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### Microstructure Simulations for Orthogonal Cutting via a Cellular Automaton Model

#### Ninggang Shen, Avik Samanta, and Hongtao Ding\*

Department of Mechanical and Industrial Engineering, University of Iowa, Iowa City, Iowa 52242, USA

\* Corresponding author. Tel.: +1-319-335-5674. E-mail address: hongtao-ding@uiowa.edu (H. Ding)

#### Abstract

In this work, a Cellular Automaton (CA) model is for the first time developed to predict material microstructure evolution during cutting processes. Prior to the CA simulation, the dynamic thermomechanical loadings of work material, Aluminum Alloy 1100, induced by various orthogonal cutting conditions are simulated by finite element-based cutting models. Evolution of dislocation density is modeled using the CA model in MATLAB for the work material subjected to these loading conditions. Multiple mechanisms of microstructure evolution are coupled in the CA model including severe plastic deformation, dynamic recovery, dynamic recrystallization, and thermally-driven grain growth.

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Keywords: Cellular Automaton; Microstructure; Dynamic Recrystallization; Cutting; Severe Plastic Deformation

#### 1. Introduction

Recently, metal material microstructure change through the cutting process has generated a great interest among manufacturing research community [1–4]. During the cutting process, complex dynamic thermomechanical loading condition accompanied with severe plastic deformation (SPD) occurs inside the work material and often induces changes in work material microstructure. For some critical cutting conditions, high cutting process temperatures can reach 80-90% of the melting point ( $T_m$ ) for the work material, accompanying with a high plastic strain and a high strain rate on the order of  $10^4 \text{ s}^{-1}$ . Under these elevated temperatures, dynamic recrystallization (DRX) subjected to SPD is considered as a main mechanism for the microstructure evolution [1,3,5].

Modeling and simulations of microstructure evolution is critical to predict the mechanical properties of metal materials after machining. DRX kinetics and thermally-driven grain growth have been developed for various metal materials [6–10]. Finite Element (FE)-based process models are often implemented to model DRX and grain growth of homogenized work material during hot working processes [11,12]. Cellular Automaton (CA) method has also been applied to simulate the microstructure evolution governed by DRX during the hot forming processes of various metals [13–17].

However, it is still a great challenge to model the microstructure evolution governed by DRX during machining processes due to the highly dynamic thermomechanical loadings. Previous CA models mainly focused on quasi-static loading conditions or conditions with low strain rates. In recent years, phenomenological relationships using Zener–Hollomon and Hall-Petch equations have been applied in FE-based cutting simulations to predict the final grain size distribution [18–23]. However, these methods are unable to capture the intricate dynamic process of recrystallization or grain refinement process.

The dislocation density-based numerical framework developed by the authors has been the first known attempt to model microstructure evolution subjected to SPD during various cutting processes, typically for temperatures well below the initiation temperature of DRX [24–26]. In this framework,

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the internal state variables were used to evaluate the dislocation generation due to plastic deformation, dislocation annihilation by dynamic recovery, and interaction between the dislocation cell interiors and cell walls. Recently, dislocation density-based approach have been adapted by more researchers to predict the microstructure evolution in machining [27–31].

In this paper, a two-dimensional (2D) CA model is for the first time developed to model microstructure evolution during orthogonal cutting. Prior to the CA simulation, the dynamic thermomechanical loadings of work material, Aluminum Alloy 1100 (AA 1100), induced by various orthogonal cutting conditions are firstly simulated by a FE-based cutting models. Then, a new model of dislocation density evolution is developed using MATLAB for the work material subjected to these loading conditions. Multiple mechanisms of microstructure evolution are coupled through dislocation density dynamics in the CA model including SPD, dynamic recovery, DRX, and thermally-driven grain growth.

#### 2. Orthogonal Cutting Process Modeling

#### 2.1 Experiments

The orthogonal cutting experiments of AA 1100 investigated in this study were performed by Ni et al. [1] using ceramic cutting tool inserts with a rake angle of  $-5^{\circ}$  at a cutting speed of 0.6 m/s, and a feed of 0.3 mm/rev. Both dry and wet cutting conditions were applied. These orthogonal cutting tests were stopped, and the work material ahead of the tool tip was obtained to evaluate any microstructure change. As shown in Fig. 1, the microstructures at two selected locations were simulated in this study: location *A* in the primary deformation zone, and location *B* in the secondary deformation zone.



Fig. 1 Optical micrograph of AA 1100 (adapted from [1]).

#### 2.2 FE process model

A 2D FE model was developed using AdvantEdge<sup>TM</sup> to evaluate the dynamic thermomechanical loadings at steady state during the cutting process. A 12 mm length of cut was simulated to achieve the steady state status. The Johnson-Cook model of AA 1100 [32] and the silicon nitride-based ceramic tool material was applied in the AdvantEdge<sup>TM</sup> model. The coolant heat transfer coefficient was determined as 1500 W/m<sup>2</sup>-K by a cutting simulation with immersed coolant enabled. The coefficient of friction was determined as 0.5 and 0.3 for the dry cutting and wet cutting, respectively. Fig. 2 shows the simulated steady-state distributions of temperature and strain rate from the AdvantEdge<sup>TM</sup> simulation for the cutting stage. The steady-state cutting temperature distribution simulated by AdvantEdge<sup>TM</sup> was then imported into ABAQUS as the initial condition for the cooling stage simulation. An implicit ABAQUS heat transfer analysis was conducted to simulate the cooling temperature history under a natural convection.



Fig. 2 Steady-state dry cutting simulation using AdvantEdge<sup>TM</sup>: (a) temperature; (b) strain rate.

## 3. Dislocation Density-Based Modeling of DRX and Grain Growth

A new dislocation density-based DRX model is developed in this study considering the dynamic thermomechanical loadings, DRX and grain growth kinetics during the cutting process. The dislocation density evolution is modeled through the approach adapted from the authors' previous work [24–26] for the work material subjected to the dynamic thermomechanical loadings during machining. The initiation of DRX at elevated temperatures is modeled using a criterion of critical dislocation density [13–17]. The dislocation density evolution model is integrated with DRX and grain growth kinetics model adapted from [15].

#### 3.1 Evolution of Dislocation Density

Under severe plastic deformation, the formation of dislocation cell structure is evaluated by the dislocation generation due to plastic deformation, dislocation annihilation by dynamic recovery, and interaction between the dislocation cell interiors and cell walls. The dislocation density evolution rate on the dislocation cell walls and cell interior are given by:

$$\dot{\rho}_{c} = \alpha^{*} \frac{1}{\sqrt{3b}} \sqrt{\rho_{w}} \cdot \dot{\gamma}_{w}^{r} - \beta^{*} \frac{6}{bd(1-f)^{1/3}} \dot{\gamma}_{c}^{r}$$

$$-k_{o} \left( \dot{\gamma}_{c}^{r} / \dot{\gamma}_{o} \right)^{-1/n} \rho_{c} \cdot \dot{\gamma}_{c}^{r}$$

$$\dot{\rho}_{w} = \beta^{*} \frac{\sqrt{3}(1-f)}{fb} \sqrt{\rho_{w}} \cdot \dot{\gamma}_{c}^{r} + \beta^{*} \frac{6(1-f)^{2}}{bdf} \dot{\gamma}_{c}^{r}$$

$$-k_{o} \left( \dot{\gamma}_{w}^{r} / \dot{\gamma}_{o} \right)^{-1/n} \rho_{w} \cdot \dot{\gamma}_{w}^{r}$$

$$(1)$$

where  $\dot{\rho}_c$  and  $\dot{\rho}_w$  are the dislocation density evolution rate in cell interior and cell walls, respectively. Dislocation evolution rate control parameters are denoted as  $\alpha^*$ ,  $\beta^*$  and  $k_o$ . *b* is the magnitude of Burgers vector, *d* is the dislocation cell size.  $\dot{\gamma}_w^r$  and  $\dot{\gamma}_c^r$  are the resolved shear strain rates for the cell walls and interiors, respectively. It is assumed that these resolved shear strain rates are equal across the cell walls and cell interiors, i.e.,

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