A Unified Material Model Including Dislocation Drag and Its Application to Simulation of Orthogonal Cutting of OFHC Copper

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Abstract

The fidelity of machining simulation models is dependent on the amount of micro-scale physics captured in the material constitutive law, microstructure evolution law(s), and the unifying scheme integrating microstructure evolution into the constitutive law. **This paper presents a unified material model that explicitly accounts for dislocation and microstructure evolution processes** as well as dislocation drag as a plausible deformation mechanism applicable at the high strain rates common in high speed cutting operations. The unified model is calibrated and implemented in the AdvantEdge™ 2-D machining simulation software and utilized to simulate the orthogonal cutting of OFHC copper. Comparison of the predicted cutting forces with experimental data reveals that the model is reasonably accurate. The experimentally observed trend of severe grain refinement in OFHC Cu chips is predicted quite well by the model. The model was further utilized to analyze the evolution of deformation field parameters, i.e. plastic strain and the Zener-Hollomon parameter, in orthogonal cutting as well as to generate microstructure-deformation maps. The model predictions of severe grain refinement in the chip at high plastic strains and low Zener-Hollomon parameter values are found to be consistent with experimental trends reported in the literature.

1. Introduction

In recent years, the finite element method (FEM) has been utilized as a powerful tool to enhance our understanding of cutting mechanics by offering the capacity to simulate *multi-physics* based machining operations. The accuracy of predictions obtained from FEM-based models of cutting is a constant concern. In particular, the fidelity of the constitutive (material) model, which describes the complex thermo-mechanical behavior of the material during the cutting operation, is central to FEM-based machining process models and has a profound influence on the prediction accuracy. Material models are often calibrated using flow stress data for deformation ranges that are not representative of metal cutting, largely due to technological limitations of the available dynamic materials characterization methods. Therefore, material models are inevitably extrapolated outside their calibration range when used in FEM-based cutting models often

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leading to poor prediction accuracy at high strain and high strain rates typical of metal machining.

It is generally accepted that the inclusion of a larger number of relevant underlying micro-scale deformation mechanisms in a material model will yield more accurate predictions outside the calibration range. The anticipated improvement in predictive capability of such *physics-based* material models makes them more appealing than *phenomenological* models, which are not physically-motivated. However, each physical mechanism brings its own parameters into the material model. Hence, there is a trade-off between the *fidelity of predictions* and the *number of model parameters*. In other words, higher fidelity is often achieved at the expense of a larger number of model parameters.

Since Johnston and Gilman's pioneering work (Johnston and Gilman, 1959) on physics-based description of the inelastic behavior of Lithium Fluoride (LiF) crystals, physics-based material models have become remarkably sophisticated in capturing underlying microscale deformation mechanisms. In recent years, the use of physics-based material models in FEM-based cutting models has received attention from researchers. Ding and Shin (2011) adopted the dislocation based material model developed by Estrin et al. (1998) and Tóth et al. (2002) (*ET model*) to simulate the chip formation and grain refinement in orthogonal cutting of commercially pure Ti (cp-Ti). Considering the dislocation cell structure as a precursor for the evolving grain structure and similar to Estrin and Kim (2007)'s work on Equal Channel Angular Pressing (ECAP), Ding and Shin traced the evolution of cell size during orthogonal cutting of cp-Ti to model the corresponding grain refinement. However, a key limitation of the ET model is that it assumes the existence of an established dislocation cell structure prior to deformation and consequently is only strictly valid for materials that have undergone sufficient straining for a cell structure to develop (Lemiale et al., 2010). Moreover, the cell/grain size in the ET model is formulated as $d = K/\sqrt{\rho_{tot}}$ where K is a constant and ρ_{tot} is the total dislocation density in the cell interior and walls. This implies that the cell/grain refinement will occur even in the absence of dynamic recrystallization if the combination of hardening and dynamic recovery mechanisms causes a net increase in ρ_{tot} . Ding et al. (2011) also applied the ET model to predict chip formation and grain refinement in orthogonal cutting of OFHC Cu under different cutting conditions. Similarly, Ding and Shin (2013) and Ding et al. (2013) used the ET model and associated dislocation density and grain size evolution laws to predict the microstructure evolution in machining of bearing steels and Al 6061-T6 alloy.

Noting that the *initial* hardness of AISI 52100 bearing steel has a major influence on the strain hardening response of the material, Umbrello et al. (2004) developed a *phenomenological* hardness-based flow stress model to simulate the orthogonal hard turning of bearing steel. They assumed the hardness to be independent of the strain and strain rate and unaffected by the high temperature in the shear zone. Therefore, the *initial* hardness of the material was used in the flow stress model and no hardness evolution with deformation was considered. The invariance of hardness contradicts other experimental evidence of severe grain refinement, phase transformation, and even hardness evolution in the machined surface reported in the literature (Ramesh and Melkote, 2008; Ramesh et al., 2005). Later, Umbrello and Filice (2009) and Umbrello (2011) introduced two *phenomenological* hardness evolution laws, termed *quenching* and *tempering*, to be used in conjunction with the hardness-based flow stress model. This model

was further enhanced by Caruso et al. (2011) to trace the grain size evolution via a Zener-Hollomon parameter (Z) based relationship reported by Yanagimoto et al. (1998) (i.e. $D = D_0 \beta Z^m$; where β and m are constants and D_0 is the initial grain size). According to this relationship, dynamic recrystallization (DRX) occurs whenever the equivalent plastic strain is larger than a critical strain (ε_{cr}) defined as $\varepsilon_{cr} = \varsigma \sqrt{D_0} Z^n$ where ς and n are constants. However, the grain size evolution in this model still does not have an explicit effect on the flow stress.

Rotella et al. (2012) used the same relationship as Caruso et al. to capture DRX in dry turning of AA7075-T651 alloy. Additionally, they applied a Hall-Petch type relation reported by Hughes et al. (1986) (i.e. $H = C_0 + C_1/\sqrt{D}$; where C_0 and C_1 are constants) to trace the hardness evolution as a result of grain refinement. The latter clearly indicates that the hardness is seen as a microstructure dependent characteristic. Also, a Zener-Hollomon parameter based flow stress model reported by Sheppard et al. (1982) (i.e. $Z = A(\sinh \alpha \sigma)^n$ where A , α , and n are constants) was used as the constitutive law. As a result, the strain and microstructure dependence of flow stress is neglected in this model. Pu et al. (2013) also adopted Yanagimoto's method to account for DRX along with the purely phenomenological Johnson-Cook flow stress model (Johnson and Cook, 1983) to simulate microstructure evolution in dry and cryogenic machining of AZ31B Magnesium alloy. Svoboda et al. (2010) adopted the physics based plasticity model developed by Lindgren et al. (2008) to simulate the orthogonal cutting of 316L stainless steel alloy. Their model is based on the dislocation glide mechanism and the flow stress is formulated as the summation of resistance to dislocation motion imposed by short range (*thermal stress*) and long range (*athermal stress*) obstacles. The dislocation density and vacancy concentration were taken as internal state variables (ISVs) and the flow stress was expressed as an explicit function of these microstructure-based ISVs. In addition, the evolution of ISVs with inelastic deformation was captured via two evolution equations. However, no evolution equation was derived for the grain size, which is indicative of the absence of grain refinement due to dynamic recrystallization effects.

To address the deficiencies of previous models, Liu et al. (2014a) recently developed a unified material model that explicitly integrates microstructure evolution (particularly due to DRX) into the constitutive law in order to describe the macro-scale material behavior during inelastic deformation. The unified model was built upon the knowledge that macro-scale inelastic deformation is the result of micro-scale interactions between mobile dislocations and various short and long range barriers. Average dislocation density and grain size evolutions laws were also formulated enabling the prediction of microstructure of the chip and machined surface. Later, Liu et al. (2014b) implemented their model in orthogonal cutting simulations to predict the cutting forces, strain field, and machining induced microstructure evolution with reasonable accuracy. However, model validation was limited to low cutting speeds where the average shear strain rate in the primary shear zone is estimated to be of the order of only $10^3/s$.

It is noted that, depending on the cutting speed, strain rates of up to $10^6/s$ can be generated in machining (Shaw, 1984). At such high deformation rates, an intensified strain rate sensitivity is often observed in the form of a sharp upturn in the flow stress versus strain rate plot, as shown in Figure 1. While an *enhanced rate of accumulation of dislocations* is reported (Follansbee and Kocks, 1988; Zerilli and Armstrong, 1992) as the primary microstructural cause for the increased strain rate sensitivity in the elbow region ($10^3 \sim 10^4/s$) in Figure 1, *dislocation drag* is considered

as the plausible microstructural cause for the increased strain rate sensitivity at higher strain rates. Dislocations can experience a drag force due to their interaction with lattice phonons and electrons as they move in the crystal lattice. This drag force may become significant at large strain rates where dislocations need to move quickly to accommodate the macroscale inelastic deformation imposed on a metal. Follansbee and Weertman (1982) estimated that the strain rate should be as high as $10^5/s$ to $10^6/s$ in a metal before dislocation drag can have a significant influence on the flow stress. The strain rate at which transition from thermal activation to drag-controlled deformation occurs is sensitive to mobile dislocation density (Regazzoni et al., 1987). Nemat-Nasser and Guo (2000) and Guo and Nemat-Nasser (2006) included the effect of dislocation drag in their physics-based material model by adding a third term to the constitutive formulation derived from thermal activation theory in order to describe the high strain rate response of commercially pure vanadium and nitronic-50 stainless steel. The grain size in the Nemat-Nasser et al. model is the initial grain size and does not evolve with the progression of inelastic deformation accompanied by continuous DRX; however, the developed unified model (Liu et al., 2014a) takes into account the evolution of microstructure via two evolutions laws and the magnitudes of dislocation density and grain size are updated iteratively with the progression of deformation.

Fig. 1 Strain rate sensitivity of OFHC Copper at room temperature and 15% strain (Regazzoni et al., 1987).

Under the premise that the inclusion of dislocation drag in the constitutive law will yield a more accurate description of deformation physics prevalent in metal cutting, Wedberg et al. (2012) modified the Lindgren model (Lindgren et al., 2008) by adding a third term representing the dislocation drag effect to the constitutive law derived from thermal activation theory and used the modified model to simulate orthogonal cutting of 316L stainless steel. The modified model still demonstrated poor predictive capability when extrapolated to strain rates higher than those common in dynamic loading experiments such as split Hopkinson pressure bar (SHPB) test. This deficiency was attributed to the inability of the Lindgren model to capture strain softening due to dynamic recrystallization at large strains.

In this paper, the unified model previously reported by Liu et al. (2014a) and validated for the low cutting speed regime, is modified to include the dislocation drag effect, which is expected to be active at high cutting speeds. The modified model is then calibrated and implemented in a commercial FEM-based machining simulation software AdvantEdge, which is used to simulate orthogonal cutting of OFHC Copper. The predicted cutting forces are compared with measurements to evaluate its effectiveness. The model is also used to analyze the cutting induced evolution of microstructure and deformation field parameters via microstructure-deformation maps.

2. The Physics-Based Unified Model with Dislocation Drag Effect

The physics-based unified material model developed by Liu et al. (2014a) is presented briefly and modified to include the dislocation drag effect. The unified model is a constitutive description of the material behavior as an explicit function of internal state variables (ISVs), i.e. grain size and dislocation density, coupled with corresponding evolution laws for the ISVs. A similar approach has been adopted by Picu and Majorell (2002), Nes and Marthinsen (2002), and Ding et al. (2011). According to the thermal activation theory (Kocks et al., 1975), the flow stress can be formulated as a superposition of an athermal (σ_a) and a thermal (σ_{th}) stress. The thermal activation controlled deformation is expected to be dominant so long as the deformation rate in the spatial domain of deformation is of the order of $10^3/s$ or less. However, in machining at high cutting speeds, strain rates of the order of 10^4 - $10^6/s$ can occur in the primary shear zone. Therefore, a transition from thermal activation to drag-controlled deformation is expected as the deforming material passes through the primary shear zone. To accommodate such a wide range of strain rates and the corresponding deformation mechanisms, a dislocation drag (σ_d) component is added to the flow stress formulation obtained from thermal activation theory to yield the following constitutive description The effect of dislocation drag is often singled out among other microstructural effects and added as a third component to the formulation derived from thermal activation theory (Guo and Nemat-Nasser, 2006; Kapoor and Nemat-Nasser, 2000; Nemat-Nasser and Guo, 2000; Wedberg et al., 2012):

$$\sigma = \sigma_{th} + \sigma_d + \sigma_a \quad (1)$$

The magnitude of σ_{th} depends on the strength of interactions between mobile dislocations and short-range barriers (e.g. interstitial impurities, substitutional alloying elements, precipitates, other dislocations, etc.). This stress component is formulated using the Kocks and Mecking (KM) model (Kocks, 1976; Mecking and Kocks, 1981) as follows:

$$\sigma_{th} = \left[1 - \left(\frac{kT}{g_0 \mu b^3} \ln \left(\frac{\dot{\epsilon}_0}{\dot{\epsilon}} \right) \right)^{1/q} \right]^{1/p} \sigma_0 \quad (2)$$

Where, k is the Boltzmann's constant, T is the temperature, g_0 is the normalized activation energy at 0 K, μ is the shear modulus, b is the magnitude of the Burgers vector, $\dot{\epsilon}_0$ is a reference strain rate, σ_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

variation of the shear modulus μ with temperature is modeled using Eqn. (3) (Follansbee and Gray, 1991) as follows:

$$\mu = \mu_0 - \sqrt{a + (T/T_r)^2} \quad (3)$$

Where μ_0 is the shear modulus at 0 K and a and T_r are material constants. Experimental observations suggest that the macroscopic flow stress (σ) typically varies linearly with strain rate over deformation rates where dislocation drag is expected to be the deformation controlling mechanism (Regazzoni et al., 1987). Hence, the dislocation drag component of flow stress is formulated as follows:

$$\sigma_d = \alpha_d \dot{\epsilon} \quad (4)$$

where α_d is the dislocation (viscous) drag coefficient. The athermal component of flow stress is derived from the interaction of mobile dislocations with long range obstacles such as grain boundaries and dislocation forests. This component is formulated in Eqn. (5) as the sum of stresses required to overcome the strain fields of dislocation forests, σ_ρ , and grain boundaries, σ_G , by an individual dislocation:

$$\sigma_a = \sigma_\rho + \sigma_G = \alpha_\rho \mu b \sqrt{\rho} + \alpha_G \mu \sqrt{\frac{b}{D}} \quad (5)$$

Here α_ρ and α_G are taken as constant parameters related to the strengths of dislocation-dislocation forest and dislocation-grain boundary interactions, respectively. The internal state variables, ρ and D , evolve during plastic deformation and knowing their values at each strain increment, the flow stress can be calculated by superposing the thermal, dislocation drag, and athermal components as indicated by Eqn. (1). The evolution law for dislocation density can be derived as follows (Liu et al., 2014a):

$$\rho_{H \& DRV} = \left[\frac{A}{B} + \left(\sqrt{\rho_0} - \frac{A}{B} \right) \exp \left(-\frac{B\epsilon}{2} \right) \right]^2 \quad (6)$$

In the above equation, A and B are the *hardening* (due to dislocation production) and *recovery* (due to dislocation annihilation) parameters, respectively. Additionally, ρ_0 is the initial dislocation density and $\rho_{H\&DRV}$ is an intermediate dislocation density determined by the competing hardening and dynamic recovery processes. Following Estrin and Mecking (1984), A was considered to be constant and B to be a temperature and strain rate dependent term as follows:

$$B = (B_1(T) + B_2(\dot{\epsilon}))^{B_3(T)} \quad (7)$$

$$B_1 = b_0 + b_1 T \quad (8)$$

$$B_2 = b_2 \log_{10} \dot{\epsilon} \quad (9)$$

$$B_3 = b_3 + b_4 T \quad (10)$$

To capture the grain size evolution during plastic deformation, the following phenomenological model was introduced by Liu et al. (2014a):

$$D = D_f + (D_0 - D_f) \tanh\left(\frac{\varepsilon_r}{\varepsilon}\right)^u \quad (11)$$

where ε_r is the critical strain at which DRX occurs, u is a temperature and strain rate dependent fitting parameter controlling the DRX rate, D_0 is the initial grain size, and D_f is the final recrystallized grain size:

$$\varepsilon_r = \varepsilon_0 (\log_{10} \dot{\varepsilon} + \varepsilon_1) e^{(\varepsilon_2/T^{\varepsilon_3})} \quad (12)$$

$$u = u_0 (\log_{10} \dot{\varepsilon} + u_1)^{u_2} e^{(u_3/T^{u_4})} \quad (13)$$

$$D_f = 10^{(C_z - m \log_{10} Z)} \quad (14)$$

Where ε_i ($i = 0 \dots 3$), u_j ($j = 0 \dots 4$), C_z and m are fitting parameters. The Zener-Hollomon parameter (Z) in Eqn. (14) is defined as follows:

$$Z = \dot{\varepsilon} e^{\left(\frac{Q}{RT}\right)} \quad (15)$$

Where Q is the activation energy for lattice self-diffusion and R is the gas constant. During DRX, dislocations are consumed to form new grain boundaries and, therefore, besides σ_G , the dislocation density and associated strengthening component (σ_ρ) are also impacted. Liu et al. (2014a) assumed that the DRX-induced change in dislocation density is proportional to the change in grain surface area per unit volume (S) as follows:

$$\Delta \rho_{DRX} = -K(\dot{\varepsilon}, T) \Delta S = K(\dot{\varepsilon}, T) \left[\frac{2}{D_0} - \frac{2}{D} \right] \quad (16)$$

$$K = K_0 (\log_{10} \dot{\varepsilon} + K_1)^{(K_2 + K_3 T)} \quad (17)$$

Where K is a proportionality parameter defining the saturation stress level (where hardening, dynamic recovery, and dynamic recrystallization processes are in equilibrium) and K_j ($j = 0 \dots 3$) are fitting parameters.

3. Calibration Procedure for the Modified Unified Material Model

Although a core idea in the development of physics-based models is to obviate the need for calibration and instead deal with material constants rather than model parameters, very often one needs to implement phenomenological descriptions for some parameters, e.g. hardening or recovery terms, that arise during model derivation. Therefore, partial calibration is inevitable even for physics-based models. In this section, the proposed model is calibrated for Oxygen-Free High Conductivity (OFHC) copper with 99.99% purity level. The initial grain size, D_0 , and dislocation density, ρ_0 , were taken to be 62 μm (Tanner and McDowell, 1999) and 10^{10} m^{-2} (Kitajima et al., 1974), respectively. The temperature dependent shear modulus of OFHC copper for $T > 100 \text{ K}$ is as follows (Follansbee and Gray, 1991):

$$\mu(T)[\text{GPa}] = 47.10 - \sqrt{0.14 + (T/60.16)^2} \quad (18)$$

In Eqn. (5), the Hall-Petch coefficient, i.e. $\kappa_G = \alpha_G \mu(T) \sqrt{b}$, was taken to be temperature dependent (Fu et al., 2008) wherein the Burgers vector magnitude (b) is 2.57×10^{-10} m. According to Hou et al. (2008) and Smith and Hashemi (2006) κ_G is equal to $\sim 100 \text{ MPa} \cdot \sqrt{\mu\text{m}}$ for annealed OFHC copper at room temperature. Replacing κ_G , μ , and b with appropriate values in the above formulation for the Hall-Petch coefficient, α_G was calculated to be 0.15 and assumed to be temperature independent. The thermal component of flow stress in Eqn. (2) adds five parameters (i.e. $\dot{\epsilon}_0$, p , q , g_0 , and σ_0) to the calibration process. The values for these parameters were taken to be equal to those reported by Nemat-Nasser and Li (1998) for annealed OFHC copper as follows: $\dot{\epsilon}_0 = 2 \times 10^{10}/\text{s}$, $p = 2/3$, $q = 2.0$, $\sigma_0 = 46 \text{ MPa}$, and $k/g_0 \mu b^3 = 5 \times 10^{-5} \text{ K}^{-1}$. The strength of dislocation-dislocation forest interactions, α_p , is temperature and rate dependent and is less than unity (i.e. $0 < \alpha_p < 1$). However, the temperature and rate dependency of α_p was assumed to be negligible at this stage of the calibration process and initialized to 0.5.

The next step is to calibrate the dislocation density and grain size evolution laws starting with the hardening (A) and recovery (B) parameters of the dislocation density evolution law in Eqn. (6). This portion of dislocation density evolution stems from the dislocation production (storage) and annihilation mechanisms in the absence of dynamic recrystallization. This is synonymous with $D = D_0$, $\Delta\rho_{\text{DRX}} = 0$, and $\sigma_G = \text{Const.}$ To eliminate the effect of DRX on the evolution of dislocation density, only portions of the experimental stress-strain curves (Tanner and McDowell, 1999) where the plastic strain is less than the critical strain (ϵ_r) were used. Additionally, since the strain rates in the selected stress-strain data are low, i.e. $0.004 \sim 1/\text{s}$, the dislocation drag stress component was expected to be negligible, i.e. $\sigma_d = 0$. Moreover, the thermal stress is constant ($\sigma_{th} = \text{Const.}$) since it is not strain dependent. For this choice of experimental stress-strain data, the only remaining stress component in the unified model that can vary with strain is σ_p . To calibrate A and B_i ($i = 1, 2, 3$) five stress-strain curves at different temperatures and strain rates were used to obtain the best fit model parameters listed in Table 1. The variation of final recrystallized grain size, D_f , with temperature and strain rate in Eqn. (14) is as follows (Kim et al., 2012):

$$D_f = 10^{(2.64 - 0.17 \log_{10} Z)}$$

The activation energy for lattice self-diffusion, Q , and the gas constant, R , were taken as 146.04 kJ/mol (Kim et al., 2012) and $8.314 \text{ J K}^{-1} \text{ mol}^{-1}$, respectively, in Eqn. (15) defining the Zener-Hollomon parameter, Z . To calibrate ϵ_r , the critical strain at which DRX occurs, and u , the DRX rate controlling parameter, in the grain size evolution law, Eqn. (11), the same set of experimental stress-strain curves used in the calibration of the hardening and dynamic recovery parameters were used except that the plastic strain was allowed to exceed the critical strain (ϵ_r) so that the effect of dynamic recrystallization present in the experimental data would be captured (this is equivalent to $D \neq D_0$, $\Delta\rho_{\text{DRX}} \neq 0$, and $\sigma_G \neq \text{Const.}$). At the macroscopic scale, dynamic recrystallization manifests itself as a flow softening behavior in the flow stress curves at large plastic strains (Blaz et al., 1983), as seen in Figure 2a. The critical strain, ϵ_r , can be readily determined from the stress-strain curves where the peak stress occurs. Revisiting Eqn. (11), it is seen that for each combination of strain rate and temperature, the DRX rate controlling parameter, u , is the only unknown left in the equation. Knowing ϵ_f , the strain value at which dynamic recrystallization effect saturates, u can be uniquely specified using Eqn. (11); ϵ_f can be determined from the stress-strain curves as the strain at which the flow stress reaches a plateau (Figure 2a). Such a plateau, occurring at large strains, is assumed to be associated with saturation

of DRX and termination of the grain refinement process (wherein the average grain size is D_f , see Figure 2b). Repeating the preceding steps, new sets of ε_r and u can be obtained for different combinations of strain rate and temperature (see Figure 2c). The data sets generated thus were used to calibrate $\varepsilon_r = \varepsilon_r(\dot{\varepsilon}, T)$ and $u = u(\dot{\varepsilon}, T)$ in Eqns. (12) and (13), respectively, by finding a set of ε_i ($i = 0 \dots 3$) and u_j ($j = 0 \dots 4$) parameters that yield the best fit to the $(\dot{\varepsilon}, T, \varepsilon_r)$ and $(\dot{\varepsilon}, T, u)$ data sets (see Figure 2d). The calibrated ε_i and u_j parameters are listed in Table 1.

Fig. 2 Schematic representation of the calibration procedure for the critical strain, ε_r , and the DRX rate controlling parameter, u , in the grain size evolution law.

The viscous drag coefficient, α_d in Eqn. (4), was calibrated using data extracted from the flow stress versus strain curves reported by Tanner and McDowell (1999) and Nemat-Nasser and Li (1998) (see Figure 3). Since the data used for calibrating the drag coefficient were obtained from low strain deformations ($\varepsilon < \varepsilon_r$), the effect of DRX on the data is assumed to be negligible. The absence of DRX translates into $D = D_0$ (or $\sigma_G = \text{Const.}$) and $\Delta\rho_{DRX} = 0$. Knowing that σ_{th} , σ_p , and the dislocation density evolution law in the absence of DRX are all calibrated prior to this step, the dislocation drag stress, σ_d , with only one unknown parameter (i.e. α_d), can be calibrated by tuning the viscous drag coefficient in the modified model to obtain the best fit to the experimental data, which results in $\alpha_d = 20$ kPa.s. As seen in Figure 3, the modification of the unified model by including dislocation drag enables it to capture the intensified strain rate sensitivity above a strain rate of $\sim 10^3$ /s.

Fig. 3 Calibration of the dislocation (viscous) drag coefficient in the modified unified model for OFHC Cu using the experimental data obtained from low strain deformations.

The last step is to calibrate the DRX-induced evolution of dislocation density in Eqn. (16). For this, the same set of experimental stress-strain curves used in calibration of the grain size evolution law wherein the plastic strain was allowed to be larger than the critical strain (ϵ_r) to account for DRX, was used in conjunction with a single cutting force data. In fact, the proportionality parameter, K , defining the saturation stress level (where hardening, dynamic recovery, and dynamic recrystallization are in equilibrium) could have been calibrated simultaneously with ϵ_r , the critical strain, and u , the DRX rate controlling parameter. However, this calibration was intentionally delayed until this juncture for the following reason. As noted earlier, DRX occurs in large strain deformations (where $\epsilon > \epsilon_r$). The strains and strain rates associated with the stress-strain data reported for OFHC Copper are limited to < 1 and $\sim 10^3/s$, respectively. However, the deformation in the primary shear zone in *high speed* cutting operations is characterized by large strains (> 1) and high strain rates ($10^4 \sim 10^6/s$). Experimental observations have confirmed the presence of DRX even under such severe deformation conditions (Brown et al., 2009). This suggests that among all the parameters in the unified model, K is the one best suited for adjustment in order to capture the evolution of microstructure over the *broad range* of strain rates characteristic of machining. Unfortunately, the stress-strain data generated from dynamic compression experiments (e.g. SHPB) do not replicate the deformation conditions typical of *high speed* cutting operations, particularly the combination of high strains and high strain rates at which DRX occurs in machining. Therefore, in order to capture the material behavior at high strains and high strain rates, it was decided to use a limited number of cutting force data in conjunction with the available stress-strain data for large strain and low strain rate conditions to calibrate the parameter K in the dislocation density evolution law.

Specifically, the available stress-strain curves corresponding to large strain, low strain rate conditions, used previously for calibration of the grain size evolution law, were used and the parameter K was tuned iteratively to achieve the best fit to the stress-strain data for each combination of strain rate and temperature. In doing so, a set of $(\dot{\epsilon}, T, K)$ data points were generated for the low strain rate deformation regime. Prior to generating similar data points for the large strain, high strain rate deformation regime, the modified material model was implemented as a user-defined material subroutine in the finite element model for orthogonal cutting (details presented in the next section) and cutting forces derived from a single *high speed* orthogonal cutting simulation were used to tune the parameter K till the predicted forces matched the measured cutting forces. This procedure yielded an extra $(\dot{\epsilon}, T, K)$ data point corresponding to the large strain, high strain rate deformation regime. Next, the generated $(\dot{\epsilon}, T, K)$ data sets were used to calibrate $K = K(\dot{\epsilon}, T)$ in Eqn. (17) by finding a set of K_j ($j = 0 \dots 4$) parameters that yielded the best fit. The calibrated K_j parameters are listed in Table 1. [Figure 4 shows a comparison of the calibrated model with and without drag against the experimental flow curves over a range of strains, strain rates, and temperatures. It can be seen that the model with drag follows the experimental data more closely than without drag thereby validating the model.](#)

Table 1. Calibrated unified model parameters for OFHC Copper

Parameter	Value	Parameter	Value
A [1/m]	6.80×10^8	u_0	5.809×10^{-3}
b_0	0.052	u_1	20.26
b_1 [1/K]	-4.87×10^{-5}	u_2	2.278
b_2	2.51×10^{-3}	u_3	1.4×10^{-5}
b_3	-0.671	u_4	-1.768
b_4 [1/K]	-8.06×10^{-5}	K_0 [1/m]	5.616×10^{18}
ϵ_0	0.243	K_1 [1/m/K]	-68.27×10^{15}
ϵ_1	9.5	K_2	10
ϵ_2	-1.863×10^{-8}	K_3	-9.528
ϵ_3	-2.696	K_4 [1/K]	9.079×10^{-3}

Fig. 4 Calibrated model (solid and dashed lines) versus experimental data (symbols; data taken from Nemat-Nasser and Li (1998)).

4. Finite Element Model of Orthogonal Cutting

To simulate the *high speed* orthogonal cutting operation, a two-dimensional finite element model was developed in AdvantEdgeTM, a specialized commercially available machining simulation software. This software uses a standard Lagrangian formulation combined with a fully automatic adaptive remeshing algorithm to simulate chip formation without any chip separation criterion (Marusich and Ortiz, 1995). The cutting tool was assumed to be rigid and **the cutting edge radius was taken to be 20 μ m, typical of the sharp cutting tools** used in the experiments employed for model validation. The contact condition at the tool/chip interface was modeled using the Coulomb friction law. The coefficient of friction, β , at the tool-chip interface was calculated for each simulation case using the measured cutting, F_c , and thrust, F_t , force data and the equation $\beta = (F_t + F_c \tan \alpha) / (F_c - F_t \tan \alpha)$ where α is the rake angle. The length of cut was sufficiently long ($L=15$ mm) to ensure that a steady state cutting condition, defined as unchanging cutting forces and chip morphology, was established. The thermo-mechanical properties of the

workpiece material used in the model are listed in Tables 2 and 3. Constrained by the high computation costs, the minimum element size was limited to about 0.02 mm. A user-defined material subroutine was developed using the FORTRAN language to implement the calibrated material model in AdvantEdge™. Orthogonal cutting simulations were performed to replicate the physical cutting tests carried out by Saldana and Chandrasekar (unpublished data) on high purity copper (99.999%; $D_0 = 900\mu\text{m}$) with zero rake angle (α), 213 μm depth-of-cut (DoC), and a range of cutting speeds (V_c) of 10.3, 26.6, 103.3, 147.6, 265.7 m/min.

Table 2 Physical properties of copper (Lampman, 1990)

E (GPa)	G (GPa)	ν	ρ (kg/m ³)	T_m (°K)
116	48	0.34	8960	1356

Table 3 Thermal parameters of copper at various temperatures (Lide, 2010; Touloukian, 1970)

Temperature (°K)	Thermal Conductivity (W/m/K)	Specific Heat (J/kg/K)	Thermal Expansion Coefficient (1/K)
200	413	356	15.2×10^{-6}
250	406	374	N/A*
300	401	385	16.5×10^{-6}
350	396	393	N/A*
400	393	399	17.6×10^{-6}
500	386	408	18.3×10^{-6}
600	379	417	18.9×10^{-6}
800	366	433	20.3×10^{-6}

* N/A: Not Available.

5. Results and Discussion

5.1. Dislocation Drag Effect on Cutting Model Predictions

The dislocation drag, as discussed before, can have a significant effect on the flow stress at strain rates higher than 10^3 - 10^4 /s, which are common in machining at high cutting speeds. The latter is evident from the simulation results listed in Table 4 wherein the cutting force, thrust force, maximum cutting temperature, chip thickness, and shear angle are compared for cases with and without dislocation drag effect. It is seen that model predictions for the case where dislocation drag effect is taken into account are in better agreement with experimental measurements provided by Chandrasekar and Saldana than the case without dislocation drag. As expected, such difference in cutting model performance with and without dislocation drag effect is negligible for low cutting speed cases.

Table 4 Predicted results with and without dislocation drag effect compared with experimental data provided by Chandrasekar and Saldana (cutting speed $V_c = 103.3$ m/min, rake angle $\alpha = 0^\circ$ and depth-of-cut $DoC = 213\mu\text{m}$)

	Without Drag	With Drag	Exp. Data
Cutting Force, F_c (N)	2420	1440	1393
Thrust Force, F_t (N)	1380	800	807
Max. Temperature ($^\circ\text{C}$)	299	244	N/A*
Chip Thickness (mm)	2.5	1.1	1.4
Shear Angle ($^\circ$)	4.9	10.9	8.4

* N/A: Not Available.

5.2. Predicted vs. Measured Cutting and Thrust Forces

Figure 5 shows a comparison of the predicted forces with measured values over the range of cutting speeds used in the experiments. Note that the cutting force data for the 103.3 m/min cutting speed was the only one used in calibrating the parameter K in Eqn. (16). It can be seen that the predicted trends and magnitudes of the cutting and thrust forces are in good agreement with the measured values over the entire range of cutting speeds. As expected, the decreasing trend in force magnitudes with cutting speed is due to the increased rate of heat generation associated with higher deformation rates and the accompanying thermal softening effect.

Fig. 5 Measured (Chandrasekar and Saldana) and predicted cutting and thrust forces for orthogonal cutting of high purity copper (99.999% pure, $D_0 = 900\mu\text{m}$) over a broad range of cutting speeds (deformation rates); Rake angle, α , and depth-of-cut, DoC , are 0° and $213\mu\text{m}$, respectively.

It is noted that the unified material model was almost entirely calibrated using stress-strain data for OFHC copper with 99.99% purity level and $62\mu\text{m}$ initial grain size, D_0 . However, the material used in the cutting experiments was a high purity copper (99.999% pure) with $900\mu\text{m}$ initial grain size. Hence, it seems reasonable to expect the test material to be mechanically softer

than the model material. This could explain the higher predicted cutting force value at the lowest cutting speed, where the quasi-static deformation rates and low cutting temperatures magnify the effect of dislocation interactions with short range barriers such as impurities. However, based on the physics of continuous DRX and dislocation drag, the discrepancy in initial grain size is not expected to have a noticeable effect on DRX or drag.

At the highest cutting speed, the dislocation drag effect is expected to be the dominant deformation controlling mechanism. Since the temperature dependency of dislocation drag (Regazzoni et al., 1987) can be significant at the high temperatures achieved in high speed cutting, the observed discrepancy in the predicted and measured cutting forces at the highest cutting speed may stem from the fact that the drag (viscous) coefficient in Eqn. (4) was taken to be a constant rather than a temperature dependent parameter. Considering the preceding discussion and noticing the broad range of cutting speeds over which the validation was exercised, the fidelity of model predictions appears to be quite good. The chip morphology is another metric used to appraise the validity of the simulations. The model predicts continuous chip morphology, as seen in the contour plots shown in Figures 6 and 7, which is corroborated by the observations made by Dr. Chandrasekar's group in their experiments on copper (Brown et al., 2002; Lee et al., 2005).

In the following section, the orthogonal cutting model is used to analyze the correlation between process parameters (cutting speed), deformation parameters (strain, strain rate, temperature), and microstructure (grain size and dislocation density) evolution.

5.3. Cutting Induced Evolution of Microstructure

The unified material model enables the prediction of microstructure evolution as the deforming material passes through various regions in the deformation field. As seen in Figure 6, the model does quite well in predicting the experimentally observed trend (Ni and Alpas, 2003; Swaminathan et al., 2005) of severe grain refinement in machining, ranging from several hundreds of micrometer before the primary shear zone (PSZ) to several tens of micrometer in the PSZ and a few micrometers after the PSZ and well into the chip. Another observation, not readily available through microscopy, is the presence of a gradient in the grain size across the chip (deformed material) thickness. Particularly, a deformed layer of submicron (nano-) sized grains is predicted by the model in the secondary deformation zone (SSZ) in the vicinity of the tool/chip interface. As the cutting speed increases, the thickness of this highly grain refined layer decreases and the grains become coarser in the chip. At higher deformation rates, the thermally activated annihilation of dislocations is expected to be more pronounced due to the higher cutting temperatures generated, which can explain the predicted grain coarsening. Also shown in Figure 6 is the evolution of dislocation density in the deformation field. It is seen that the dislocation density increases as the material approaches the PSZ and, when in the chip, it exhibits a gradient across the thickness. This dislocation density gradient across the chip thickness is consistent with the corresponding gradient in grain size, i.e. the regions with finer grain size are characterized by lower dislocation density due to continuous DRX. The evolutions of grain size and dislocation density are co-occurring events during continuous DRX. The gradient in intensity of DRX from the secondary shear zone to the chip free surface results in comparatively lower dislocation density and finer grains in the secondary shear zone since dislocations are annihilated during

DRX leading to grain refinement. This observation is consistent with the underlying physics of *continuous* DRX (Gourdet and Montheillet, 2003). During severe plastic deformation and as DRX occurs, low angle grain boundaries (LABs) nucleate and their misorientation angles grow due to dislocation production and accumulation mechanisms until those LABs transition into high angle grain boundaries (HABs) and form new grains (Gourdet and Montheillet, 2003).

Fig. 6 Cutting induced evolution of grain size and dislocation density in OFHC copper over a broad range of cutting speeds.

5.4. Evolution of Deformation Parameters in Orthogonal Cutting

Figures 7a, 7c, and 7e map the strain, strain rate, and temperature evolution in the spatial domain of deformation in orthogonal cutting for a representative case, i.e. 103.3 m/min. The strain field shows that the material is severely deformed as it passes through the PSZ with some additional deformation in the SSZ resulting in a descending gradient in the plastic strain across the chip thickness moving away from the tool/chip interface. The deformation rate peaks at the PSZ, as shown in the strain rate field, while it is not distributed uniformly across this region and reaches

its maximum value in the close proximity of the cutting edge. According to the temperature field, the cutting temperature increases as the deforming material passes through the PSZ with additional temperature rise in the proximity of the tool/chip interface in the SSZ due to frictional heat generation. The preceding qualitative observations of the strain, strain rate, and temperature fields are consistent with current understanding of the mechanics of evolution of the deformation field parameters in machining and hence confirm the ability of the complex model to accurately describe expected behavior.

Fig. 7 Evolution of deformation parameters in orthogonal cutting of high purity copper (rake angle $\alpha = 0^\circ$ and depth-of-cut $DoC = 213\mu\text{m}$); (a, c, e) representative plastic strain, strain rate, and temperature fields; (b, d, f) evolution of plastic strain, strain rate, and temperature along path ABC for different cutting speeds; (g) shear strain versus shear angle variation according to classical theory of cutting; (h) evolution of Zener-Hollomon parameter along path ABC for different cutting speeds.

It is, however, expected that a quantitative analysis of strain, strain rate, and temperature fields can provide further insight into the evolution of the deformation parameters as the material approaches the PSZ, passes through the PSZ, and enters the chip. To do so and as shown in Figures 7a, 7c, and 7e, an imaginary path *ABC* was defined in the spatial domain of the deformation field and the strain, strain rate, and temperature evolutions from point *A* to point *B* and finally to point *C* were examined. It is seen in Figure 7b that the strain gradually increases as it approaches the PSZ, rises sharply as it passes through the PSZ, and, as expected, levels off at an almost constant value in the chip. Another observation made from model predictions is that the strain level, particularly in the chip, decreases at higher cutting speeds. The latter is also corroborated by the classical theory of cutting mechanics (Merchant, 1945) as follows. According to this theory, the average strain, ε , in the chip can be approximated using the following equation

$$\varepsilon = \frac{\gamma}{\sqrt{3}} = \frac{1}{\sqrt{3}} \cdot \frac{\cos \alpha}{\sin \phi \cos(\phi - \alpha)}$$

Where γ is the average shear strain, α is the tool rake angle, and ϕ is the shear plane angle. For the cases considered here, the rake angle is zero. Hence, the above equation reduces to

$$\varepsilon = \frac{\gamma}{\sqrt{3}} = \frac{1}{\sqrt{3}} \cdot \frac{1}{\sin \phi \cos \phi}$$

Plotting the above equation in Figure 7g over a wide range of hypothetical shear angles reveals that the average strain in the chip decreases as the shear angle increases. Therefore, it seems that higher cutting speeds should be associated with larger shear angles for the model predictions of the average chip strain in Figure 7b to be accurate. Revisiting the contour plots in Figure 6 reveals that, indeed, the shear angle is larger for higher cutting speeds. The latter can be explained by noting that higher strain rates and lower cutting temperatures before the PSZ at higher cutting speeds, as seen in Figures 7d and 7f, render the material mechanically stronger since strain rate hardening is expected to prevail over thermal softening in the region before the

PSZ. On the other hand, it is known that mechanically stronger materials deform over larger shear angles in orthogonal cutting. Hence, the higher the cutting speed, the larger the shear angle.

While the presence of higher strain rates in and around the PSZ at higher cutting speeds, as seen in Figure 7d, is intuitive, the observed trend in corresponding temperature gradients, seen in Figure 7f, is not and requires further elaboration. According to Figure 7f, higher cutting speeds result in lower cutting temperatures before the PSZ while this trend is reversed after the PSZ. A plausible explanation for this observation is as follows. Since the material is severely sheared in the PSZ, a significant amount of heat generation is anticipated in the PSZ. At low cutting speeds, the heat generated in the PSZ will have more time to diffuse along the *BA* segment of the defined path in Figure 7e and hence the temperatures are anticipated to be higher compared to those at high speeds. However, after the PSZ and along the *BC* segment of the defined path, the lack of sufficient time for heat diffusion at high cutting speeds is compensated by more heat generation in the SSZ resulting in higher temperatures over the *BC* segment of the path. Additionally, an inflection point is present in Figure 7f. This interesting observation translates into the existence of a location right before the hypothetical shear plane where the cutting temperature does not change, notwithstanding the cutting speed magnitude.

Another interesting observation is the evolution of the Zener-Hollomon (*Z*) parameter in the cutting induced deformation field along the path *ABC*, as shown in Figure 7h. This parameter combines the evolution of strain rate and temperature and is larger for lower temperature, higher rate deformation. The latter is obvious from Figure 7h where *Log Z* decreases along the path. While higher cutting speeds are associated with larger *Z* values before the PSZ, the corresponding *Z* values are smaller after the PSZ, which is consistent with the observed evolutions of strain rate and the temperature fields along the path in Figures 7d and 7f and the definition of *Z* in Eqn. (15). It is seen that an inflection point exists on the hypothetical shear plane where the Zener-Hollomon parameter does not change, notwithstanding the cutting speed magnitude. This insight is expected to be beneficial in analyzing the deformed microstructures produced in the deformation zone where an understanding of the combined evolution of strain rate and temperature will be instrumental in explaining the observed microstructures and identifying favorable deformation conditions.

5.5. Correlation between Cutting Induced Microstructure and Deformation Parameters

The generation of maps correlating the process induced microstructure to deformation field parameters is essential for controlled production of a desired microstructure. The cutting process can be used to generate such maps since it can produce a broad range of strains, strain rates, and temperatures in a single pass of the cutting tool (Brown et al., 2009; Swaminathan et al., 2005). In this context, the model presented in this paper can be used to easily generate such maps in contrast to costly experiments. As discussed before, the deformation field can be characterized by the set of inelastic strains, ϵ , and Zener-Hollomon parameter, *Z*, values at any point in the deformation field. Maps, such as those shown in Figure 8, can be produced by tracing the evolution of the deformation parameters, i.e. ϵ and *Z*, and the resulting microstructure along imaginary paths, such as *ABC* in Figure 7, under different cutting conditions, in this case cutting speed. It is evident from Figure 8 that severe grain refinement occurs in the low Zener-Hollomon and high strain region of the map, which is associated with high dislocation density structure

compared to the undeformed material. The versatility of such maps stems from the fact that each value of Zener-Hollomon parameter can be achieved by a wide array of strain rate and temperature combinations, from low strain rate, high temperature deformations to high strain rate, cryogenic processes.

Fig. 8 Maps correlating the cutting induced microstructure to deformation field parameters.

6. Conclusions

A unified material model including the effect of dislocation drag, which is a deformation controlling mechanism at the deformation rates prevalent in high speed cutting operations, was presented and evaluated using orthogonal cutting simulations of OFHC Copper. The model was experimentally validated over a wide range of cutting speeds and shown to yield good results. The model also enabled the prediction of microstructure evolution as the deforming material passes through the deformation field. The model did quite well in predicting the commonly observed trend of severe grain refinement in orthogonal cutting of OFHC Cu. Cutting simulations carried out using the model showed that the strain level in the deforming material decreases, particularly in the chip, as the cutting speed increases, a trend that was found to be in accord with the classical theory of cutting mechanics. It was also shown that higher cutting speeds resulted in lower cutting temperatures in the deforming material before the primary shear zone (PSZ), while this trend is reversed after the PSZ. The latter observation was explained by the mechanics of heat generation and diffusion in and around the PSZ. Additionally, the Zener-Hollomon parameter was found to follow a decreasing trend when moving along a deformation path that passes through the PSZ and into the chip. An inflection point was identified on the shear plane where the Zener-Hollomon parameter did not change even with variation in cutting speed. It was also shown that versatile microstructure-deformation maps can be generated from the model. As demonstrated by Chandrasekar and his co-workers (Brown et al., 2009; Swaminathan et al., 2005), such maps can be very useful in identifying the deformation parameters necessary to engineer desired microstructures. In closing, the unified model was developed with the machining type application in mind; however, it is expected to work fine under other deformation regimes so long as strains, strain rates, and temperature do not surpass those transpiring in machining operations. Moreover, noting that formulations used for constitutive description and evolution laws are not lattice specific, the unified model should be

applicable to other lattice structures so long as the underlying physical mechanisms for inelastic deformation are identical. The applicability of the unified model to other lattice structures remains to be verified.

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