Mechanics of Materials 109 (2017) 67–81

Contents lists available at ScienceDirect

Mechanics of Materials

journal homepage: www.elsevier.com/locate/mechmat

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

ARTICLE INFO

Article history:
Received 29 February 2016
Revised 7 January 2017
Available online 30 March 2017

Keywords:
Machining
Constitutive modeling
Titanium
Chip segmentation
Grain boundary sliding
Microstructure sensitive

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.

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 (Minnaar and Zhou, 1998) as well as conventional ductile failure caused by void coalescence and growth (Cho et al., 1990; Lee et al., 1993; Cho et al., 1993; Liao and Duffy, 1998). 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. (1982) 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. (2015) 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 (Molinari et al., 2002). 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 (2002) developed an analytical machining model for Ti-6Al-4V based on a plastic instability failure mechanism associated with thermal softening. Molinari et al. (2013) 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 (Sima and Özel, 2010) as well as fracture criteria (Marusich and Ortiz, 1995). A counter argument to the ductile fracture argument is that it is well known that ductility is heavily dependent on stress triaxiality (Rice and Tracey, 1969) and so the intense shearing of the primary deformation zone superimposed with large compressive hydrostatic stresses may limit ductile failure under

---

* Corresponding author.
E-mail addresses: pfz3@gatech.edu, patxifernandezzelaia@gmail.com (P. Fernandez-Zelaia).

http://dx.doi.org/10.1016/j.mechmat.2017.03.018
0167-6636/

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 (Sun and Guo, 2008). The same was found to be true of shear bands in Ti-6Al-4V subject to ballistic plug testing (Murr et al., 2009). 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 (Brown et al., 2009; Shankar et al., 2005; Shankar et al., 2006). Deformation mechanisms active at the nanocrystalline scale are vastly different than those present at higher length scales (Meyers et al., 2006; Gleiter, 1989; Suryanarayana, 1995). Recent micro-mechanical inspired modeling work by Melkote et al. (2015) incorporated a phenomenological inverse Hall–Petch (Chokshi et al., 1989) 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 (Yamakov et al., 2002; Schiøtz, 2004). Recent work by Sagapuram et al. (2016) 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 (Molinari et al., 2013; Sima and Özel, 2010; Miguélez et al., 2013; Ye et al., 2013). Many of these models are based on the classic Johnson–Cook model (Johnson and Cook, 1983) 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. Furthermore, 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 (Melkote et al., 2015; Ding et al., 2011; Ding and Shin, 2011; Ding and Shin, 2012; Ding and Shin, 2013; Liu et al., 2014; Liu et al., 2015). 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 (AdvantEdge 2015) 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 (Welsch et al., 1993). 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 (2002). 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 Eq. (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 Peierel'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 (Christian and Mahajan, 1995). There is evidence that twin boundaries behave as obstacles for propagating dislocations and have an effect on the strength and strain hardening characteristics (Christian and Mahajan, 1995; Salem et al., 2002; Salem et al., 2005; Salem et al., 2006). Conversely, a study on the role of