A physically based constitutive model for simulation of segmented chip formation in orthogonal cutting of commercially pure titanium

Shreyes N. Melkote (2)a, Rui Liu a, Patxi Fernandez-Zelaia a, Troy Marusich b

a George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA, USA
b Third Wave Systems LLC, Minneapolis, MN, USA

ARTICLE INFO
Keywords:
Machining
Modelling
Segmented chip

ABSTRACT

The accuracy of cutting simulations depends on the knowledge of micro-scale physics included in the constitutive and microstructure evolution models of the cutting process. This paper presents an enhanced physically based model that accounts for microstructure evolution induced flow softening due to the inverse Hall–Petch effect below a critical grain size. The model’s ability to simulate segmented chip formation and grain refinement in the shear bands produced in orthogonal cutting of commercially pure titanium is evaluated through finite element simulations and experiments. Results show good prediction accuracy for the cutting and thrust forces, chip morphology, and segmentation frequency.

© 2015 CIRP.

1. Introduction

A segmented chip is commonly observed in cutting materials with low thermal conductivity (e.g. titanium and its alloys). The low thermal conductivity gives rise to heat accumulation in the primary shear zone, which causes localized softening, and shear localization and chip segmentation [1]. This in turn can cause undesirable oscillations in the cutting force and associated vibrations that can inhibit tool life and yield poor surface quality and dimensional accuracy of the machined feature.

Segmented chip formation has been simulated by several researchers using different modelling approaches that are well-documented in a recent CIRP keynote paper [2]. Based on observations of voids and cracks in the shear band, Uhlmann et al. [3] simulated segmented chip formation by incorporating a ductile fracture mechanism in their model. Hua and Shivpuri [4] used an energy-based ductile fracture criterion to simulate segmented chip formation in cutting of Ti-6Al-4V. More recently, Calamaz et al. [5] proposed a phenomenological modification to the popular Johnson–Cook flow stress model to simulate chip segmentation in cutting of Ti-6Al-4V. This model was further refined by Özel and his co-workers for different applications [6,7]. Rotella and Umbrello [8] used a similar flow stress model in conjunction with evolution equations for grain size and hardness variation to predict microstructure changes due to dynamic recrystallization (DRX) in dry and cryogenic machining of Ti-6Al-4V. Calamaz et al. [5] also noted that strain softening can be attributed to microstructural changes induced by dynamic recovery (DRV) and/or DRX processes active during severe plastic deformation. Ding and Shin [9] presented a physically based model that accounts for these effects using dislocation density as the sole internal state variable. However, they only simulated continuous chip formation with their model.

In this paper, a recently developed physically based constitutive model [10], which is motivated by the mechanics of interaction of mobile dislocations with microstructural barriers, is extended by incorporating an additional deformation mechanism to allow for accurate simulation of segmented chip formation in cutting of commercially pure titanium (CP-Ti). Specifically, in order to describe the material constitutive behaviour when ultrafine grains are formed in the shear band during cutting of CP-Ti, the inverse Hall–Petch effect (IHPE), commonly attributed to grain boundary sliding [11], is introduced in the model. This enables the material model to capture flow softening below a critical grain size. The model is implemented as a user-defined subroutine in a FEM-based machining simulation software AdvantEdge™ (Third Wave Systems, USA) and is used to simulate orthogonal cutting of CP-Ti. Orthogonal cutting experiments are conducted to determine the cutting forces and chip characteristics, which are compared with simulation results to evaluate the performance of the enhanced model.

2. Physically based constitutive model

This section briefly summarizes key aspects of the previously developed constitutive model [10], which deals with simulation of continuous chip formation, and discusses the IHPE model enhancement. Following thermal activation theory [12], the flow strength of a metal undergoing plastic deformation is formulated as a linear superposition of an athermal stress, \( \sigma_a \), a thermal stress, \( \sigma_t \), and a dislocation drag stress, \( \sigma_d \), as follows:

\[
\sigma = \sigma_a + \sigma_t + \sigma_d
\]  

(1)
The magnitude of $\sigma_{th}$ depends on the strength of interactions of mobile dislocations with short-range barriers such as lattice friction and solute atoms. This component is modelled using the formulation proposed by Mecking and Kocks [13] as follows:

$$\sigma_{th} = \left[1 - \left(\frac{kT}{g0\mu b \ln\left(\frac{b}{c}\right)}\right)^{1/q}\right]^{1/P} \sigma_0$$

(2)

where, $k$ is the Boltzmann’s constant, $T$ is the absolute temperature, $g0$ is the normalized activation energy at 0 K, $\mu$ is the temperature-dependent shear modulus, $b$ is the magnitude of the Burgers vector, $c$ is a reference strain rate, $\sigma_0$ is the stress required to overcome short range obstacles at 0 K, and $p$ and $q$ are parameters defining the shape of energy barriers associated with short range obstacles.

The athermal stress, $\sigma_{at}$, is formulated as the sum of stresses required to overcome the resistance to dislocation motion offered by grain boundaries, $\sigma_C$, and dislocation forest, $\sigma_P$, as follows:

$$\sigma_a = \sigma_C + \sigma_P = \frac{\alpha_C \mu \sqrt{b}}{\sqrt{D}} + \alpha_P \mu b \sqrt{\rho}$$

(3)

where $\alpha_C$ and $\alpha_P$ are parameters related to the strength of mobile dislocation-grain boundary and dislocation-dislocation forest interactions, respectively. The two internal state variables, dislocation density, $\rho$, and average grain size, $D$, evolve with deformation.

In the grain boundary contribution term, $\sigma_C$ in Eq. (3), the parameter $\alpha_C$ equals a constant, $\alpha_C^0$, which is independent of grain size in the deformation regime where the conventional Hall–Petch effect is active. Below a critical grain size ($D_C$), which is a function of temperature, the IHPE is observed in many metals and is accompanied by a decrease in flow stress with decreasing grain size (Fig. 1). In order to capture this softening, $\sigma_C$ is modelled using the phenomenological equation:

$$\sigma_C = \sigma_C^0 \tan h\left(\frac{d}{D^{0.7}}\right)^{10}$$

(4)

where $d$ and $v$ are temperature-dependent parameters with forms given in Table 2. For this combination of $d$ and $v$, the resultant $D_C$, at room temperature is ~10 nm, which is in agreement with values reported for various metals [14].

![Fig. 1. Schematic representation of IHPE on flow stress.](image)

Evolution (refinement) of grain size, $D$, due to continuous DRX, which occurs in severe plastic deformation of titanium [15], is modelled as follows:

$$D = D_f + (D_0 - D_f) \tan h\left(\frac{\sigma_C^0}{\mu}\right)^{u}$$

(5)

where $\sigma_C$ and $u$ are temperature and strain rate dependent parameters, $D_0$ is the initial grain size, and $D_f$ is the final recrystallized grain size defined as a function of the Zener-Hollomon parameter, $Z = \dot{\varepsilon} exp(Q/RT)$, as follows:

$$D_f = C_2 Z^{-m}$$

(6)

where $C_2$ and $m$ are material dependent parameters.

In the term representing the contribution of dislocation forests, $\sigma_P$, the evolution of dislocation density is modelled as follows:

$$\rho = \rho_k + \left(\rho_{DRX} - \rho_k\right) \left(\frac{D_f}{D_0}\right)^{0.5}$$

(7)

where $\rho_{DRX}$ is the dislocation density due to slip-induced hardening and dynamic recovery processes (but in the absence of DRX) and is given by the following closed-form expression:

$$\rho_{DRX} = \left[A \left(\sqrt{B - \rho_0} - B\right)^2\right]^{(2/3)}$$

(8)

where $\rho_0$ is the initial dislocation density, and $A$ and $B$ are the hardening and dynamic recovery parameters, respectively. $\rho_k$ is the dislocation density corresponding to the fully recrystallized grain structure. With increasing plastic strain, dislocations are consumed to form new cell/grain boundaries during the DRX process [16], which is modelled by Eq. (7).

At high strain rates (>10$^2$ s$^{-1}$), the deformation is known to be influenced by viscous drag type effects, which impede the motion of dislocations [17]. Hence, the dislocation drag component of flow stress is modelled as follows [10]:

$$\sigma_d = \sigma_{d,0}$$

(9)

where $\sigma_{d,0}$ is the dislocation (viscous) drag coefficient.

3. Model calibration

The twelve known material parameters and constants for CP-Ti, derived from literature and/or from the material used in the experiments, are listed in Table 1. The remaining eleven free parameters, which are not available in the literature, are calibrated using available data as described in [18] and given in Table 2.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Ref.</th>
<th>Parameter</th>
<th>Value</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_0$ (MPa)</td>
<td>140</td>
<td>[19]</td>
<td>$\alpha_C$</td>
<td>0.5</td>
<td>[20]</td>
</tr>
<tr>
<td>$k/g_0$ (K)</td>
<td>4.8 $\times$ 10$^{-5}$</td>
<td>[19]</td>
<td>$D_0$ (m)</td>
<td>40</td>
<td></td>
</tr>
<tr>
<td>$b$ (m)</td>
<td>2.95 $\times$ 10$^{-10}$</td>
<td>[19]</td>
<td>$\rho_0$ (m$^{-3}$)</td>
<td>10$^{13}$</td>
<td>[21]</td>
</tr>
<tr>
<td>$d$ (m)</td>
<td>4 $\times$ 10$^8$</td>
<td>[19]</td>
<td>$Q$ (kJ/mol)</td>
<td>146.04</td>
<td>[22]</td>
</tr>
<tr>
<td>$p$</td>
<td>2/3</td>
<td>[19]</td>
<td>$R$ (kJ/mol)</td>
<td>8.314</td>
<td>[22]</td>
</tr>
<tr>
<td>$q$</td>
<td>2</td>
<td>[19]</td>
<td>$\sigma_d$ (kPa s)</td>
<td>4.5</td>
<td>[23]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu$ (GPa)</td>
<td>(48.66–0.03223T)</td>
</tr>
<tr>
<td>$\alpha_C^0$</td>
<td>0.4544</td>
</tr>
<tr>
<td>$C_2$</td>
<td>5.1 $\times$ 10$^8$</td>
</tr>
<tr>
<td>$m$</td>
<td>6.3</td>
</tr>
<tr>
<td>$A$ (m$^{-1}$)</td>
<td>1.2 $\times$ 10$^9$</td>
</tr>
<tr>
<td>$B$ (m$^{-1}$)</td>
<td>(15.66 + 0.097) $e^{-0.2979x + 0.10^6\log_{10}(x)}$</td>
</tr>
<tr>
<td>$\dot{\varepsilon}$</td>
<td>0.237 + 0.00724 $\log_{10}(\frac{\rho_0}{12})$</td>
</tr>
<tr>
<td>$u$</td>
<td>7.4 – 2.44 $\log_{10}(\frac{\rho_0}{12})$ $^{-1.14}$</td>
</tr>
<tr>
<td>$\rho_{k}$ (m$^{-3}$)</td>
<td>4 $\times$ 10$^5$</td>
</tr>
<tr>
<td>$d$ (m$^{-2.5}$)</td>
<td>4 $\times$ 10$^{14}$</td>
</tr>
<tr>
<td>$\nu$</td>
<td>2 $\times$ 0.005(T – 293)</td>
</tr>
</tbody>
</table>

4. Experiments

Orthogonal tube cutting experiments were performed on a Hardinge T-42 SP CNC lathe using commercially pure titanium (grade 2) with an as-received microstructure consisting of...
equiaxed α-phase grains of average diameter 40 μm. To ensure plane strain conditions, the tube wall thickness was restricted to 2 mm. To probe a wide range of strains and strain rates, three feeds (t = 0.1, 0.2, 0.3 mm) and five cutting speeds (vc = 20, 60, 100, 140, 180 m/min) were used. Each test condition was replicated twice. Also, each test was conducted with a 0° rake angle tool and a new uncoated tungsten carbide insert (Kennametal TCMW3251, KCK20) with an up-sharp cutting edge (~10 μm). No cutting fluid was used. The cutting force, Fz, and thrust force, Fy, were measured using a piezoelectric force dynamometer (Kistler Model 9257B). The cut chips were cold mounted in epoxy, ground and polished to a 0.05 μm finish. Kroll’s reagent, a mixture of 1 ml hydrofluoric acid (HF, 40%), 2 ml nitric acid (HNO3, 40%) and 247 ml de-ionized water, was used to etch and reveal the chip microstructure.

5. Finite element model

To simulate orthogonal cutting, a 2-D finite element model was built in AdvantEdge™ (Third Wave Systems, USA), a physics-based machining simulation code. The enhanced constitutive model presented earlier was implemented in the software via a user-defined yield surface routine coded in FORTRAN. The contact condition at the tool/chip interface was modelled using the Coulomb friction law. The mean coefficient of friction, β, at the tool/chip interface for each simulation (listed in Table 3) was computed from the measured Fz and Fy and the equation $\beta = (F_z + F_t \tan \alpha)/(F_z - F_t \tan \alpha)$, where α is the rake angle.

Table 3

<table>
<thead>
<tr>
<th>$v_c$ (m/min)</th>
<th>$t_a$ (0.1 mm)</th>
<th>$t_a$ (0.2 mm)</th>
<th>$t_a$ (0.3 mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.63</td>
<td>0.50</td>
<td>0.44</td>
</tr>
<tr>
<td>60</td>
<td>0.52</td>
<td>0.40</td>
<td>0.34</td>
</tr>
<tr>
<td>100</td>
<td>0.49</td>
<td>0.37</td>
<td>0.30</td>
</tr>
<tr>
<td>140</td>
<td>0.46</td>
<td>0.31</td>
<td>0.28</td>
</tr>
<tr>
<td>180</td>
<td>0.42</td>
<td>0.29</td>
<td>0.27</td>
</tr>
</tbody>
</table>

6. Results

The simulated $F_z$ and $F_t$ are compared with experimental results in Fig. 2. The measured $F_z$ and $F_t$ decrease with increasing $v_c$ and decreasing $t_a$. The simulated results show a similar trend with less than 5% prediction error for $F_z$ and 10–20% error for $F_t$. The higher error in $F_t$ is attributed to the simple Coulomb friction model used and the absence of tool wear in the finite element model, which is invariably present when cutting titanium.

The simulated peak (S1) and valley (S2) thicknesses of the segmented chips (see Fig. 4) are compared with measurements in Fig. 3. Note that only fully formed shear bands were included in the measurements. Generally, the measured chip thickness decreases with increasing $v_c$ and decreasing $t_a$. The simulated values show a similar trend but tend to overestimate the thickness, especially S2, for most of the cutting conditions. One reason for this is the lack of a ductile fracture mechanism in the model to account for cracks often observed at the free surface of the chip in the vicinity of the shear band (see Fig. 6(a)). Detailed comparisons of the chip morphology are shown in Fig. 4. It can be seen that the major features of segmented chips are captured by the simulations.

Fig. 2. Mean and variation of experimental (EXP) and mean of simulated (SIM) cutting ($F_z$) and thrust ($F_t$) forces for different cutting conditions.

Fig. 3. Mean and variation of experimental (EXP) and mean of simulated (SIM) peak (S1) and valley (S2) thicknesses of the machined chip for different cutting conditions. Note: due to irregularity in chip geometry, the mean estimator and mean estimator variance of S1 and S2 were calculated using a bootstrapping method applied to 10–15 data points per chip.

Fig. 4. Comparison of measured and simulated chip shapes.
7. Conclusions

The paper presented an enhanced physics-based constitutive model for simulation of segmented chips formed in cutting of commercially pure titanium (CP-Ti). The model incorporates the inverse Hall–Petch effect (IHPE) to describe the softening effect of ultrafine grain structure in the shear band on the material flow strength. The flow strength is an explicit function of the grain size and dislocation density, which evolve with deformation. In order to validate the simulation results, orthogonal cutting experiments were performed over a range of feeds and speeds. The model simulations yield reasonably accurate predictions of the cutting force (≤5% error), thrust force (10–20% error), segmentation frequency, and chip morphology. Additionally, the model is able to simulate the spatial distribution of grain size and dislocation density, which are shown to be in good qualitative agreement with the observed chip microstructure. Future work will focus on adding a ductile fracture mechanism to the model to capture crack formation in the shear band region.

References