A microstructure sensitive grain boundary sliding and slip based constitutive model for machining of Ti-6Al-4V

Patxi Fernandez-Zelaia^{a,*}, Shreyes Melkote^a, Troy Marusich^b, Shuji Usui^b

^a George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA, United States

^b Third Wave Systems, Minneapolis, MN, United States

* Corresponding author at: George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA, United States. Tel.: +1 404 894 0368; fax: +1 404 984 9342. E-mail address: pfz3@gatech.edu (P. Fernandez-Zelaia).

Abstract

A composite dual phase internal state variable constitutive model was developed for Ti-6Al-4V. The proposed model includes diffusion assisted grain boundary sliding based physics in addition to a traditional slip-based plasticity. Influence of microstructure on the flow stress is introduced via dislocation density and mean grain size internal state variables. The dislocation density evolves according to a physics based law that considers dislocation nucleation and annihilation processes. Grain refinement is driven by dynamic recrystallization, which is modeled phenomenologically. The model is calibrated with uniaxial stress-strain data that ranges between quasi-static and dynamic rates across a wide range of temperatures. Validation against machining data shows that the model predicts chip segmentation frequency, machining forces, and tool temperatures reasonably well. The newly introduced grain boundary sliding physics was found to dominate deformation following sufficient grain refinement. This deformation mode provides softening at the constitutive level without the need for invoking damage based softening mechanisms. This physical interpretation is something that has not previously been explored in the machining literature.

Keywords: machining, constitutive modeling, titanium, chip segmentation, grain boundary sliding, microstructure sensitive

1. Introduction

Segmented chips are often observed in the machining of high strength and low thermal conductivity materials. High rate shear band failure in ductile metals has been traditionally associated with a competition between thermal softening and rate hardening [1] as well as conventional ductile failure caused by void coalescence and growth [2-5]. At high rates titanium is particularly susceptible to shear band failure as (1) its high strength drives heat generation during large strain plastic deformation, and (2) the low thermal conductivity impedes conduction of heat away from the band. Komanduri et al. [6] studied chip segmentation and observed that these instabilities were correlated with increased tool wear and deleterious effects on component precision. Recent work by Sagapuram et al. [7] studied segmentation processes via in-situ digital image correlation (DIC) techniques and showed that the workpiece surface itself inherited heterogeneous strain fields from the chip segmentation process. Counter arguments exist, which argue that chip segmentation may have some desirable effects; segmentation instantaneously decreases cutting forces acting on the tool and may also improve chip evacuation [8]. Therefore, it is clear that a need exists to: (1) understand the fundamental physical mechanisms responsible for serrated chip formation, and (2) to develop predictive computational tools that engineers can use to simulate chip segmentation in metal cutting.

The literature contains a large body of work dedicated to modeling of the chip segmentation process. Komanduri and Hou [9] developed an analytical machining model for Ti-6Al-4V based on a plastic instability failure mechanism associated with thermal softening. Molinari et al. [10] performed a thorough study of shear banding in Ti-6Al-4V using both finite element analysis (FEA) and analytical techniques. In their work, thermal softening, which results in the loss of load carrying capacity, along with ductile fracture were the mechanisms attributed to producing shear bands in chips. Many FEA based machining models have been proposed that introduce softening via damage accumulation [11] as well as fracture criteria [12]. A counter argument to

the ductile fracture argument is that it is well known that ductility is heavily dependent on stress triaxiality [13] and so the intense shearing of the primary deformation zone superimposed with large compressive hydrostatic stresses may limit ductile failure under certain machining conditions. Sun and Guo characterized Ti-6Al-4V chips produced in end milling and found that hardness within the shear bands was high relative to the surrounding medium [14]. The same was found to be true of shear bands in Ti-6Al-4V subject to ballistic plug testing [15]. This suggests that the shear bands, at least in the cases studied, may not be weakened by ductile damage.

The microstructures of machined chips have been observed to contain highly refined submicron grain structures that are likely generated by a continuous dynamic recrystallization (DRX) process [16-18]. Deformation mechanisms active at the nanocrystalline scale are vastly different than those present at higher length scales [19-21]. Recent micro-mechanical inspired modeling work by Melkote et al. [22] incorporated a phenomenological inverse Hall-Petch [23] relationship, which provided the mechanism for flow softening following sufficient DRX grain refinement. Experimental studies focused on nanocrystalline deformation mechanics under machining conditions (high rates and temperatures) do not exist in the current literature. However, there are molecular dynamics studies which suggest that grain boundary driven mechanisms can accommodate a significant fraction of total deformation under such extreme conditions [24, 25]. Recent work by Sagapuramet al. [26] utilized a novel experimental technique to measure the relative displacement of adjacent chip segments. Despite the expected temperature in the shear bands being below liquidus, they found that the relative sliding can be explained well using a viscous slider model. This experimental observation seems to suggest that shear bands deform in a viscous manner following nucleation.

It is important to note that various models currently exist that are capable of predicting shear banding as well as the corresponding forces in machining of Ti-6Al-4V [10, 11, 27, 28]. Many of these models are based on the classic Johnson-Cook model [29] with the addition of additional terms (damage for example). The Johnson-Cook model phenomenologically captures various modes of expected material behavior; strain hardening, rate hardening, and thermal softening. Inclusion of damage or other softening terms can further bolster the robustness of the constitutive law. Secondly, the Johnson-Cook model is computationally inexpensive to evaluate from within the FEA framework. Therefore, from an engineering perspective, Johnson-Cook type models are very attractive. What the standard Johnson-Cook approach lacks is the ability to capture the evolution of the material state. The material state can be represented by physically relevant variable(s) (besides strain) important to the underlying physics; examples include mean dislocation density, mean grain size, phase volume fraction, twinning density, crystallographic texture, etc. Therefore, researchers in the machining community have begun to develop physically inspired constitutive models [22, 30-35]. The motivation for this work is to expand on the capabilities of machining regime constitutive models by incorporating the evolution of state variables via a micro-mechanics framework. Admittedly, this approach is computationally more expensive. Nevertheless, both modeling strategies have their place in engineering; the simpler phenomenological models can be utilized by manufacturers for quickly determining tooling requirements and the more complex physically based models may be more appropriate for detailed functional surface design.

In this work we develop a composite dual phase internal state variable constitutive model for Ti-6Al-4V. The proposed model includes diffusion assisted grain boundary sliding (GBS) based

physics in addition to a traditional slip based plasticity model. Microstructure influence is captured via dislocation density and mean grain size internal state variables (ISVs). The dislocation density state evolves according to a physics based law that considers nucleation and annihilation as well as DRX. Grain refinement is driven by DRX which is modeled phenomenologically. The model is calibrated with uniaxial stress-strain data that spans quasi-static and dynamic rates across a wide range of temperatures. Machining simulations are performed in Thirdwave Systems' AdvantEdge finite element method (FEM) based software [36] and validated against machining experiments reported in the literature.

2. Material model development

2.1. Ti-6Al-4V metallurgy

Ti-6Al-4V is a dual phase $\alpha + \beta$ alloy with a microstructure that is very sensitive to prior processing conditions [37]. Alloying elements Al and V behave as α and β stabilizers, respectively. During cooling from above the β transus, alloying elements Al and V partially segregate into α and β phases, respectively. These alloying elements and any impurity elements such as O, C, and N provide the alloy with solid solution strengthening. Upon sufficiently slow cooling from above the β transus (1270 K) the bcc β transforms to hcp α via diffusion and forms a coarse lamellar microstructure. Air cooling can produce fine needle-like microstructures. Quenching from the $\alpha + \beta$ region can even yield hcp martensite (α') or orthorhombic martensite (α''). Mechanical working in the $\alpha + \beta$ region can result in breakup of the lamellar structures producing an equiaxed microstructure. The following study will focus on a microstructure composing of: (1) equiaxed primary α grains and (2) secondary α grains with a small volume fraction of β dispersed between secondary α .

2.2. Composite constitutive material model

The bulk Ti-6Al-4V response is modeled as the homogenized response of the individual $\alpha + \beta$ composite phases. The physics associated with each individual phase follows a similar approach to that developed by Picu and Majorell [38]. The α phase is assumed to deform due to dislocation based mechanisms as well as a GBS based mechanism. The dislocation deformation based flow stress is composed of thermal and athermal terms. The thermal portion of the α phase model contains two terms ($i=2$ in equation (1)) which represent contributions from Al solid solution strengthening and impurities (oxygen equivalent). The athermal terms represent Taylor hardening and Hall-Petch hardening which contain the influence of the microstructure ISVs (dislocation densities and mean grain diameter) on the flow stress. The GBS portion of the α model becomes dominant when the mean grain size is sufficiently small such that GBS can accommodate the imposed deformation rates at the corresponding temperature. The β phase response is modeled using an athermal dislocation drag term and a thermal stress component. The thermal component for the β phase contains only one term, which represents Peierl's forces associated with V solid solution strengthening.

2.3. Dislocation based deformation mechanisms

Metals with hcp lattice structures have long been observed to deform via a combination of dislocation slip and twinning [39]. There is evidence that twin boundaries behave as obstacles for propagating dislocations and have an effect on the strength and strain hardening characteristics

[39-42]. Conversely, a study on the role of twinning in single crystal Ti-Al alloys under quasi-static conditions found that twinning decreases with increasing Al content and increasing temperature [43]. Therefore, in the proposed model, deformation twinning is neglected. Instead, it is argued here that in machining the plastic strains in the primary shear zone are large and occur over very short time spans, thereby producing elevated temperatures that activate additional slip systems, which obviate the need for twinning based deformation.

The polycrystalline deformation response associated with dislocation slip processes can be categorized into thermal and athermal terms. Short range interactions, such as Peierel's forces, represent thermal barriers to dislocation motion and are quantified using a form introduced by Follansbee and Kocks [44],

$$\sigma = \sum_i \sigma_i \left\langle 1 - \left(kTQ_i^{-1} \log \left(\dot{\varepsilon}_{oi} / \dot{\varepsilon}^p \right) \right)^{\frac{1}{q_i}} \right\rangle^{\frac{1}{p_i}} \quad (1)$$

where σ is the equivalent uniaxial tensile stress, σ_i is the stress required to overcome the i^{th} obstacle at 0 K, k is the Boltzman constant, T is the temperature, Q_i is the activation energy of the i^{th} barrier, $\dot{\varepsilon}_{oi}$ is a constant, $\dot{\varepsilon}^p$ is the strain rate associated with dislocation slip based deformation, q_i and p_i are constants that statistically characterize the i^{th} obstacle energy profile. The summation is over all thermally activated obstacles which for an alloy may include multiple solid solution alloying elements or impurities; $\langle \rangle$ represent Macaulay brackets.

The athermal sources of strengthening are not thermally activated and represent interactions between dislocations and long range obstacles. In this work we consider Taylor hardening, Hall-Petch hardening and drag stress strengthening. Taylor hardening models the effects of dislocation-dislocation interactions and follows the following form [45],

$$\sigma = \alpha_p \mu b \sqrt{\rho} \quad (2)$$

where α_p is a parameter on the order of unity (1.04 [46]), μ is the shear modulus, b is the burgers vector magnitude ($3.47 \cdot 10^{-10} m$ calculated from ECAP processed Ti [46]) and ρ is the average dislocation density. Hall-Petch strengthening is attributed to a pile-up mechanism at grain boundaries and is modeled as,

$$\sigma = \alpha_{HP} \mu \sqrt{b/d} \quad (3)$$

where α_{HP} is a parameter on the order of unity (calculated as 0.413 [47]) and d is the mean grain size. Dislocation drag is believed to be a viscous mechanism that occurs at very high rates ($\sim 10^3 s^{-1}$ and above) where dislocations interact with lattice phonons thereby significantly increasing the strain rate sensitivity [48-50]. There is however another school of thought that attributes the apparent increase in strain rate sensitivity at high rates to a drastic increase in the dislocation nucleation rate [44, 51, 52]. Nevertheless, we chose to utilize the following

phenomenological form, introduced by Nemat-Nasser et al. [49], to account for an assumed dislocation drag phenomenon,

$$\sigma = \tau_d \left(1 - \exp(-\alpha_d \dot{\epsilon}^p)\right) \quad (4)$$

where τ_d and α_d are material constants. The total flow stress expression is a sum of all thermal and athermal terms,

$$\sigma = \sum_i \sigma_i \left\langle 1 - \left(kTQ_i^{-1} \log(\dot{\epsilon}_{oi}/\dot{\epsilon}^p) \right)^{\frac{1}{q_i}} \right\rangle^{\frac{1}{p_i}} + \alpha_\rho \mu b \sqrt{\rho} + \alpha_{HP} \mu \sqrt{b/d} + \tau_d \left(1 - \exp(-\alpha_d \dot{\epsilon}^p)\right) \quad (5)$$

2.4. Grain boundary sliding

Grain boundary sliding (GBS) is a deformation mechanism where rigid-body sliding displacements occur between adjacent grains [53, 54]. Materials deforming in the GBS regime may achieve tensile strain elongations up to several thousand percent and are said to undergo superplasticity [55-57]. For a polycrystalline material, the schematic shown in Figure 1 illustrates the relationships between the imposed deformation rate, mean grain size, and the active deformation mechanism; not shown is the dependence on temperature. Fine grained materials facilitate superplastic deformation at lower temperatures as the refined grain structure promotes additional GBS [58]. Experimental studies of superplasticity and GBS however are limited to strain rates below 10^0 - $10^{-1} s^{-1}$ and therefore it is unclear if GBS is active during machining. Furthermore, studies on nanocrystalline microstructures at elevated temperatures are experimentally challenging as these microstructures are usually thermally unstable [59] and grain growth alters the initial microstructure [60]. Molecular dynamics (MD) studies however provide physical insight regarding the deformation mechanisms active during machining e.g. nanocrystalline grain structures deforming at elevated temperatures and high rates. MD studies investigating deformation characteristics in the nanocrystalline range have shown that at elevated temperatures (1200K) and high deformation rates ($\sim 10^7 s^{-1}$) both GBS and Coble creep can contribute significantly to bulk deformation [61, 62]. As the mean grain size decreases, grain boundary dependent deformation mechanisms become active as the intercrystalline region volume fraction increases [20, 63]. Comprehensive reviews of nanocrystalline materials and their properties have been published by Meyers [19], Suryanarayana [21], and Gleiter [20].

Figure 1. Schematic illustrating grain size dependent GBS-slip competition. Reproduced from [56].

The physics associated with GBS deformation is incorporated into our model using a formulation developed by Ashby and Verrall [54]. This model considers a diffusion assisted GBS mechanism where diffusive mass transport, via the lattice and grain boundaries, facilitates the transport of mass such that sliding grains always remain geometrically compatible with adjacent grains. It is critical to make the distinction that this model only requires mass transport to facilitate GBS and hence requires much less mass transport than traditional diffusion based creep processes. The final form of the equation developed by Ashby and Verrall is,

$$\dot{\epsilon}^{gbs} = 100 \frac{\Omega}{kTd^2} (\sigma - \bar{\sigma}^{gbs}) D_v \left(1 + \frac{3.3\delta}{d} \frac{D_B}{D_v} \right) \quad (6)$$

where d is the mean grain size, Ω is the atomic volume ($1.76 \cdot 10^{-29} m^{-3}$ [64]), $\bar{\sigma}^{gbs}$ the threshold stress necessary for GBS, D_v is the lattice diffusion coefficient, D_B is the grain boundary diffusion coefficient and δ is the grain boundary thickness (assumed to be $2b$). In the limit where the grain size becomes extremely refined, this expression approaches the familiar Coble creep expression [65]. The diffusion parameters introduce additional temperature dependency via the following Arrhenius equation,

$$D_i = D_{o,i} \exp(-Q_i/kT) \quad (7)$$

The subscripts in this expression correspond to diffusion along boundaries ($i = B$) and the lattice ($i = v$). There are a number of papers that provide values for the activation energy and pre-exponential for self-diffusion and grain boundary diffusion in Ti-6Al-4V, α , and β [64, 66-70].

The following values were taken from the ranges provided in these works: $D_v = 10^{-9} m^2 s^{-1}$, $D_B = 8 \cdot 10^{-5} m^2 s^{-1}$, $Q_v = 260 kJ \cdot mol^{-1}$, and $Q_B = 80 kJ \cdot mol^{-1}$. Note that the selected boundary activation energy is 20% lower than the lower limit for grain boundary self-diffusion in α -Ti (

$97 \text{ kJ} \cdot \text{mol}^{-1}$). We justify this by noting that it has been shown that the presence of non-equilibrium grain boundaries in Al and Mg alloys have been observed to accelerate diffusion rates by an order of magnitude [71, 72]. Horvath and Gleiter [73] showed that in nanocrystalline Cu produced via vapor condensation, the apparent activation energy decreased by 40% relative to coarse grain Cu. Since the structures produced by DRX are not expected to behave like the coarse grain parent material, we are utilizing a slightly lower activation energy to forgo introducing any additional complexity to the model. This assumed value will of course affect machining simulations results. An activation energy that is too high will totally suppress GBS, eliminating softening and therefore potentially suppressing chip segmentation. Likewise, an activation energy that is too low will facilitate GBS even at large grain size values, and therefore the softening mechanism will be always active. Therefore, in lieu of additional experimental nanocrystalline diffusion data or a more complex physical model, we use an assumed value that yields reasonable results.

The threshold stress, $\bar{\sigma}^{gbs}$, characterizes the necessary applied mechanical work needed to overcome an energetic barrier associated with temporarily creating grain boundary surfaces during the intermediate sliding state. This interpretation represents a lower bound for the true threshold stress as other mechanisms may also inhibit GBS. For our model, a threshold stress developed by Hahn and Padmanabhan is used [74]. In addition to the grain boundary surface energy, their formulation also accounts for the viscous mechanical work associated with grain surfaces shearing relative to one another and is given by:

$$\bar{\sigma}^{gbs} = \left(\frac{2\mu\Gamma\Delta A / A}{\alpha_f (NA)^{1/2}} \right)^{1/2} \quad (8)$$

Here, Γ is the specific grain boundary energy, ΔA is the increase in grain boundary surface area at the intermediate configuration, A is the total grain boundary surface area, N is the number of grains participating in a sliding event, and α_f is a shape factor. The specific grain boundary energy values reported by Ashby and Verral [54] correspond to $0.1 \text{ J} \cdot \text{m}^{-2}$ and $0.25 \text{ J} \cdot \text{m}^{-2}$ for relatively coarse grain zinc and lead, respectively. Note that there is evidence that this energy value may be larger for nanocrystalline materials relative to their coarse grain counterparts; a detailed review of both arguments can be found in [21]. For the implementation of this model, a constant value of $0.1 \text{ J} \cdot \text{m}^{-2}$ was used. Expressions for both ΔA and A can be found in Hahn and Padmanabhan's [74] original work as functions of the grain size and grain boundary width $\mathcal{S}$. The number of grains participating in a sliding event can be expressed as,

$$N = (d_v/d)^3 \quad (9)$$

where d_v represents the diameter of an invariant spherical volume element. For the implementation of this model we have chosen $d_v = 10 \mu\text{m}$ such that this number shall never be less than unity. Note that the model is sensitive to this selection but will be accounted for later by via the shape factor α_f ; the two could be lumped together, however, we chose to retain some of the physical meaning introduced by Hahn and Padmanabhan [74].

2.5. Microstructure state variable evolution

The influence of microstructure on deformation is introduced by treating the average grain size and dislocation density parameters as evolving ISVs. These ISVs provide a physical basis for the evolution of flow stress. During deformation, the statistically stored dislocation density evolves due to nucleation of additional dislocations at lattice defects, annihilation due to thermally activated dynamic recovery mechanisms, and segregation of dislocations into cellular structures. At high dislocation densities, these cell walls form to reduce the stored energy of the system [75]. In our development of the model we have chosen to decouple the total dislocation density into cell-interior (ρ_c) and cell-wall (ρ_w) densities [76]:

$$\rho = \rho_c + \rho_w \quad (10)$$

The cell interior dislocation density, ρ_c , is the dependent variable used in the Taylor hardening expression (equation (2)) and the mean grain size, d , is utilized in the Hall-Petch expression (equation (3)). DRX is the driving force associated with grain refinement which has been observed to induce microstructure evolution during severe plastic deformation (SPD) [15, 16, 77]. Continuous DRX first requires dislocation cell structure formation followed by sub-cell lattice rotations, which produce a severely refined high angle grain boundary structure [77]. Note that we do not use the cell wall dislocation density, ρ_w , to describe the flow stress as it is these cell wall dislocations that physically contribute to the formation of the grain boundaries.

The cell-interior evolution follows a form developed by Estrin and Mecking [78] with an additional term to account for cell-wall dislocation evolution,

$$\frac{\partial \rho_c}{\partial \bar{\epsilon}} = A\sqrt{\rho_c} - B\rho_c - \frac{\partial \rho_w}{\partial \bar{\epsilon}} \quad (11)$$

where A and B represent nucleation and annihilation terms. The evolution equations are with respect to the accumulated slip strain, $\bar{\epsilon} = \int \dot{\epsilon}^p dt$. It is critical to introduce this distinction as these mechanisms are driven solely by slip based inelastic deformation mechanism i.e. GBS does not contribute to ISV evolution. The cell-wall density evolution is influenced by the grain size evolution as the grain boundary surface area ($\propto d^{-2}$) is assumed to be composed of cell-wall dislocations. In our model no distinction is made between low angle and high angle grain boundaries; others have included this distinction [79]. A differential form of the expression presented by Liu et al. [34] is adopted here,

$$\left. \frac{\partial \rho_w}{\partial \bar{\epsilon}} \right|_{DRX} = -\frac{2K}{d^2} \frac{\partial d}{\partial \bar{\epsilon}} \quad (12)$$

where K is a scaling parameter. Calibration of K is difficult as a value that is too large can numerically drive the cell interior dislocation density to be negative. To circumvent this problem, an expression for K was developed by imposing an additional constraint; K is selected such that, for an assumed constant rate-temperature condition, all newly nucleated dislocations will eventually be driven from the cell interior to the cell walls.

$$\lim_{d_n \rightarrow d_f}(\rho_w) = \rho_{c,ss} - \rho_{c,o} = (A/B)^2 - \rho_{c,o} \quad (13)$$

where $\rho_{c,o}$ is the initial cell interior dislocation density ($10^{10}m^{-2}$ is considered the annealed state's initial density), and $\rho_{c,ss}$ is the steady state cell interior dislocation density. The steady state cell interior dislocation density refers to the dislocation density saturation value in the cell interior if DRX were not present. This saturation value corresponds to equilibrium between nucleation and annihilation processes (recovery). For constant rate-temperature conditions, and in the absence of DRX, $\rho_{c,ss}$ can be found from equation (11) to be $(A/B)^2$. The integral form of equation (12) is used to develop an expression for K as follows,

$$\int_{\rho_{w,n}}^{\rho_{ss}} \partial \rho_w = \int_{d_n}^{d_f} \frac{\partial \rho_w}{\partial \bar{\varepsilon}} \frac{\partial \bar{\varepsilon}}{\partial D} dD = \int_{d_n}^{d_f} -\frac{2K}{D^2} dD \quad (14)$$

$$K = \frac{1}{2} \left\langle \left(\frac{A}{B} \right)^2 - \rho_{c,o} - \rho_{w,n} \right\rangle \left(\frac{1}{d_f} - \frac{1}{d_n} \right)^{-1} \quad (15)$$

where d_f is the final recrystallized grain size and d_n refers to the grain size at time t_n . This expression implicitly accounts for rate, temperature, and ISV history dependencies. To accommodate temporal changes in the imposed rate and temperature, K is recalculated (explicitly) at each integration time step. The final grain size represents the grain size that would be achieved with sufficient straining at constant rate and temperature.

It is likewise assumed that for constant rate-temperature conditions there exists a dislocation cell diameter that is reached after sufficient straining. During continuous DRX the lattice within dislocation cells continuously rotates relative to the adjacent cells forming high angle grain boundaries. Experimentally the dislocation cell diameter was shown by Holt to have the following dependence [75]:

$$d_{cell} \approx K_c / \sqrt{\rho} \quad (16)$$

K_c is a scaling parameter found experimentally to be 10-20 in [80] and 10 in [81]. Ding and Shin developed a dislocation dynamics based constitutive model for machining applications and utilized a value of 10 [33]. These authors' approach use equation (16) to explicitly predict the mean grain size as a function of the instantaneous values of the two evolving dislocation density state variables. Our modeling approach is physically based on the relationship in equation (16) yet contains nuanced differences. In our approach, we have two evolving dislocation density state variables as well as a third evolving mean grain size state variable. Our methodology assumes that grain refinement doesn't occur instantaneously but rather requires time, which is associated with cell lattice rotation; low angle grain boundaries form by rotating dislocation cell lattices, which, with sufficient deformation, eventually transform to high angle grain boundaries. We do not explicitly account for grain boundary misorientation, but a more rigorous modeling treatment of this phenomena may be found in the work of Gourdet and Montheillet [79]. The

evolution law for the mean grain size follows a phenomenological law where the mean grain size is driven toward d_f ,

$$\frac{\partial d}{\partial \bar{\varepsilon}} = C \langle d - d_f \rangle^u \bar{\varepsilon} \exp\left(-(\bar{\varepsilon} - \varepsilon_r)^2\right) \quad (17)$$

where u and ε_r are fitting parameters. The grain diameter term describes a refinement driving force between the current grain size and the final grain size. The accumulated slip strain dependent term represents a driving force induced by slip based inelastic straining. The final grain size follows the form of equation (16); $d_f \approx K_c / \sqrt{\rho_{c,ss}}$. Note that this is an explicit function of the steady state cell interior dislocation density, which has a known form. This modeling formulation implicitly assumes that neither the current grain size (d_n) nor final realizable grain size correspond to the instantaneous values of dislocation densities. The instantaneous value of the grain size is solved for by integration of equation (17). Using a value of 10 for K_c we found that the final grain size in the sheared bands are fairly large (1-10 μm). This is in part because the mean grain diameter ISV does not evolve quickly enough to reach the final realizable grain size. A value of 0.1 was used to give reasonable results in the 100-500nm range. It is also important to note that in our formulation the final grain size is dependent on the steady state dislocation density $\rho_{c,ss} = A/B$. The calibration of the dislocation evolution laws is done using experimental flow stress data (see section 2.7) and therefore the grain refinement model is subject to the non-unique hardening evolution fitting parameters. C in equation (17) is solved for by assuming that, in the limit, the grain size asymptotically approaches the final recrystallized grain size:

$$\int_{d_n}^{d_f} \frac{\partial d}{\langle d - d_f \rangle^u} = C \int_{\bar{\varepsilon}_n}^{\infty} \bar{\varepsilon} \exp\left(-(\bar{\varepsilon} - \varepsilon_r)^2\right) \partial \bar{\varepsilon} \quad (18)$$

The form of the strain dependent portion of equation (17) was intentionally chosen such that the integral on the right hand side of equation (18) can be evaluated analytically and remains bounded. For the expression in equation (17) to be physically meaningful $u > 0$ and for the integrand on the left hand side of equation (18) to remain bounded, $u < 1$. Given these constraints the integrals can be evaluated analytically and the following expression for C can be solved for,

$$C = -\frac{2}{-u+1} \frac{\langle d_n - d_f \rangle^{-u+1}}{\sqrt{\pi} \varepsilon_r - \sqrt{\pi} \varepsilon_r \text{erf}(\bar{\varepsilon}_n - \varepsilon_r) + \exp(-\bar{\varepsilon}_n^2 - \varepsilon_r^2 + 2\bar{\varepsilon}_n \varepsilon_r)} \quad (19)$$

Much like the derivation for K , C implicitly contains rate, temperature, and history dependency. Analogous to K , the constant C is revaluated (explicitly) at each time integration point to account for the evolution of the thermomechanical process history. The benefit of this approach is that numerically DRX may be automatically halted if a material point reaches a thermomechanical state where $d_n < d_f$; i.e. rates suddenly slow or temperatures increase significantly as a material

point exists the primary deformation zone. The behavior of the model and its dependency on (u, ε_r) can be seen in Figure 2.

Figure 2. Grain refinement model behavior with $d_f = 50 \text{ nm}$ and $d_o = 10 \text{ } \mu\text{m}$.

An attempt at calibrating the remaining parameters (u, ε_r) to data in the literature from various large strain deformation processes (e.g. equal channel angular pressing, high pressure torsion, multi-pass rolling, machining) was made; however uncertainties in the associated imposed rates and strains yielded insufficient confidence in the compiled dataset. Studies have shown that significant refinement can occur with as little straining as ~ 1 [82], therefore u and ε_r were chosen to be 0.95 and 0.05, respectively. These parameters were not optimized in any way, however it is important to note that the model is sensitive to the choice of these parameters. For example, choosing a u that is too small or ε_r that is too large would require extremely large strains to drive DRX. Hence DRX, under some machining conditions, would effectively be suppressed.

2.6. Thermal and elastic properties

The machining problem is complex and includes physics that requires the solution of a coupled heat transfer problem. Therefore it is necessary to specify thermal properties as well as temperature dependent constitutive properties. The following thermal properties were used for all simulations; thermal conductivity of $6.7 \text{ W}\cdot\text{m}^{-1}\cdot\text{C}^{-1}$ [9], heat capacity of $520 \text{ J}\cdot\text{kg}^{-1}\cdot\text{C}^{-1}$ [83], and a coefficient of thermal expansion of $9\cdot 10^{-6}$ [84]. A density of $4430 \text{ kg}\cdot\text{m}^{-3}$ [28] was used. The temperature dependency of the properties was neglected. Poisson's ratio, ν , was taken as 0.3. For simplicity the CP-Ti α modulus was used for both α and β phases [85]:

$$\mu = 43.6 \left[1 - \frac{1.2(T - 300)}{1923} \right] \text{ GPa} \quad (19)$$

2.7. Model Calibration

Model calibration was performed using experimental uniaxial data collected from the literature. Special care was taken to only consider experiments performed on similar microstructures of similar morphology. A calibration methodology similar to that described by Picu and Majorell was implemented [38]; first the thermal stress components of the yield surface are calibrated followed by the hardening equations. A standard non-linear regression technique was utilized with an objective function defined by the total error associated with stress prediction. A linear law of mixtures was used to calculate the aggregate uniaxial homogenized Ti-6Al-4V response. For these uniaxial calculations the volume fraction of each respective phase is assumed to follow equilibrium kinetics (as samples were allowed to reach equilibrium) and therefore varies with temperature [38]:

$$f_{\beta} = (T/1270)^{10} \quad (20)$$

First the β phase model was calibrated to Ti-6Al-4V experiments performed above the β transus [86-92]. A dislocation drag term, equation (4), was utilized to capture the observed increase in strain rate sensitivity, as illustrated in Figure 3.

Figure 3. β -phase initial yield at temperatures above transus.

The β thermal stress expression, equation (1), required only one term in the sum; $\sigma_{\beta 0} = 1000 \text{ MPa}$, $p_{\beta} = 0.3$, $q_{\beta} = 1.3$, $Q_{\beta} = 500 \text{ kJ} \cdot \text{mol}^{-1}$, $\dot{\epsilon}_{o\beta} = 3.61 \cdot 10^{10} \text{ s}^{-1}$. The drag stress, equation (4), was fit with $\tau_d = 225 \text{ MPa}$ and $\alpha_d = 10^{-3} \text{ s}$. It is clear from the available data that at high rates there is a significant increase in strain rate sensitivity that cannot be captured with a single thermal stress term.

The α -phase thermal stress model, equation (1), can be fit assuming constant structure at incipient yielding; evolution of the microstructure can only be driven by inelastic deformation and therefore it is possible to decouple these equations. As Ti-6Al-4V and CP-Ti have similar

impurity concentrations the oxygen-equivalent thermal stress expression was fit to experimental data available for commercial purity titanium (CP-Ti) [50, 93, 94]. This physics corresponds to the first term in the summation in equation (1). The best fit was obtained with the following values: $\sigma_{\alpha 0} = 853.6 \text{ MPa}$, $p_{\alpha 0} = 0.503$, $q_{\alpha 0} = 1.591$, $Q_{\alpha 0} = 422 \text{ kJ} \cdot \text{mol}^{-1}$, $\dot{\epsilon}_{\alpha \alpha 0} = 8.91 \cdot 10^{12} \text{ s}^{-1}$. The remaining Al solid solution strengthening term, the second term in the summation in equation (1), was calibrated using Ti-6Al-4V data across a range of temperatures and rates [1, 86, 87, 90, 91, 95-101]. As described by Picu and Majorell, a temperature dependent activation energy is necessary in this term for capturing the apparent discontinuity in yield stress observed around 800 K [38]. This discontinuity is unique to the alloyed α phase as neither the β phase nor CP-Ti exhibit this behavior. The expression used has the following form:

$$Q_{\alpha 1} = \left(\frac{1}{Q_{Al,1}^2} + \frac{1}{Q_{Al,2}^2} \left\langle 1 - \frac{T_c}{T} \right\rangle^2 \right)^{-1/2} \quad (21)$$

The best fit parameters are: $\sigma_{\alpha 1} = 955.4 \text{ MPa}$, $p_{\alpha 1} = 1.0$, $q_{\alpha 1} = 1.695$, $\dot{\epsilon}_{\alpha \alpha 1} = 10^8 \text{ s}^{-1}$, $Q_{Al,1} = 303.8 \text{ kJ} \cdot \text{mol}^{-1}$, $Q_{Al,2} = 102 \text{ kJ} \cdot \text{mol}^{-1}$, and $T_c = 822 \text{ K}$. No drag stress was required in the α portion of the model. The calibrated Ti-6Al-4V yield surface model is shown in Figure 4.

Figure 4. Initial yield stress calibration results for aggregate Ti-6Al-4V response.

The hardening portion of the model was calibrated in a similar fashion using a total of 100 uniaxial loading experimental data sets gathered from the literature [86, 87, 91, 98-100, 102-105]. During calibration, we assumed that all hardening comes from Taylor hardening and therefore only from dislocation evolution; grain refinement and DRX are insignificant in these experiments. This is justifiable since strains in the dynamic tests used in this study are small and the Zener-Holloman parameter is relatively low in the large strain compression experiments. We assume that no GBS occurs in any of the experiments in the calibration set as the grains are assumed to remain large. Using a shape factor of unity in equation (8) predicts threshold stresses

on the order of 30 MPa for a coarse grain microstructure (10 μ m) at room temperature. This low value of threshold value artificially softens the simulated flow stress, particularly at quasi-static high temperature conditions. Our strategy was to select the largest shape factor possible that eliminates the influence of GBS in all of the uniaxial flow stress predictions. This shape factor value ($\alpha_f = 6 \cdot 10^{-4}$) is implicitly tied to our selection of the volume element ($d_v = 10 \mu\text{m}$); in fact, the two can be lumped together in Equation (8) but in doing so physical meaning is lost.

The remaining unknown constants correspond to terms in the cell-interior dislocation density evolution, equation (11). The nucleation term, A , is commonly assumed to be constant (calibrated to $1.18 \cdot 10^8$). The temperature-rate dependency associated with dynamic recovery is captured through B with the following expression,

$$B = \left(\frac{\dot{\varepsilon}_d}{\dot{\varepsilon}^\rho} \right)^n \exp \left(-\frac{Q_d}{kT} \right) \quad (22)$$

which, with $n=1$, is identical in form to the work of Klepaczko and Chiem [106]. The expression captures the thermally activated nature of dynamic recovery through an Arrhenius form. $\dot{\varepsilon}_d$, n , and Q_d are calibration parameters. $\dot{\varepsilon}^\rho$ is the inelastic slip strain rate. In the optimization routine, high rate data ($> 10^3 \text{ s}^{-1}$) was weighted more heavily during regression as the objective function is otherwise biased by the larger set of slow and moderate rate data. The best-fit was achieved with $n = 0.169$, $Q_d = 8.88 \text{ kJ} \cdot \text{mol}^{-1}$, and $\dot{\varepsilon}_d = 5.1 \cdot 10^{15} \text{ s}^{-1}$. A visualization of the calibrated results is shown in Figure 5. Note that due to the limitations of dynamic testing techniques, high rate experiments cannot impose strains beyond ~ 0.3 .

Figure 5. Stress prediction results at various strains, temperatures, and strain rates following calibration of the hardening parameters. Note that the tolerance bands in each figure represent a 50% deviation.

A summary of all model parameters utilized in this work can be found in Table 1 of the Appendix.

3. Continuum update framework

The material constitutive model presented in Section 2 is implemented as a total deformation material user-defined subroutine for use within the commercially available FEM-based machining software AdvantEdge [36]. The AdvantEdge engine passes the subroutine the previous step's (t_n) total deformation gradient ($\mathbf{F}_n$), the relative deformation gradient for the update ($\mathbf{f}_{n+1}$), the previous homogenized Cauchy stress ($\mathbf{T}_n$), the time step (Δt), and all solution dependent variables (SDVs). SDVs include microstructure sensitive ISVs as well as individual phase continuum variables ($\mathbf{F}_{n,\alpha}$, $\mathbf{F}_{n,\beta}$, $\mathbf{T}_{n,\alpha}$, $\mathbf{T}_{n,\beta}$, etc.). The subroutine must return the updated homogenized Cauchy stress and SDVs.

3.1. Large deformation kinematics

A large deformation continuum kinematic framework is needed to perform the necessary subroutine updates. An implementation similar to those found in [12, 107, 108] is utilized. Thermal dilatation is handled internally by the AdvantEdge engine and is accounted for in the relative deformation gradient $\mathbf{f}_{n+1}$. Neglecting thermally imposed deformations, the total deformation gradient at the end of time step $n+1$ can be decomposed multiplicatively into elastic and inelastic components:

$$\mathbf{F}_{n+1} = \mathbf{F}_{n+1}^e \mathbf{F}_{n+1}^p \quad (23)$$

A logarithmic strain measure was chosen for this study:

$$\bar{\mathbf{E}} = \frac{1}{2} \ln(\mathbf{F}^T \mathbf{F}) \quad (24)$$

Assuming isotropic behavior (the spin component of the velocity gradient ($skw\mathbf{L}^p$) is identically zero) a forward Euler time integration procedure yields the following updates,

$$\mathbf{F}_{n+1}^p = \exp(\Delta t \dot{\boldsymbol{\varepsilon}}_{n+1}^{in} \cdot \mathbf{n}_{n+1}) \cdot \mathbf{F}_n^p \quad (25)$$

$$\mathbf{F}_{n+1}^e = \exp(-\Delta t \dot{\boldsymbol{\varepsilon}}_{n+1}^{in}) \cdot \mathbf{F}_{n+1} \cdot \mathbf{F}_n^{p-1} \cdot \exp(-\mathbf{n}_{n+1}) \quad (26)$$

where $\dot{\boldsymbol{\varepsilon}}^{in}$ is the total inelastic strain rate, $\dot{\boldsymbol{\varepsilon}}_{n+1}^{in} = \dot{\boldsymbol{\varepsilon}}_{n+1}^p + \dot{\boldsymbol{\varepsilon}}_{n+1}^{gbs}$, and the tensor quantity $\mathbf{n}$ describes the direction of inelastic flow,

$$\mathbf{n} = \bar{\mathbf{T}}' / \|\bar{\mathbf{T}}'\| \quad (27)$$

where $\bar{\mathbf{T}}'$ is a deviatoric stress measure conjugate to the logarithmic strain.

3.2. Time integration scheme

When discretized, the proposed system of differential equations (equations (5),(6),(11),(12), and (17)) are numerically stiff. To ensure numerical stability during integration, an implicit forward Euler scheme is adopted. In this scheme stress updates are performed through the deviatoric isotropic elasticity relation,

$$\bar{\mathbf{T}}'_{n+1} = 2\mu\bar{\mathbf{E}}'^e_{n+1} \quad (28)$$

where μ is the shear modulus and $\bar{\mathbf{E}}'^e_{n+1}$ is the deviatoric elastic logarithmic strain. Using arguments from [107] equation (28) can be expressed in an equivalent scalar form,

$$\sigma_{n+1} = \sigma_{n+1}^* - \sqrt{6}\mu\Delta t \dot{\epsilon}_{n+1}^{in} \quad (29)$$

where $\sigma_{n+1} = \sqrt{\frac{3}{2}\bar{T}'_{n+1,ij}\bar{T}'_{n+1,ij}}$ and σ_{n+1}^* is the analogous elastic predictor. The scalar stress measures represent equivalent uniaxial tensile stresses. After computation of the elastic stress predictor, the stress tensor can be updated by,

$$\bar{\mathbf{T}}'_{n+1} = \eta_{n+1} \bar{\mathbf{T}}'^*_{n+1} \quad (30)$$

$$\eta_{n+1} = \sigma_{n+1} / \sigma_{n+1}^* \quad (31)$$

where η is the radial return factor. Equation (29) coupled with the discretized implicit forms of equations (5), (6), and (11) forms a system of simultaneous nonlinear equations:

$$\begin{aligned} \sigma_{n+1}^* - \sqrt{6}\mu\Delta t (\dot{\epsilon}_{n+1}^\rho + \dot{\epsilon}_{n+1}^{gbs}) &= \alpha_{HP}\mu\sqrt{b/d_{n+1}} + \alpha_\rho\mu b\sqrt{\rho_{c,n+1}} + \tau_d \left(1 - \exp(-\alpha_d \dot{\epsilon}_{n+1}^\rho)\right) \\ &+ \sum_i \sigma_i \left\langle 1 - \left(kTQ_i^{-1} \log\left(\frac{\dot{\epsilon}_{oi}}{\dot{\epsilon}_{n+1}^\rho}\right)\right)^{q_i} \right\rangle^{\frac{1}{p_i}} \end{aligned} \quad (32)$$

$$\sigma_{n+1}^* - \sqrt{6}\mu\Delta t (\dot{\epsilon}_{n+1}^\rho + \dot{\epsilon}_{n+1}^{gbs}) = \frac{\dot{\epsilon}_{n+1}^{gbs} kT d_{n+1}^2}{100\Omega D_v \left(1 + \frac{3.3\delta}{d_{n+1}} \frac{D_B}{D_v}\right)} + \bar{\sigma}_{n+1}^{gbs}(d_{n+1}, T) \quad (33)$$

$$\rho_{c,n+1} = \rho_{c,n} + \Delta t \cdot \dot{\epsilon}_{n+1}^\rho \left. \frac{\partial \rho_c}{\partial \bar{\epsilon}} \right|_{n+1} \quad (34)$$

These equations are solved simultaneously for $\dot{\epsilon}_{n+1}^\rho$, $\dot{\epsilon}_{n+1}^{gbs}$ and $\rho_{c,n+1}$ using a Newton-Raphson (NR) solver. Convergence is met when each of the residuals corresponding to equations (32)-(34) falls below 1 MPa, 1 MPa, and $10^7 m^{-2}$, respectively. Due to the simplified nature of the β portion of the model, only equation (32) needs to be solved when performing the β phase

updates. As equation (32) contains highly nonlinear $\log(\dot{\epsilon}_{n+1}^\rho)$ terms convergence using a linear expansion of the residuals in $\dot{\epsilon}_{n+1}^\rho$ was found to be extremely slow. A log-linear expansion of the residuals in $\dot{\epsilon}_{n+1}^\rho$ was found to greatly accelerate convergence by allowing trial solutions of $\dot{\epsilon}_{n+1}^\rho$ to traverse values by orders of magnitude. This alternate formulation reduced the number of iterations for achieving convergence by roughly an order of magnitude. Additionally this expansion maintains $\dot{\epsilon}_{n+1}^\rho > 0$ during solving which alleviates numerical issues.

Following convergence of the NR-solver all relevant quantities are known and the continuum updates presented in section 3.1 can be performed. For a detailed algorithmic procedure corresponding to the continuum updates see [107, 108].

3.3. Homogenization

In this work we have utilized a Taylor criteria [109] for homogenization of the Ti-6Al-4V response. This assumption requires that the deformation gradient in both α and β phases are equal to the imposed aggregate deformation gradient:

$$\mathbf{F}_i = \mathbf{F} \quad \text{for } i = \alpha, \beta \quad (35)$$

The homogenized stress is then computed using a linear rule of mixtures in the reference configuration e.g. in terms of the first Piola-Kirchoff stress:

$$\mathbf{P} = f_\alpha \mathbf{P}_\alpha + (1 - f_\alpha) \mathbf{P}_\beta \quad (36)$$

In all machining simulations the phase fractions of α and β are assumed to remain constant. Our argument is that bulk lattice diffusion is necessary to allow for a $\alpha \leftrightarrow \beta$ transformation and that there is simply not enough time for this occur to during machining.

3.4. Solution dependent variable transfer

AdvantEdge automatically implements a continuous adaptive remeshing routine which enables modeling of unconstrained inelastic deformation processes within a Lagrangian framework. To maintain simulation stability and accuracy special care is required in the transfer of ISVs and other SVDs ($\mathbf{F}$, $\mathbf{T}$). This is particularly important following remeshing. As an example consider that element-wise transfer of the plastic deformation gradient, $\mathbf{F}^p$, fails to preserve plastic incompressibility i.e. $\det \mathbf{F}^p \neq 1$. The transfer operators used in our study were developed and presented in greater detail in [110].

The transfer operator for updating the deviatoric conjugate stress tensor, $\bar{\mathbf{T}}'_n$, assumes a scalar multiple of the transferred deviatoric conjugate stress, $\hat{\mathbf{T}}'_n$,

$$\bar{\mathbf{T}}'_n = \theta \hat{\mathbf{T}}'_n \quad (37)$$

where the transferred deviatoric conjugate stress is not explicitly transferred but rather is calculated via the strain (24) and elasticity (28) relations from the explicitly transferred elastic deformation gradient. The equivalent scalar relation is:

$$\theta = \sigma_n / \hat{\sigma}_n \quad (38)$$

The numerator, σ_n , is saved as a SDV at the end of each time step for each individual phase. The denominator is computed from $\sqrt{\frac{3}{2} \hat{\mathbf{T}}'_{n,ij} \hat{\mathbf{T}}'_{n,ij}}$. The scalar value θ may be determined from equation (38) and is used to update $\bar{\mathbf{T}}'_n$ in equation (37). The volumetric portion of the conjugate stress measure is unchanged due to this operation and hence the complete Cauchy stress can be recovered. Following this operation, the elastic and inelastic deformation gradients need to be updated to ensure compatibility of the elasticity equations ((24) and (28)) and the multiplicative decomposition (23). Without this operation interpolation errors introduced in the transferred deformation gradients propagate into the Cauchy stress. Following remeshing these errors can artificially generate stresses on the order of 10 *GPa* which yields the subroutine unstable.

4. Machining Validation

The proposed constitutive model was validated against a variety of Ti-6Al-4V data found in the literature: cutting forces [11, 111], serration frequency [8], and maximum tool temperature [112]. The initial assumed grain size corresponding to α -grains was $10\mu\text{m}$. Numerical simulations were performed to exactly match the process conditions reported in these studies; force results and all process parameters are shown in Figure 6 and Figure 7. These experimental studies utilized uncoated carbide tools with sharp cutting edge radii ($\sim 5\mu\text{m}$). Numerical simulations were performed using uncoated cemented-carbide tool with a $5\mu\text{m}$ edge radius. Coulomb friction coefficients were estimated using Merchant's model from each individual experiment and used as input to the corresponding simulations, see Table 1 in the Appendix. Validation simulations corresponding to data from Cotterell and Byrne [111] used a constant value of 0.50 across all simulations as this value is within the bounds of experimental error seen in Figure 7. We purposefully chose a simple friction model as our focus in this paper is on the constitutive behavior. Fundamentally, this simplification neglects complex tribological interactions between the chip and rake face [113].

Chip segmentation frequency validation is shown in Figure 8. These segmentation frequency experiments were performed using a planing-type process at a feed of 0.12 mm and a rake angle of $\alpha = 0^\circ$. Our simulated results are slightly below 0.12 mm however, note that these authors suggest that the chip segmentation frequency data is only weakly dependent on the feed. Additionally, note that the physical experiments were performed with a rake angle of $\alpha = 0^\circ$ whereas the numerical simulations correspond to 5° and 6.5° . Here, we are assuming that the difference in rake angles is sufficiently small so as to not significantly affect the chip segmentation frequency.

Tool temperature validation is shown in Figure 9. The study referenced focused on quantification of the uncertainties associated with in-situ temperature measurements of the tool. Their work concluded that at 500°C the measurement uncertainty is 15% and at 1000°C it is 8%;

the error bars shown in Figure 9 reflect these values. Estimation of the maximum tool temperature in cutting via simulation is difficult because the tool temperatures generally require much longer times to reach steady state relative to the cutting forces. Experimentally, the steady state temperatures are conservatively estimated to reach steady state after 5 seconds [112]; performing simulations of this length proved to be computationally intractable. Therefore, we employed a strategy proposed in [114] where, by numerically decreasing the tool material's heat capacity, the steady state temperature in the tool can be achieved much faster. For the four validation test cases considered, the tool was modeled to have a thermal conductivity of $80 \text{ W}\cdot\text{m}^{-1}\cdot\text{C}^{-1}$, heat capacity of $10 \text{ J}\cdot\text{kg}^{-1}\cdot\text{C}^{-1}$ and a density of $15,000 \text{ kg}\cdot\text{m}^{-3}$ [114]. The results in Figure 9 show that the absolute tool temperature prediction errors range from 2.3% to 9.5% at the lower cutting speed (40 m/min) and from 14.9% to 21.8% at the higher cutting speed (80 m/min).

Figure 6. Force validation using experimental data from Sima and Özel [11].

Figure 7. Force validation using experimental data from Cotterell and Byrne [111].

Figure 8. Chip segmentation frequency validation using experimental data from Molinari et al. [8].

Figure 9. Maximum tool temperature predictions using experimental data from Soler et al. [112].

Machining constitutive models may also be validated using peak-valley measurements of segmented chips (or equivalently the segmentation intensity ratio [10, 115]) in Ti and Ti-alloys [11]. Morphological chip features amongst our collected dataset are limited to that found in [11]. For a cutting speed of $121.9 \text{ m} \cdot \text{min}^{-1}$, feed of $0.1270 \text{ mm} \cdot \text{rev}^{-1}$, and an uncoated WC tool with a 5° rake, the reported experimental peak and valley chip thickness values in [11] are 0.230 mm and 0.156 mm , respectively. Our simulated predictions are 0.165 mm and 0.130 mm , respectively. The simulated values in that paper, corresponding to a modified Johnson-Cook model, are 0.171 mm and 0.135 mm .

5. Results and discussion

At high cutting speeds the force predictions are very accurate across all the tested conditions. However, at the lowest speed cutting forces are over-predicted by 25% at $f = 0.1 \text{ mm}$, $V = 13.77 \text{ m} \cdot \text{min}^{-1}$, $\alpha = -6^\circ$ (Figure 7). We hypothesize that the observed variation may be due to tribological influences, such as stick-slip, present at lower speeds. The chip segmentation frequency follows the experimental trend very well. Cutting temperatures are reasonable with the exception of process conditions corresponding to $0.25 \text{ mm} \cdot \text{rev}^{-1}$ and $80 \text{ m} \cdot \text{min}^{-1}$. It is important to note that temperatures in the tool are driven by tribological effects which we are not attempting to address in this work. Overall, given that the calibration was performed with uniaxial data only, the model performs reasonably well.

The GBS physics in the model is introduced to provide a competing deformation mechanism to slip as the grain structure becomes sufficiently refined. Following refinement, for a given strain rate, the required stress to drive GBS deformation may be lower than that required to drive slip based processes (Figure 1) e.g. GBS serves as a softening mechanism. The role of temperature is critical as higher temperatures drive additional grain boundary diffusion, which facilitates GBS based deformation. The hypothesis is that high strength and low thermal conductivity metals (such as Ti and its alloys) may deform via this mechanism during high speed machining and hence, in the absence of ductile fracture, it may be GBS that causes segmented chip behavior.

To illustrate key temporal effects, a sampling point was selected in the FEM model $50 \mu\text{m}$ ahead and above the tool tip as shown in Figure 10. Relevant SDV time histories from this sample point were analyzed to interpret the simulated results. The GBS rate, slip rate, and von Mises stress histories from this location are shown in Figure 11.

Figure 10. Time history sampling point.

Figure 11. Simulated GBS rate, slip rate, and von Mises stress for $f = 0.1 \text{ mm}$, $V = 30 \text{ m} \cdot \text{min}^{-1}$, $\alpha = 6.5^\circ$ at a location $50 \mu\text{m}$ above and ahead of the tool tip.

The time histories reveal that the model does indeed periodically alternate between slip and GBS as dominant mechanisms. Additionally, under these conditions, GBS reduces the effective von Mises stress by $\sim 50\%$ at the selected location. To further interpret these results, additional SDV time histories are shown in Figure 12.

Figure 12. Simulated GBS, grain size, α -phase slip strain, total homogenized strain and temperature time histories at a location $50 \mu\text{m}$ above and ahead of the tool tip for $f = 0.1 \text{ mm}$, $V = 30 \text{ m} \cdot \text{min}^{-1}$, $\alpha = 6.5^\circ$.

The SDV evolution histories show that it is grain refinement that is critical to this process. At first slip based deformation is dominant which drives grain refinement which leads to an increase

in flow stress. The increase in flow stress accelerates heat generation, which cannot efficiently diffuse away due to low thermal conductivity, and drives a rapid increase in temperature. This grain refinement continues until the mean grain size and temperature are sufficient to activate GBS based deformation. At this point GBS accommodates all deformation, which retards further grain refinement, and lowers the effective flow stress. Finally, as fresh (unrefined) material enters the primary deformation zone, the sequence begins again and generates the observed periodic behavior. Contour maps illustrating the spatial fields relevant to this process are shown in Figure 13 and Figure 14. Snap shots in Figure 13 are taken at the beginning of this process and Figure 14 shows the process 50 μ s thereafter.

Figure 13. Contours of (a) von Mises stress, (b) mean grain size, (c) α -phase slip rate, and (d) α -phase slip rate during incipient shear band formation. $f = 0.1 \text{ mm}$, $V = 30 \text{ m} \cdot \text{min}^{-1}$, $\alpha = 6.5^\circ$.

At this time step the shear band is beginning to develop. Ahead of the deformation zone, and near the free surface adjacent to the developing band, slip is dominant (Figure 13c) which drives refinement (Figure 13b). Grain refinement within the primary deformation zone (beginning at the chip-tool interface) induces a propagating front of GBS deformation (Figure 13d). This propagating band also begins to reduce the flow stress starting at the tool-chip interface (Figure 13a).

Figure 14. Contours of (a) von Mises stress, (b) mean grain size, (c) α -phase slip rate, and (d) α -phase slip rate $50\mu s$ after incipient shear band formation. $f = 0.1\text{ mm}$, $V = 30\text{ m}\cdot\text{min}^{-1}$, $\alpha = 6.5^\circ$.

After $50\mu s$ has elapsed, the shear band forms and a heterogeneous feature begins to form on the free surface of the chip. At this point slip contributes negligibly (Figure 14c) and GBS is the dominant deformation mode (Figure 14d). The von Mises stress within the shear band has softened considerably as have stresses ahead of the shear band (Figure 14a). The final shear band grain size predicted by the simulation is roughly 100 nm (Figure 14b), which is reasonable compared to experimental observations on Al [17], Cu [16], and commercially purity titanium [18].

The homogenized total accumulated plastic strain is shown in Figure 15. This includes strain contributions from both α , comprising of slip and GBS modes, and β , which is assumed to deform by slip only.

Figure 15. Total accumulated plastic strain distribution for
 $f = 0.1 \text{ mm}$, $V = 30 \text{ m} \cdot \text{min}^{-1}$, $\alpha = 6.5^\circ$.

The heterogeneous distribution of strain is expected in segmented chips. Additionally a very pronounced secondary shear zone is predicted. This can be common depending on the workpiece material, tool, and process parameters.

6. Conclusions

A composite dual phase internal state variable constitutive model was developed for Ti-6Al-4V. The proposed model includes grain boundary sliding based physics in addition to a traditional slip based plasticity. Microstructural influences are incorporated into the model by introducing dislocation density and the mean grain size as internal state variables which evolve with plastic deformation. The model was calibrated to uniaxial stress-strain data that spanned quasi-static to dynamic rates across a wide range of temperatures. Validation against machining data showed that the model predicted chip segmentation, machining forces, and tool temperatures reasonably well over a range of feeds and speeds. The newly introduced GBS physics was shown to dominate deformation following sufficient grain refinement. This deformation mode provides softening at the constitutive level without the need for invoking a ductile failure based softening mechanism. This physical interpretation is something that has not previously been explored in the machining community.

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Appendix

Table 1. Model Parameters.

Model Component	Variables	Description
Calibrated Model Parameters		
β -thermal and drag stress	$\sigma_{\beta 0}, p_{\beta}, q_{\beta}, Q_{\beta}, \dot{\varepsilon}_{o\beta}, \tau_d, \alpha_d$	Ti-6Al-4V initial yield data above β -transus [86-92]
α oxygen equivalent thermal stress	$\sigma_{\alpha 0}, p_{\alpha 0}, q_{\alpha 0}, Q_{\alpha 0}, \dot{\varepsilon}_{o\alpha 0}$	CP-Ti initial yield data below β -transus [50, 93, 94]
α solid solution thermal stress	$\sigma_{\alpha 1}, p_{\alpha 1}, q_{\alpha 1}, Q_{\alpha 1}, \dot{\varepsilon}_{o\alpha 1}, Q_{Al,1}, Q_{Al,2}, T_c$	Ti-6Al-4V initial yield data below β -transus [1, 86, 87, 90, 91, 95-101].
α phase dislocation density evolution law	$A, B, \dot{\varepsilon}_d, Q_d, n$	Ti-6Al-4V uniaxial stress-strain below β -transus [1, 86, 87, 90, 91, 95-101].
Model Parameters from Literature		
Taylor hardening factor	α_p	ECAP processed CP-Ti [46]
Burgers vector magnitude	b	ECAP processed CP-Ti [46]
Grain boundary width	δ	Assumed to be $2b$ [54]
Hall-Petch hardening slope	α_{HP}	Pure Ti grain sizes 6-100 μ m [47]
GBS atomic volume	Ω	Ti-6Al-4V superplasticity study [64]
Diffusion GBS parameters	D_v, D_B, Q_v	Ti-6Al-4V and Ti [64, 66-70]
Specific grain boundary energy	Γ	0.1 and 0.25 $J \cdot m^{-2}$ for Zn and Pb [54]
Elastic constants	μ, ν	Shear modulus and Poisson's ratio [85]
Physical properties	thermal conductivity, heat capacity, coefficient of thermal expansion, density	Taken from literature [9, 28, 83, 84]
Assumed Model Parameters		
Boundary self-diffusion activation energy	Q_B	Assumed $Q_B = 80 \text{ kJ} \cdot \text{mol}^{-1}$ (see section 2.4)
Invariant material volume diameter undergoing GBS	d_v	10 μ m chosen (see section 2.4)
Shape factor	α_f	$6 \cdot 10^{-4}$ produced reasonable GBS threshold stress values (see section 2.7)
Dislocation cell diameter factor	K_c	0.1 (see section 2.5)
Grain refinement evolution equation constants	u, ε_r	0.95 and 0.5, respectively (see section 2.5)
Analytically Derived Expressions		
DRX multiplicative factor	K	equation (13-15)
Grain evolution multiplicative factor	C	equation (17-19)

Table 2. Coulomb friction values used in simulations

(Figure 6) rake = 5° speed = 121.90 m·min ⁻¹		(Figure 7) rake = 6.5° feed = 0.1000 mm·rev ⁻¹		(Figure 8) Frequency Validation			
Feed (mm·rev ⁻¹)	μ	Speed (m·min ⁻¹)	μ	Feed (mm·rev ⁻¹)	Speed (m·min ⁻¹)	Rake	μ
0.0254	0.76	12.00	0.50	0.0762	139.00	5.0°	0.53
0.0508	0.59	30.00	0.50	0.1000	112.00	6.5°	0.50
0.0762	0.53	57.00	0.50	0.1000	84.00	6.5°	0.50
0.1016	0.48	84.00	0.50	0.1000	57.00	6.5°	0.50
0.1270	0.45	112.00	0.50	0.1000	30.00	6.5°	0.50
		139.00	0.50	0.0800	13.77	-6.0°	0.71

(Figure 9) Temperature Validation Rake = 7.0°		
Speed (m·min ⁻¹)	Feed (mm·rev ⁻¹)	μ
40.00	0.1000	0.50
40.00	0.2500	0.50
80.00	0.1000	0.50
80.00	0.2500	0.50

References

1. Minnaar, K. and M. Zhou, *An analysis of the dynamic shear failure resistance of structural metals*. Journal of the Mechanics and Physics of Solids, 1998. **46**(10): p. 2155-2170.
2. Cho, K., Y. Chi, and J. Duffy, *Microscopic observations of adiabatic shear bands in three different steels*. Metallurgical Transactions A, 1990. **21**(4): p. 1161-1175.
3. Lee, S., et al., *Dynamic fracture initiation behavior of an HY-100 steel*. Metallurgical Transactions A, 1993. **24**(4): p. 901-912.
4. Cho, K.-M., et al., *Adiabatic shear band formation during dynamic torsional deformation of an HY-100 steel*. Acta metallurgica et materialia, 1993. **41**(3): p. 923-932.
5. Liao, S.-c. and J. Duffy, *Adiabatic shear bands in a Ti-6Al-4V titanium alloy*. Journal of the Mechanics and Physics of Solids, 1998. **46**(11): p. 2201-2231.
6. Komanduri, R., et al., *On the Catastrophic Shear Instability in High-Speed Machining of an AISI 4340 Steel*. Journal of Engineering for Industry, 1982. **104**(2): p. 121-131.
7. Sagapuram, D., et al., *On control of flow instabilities in cutting of metals*. CIRP Annals-Manufacturing Technology, 2015. **64**(1): p. 49-52.
8. Molinari, A., C. Musquar, and G. Sutter, *Adiabatic shear banding in high speed machining of Ti-6Al-4V: experiments and modeling*. International Journal of Plasticity, 2002. **18**(4): p. 443-459.

9. Komanduri, R. and Z.-B. Hou, *On thermoplastic shear instability in the machining of a titanium alloy (Ti-6Al-4V)*. Metallurgical and Materials Transactions A, 2002. **33**(9): p. 2995-3010.
10. Molinari, A., X. Soldani, and M. Miguélez, *Adiabatic shear banding and scaling laws in chip formation with application to cutting of Ti-6Al-4V*. Journal of the Mechanics and Physics of Solids, 2013. **61**(11): p. 2331-2359.
11. Sima, M. and T. Özel, *Modified material constitutive models for serrated chip formation simulations and experimental validation in machining of titanium alloy Ti-6Al-4V*. International Journal of Machine Tools and Manufacture, 2010. **50**(11): p. 943-960.
12. Marusich, T. and M. Ortiz, *Modelling and simulation of high - speed machining*. International Journal for Numerical Methods in Engineering, 1995. **38**(21): p. 3675-3694.
13. Rice, J.R. and D.M. Tracey, *On the ductile enlargement of voids in triaxial stress fields**. Journal of the Mechanics and Physics of Solids, 1969. **17**(3): p. 201-217.
14. Sun, J. and Y.B. Guo, *A new multi-view approach to characterize 3D chip morphology and properties in end milling titanium Ti-6Al-4V*. International Journal of Machine Tools and Manufacture, 2008. **48**(12-13): p. 1486-1494.
15. Murr, L.E., et al., *Microstructure evolution associated with adiabatic shear bands and shear band failure in ballistic plug formation in Ti-6Al-4V targets*. Materials Science and Engineering: A, 2009. **516**(1-2): p. 205-216.
16. Brown, T.L., et al., *A study of the interactive effects of strain, strain rate and temperature in severe plastic deformation of copper*. Acta Materialia, 2009. **57**(18): p. 5491-5500.
17. Shankar, M.R., et al., *Characteristics of aluminum 6061-T6 deformed to large plastic strains by machining*. Materials Science and Engineering: A, 2005. **410-411**(0): p. 364-368.
18. Shankar, M.R., et al., *Severe plastic deformation (SPD) of titanium at near-ambient temperature*. Acta Materialia, 2006. **54**(14): p. 3691-3700.
19. Meyers, M.A., A. Mishra, and D.J. Benson, *Mechanical properties of nanocrystalline materials*. Progress in Materials Science, 2006. **51**(4): p. 427-556.
20. Gleiter, H., *Nanocrystalline materials*. Progress in materials science, 1989. **33**(4): p. 223-315.
21. Suryanarayana, C., *Nanocrystalline materials*. International Materials Reviews, 1995. **40**(2): p. 41-64.
22. Melkote, S.N., et al., *A physically based constitutive model for simulation of segmented chip formation in orthogonal cutting of commercially pure titanium*. CIRP Annals - Manufacturing Technology, 2015. **64**(1): p. 65-68.
23. Chokshi, A.H., et al., *On the validity of the hall-petch relationship in nanocrystalline materials*. Scripta Metallurgica, 1989. **23**(10): p. 1679-1683.
24. Yamakov, V., et al., *Grain-boundary diffusion creep in nanocrystalline palladium by molecular-dynamics simulation*. Acta Materialia, 2002. **50**(1): p. 61-73.
25. Schiøtz, J., *Atomic-scale modeling of plastic deformation of nanocrystalline copper*. Scripta Materialia, 2004. **51**(8): p. 837-841.
26. Sagapuram, D., et al. *Geometric flow control of shear bands by suppression of viscous sliding*. in *Proc. R. Soc. A*. 2016. The Royal Society.
27. Miguélez, M., X. Soldani, and A. Molinari, *Analysis of adiabatic shear banding in orthogonal cutting of Ti alloy*. International Journal of Mechanical Sciences, 2013. **75**: p. 212-222.

28. Ye, G.G., et al., *Modeling periodic adiabatic shear band evolution during high speed machining Ti-6Al-4V alloy*. International Journal of Plasticity, 2013. **40**(0): p. 39-55.
29. Johnson, G.R. and W.H. Cook. *A constitutive model and data for metals subjected to large strains, high strain rates and high temperatures*. in *Proceedings of the 7th International Symposium on Ballistics*. 1983. The Netherlands.
30. Ding, H., N. Shen, and Y.C. Shin, *Modeling of grain refinement in aluminum and copper subjected to cutting*. Computational Materials Science, 2011. **50**(10): p. 3016-3025.
31. Ding, H. and Y.C. Shin. *Dislocation density-based grain refinement modeling of orthogonal cutting of commercially pure titanium*. in *ASME 2011 International Manufacturing Science and Engineering Conference*. 2011. American Society of Mechanical Engineers.
32. Ding, H. and Y.C. Shin, *A Metallo-Thermomechanically Coupled Analysis of Orthogonal Cutting of AISI 1045 Steel*. Journal of Manufacturing Science and Engineering, 2012. **134**(5): p. 051014-051014.
33. Ding, H. and Y.C. Shin, *Multi-physics modeling and simulations of surface microstructure alteration in hard turning*. Journal of Materials Processing Technology, 2013. **213**(6): p. 877-886.
34. Liu, R., et al., *A unified internal state variable material model for inelastic deformation and microstructure evolution in SS304*. Materials Science and Engineering: A, 2014. **594**(0): p. 352-363.
35. Liu, R., et al., *A unified material model including dislocation drag and its application to simulation of orthogonal cutting of OFHC Copper*. Journal of Materials Processing Technology, 2015. **216**: p. 328-338.
36. AdvantEdge, 2015. Thirdwave Systems, Minneapolis, MN, v7.0.
37. Welsch, G., R. Boyer, and E. Collings, *Materials properties handbook: titanium alloys*. 1993: ASM international.
38. Picu, R.C. and A. Majorell, *Mechanical behavior of Ti-6Al-4V at high and moderate temperatures—Part II: constitutive modeling*. Materials Science and Engineering: A, 2002. **326**(2): p. 306-316.
39. Christian, J.W. and S. Mahajan, *Deformation twinning*. Progress in materials science, 1995. **39**(1): p. 1-157.
40. Salem, A.A., S.R. Kalidindi, and R.D. Doherty, *Strain hardening regimes and microstructure evolution during large strain compression of high purity titanium*. Scripta Materialia, 2002. **46**(6): p. 419-423.
41. Salem, A.A., S.R. Kalidindi, and S.L. Semiatin, *Strain hardening due to deformation twinning in α -titanium: Constitutive relations and crystal-plasticity modeling*. Acta Materialia, 2005. **53**(12): p. 3495-3502.
42. Salem, A.A., et al., *Strain hardening due to deformation twinning in α -titanium: mechanisms*. Metallurgical and Materials Transactions A, 2006. **37**(1): p. 259-268.
43. Williams, J., R. Baggerly, and N. Paton, *Deformation behavior of HCP Ti-Al alloy single crystals*. Metallurgical and Materials Transactions A, 2002. **33**(13): p. 837-850.
44. Follansbee, P.S. and U.F. Kocks, *A constitutive description of the deformation of copper based on the use of the mechanical threshold stress as an internal state variable*. Acta Metallurgica, 1988. **36**(1): p. 81-93.

45. Taylor, G.I., *The mechanism of plastic deformation of crystals. Part I. Theoretical.* Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character, 1934: p. 362-387.
46. Zhu, Y., et al., *Nanostructures in Ti processed by severe plastic deformation.* Journal of materials research, 2003. **18**(08): p. 1908-1917.
47. Lederich, R.J., et al., *The effect of grain size on yield stress and work hardening of polycrystalline titanium at 295 K and 575 K.* Materials Science and Engineering, 1978. **33**(2): p. 183-188.
48. Kumar, A. and R.G. Kumble, *Viscous Drag on Dislocations at High Strain Rates in Copper.* Journal of Applied Physics, 1969. **40**(9): p. 3475-3480.
49. Nemat-Nasser, S., W.-G. Guo, and D.P. Kihl, *Thermomechanical response of AL-6XN stainless steel over a wide range of strain rates and temperatures.* Journal of the Mechanics and Physics of Solids, 2001. **49**(8): p. 1823-1846.
50. Nemat-Nasser, S., W.G. Guo, and J.Y. Cheng, *Mechanical properties and deformation mechanisms of a commercially pure titanium.* Acta Materialia, 1999. **47**(13): p. 3705-3720.
51. Zerilli, F.J. and R.W. Armstrong, *The effect of dislocation drag on the stress-strain behavior of F.C.C. metals.* Acta Metallurgica et Materialia, 1992. **40**(8): p. 1803-1808.
52. Molinari, A. and G. Ravichandran, *Constitutive modeling of high-strain-rate deformation in metals based on the evolution of an effective microstructural length.* Mechanics of Materials, 2005. **37**(7): p. 737-752.
53. Raj, R. and M. Ashby, *On grain boundary sliding and diffusional creep.* Metallurgical transactions, 1971. **2**(4): p. 1113-1127.
54. Ashby, M. and R. Verrall, *Diffusion-accommodated flow and superplasticity.* Acta Metallurgica, 1973. **21**(2): p. 149-163.
55. Sherby, O.D. and J. Wadsworth, *Superplasticity—Recent advances and future directions.* Progress in Materials Science, 1989. **33**(3): p. 169-221.
56. Nieh, T., et al., *High strain rate superplasticity in a continuously recrystallized Al-6% Mg-0.3% Sc alloy.* Acta materialia, 1998. **46**(8): p. 2789-2800.
57. Ko, Y.G., et al., *Microstructural influence on low-temperature superplasticity of ultrafine-grained Ti-6Al-4V alloy.* Materials Science and Engineering: A, 2005. **410-411**(0): p. 156-159.
58. McFadden, S., et al., *Observations of low-temperature superplasticity in electrodeposited ultrafine grained nickel.* Materials Letters, 2000. **45**(6): p. 345-349.
59. Saldana, C., A.H. King, and S. Chandrasekar, *Thermal stability and strength of deformation microstructures in pure copper.* Acta Materialia, 2012. **60**(10): p. 4107-4116.
60. McFadden, S., et al., *Low-temperature superplasticity in nanostructured nickel and metal alloys.* Nature, 1999. **398**(6729): p. 684-686.
61. Wolf, D., et al., *Deformation of nanocrystalline materials by molecular-dynamics simulation: relationship to experiments?* Acta Materialia, 2005. **53**(1): p. 1-40.
62. Schiøtz, J., F.D. Di Tolla, and K.W. Jacobsen, *Softening of nanocrystalline metals at very small grain sizes.* Nature, 1998. **391**(6667): p. 561-563.
63. Suryanarayana, C., et al., *Grain size effects in nanocrystalline materials.* Journal of Materials Research, 1992. **7**(08): p. 2114-2118.

64. Pilling, J., et al., *Solid state bonding in superplastic Ti-6Al-4V*. Metal Science, 1984. **18**(3): p. 117-122.
65. Coble, R., *A model for boundary diffusion controlled creep in polycrystalline materials*. Journal of Applied Physics (US), 1963. **34**.
66. Köppers, M., et al., *Intrinsic self-diffusion and substitutional Al diffusion in α -Ti*. Acta Materialia, 1997. **45**(10): p. 4181-4191.
67. Malakondaiah, G. and P. Rama Rao, *Creep of Alpha-Titanium at low stresses*. Acta Metallurgica, 1981. **29**(7): p. 1263-1275.
68. De Reza, N.E.W. and y. C.M. Libanati, *Autodifusion de titanio beta y hafnio beta*. Acta Metallurgica, 1968. **16**(10): p. 1297-1305.
69. Arieli, A. and A. Rosen, *Superplastic deformation of Ti-6Al-4V alloy*. Metallurgical Transactions A, 1977. **8**(10): p. 1591-1596.
70. Mishra, R.S., et al., *Mechanical behavior and superplasticity of a severe plastic deformation processed nanocrystalline Ti-6Al-4V alloy*. Materials Science and Engineering: A, 2001. **298**(1-2): p. 44-50.
71. Valiev, R., R.S. Musalimov, and N. Tsenev, *The non - equilibrium state of grain boundaries and the grain boundary precipitations in aluminium alloys*. Physica status solidi (a), 1989. **115**(2): p. 451-457.
72. Valiev, R.Z., N. Krasilnikov, and N. Tsenev, *Plastic deformation of alloys with submicron-grained structure*. Materials Science and Engineering: A, 1991. **137**: p. 35-40.
73. Horváth, J., R. Birringer, and H. Gleiter, *Diffusion in nanocrystalline material*. Solid State Communications, 1987. **62**(5): p. 319-322.
74. Hahn, H. and K.A. Padmanabhan, *A model for the deformation of nanocrystalline materials*. Philosophical Magazine Part B, 1997. **76**(4): p. 559-571.
75. Holt, D.L., *Dislocation Cell Formation in Metals*. Journal of Applied Physics, 1970. **41**(8): p. 3197-3201.
76. Estrin, Y., et al., *A dislocation-based model for all hardening stages in large strain deformation*. Acta Materialia, 1998. **46**(15): p. 5509-5522.
77. Ni, H. and A.T. Alpas, *Sub-micrometer structures generated during dry machining of copper*. Materials Science and Engineering: A, 2003. **361**(1-2): p. 338-349.
78. Estrin, Y. and H. Mecking, *A unified phenomenological description of work hardening and creep based on one-parameter models*. Acta Metallurgica, 1984. **32**(1): p. 57-70.
79. Gourdet, S. and F. Montheillet, *A model of continuous dynamic recrystallization*. Acta Materialia, 2003. **51**(9): p. 2685-2699.
80. Murr, L.E. and D. Kuhlmann-Wilsdorf, *Experimental and theoretical observations on the relationship between dislocation cell size, dislocation density, residual hardness, peak pressure and pulse duration in shock-loaded nickel*. Acta Metallurgica, 1978. **26**(5): p. 847-857.
81. Kuhlmann-Wilsdorf, D. and J.H. Van Der Merwe, *Theory of dislocation cell sizes in deformed metals*. Materials Science and Engineering, 1982. **55**(1): p. 79-83.
82. Sagapuram, D., et al., *Controlling texture in magnesium alloy sheet by shear-based deformation processing*. Acta Materialia, 2013. **61**(18): p. 6843-6856.
83. Abele, E. and B. Fröhlich, *High speed milling of titanium alloys*. Advances in Production Engineering & Management, 2008. **3**(3): p. 131-140.
84. Zhang, Y., *Numerical simulation approaches and methodologies for multi-physic comprehensions of titanium alloy (Ti-6Al-4V) CUTTING*. 2011, INSA de Lyon.

85. Chichili, D.R., K.T. Ramesh, and K.J. Hemker, *The high-strain-rate response of alpha-titanium: experiments, deformation mechanisms and modeling*. Acta Materialia, 1998. **46**(3): p. 1025-1043.
86. Seshacharyulu, T., et al., *Hot working of commercial Ti-6Al-4V with an equiaxed α - β microstructure: materials modeling considerations*. Materials Science and Engineering: A, 2000. **284**(1-2): p. 184-194.
87. Seo, S., O. Min, and H. Yang, *Constitutive equation for Ti-6Al-4V at high temperatures measured using the SHPB technique*. International Journal of Impact Engineering, 2005. **31**(6): p. 735-754.
88. Cai, J., et al., *Constitutive equations for elevated temperature flow stress of Ti-6Al-4V alloy considering the effect of strain*. Materials & Design, 2011. **32**(3): p. 1144-1151.
89. Ding, R., Z.X. Guo, and A. Wilson, *Microstructural evolution of a Ti-6Al-4V alloy during thermomechanical processing*. Materials Science and Engineering: A, 2002. **327**(2): p. 233-245.
90. Luo, J., et al., *The variation of strain rate sensitivity exponent and strain hardening exponent in isothermal compression of Ti-6Al-4V alloy*. Materials & Design, 2010. **31**(2): p. 741-748.
91. Lee, W.-S. and C.-F. Lin, *Plastic deformation and fracture behaviour of Ti-6Al-4V alloy loaded with high strain rate under various temperatures*. Materials Science and Engineering: A, 1998. **241**(1-2): p. 48-59.
92. Li, L.X., et al., *Flow stress behavior and deformation characteristics of Ti-3Al-5V-5Mo compressed at elevated temperatures*. Materials & Design, 2002. **23**(5): p. 451-457.
93. Harding, J., *The temperature and strain rate sensitivity of alpha-titanium*. Archiwum Mechaniki Stosowanej, 1975. **27**(5): p. 715-732.
94. Meyers, M.A., et al., *Evolution of microstructure and shear-band formation in α -hcp titanium*. Mechanics of Materials, 1994. **17**(2-3): p. 175-193.
95. De Meester, B., M. Döner, and H. Conrad, *Deformation kinetics of the Ti-6Al-4V alloy at low temperatures*. Metallurgical Transactions A, 1975. **6**(1): p. 65-75.
96. Combres, Y. and J.-J. Blandin, *Comparison of the beta-CEZ and Ti-64 superplastic properties*. Titanium'95- Science and technology, 1996: p. 864-871.
97. Nemat-Nasser, S., et al., *Dynamic response of conventional and hot isostatically pressed Ti-6Al-4V alloys: experiments and modeling*. Mechanics of Materials, 2001. **33**(8): p. 425-439.
98. Schroeder, G. and T.W. Duerig, *Forgeability of Beta - Titanium Alloys under Isothermal Forging Conditions*. Titanium: Science and technology, 1985: p. 585-592.
99. Follansbee, P.S. and G.T. Gray, *An analysis of the low temperature, low and high strain-rate deformation of Ti-6Al-4V*. Metallurgical Transactions A, 1989. **20**(5): p. 863-874.
100. Majorell, A., S. Srivatsa, and R.C. Picu, *Mechanical behavior of Ti-6Al-4V at high and moderate temperatures—Part I: Experimental results*. Materials Science and Engineering: A, 2002. **326**(2): p. 297-305.
101. Paton, N., J. Williams, and G. Rauscher, *The deformation of alpha-phase titanium*. Titanium science and technology, 1973: p. 1049-1069.
102. Meyer, L.W., *Titanium Science and Technology*. Deutsche Gesellschaft for Metallkunde, 1984: p. 1851-58.
103. Nicholas, T., *Experimental Mechanics*. 1981. **38**: p. 177-85.

104. Lee, W.-S. and C.-F. Lin, *High-temperature deformation behaviour of Ti6Al4V alloy evaluated by high strain-rate compression tests*. Journal of Materials Processing Technology, 1998. **75**(1–3): p. 127-136.
105. Jiao, L., L. Miaoquan, and Y. Weixin, *Microstructure Evolution during High Temperature Deformation of Ti-6Al-4V Alloy*. Rare Metal Materials and Engineering, 2010. **39**(8): p. 1323-1328.
106. Klepaczko, J.R. and C.Y. Chiem, *On rate sensitivity of f.c.c. metals, instantaneous rate sensitivity and rate sensitivity of strain hardening*. Journal of the Mechanics and Physics of Solids, 1986. **34**(1): p. 29-54.
107. Weber, G. and L. Anand, *Finite deformation constitutive equations and a time integration procedure for isotropic, hyperelastic-viscoplastic solids*. Computer Methods in Applied Mechanics and Engineering, 1990. **79**(2): p. 173-202.
108. Srikanth, A. and N. Zabaras, *A computational model for the finite element analysis of thermoplasticity coupled with ductile damage at finite strains*. International Journal for Numerical Methods in Engineering, 1999. **45**(11): p. 1569-1605.
109. Taylor, G.I., *Plastic strain in metals*. J. Inst. Metals, 1938(62): p. 307–324.
110. Camacho, G. and M. Ortiz, *Adaptive Lagrangian modelling of ballistic penetration of metallic targets*. Computer methods in applied mechanics and engineering, 1997. **142**(3): p. 269-301.
111. Cotterell, M. and G. Byrne, *Characterisation of chip formation during orthogonal cutting of titanium alloy Ti–6Al–4V*. CIRP Journal of Manufacturing Science and Technology, 2008. **1**(2): p. 81-85.
112. Soler, D., et al., *Uncertainty of temperature measurements in dry orthogonal cutting of titanium alloys*. Infrared Physics & Technology, 2015. **71**: p. 208-216.
113. Molinari, A., R. Cheriguene, and H. Miguélez, *Numerical and analytical modeling of orthogonal cutting: the link between local variables and global contact characteristics*. International journal of mechanical sciences, 2011. **53**(3): p. 183-206.
114. Deshpande, A. and V. Madhavan, *A novel approach to accelerate attainment of thermal steady state in coupled thermomechanical analysis of machining*. International Journal of Heat and Mass Transfer, 2012. **55**(13–14): p. 3869-3884.
115. Atlati, S., et al., *Analysis of a new Segmentation Intensity Ratio “SIR” to characterize the chip segmentation process in machining ductile metals*. International Journal of Machine Tools and Manufacture, 2011. **51**(9): p. 687-700.