolves between a starting value  $f_{m0}$  and an asymptotic value  $f_{ma}$  [38]. Finally, an empirical law is used to define the relation between the densities of the total dislocations and the cumulative plastic strain.

$$\rho_m = f_m \rho_t; \qquad \rho_t = \rho_0 + C_\rho p_\beta \tag{21}$$

where  $C_{\rho}$  and  $a_{\rho}$  are material parameters.

The strain rate had a significant influence on the yield point phenomenon, therefore, the following time evolution of  $f_m$  is assumed (Equation 22).

$$\dot{f}_m = -\lambda \dot{p}^{\kappa}_{\beta} \left( f_m - f_{ma} \right) \tag{22}$$

with:  $f_m(t=0) = f_{m0}$  and  $\lambda$  and  $\kappa$  are material parameters.

This equation differs from the literature [14]. Indeed, in the present study, the yield point phenomenon increases with the strain rate, which is an effect that has not been observed on steels [24, 25] or on metastable  $\beta$ -titanium alloys [21, 22].

As shown previously, the tensile dwell time induces a stress relaxation which 268 can be reproduced by introducing a static recovery term into the isotropic hard-269 ening component. This phenomenon involves a dislocations rearrangement with a 270 decrease in the dislocation density [39–41]. Moreover, during this dwell time at 271 high temperature, some interstitial atoms can diffuse back around the dislocations, 272 leading to the re-pinning of dislocations in the Cottrel atmosphere. Therefore, the 273 yield point phenomenon is again observed during the second loading. In order to 274 account for this effect in the model formulation, Eq. 22 is modified by Eq. 23 and 275 a static recovery term is added, describing the decrease in the density of the mobile 276 dislocations during dwell time. 277

$$\dot{f}_m = -\lambda \dot{p}^{\kappa}_{\beta} \left( f_m - f_{ma} \right) - \mu f^{\delta}_m \tag{23}$$

<sup>278</sup> where  $\mu$  and  $\delta$  are material parameters.

279

All the constitutive equations are given in Appendix A (table A.1).

#### 281 4. Results

- 282 4.1. Identification Strategy
- 283 4.1.1. Young's Modulus

The evolution of Young's modulus with the temperature is obtained by using the relationship given by Eq. 24.

$$E = (Z_{\alpha_I} + Z_{\alpha_{II}})E_\alpha + Z_\beta E_\beta \tag{24}$$

The same values are assumed for  $\alpha_I$  nodules and  $\alpha_{II}$  lamellae. A tensile test at 1030°C was performed to determine the modulus of the  $\beta$ -treated alloy. A literature review [15, 42–45] allows Young's modulus evolution to be determined at lower temperatures. Then, knowing the phase fraction  $Z_{\phi}$ , the Young's modulus values of the  $\alpha$  phase are deduced from Eq. 24. The results obtained are in a good agreement with the values found in the literature, as shown in Fig. 10.



Figure 10: Temperature evolution of Young's modulus for  $\alpha$  and  $\beta$  phases: (a) literature (b) values used in this study

#### 292 4.1.2. Time-dependent parameters

The tensile tests performed with a cooling rate of  $60^{\circ}C/min$  were used to iden-293 tify the viscous parameters  $K_{\phi}$  and  $n_{\phi}$ . The stress relaxation curves  $\sigma - \sigma_i = f(time)$ 294 were plotted in a bi-logarithmic diagram to determine these parameters for temper-295 ature level, where  $\sigma_i$  is the non-viscous stress corresponding to the stabilized stress 296 value at the end of the relaxation time. The static recovery term  $a_{\phi}$  of the isotropic 29 hardening variable allows a better description of the relaxation curve, as shown in 298 Fig. 11. This term  $a = a_{\phi}$  is assumed to be equal for each phase and is obtained by 299 an optimization procedure for each temperature level. 300

The curve gives the value of  $n = n_{\phi}$ , which is assumed to be the same for each phase. The  $K_{\phi}$  parameter depends on the phase, as shown in Eq. 19 and 20. Assuming  $K_{\alpha_I} = K_{\alpha_{II}}$  given by the bi-logarithmic curve, L (provided by Eq. 1) and  $d_{\alpha_I}$ , obtained by image analysis, one can determine, on the one hand,  $K_1$ for the  $\alpha_I$  nodules, and on the other hand,  $K_2$  and  $n_L$  for the  $\alpha_{II}$  lamellae. It can be observed that Eq. 19 corresponds to a Hall-Petch law and the coefficient



Figure 11: Comparison between the relaxation range provided by the model and the experiment for a cooling rate of  $60^{\circ}C/min$  and a temperature of  $700^{\circ}C$ 

 $n_d$  is equal to 0.5. Moreover, the D parameter for the  $\beta$  phase is obtained by 307 taking  $Z_{\beta} = 1$ . Then, a rule of mixtures between phases gives a weighting of the 308 parameters related to each phase. To consider the yield point phenomenon in the 309 model formulation induced at high temperature, some additional parameters need 310 to be identified. The values of the Burgers vector  $b_{\rho}$  and of the Taylor factor M 311 come from the work of Wang for a titanium alloy [21]. Moreover, the parameters 312 related to the dislocation densities  $\rho_0, C_\rho$  and  $f_{m0}$  are also found in the literature 313 [22]. Lastly, the parameter  $a_{\rho}$  is identified from the tests performed at 950°C and 314 900°C, its value is usually between 0.7 and 1.5 [24, 37, 39]. The parameters  $\lambda$ ,  $\delta$ , 315  $\kappa$  and  $\mu$  related to the volume fraction of mobile dislocation are also identified at 316  $950^{\circ}C$  and  $900^{\circ}C$  where the yield point phenomenon is observed, they are selected 317 to fit the stress-strain curve and are determined by an optimization procedure. The 318 volume fraction of mobile dislocations  $f_m$  evolves between an initial value  $f_{m0}$  and 319 an asymptotic one  $f_{ma}$  [24, 25].  $f_{m0}$  is constant with the temperature, whereas 320  $f_{ma}$  decreases in order to take into account the decrease in the mobile dislocations 321 density at lower temperatures. This evolution will only be activated at  $950^{\circ}C$  and 322  $900^{\circ}C$  in order to consider the yield point phenomenon. For the other temperature 323 levels, this phenomenon vanishes by taking  $f_{ma} = f_{m0}$ . 324

325 4.1.3. Hardening parameters

The parameters  $Q = Q_{\phi}$  and  $b = b_{\phi}$  of the isotropic hardening variable and the elasticity limit  $\sigma^0 = \sigma_{\phi}^0$  are assumed to be equal for each phase. An optimization procedure is used for a cooling rate of  $60^{\circ}C/min$  considering the whole database.

329 4.2. Results

330 4.2.1. Model prediction on  $(\alpha + \beta)$  Ti-6Al-4V

Fig. 12 illustrates a comparison between simulation and experiment at  $950^{\circ}C$ . At this temperature, the mechanism related to the  $\beta$  phase is predominant and the modified version of the Yoshida model (Eq. 15, 21, 22) presented in the previous section allows a good description of the behavior at different strain rates.



Figure 12: Yield point prediction at  $950^{\circ}C$  and several strain rates (*line*: simulation, *marker*: experiment

For a cooling rate of  $60^{\circ}C/min$  the model response is in a good agreement with the experiment at lower temperatures and different strain rates, as shown in Fig. 13a at  $800^{\circ}C$  and in Fig. 13b at  $700^{\circ}C$ .



Figure 13: Computed Strain-Stress data (*line*) compared to Experimental results (*marker*) for several strain rates and at  $\theta = 800^{\circ}C$  (a);  $\theta = 700^{\circ}C$  (b).

Lastly, the model predictions for several cooling rates are illustrated in Fig. 14 at  $\theta = 500^{\circ}C$  (a) and at  $\theta = 20^{\circ}C$  (b).

All the values of the model parameters are given in Appendix B (Tables B.2-B.6).

#### 341 4.2.2. Model extension on $\beta$ -treated Ti-6Al-4V

In this section, the model is extended to a  $\beta$ -treated alloy. For this purpose, an experimental test campaign similar to the previous one was performed. It used the same starting samples obtained after the Forging operation (see Fig. 1) but the experimental procedure was changed by considering a solution annealing at



Figure 14: Computed Strain-Stress data (*line*) compared to Experimental results (*marker*) for several cooling rates and at  $\theta = 500^{\circ}C$  (a);  $\theta = 20^{\circ}C$  (b).

1030°C above the  $\beta$ -transus temperature ( $T_{\beta} = 1000^{\circ}C$ ). In this case, all the 346 model parameters related to the  $\beta$ -phase are identified at 1030° C (see table C.7). At 347 this temperature, the parameters of the mechanical model are  $\alpha$ -phase independent, 348 therefore  $Z_{\alpha_I} = Z_{\alpha_{II}} = 0$ . For the other temperature levels, the model prediction was 349 made by maintaining the values of almost all the model parameters identified for the 350  $(\alpha + \beta)$  heat treatment (Tables B.2-B.6). Only the microstructural parameters (Table 351 C.8) related to the phase fractions  $Z_{\Phi}$  and the evolution of lamellae morphology L 352 with the cooling rate needed to be identified again from SEM image analysis in order 353 to investigate the  $\beta$ -heat-treated alloy. The mechanism related to the  $\alpha_I$  nodules 354 vanished in this case  $(Z_{\alpha_I} = 0)$ , as during the solid solution annealing at 1030°C 355 where all the  $\alpha_I$  nodules were transformed into  $\beta$ . Then, during cooling below the 356  $\beta$ -transus temperature, the  $\beta$  phase was finally transformed into a fully lamellar 357  $(\alpha + \beta)$  microstructure. 358



Figure 15: Computed Strain-Stress data (*line*) compared to Experimental results (*marker*) at  $\theta = 950^{\circ}C$  and several strain rates (a); at  $\theta = 700^{\circ}C$  and several cooling rates (b).



Figure 16: Computed Strain-Stress data (*line*) compared to Experimental results (*marker*) for several cooling rates and at  $\theta = 500^{\circ}C$  (a);  $\theta = 20^{\circ}C$  (b).

Fig. 15 and Fig. 16 illustrate the comparison between the computed Strain-359 Stress data and experimental results in the case to the  $\beta$ -heat treated Ti-6Al-4V, 360 at 950°C and for several strain rates (Fig. 15a), at intermediate temperatures 361  $(T = \{20, 500, 700\}^{\circ}C)$  and for several cooling rates (Fig. 15b and 16a-b). Aside 362 from the temperature of  $950^{\circ}C$  where the stress levels are very low, discrepancies 363 between the model response and the experiment were less than 15% for the other 364 test conditions. This is guite acceptable since the only parameters that have to 365 be changed concern microstructural features of the  $\beta$ -heat treated alloy. 366

#### 367 4.3. Discussion

The quenching of industrial parts generates transient temperature variations 368 that induce plastic straining due to thermal self-constraining. The degree of self-369 constraining depends on the dimensions of a part and on the heat transfer mecha-370 nisms between the part and the quenching environment (for example oil or water 371 quenching ...) that control the mean global cooling rate [46]. In general the residual 372 stresses are investigated at room temperature, and can be measured through X-Ray 373 Diffraction or hole drilling methods. In-situ measurements of the residual stresses 374 are not possible and the only rational manner is to use advanced thermo-mechanical 375 modeling and numerical simulations analysis. Therefore relevant and reliable consti-376 tutive laws have to be developed. However, alloys such as Ti-6Al-4V alloy are very 377 much prone to microstructural evolution at high temperature or during transient 378 temperature-time conditions. In many approaches, the reliability of the constitutive 379 laws is examined by laboratory testing of heat-treated alloys. The high temperature 380 assessments are thus run on specimens heated up again to a prescribed temperature 381 for mechanical testing. In the present investigation, the main objective was to assess 382 and to model the thermo-mechanical behavior of Ti-6Al-4V alloy, through stepwise-383 temperature mechanical testing by first conducting an in-situ heat-treatment and 384 then by quenching with a controlled rate to a prescribed temperature and finally 385 by conducting the mechanical testing at this temperature. Such combining of time-386 temperature-mechanical scenarios are not commonly reported in the literature and 387 often absent in the open literature. Although, many investigations deal with the 388

mechanical behavior of Titanium alloys especially Ti-6Al-4V alloy, most of them
consider the thermodynamic equilibrium conditions. However, some comparisons
can be made with the present study considering the influence of the microstructure
on the mechanical response of the material.

First, the phase analysis (Fig. 8) illustrates a drastic decrease of the  $\beta$  phase 393 from 950 to  $800^{\circ}C$  with a  $\beta$  phase around 78% at 950°C. Similar results are found in 394 the literature at this temperature [32, 33]. This means that the role of the  $\beta$  phase 395 cannot be neglected and the plasticity induced has to be linked to this phase. The 396 yield point phenomenon illustrated in Fig. 12 is observed on many Body-Centered 397 Cubic (BCC) materials [39, 41] such as the  $\beta$  phase for titanium alloys. It can be 398 related to the dislocations locked by the solute atoms then broken away from the 399 pinning points at a high stress level. It is also associated with discontinuous yielding 400 with the increase of new mobile dislocations generated from the grain boundary 401 [20, 21, 47, 48]. The behavior model implemented in the present study is based on 402 a rule of mixture between two mechanisms, one related to the  $\alpha$  phase (divided in 403 primary and secondary phases), the second to the  $\beta$  phase. At high temperatures, 404 the constitutive equations associated with the  $\beta$  phase are predominant, and the 405 formulation is based on the works performed by Yoshida et al on BCC materials 406 [21, 22, 24, 25]. As discussed previously, these equations are modified to take into 407 account some particular effects observed, such as the increase of the yield point with 408 the strain rate and the dislocations rearrangement with a decrease in the dislocation 409 density during dwell times (see Eq. 23). 410

Secondly, at lower temperatures, the effect of the  $\alpha$  phase increases while that 411 of the  $\beta$  phase decreases. Moreover, Fig. 4 shows a decrease of the  $\alpha_{II}$ -lamellar 412 thickness with the cooling rate involving an increase of the flow stress (Fig. 5). 413 This result is induced by an increase of the  $\alpha/\beta$  boundaries acting as obstacles to 414 the dislocation movements. These results are also shown in several investigations 415 [28, 35, 49]. This effect is described in the constitutive equations through the viscous 416 flow where the  $K_{\Phi}$  ( $\Phi = \{\alpha_I, \alpha_{II}\}$ ) parameter evolves with the thickness of the  $\alpha_{II}$ 417 lamellae L (see Eq. 20), itself related to the cooling rate, or with the average size of 418 the primary  $\alpha$  nodules  $d_{\alpha_I}$  (Eq. 19). 419

Finally, the strain rate sensitivity is reduced for temperatures inferior to  $500^{\circ}C$ [8] involving a significant hardening effect which is assumed similar for each phase. On the other hand, Fig. 12 and 13 show an important strain rate effect for the temperatures exceeding  $600^{\circ}C$  as mentioned in [3] compared to the hardening effect.

#### 424 5. Conclusions

In the present work, an experimental device was developed to reproduce the mechanical behavior of Ti-6Al-4V throughout the die-forging operation. A nonunified behavior model was implemented and the following conclusions can be drawn.

- For a  $(\alpha + \beta)$  dual-phase alloy, the phase transformation is greatly influenced by the cooling rate conditions, which themselves play an important role in the strain-stress response of the material.
- The non-unified behavior model is able to predict the mechanical behavior, assuming an initial phase proportion  $(\alpha_I, \alpha_{II} \text{ or } \beta)$ .

• Depending on the test temperature, the model gives a good prediction of the 433 strain rate and hardening effects. Moreover, based on a modified Yoshida 434 model formulation, it can describe the yield point phenomenon observed at 435 high temperature and the static recovery effect exhibited during the dwell 436 times. 437

438

• Lastly, the model was successfully extended to the behavior prediction of a  $\beta$ -treated Ti-6Al-4V alloy. 439

#### Acknowledgement 440

The authors very much acknowledge the financial support received through an 441 FUI grant in the framework of the collaborative project TiMaS (Titanium Machining 442 and Simulation), led by Airbus. The authors also gratefully acknowledge Figeac Aéro 443 for the machining of samples. 444

# 445 Appendix A. Model summary

# The table A.1 summarizes the model formulation.

	Multi-axial formulation	Uni-axial formulation					
Yield criterion	$f_{\phi} = \sigma_{\phi}^{eq} - R_{\phi} - \sigma_{\phi}^{0}  \forall \phi$	$f_{\phi} =  \sigma_{\phi}  - R_{\phi} - \sigma_{\phi}^{0}  \forall \phi$					
Hooke's law	$\underline{\sigma_{\phi}} = \underline{C_{\phi}} \left( \underline{\varepsilon_{\phi}^{t}} - \underline{\varepsilon_{\phi}^{p}} \right)  \forall \phi$	$\sigma_{\phi} = E_{\phi} \left( \varepsilon_{\phi}^{t} - \varepsilon_{\phi}^{p} \right)  \forall \phi$					
	$\underline{\dot{arepsilon}^p} = \sum_{\phi} Z_{\phi}^2 rac{3}{2} rac{\sigma_{\phi}}{\sigma_{\perp}^{eq}} \dot{p}_{\phi}  orall \phi$	$\dot{\varepsilon}^p = \sum_{\phi} Z_{\phi} \ \dot{p}_{\phi} \ sign(\sigma_{\phi})  \forall \phi$					
Flow rules	with $\dot{p}_{\alpha} = \left\langle \frac{f_{\alpha}}{K_{\alpha}} \right\rangle^{n_{\alpha}^{-\phi}} \forall \alpha = \alpha_{I}, \alpha_{II}$	with $\dot{p}_{\alpha} = \left\langle \frac{f_{\alpha}}{K_{\alpha}} \right\rangle^{n_{\alpha}}$					
	and $\dot{p}_{\beta} = \frac{\dot{b}_{\rho} \ \rho_m}{M} \left\langle \frac{f_{\beta}}{D} \right\rangle^{n_{\beta}}$	and $\dot{p}_{\beta} = \frac{b_{\rho} \ \rho_m}{M} \left\langle \frac{f_{\beta}}{D} \right\rangle^{n_{\beta}}$					
Microstructural	$K_{\alpha_I} = K_1$ of	$d_{\alpha_I}^{\ -n_d}$					
parameters	$K_{\alpha_{II}} = K_2 \ L^{-n_L}  \text{w}$	with $L = B \dot{\theta}^{-1}$					
Metallurgical	$ ho_m = f_m \;  ho_t;   ho_t$ =	$= \rho_0 + C_\rho \ p_\beta$					
parameters	$\dot{f_m} = -\lambda \ \dot{p}^\kappa_eta \left( f_m - f_{ma}  ight) - f_{ma}$	$\mu f_m^{\delta};  f_m\left(0\right) = f_{m0}$					
Isotropia hordoning	$\dot{r} = -\sum_{\phi} Z_{\phi} \ \dot{r}_{\phi} \ \text{with} \ \dot{r}_{\phi} = \dot{p}_{\phi} \left(1 - b_{\phi} \ r_{\phi}\right) - a_{\phi} \ r_{\phi}$						
isotropic nardening	and $R_{\phi} = b_{\phi} Q$	$\phi r_{\phi}  \forall \phi$					

### <sup>447</sup> Appendix B. Model coefficients for $\alpha + \beta$ treated Ti-6Al-4V

Table B.2 illustrates the phase-independent model parameters, tables B.3 and B.4 the  $\alpha$ -phase dependent model parameters and tables B.5 and B.6  $\beta$ -phase dependent model parameters

$\theta \ [^{\circ}C]$	950	900	800	700	600	500	400	300	20
$\sigma^0 \ [MPa]$	1	1	3	10	34	145	327	386	650
$Q \ [MPa]$	1	2	55	85	92	97	100	101	103
b	1	5	190	317	400	425	433	434	435
$a  [s^{-1}]$	$5 \ 10^{-1}$	$2.5 \ 10^{-1}$	8. $10^{-2}$	$2 \ 10^{-2}$	$8 \ 10^{-3}$	$3 \ 10^{-3}$	$2 \ 10^{-4}$	$1.4 \ 10^{-4}$	$4 \ 10^{-5}$
n	3.3	3.4	3.6	4.9	7.8	9.8	11.2	11.7	12

Table B.2: Phase independent and temperature dependent model parameters

Table B.3:  $\alpha$ -phase and temperature dependent model parameters (1)

$\theta \ [^{\circ}C]$	950	900	800	700	600	500	400	300	20	
$E_{\alpha} \ [GPa]$	35	47	60.7	70	77.4	86	85.1	84.1	109.5	
$Z_{\alpha_{II}}$	0	0.22		0.44						
$K_1$	23.7	24	62.8	77.3	73.5	51.5	20.8	20.2	32.3	
$K_2$	95	96	251	309	294	208	83	81	131	

Table B.4:  $\alpha$ -phase dependent model parameters (2)

$Z_{\alpha_I}$	$d_{\alpha_I} \ [mm]$	$n_d$	$n_L$	В
0.22	$15.10^{-3}$	0.5	0.105	$66.7 \ 10^{-3}$

Table B.5:  $\beta$ -phase and temperature dependent model parameters (1)

$\theta \ [^{\circ}C]$	950	900	800	700	600	500	400	300	20
$E_{\beta} \ [GPa]$	39.3	48.2	60.7	69	74	81	79	78	90
D	181	182	370	472	493	372	160	148	290
$Z_{eta}$	0.78	0.56	0.18						
$f_{ma}$	5. $10^{-3}$	$1.\ 10^{-3}$	5.5 $10^{-4}$ 4.5 $10^{-4}$ 4.10 <sup>-4</sup>						

Table B.6:  $\beta$ -phase dependent model parameters (2)

$b_{ ho} \ [cm]$	M	$\rho_0 \ [cm^{-2}]$	$C_{ ho} \ [cm^2]$	$f_{m0}$	$\lambda$	κ	$\mu$	δ
$2.5  10^{-8}$	2.76	$6.4 \ 10^{10}$	$2.1  10^{11}$	$4 \ 10^{-4}$	$18 \ 10^3$	2	1.25	2

## <sup>451</sup> Appendix C. Model coefficients updated for $\beta$ treated Ti-6Al-4V

<sup>452</sup> Table C.7 gives the values of the model parameters at 1030° C and table C.8 the <sup>453</sup> temperature evolution of the microstructural parameters identified for the  $\beta$ -heat <sup>454</sup> treated titanium alloy.

$\sigma^0 \ [MPa]$	$Q \ [MPa]$	b	$a \ [s^{-1}]$	n	$E_{\beta} \ [GPa]$	$D \ [MPa]$	$f_{ma}$
0	1	1	1.1	3	35	85	$1 \ 10^{-1}$

Table C.7: Temperature model parameters at  $1030^\circ C$ 

Table C.8: Updated microstructural parameters for the  $\beta\text{-treated Ti-6Al-4V}$ 

$\theta \ [^{\circ}C]$	1030	950	900	800	700	600	500	400	300	20	
$Z_{\alpha_I}$	0										
$Z_{\alpha_{II}}$	0	0 0.22 0.44 0.82									
$Z_{\beta}$	1	0.78	0.56	0.18							
В		80.6 10 <sup>-3</sup>									

#### 455 References

#### 456 References

- [1] R. Boyer, E. Collings, G. Welsch, Materials Properties Handbook: Titanium
   Alloys, 4th Edition, ASM International, 2007.
- [2] A. Majorell, S. Srivatsa, R. Picu, Mechanical behavior of Ti-6Al-4V at high and
  moderate temperatures Part I: Experimental results, Materials Science and
  Engineering: A 326 (2) (2002) 297–305.
- [3] M. Vanderhasten, Ti-6Al-4V: Deformation map and modelisation of tensile be haviour, thése de Doctorat, Katholieke Universiteit Leuven, 2007.
- [4] R. Picu, A. Majorell, Mechanical behavior of Ti-6Al-4V at high and moderate
  temperatures Part II: constitutive modeling, Materials Science and Engineering: A 326 (2002) 306-316.
- 467 [5] B. Cheong, J. Lin, A. Ball, Modelling of hardening due to grain growth for
  468 a superplastic alloy, Journal of Materials Processing Technology 119 (2001)
  469 361–365.
- [6] S. Semiatin, F. Montheillet, G. Shen, J. Jonas, Self-consistent modeling of the
  flow behavior of wrought alpha/beta titanium alloys under isothermal and nonisothermal hot-working conditions, Metallurgical and Materials Transactions A
  33 (2002) 2719–2727.
- 474 [7] Y. Robert, Simulation numérique du soudage du TA6V par laser YAG impul475 sionnel: caractérisation expérimentale et modélisation des aspects thermomé476 caniques associés à ce procédé, thèse de Doctorat, École des Mines de Paris,
  477 2007.
- [8] Z. Tao, H. Yang, H. Li, X. Fan, Quasi-static tensile behavior of large-diameter
  thin-walled Ti-6Al-4V tubes at elevated temperature, Chinese Journal of Aeronautics 29 (2) (2016) 542–553.
- [9] O. Bouaziz, Revisited storage and dynamic recovery of dislocation density evolution law: Toward a generalized kocks-mecking model of strain-hardening, Advanced Engineering Materials 14 (9) (2012) 759–761.
- [10] H. Mecking, B. Nicklas, N. Zarubova, U. Kocks, A *universal* temperature scale for plastic flow, Acta Metallurgica 34 (3) (1986) 527–535.
- [11] J. Lin, T. Dean, Modelling of microstructure evolution in hot forming using
  unified constitutive equations, Journal of Materials Processing Technology 167
  (2005) 354–362.
- [12] J. Lin, J. Yang, GA-based multiple objective optimisation for determining vis coplastic constitutive equations for superplastic alloys, International Journal of
   Plasticity 15 (11) (1999) 1181–1196.

- [13] X. Fan, H. Yang, Internal-state-variable based self-consistent constitutive modeling for hot working of two-phase titanium alloys coupling microstructure evolution, International Journal of Plasticity 27 (11) (2011) 1833–1852.
- [14] J. Teixeira, B. Denand, E. Aeby-Gautier, S. Denis, Simulation of coupled temperature, microstructure and internal stresses evolutions during quenching of a  $\beta$ -metastable titanium alloy, Materials Science and Engineering A 651 (2016) 615–625.
- [15] J. Teixeira, B. Denand, E. Aeby-Gautier, S. Denis, Influence of the  $\beta \rightarrow \alpha + \beta$ transformation on the stresses and strains evolutions during quenching of the Ti17 alloy from the  $\beta$  phase field, in: Thermal Process Modeling: Proceedings from the 5th International Conference on Thermal Process Modeling and Computer Simulation, ASM International, 2014, pp. 199–209.
- [16] V. Velay, H. Matsumoto, V. Vidal, A. Chiba, Behavior modeling and microstructural evolutions of Ti-6Al-4V alloy under hot forming conditions, International Journal of Mechanical Sciences 108-109 (2016) 1 – 13.
- [17] E. Alabort, P. Kontis, D. Barba, K. Dragnevski, R. Reed, On the mechanisms of superplasticity in Ti-6Al-4V, Acta Materialia 105 (2016) 449 463.
- <sup>509</sup> [18] A. Laasraoui, J. Jonas, Prediction of steel flow stresses at high temperatures and strain rates, Metallurgical Transactions A 22A (7) (1991) 1545–1558.
- [19] H. Mecking, Strain hardening and dynamic recovery, in: Dislocation Modelling
   of Physical Systems, Pergamon, 1981, pp. 197–211.
- [20] A. Momeni, S. Abbasi, M. Morakabati, A. Akhondzadeh, Yield point phenomena in TIMETAL 125 beta Ti alloy, Materials Science and Engineering: A 643
  (2015) 142–148.
- [21] X. Wang, H. Hamasaki, M. Yamamura, R. Yamauchi, T. Maeda, Y. Shirai,
  F. Yoshida, Yield-Point Phenomena of Ti-20V-4Al-1Sn at 1073 K and Its Constitutive Modelling, Materials Transactions 50 (6) (2009) 1576–1578.
- [22] X. Wang, H. Hamasaki, M. Yamamura, R. Yamauchi, T. Maeda, Y. Shirai,
  F. Yoshida, A Study of High Temperature Viscoplastic Deformation of Beta Titanium Alloy Considering Yield-point Phenomena, Key Engineering Materials 410-411 (2009) 177–185.
- F. Montheillet, Comportement rhéologique des matériaux métalliques multi phasés, Techniques de l'Ingénieur m3010 (2012) 24.
- F. Yoshida, A constitutive model of cyclic plasticity, International Journal of Plasticity 16 (2000) 359–380.
- F. Yoshida, Y. Kaneda, S. Yamamoto, A plasticity model describing yield-point
   phenomena of steels and its application to FE simulation of temper rolling,
   International Journal of Plasticity 24 (2008) 1792–1818.

- E. Taleff, C. Syn, D. Lesuer, O. Sherby, Pearlite in ultrahigh carbon steels: Heat
  treatments and mechanical properties, Metallurgical and Materials Transactions
  A 27 (1) (1996) 111–118.
- <sup>533</sup> [27] F. Perdrix, M. Trichet, J. Bonnentien, M. Cornet, J. Bigot, Influence of cooling
  <sup>534</sup> rate on microstructure and mechanical properties of a Ti-48Al alloy, Inter<sup>535</sup> metallics 7 (12) (1999) 1323–1328.
- [28] F. Perdrix, M. Trichet, J. Bonnentien, M. Cornet, J. Bigot, Influence of nitrogen on the microstructure and mechanical properties of Ti-48Al alloy, Intermetallics 9 (2001) 147–155.
- <sup>539</sup> [29] H. Ishii, K. Ohkubo, S. Miura, T. Mohri, Mechanical Properties of  $\alpha + \kappa$  Two-<sup>540</sup> phase Lamellar Structure in Fe-Mn-Al-C Alloy, Materials Transactions 44 (9) <sup>541</sup> (2003) 1679–1681.
- [30] R. Julien, V. Velay, V. Vidal, Y. Dahan, R. Forestier, F. Rézaï-Aria, Tensile
  behaviour of high temperature forged ti-6al-4v during in-situ heat treatments,
  Materials Letters 208 (Supplement C) (2017) 7 9.
- [31] I. Katzarov, S. Malinov, W. Sha, Finite Element Modeling of the Morphology of  $\beta$  to  $\alpha$  Phase Transformation in Ti-6Al-4V Alloy, Metallurgical and Materials Transactions A 33 (4) (2002) 1027–1040.
- [32] J. Elmer, T. Palmer, S. Babu, E. Specht, In situ observations of lattice expansion and transformation rates of  $\alpha$  and  $\beta$  phases in Ti-6Al-4V, Materials Science and Engineering A 391 (1-2) (2005) 104–113.
- <sup>551</sup> [33] I. Lonardelli, N. Gey, H.-R. Wenk, M. Humbert, S. Vogel, L. Lutterotti, In <sup>552</sup> situ observation of texture evolution during  $\alpha \to \beta$  and  $\beta \to \alpha$  phase transfor-<sup>553</sup> mations in titanium alloys investigated by neutron diffraction, Acta Materialia <sup>554</sup> 55 (17) (2007) 5718 - 5727.
- <sup>555</sup> [34] Y. Sui, A. Liu, B. Li, J. Guo, Relationship between Thickness of Lamellar <sup>556</sup>  $\alpha + \beta$  Phase and Mechanical Properties of Titanium Alloy, Advanced Materials <sup>557</sup> Research 311-313 (2011) 1916–1919.
- <sup>558</sup> [35] F. Gil, M. Ginebra, J. Manero, J. Planell, Formation of  $\alpha$ -Widmanstätten struc-<sup>559</sup> ture: effects of grain size and cooling rate on the Widmanstätten morphologies <sup>560</sup> and on the mechanical properties in Ti6Al4V alloy, Journal of Alloys and Com-<sup>561</sup> pounds 329 (2001) 142–152.
- [36] A. Cottrell, B. Bilby, Dislocation Theory of Yielding and Strain Ageing of Iron,
   Proceedings of the Physical Society. Section A 62 (1) (1948) 49–62.
- <sup>564</sup> [37] G. Hahn, A model for yielding with special reference to the yield-point phenomena of iron and related BBC metals, Acta Metallurgica 10 (8) (1962) 727–738.

- [38] F. Yoshida, Constitutive modeling of large-strain cyclic plasticity for anisotropic
  metals, in: Hardening and Damage of Materials under Finite Deformations :
  Constitutive Modeling and Numerical Implementation, Dortmund, 2012, pp.
  1-67.
- [39] D. Hull, D. Bacon, Introduction to Dislocations, 5th Edition, Vol. 36, Elsevier, 2011.
- [40] C. Kerisit, R. E. Loge, S. Jacomet, V. Llorca, N. Bozzolo, EBSD coupled to SEM
  in situ annealing for assessing recrystallization and grain growth mechanisms
  in pure tantalum, Journal of Microscopy 250 (3) (2013) 189–199.
- [41] R. Smallman, A. Ngan, Modern Physical Metallurgy, 8th Edition, Elsevier, 2014.
- <sup>577</sup> [42] V. Joshi, Titanium Alloys : An Atlas of Structures and Fracture Features, CRC
   <sup>578</sup> Taylor & Francis, 2006.
- [43] M. Brandes, M. Baughman, M. Mills, J. Williams, The effect of oxygen and
  stress state on the yield behavior of commercially pure titanium, Materials
  Science and Engineering A 551 (2012) 13–18.
- [44] V. Vidal, Y. Balcaen, F. Pettinari-Sturmel, J. Douin, P. Lours, V. Velay,
  L. Robert, Experimental Study of the Deformation Mechanisms in Textured
  Alpha-titanium Alloy Sheets, in: Zhou, L and Chang, H and Lu, Y and Xu, D
  (Ed.), Ti-2011: Proceedings of the 12<sup>th</sup> world conference on Titanium, Vol. II,
  2012, pp. 1290–1293.
- [45] S. Fréour, D. Gloaguen, M. François, R. Guillén, Application of inverse models and XRD analysis to the determination of Ti-17  $\beta$ -phase coefficients of thermal expansion, Scripta Materialia 54 (2006) 1475–1478.
- [46] B. Bourouga, J. Gilles, Roles of heat transfer modes on transient cooling by
  quenching process, International Journal of Material Forming 3 (2) (2010) 77–
  88.
- [47] Y. Duan, P. Li, K. Xue, Q. Zhang, X. Wang, Flow behavior and microstructure evolution of TB8 alloy during hot deformation process, Transactions of Nonferrous Metals Society of China 17 (6) (2007) 1199 – 1204.
- [48] L. Li, Y. Lou, L. Yang, D. Peng, K. Rao, Flow stress behavior and deformation
  characteristics of Ti-3Al-5V-5Mo compressed at elevated temperatures, Materials and Design 23 (5) (2002) 451 457.
- [49] S. Semiatin, T. Bieler, The effect of alpha platelet thickness on plastic flow
  during hot working of Ti-6Al-4V with a transformed microstructure, Acta Materialia 49 (17) (2001) 3565 3573.