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Procedia CIRP 58 (2017) 370 – 374

www.elsevier.com/locate/procedia

16th CIRP Conference on Modelling of Machining Operations

Thermodynamics-based interpretation of white layer formation in metal cutting

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Abstract

In metal cutting, the formation of white layers in the machined surface is a common phenomenon and refers to severe grain refinements, which appear white in etched micrographs. Due to the resulting modifications of the mechanical properties in the workpiece surface, understanding the initiation and evolution of white layer formation is of great interest for the industry. In order to save time as well as costs during tool and process design, the industry therefore demands valid predictive models of white layer formation. This requires the theoretical understanding of the underlying metal-physical mechanisms governing these structural material modifications. The relevant mechanisms include dynamic recrystallization (DRX), shearing and possibly phase transformations. Recently it was shown that DRX is predictable by thermodynamic potentials such as the Helmholtz free energy, which describe white layer formation as chains of spontaneous, irreversible state changes. In this paper, we provide a new interpretation of the energy transformations governing these thermodynamic state changes in the machined surface. The individual impacts of dissipation, heat conduction, mechanical work as well as the associated flow and production of entropy on the initiation and kinetics of DRX during cutting are discussed. The interpretation provides new fundamental insight into white layer formation by the example of orthogonal cutting quenched/tempered AISI 4140 using cemented carbide tools.

Keywords: Cutting; White layer; Microstructure; Energy

1. Introduction

The functionalities of parts in mechanical engineering may severely be determined by their topographical as well as metallurgical and mechanical surface characteristics [1,2]. These properties include surface roughness as well as properties such as residual stresses, hardness, mechanical strength, chemical stability and corrosion resistance [3]. Often these combined properties are summarized by the term surface integrity [2]. Depending on the workmaterial properties and the thermo-mechanical loads during metal cutting, alterations of the surface integrity through different physical mechanisms may occur, including severe plastic deformation, dynamic recrystallization and chemical effects [2]. In this respect the formation of white layers is of special interest. White layers refer to layers, which appear white in etched micrographs of the machined surface. White layers usually differ significantly from the bulk material in terms of structure and mechanical properties. In particular the higher hardness and lower ductility are responsible for increased formations and propagations of cracks, which therefore decrease the fatigue resistance of dynamically loaded components [4-7]. A considerable amount of work has been dedicated to the identification of the white layer formation mechanisms. Table 1 summarizes some empirical results for steel. As shown, grain refinement towards nano-crystalline structures through dynamic recrystallization (DRX) constitutes the main mechanism of white layer formation.

Modelling approaches of white layer formation in metal cutting considered the empirical findings from Table 1 and incorporated models of dynamic recrystallization in Finite Element (FE) simulation models. The majority of these works

doi:10.1016/j.procir.2017.03.328

used approaches based on the Zener-Hollomon parameter Z to calculate the critical strain at DRX initiation and the developing grain sizes, e.g. [8-12]. These approaches have in common that many material parameters have to be calibrated simultaneously, whose values are therefore difficult to interpret physically.

Table 1: Characterization of white layer formation in metal cutting

Material	Process	Structural modifications and mechanisms
AISI 52100 and 4340	Turning	nano-crystalline structure (d ≈ 30-500 nm): Dynamic recrystallization, cementite decomposition and dissolution [13]
AISI 4340, BS817M40	Turning	nano-crystalline structure (d ≈ 10-100 nm): Phase transformations (retained austenite), dynamic recovery, dynamic recrystallization [14,15]
AISI 52100	Turning	nano-crystalline structure (d ≈ 5-20 nm): Grain refinement through severe plastic deformation (moderate cutting speeds), phase transformations (high speeds) [16]
Annealed steels	Turning	severe grain refinement through plastic deformation, decomposition of ferrite and carbides into austenite, presence of retained austenite and martensite in white layer [17]
AISI 4140	Orthogonal cutting	nano-crystalline structure (d ≈ 100-200 nm): Dynamic recrystallization [18]

Buchkremer and Klocke developed a DRX model based on irreversible thermodynamics, which aimed at overcoming these difficulties [19]. The model is based on the free Helmholtz energy, whose sign of its differential signals whether a thermodynamic state change occurs spontaneously or not. Buchkremer and Klocke's model is used in this work for the thermodynamics-based interpretation of white layer formation in metal cutting. The paper is organized as follows: First, Buchkremer and Klocke's model and its validation are summarized. In the following, the interpretation of the energy and entropy terms of the model is presented, which constitutes the originality of the present paper.

2. Modelling dynamic recrystallization based on the free Helmholtz energy

Buchkremer and Klocke's model of dynamic recrystallization was published earlier and is summarized in the following [19]. For the considered material quenched/tempered AISI 4140 it was shown by X-ray diffraction that the phase transformations within the white layers were insignificant and could be neglected. The model will be used in the subsequent section for interpretation of the energy terms and entropy flow/production in the machined surface during cutting. In the model, DRX is described by a chain of irreversible thermodynamic state changes. In this context, DRX constitutes the transformation of mechanical energy, which is stored around dislocations, into interface energy, whose total amount scales reversely with the grain size. The question, whether this energy transformation occurs spontaneously or not, is indicated by the sign of the differential of the Helmholtz energy df (small letters indicate volume specific values hereinafter). If the Helmholtz energy decreases ($df \leq 0$) spontaneous transformation is possible:

$$f = u - T \cdot s \tag{1}$$

with u as the internal energy, T as the absolute temperature and s as the as entropy. The differential of f reads as follows:

$$df = du - dT \cdot s - T \cdot ds \tag{2}$$

where du incorporates the increments of the mechanical energy de_{me}, thermal energy de_{th} and interface energy de_a:

$$du = de_{me} + de_{th} + de_a \tag{3}$$

The entropy increment ds constitutes the sum of entropy flow ds_{th} due to heat conduction and entropy production ds_{diss} due to dissipation of mechanical into thermal energy. Using Clausius' entropy definition ds can therefore be written as

$$ds = ds_{th} + ds_{diss} = \frac{de_{diss}}{T} + \frac{de_{th}}{T} \tag{4}$$

where de_{diss} describes the dissipated mechanical energy and de_{th} the thermal energy increment due to heat conduction. The energy term de_{diss} was assumed to be linear proportional to the mechanical energy increment de_{me} by the Taylor-Quinney coefficient $\beta = de_{diss}/de_{me}$. The value of β was adopted from the literature as 0.9 [20]. The mechanical energy increment de_{me} was formulated as the integral of the yield stress σ_{yld} over the equivalent strain ϵ, where σ_{yld} was calculated using the constitutive model of Johnson-Cook [21]:

$$\Delta e_{me} = \int_{\epsilon_t}^{\epsilon_{t+1}} \sigma_{yld}(\epsilon, \dot{\epsilon}, T) \cdot d\epsilon = \left(1 + C \cdot \ln\left(\frac{\bar{\dot{\epsilon}}}{\dot{\epsilon}_0}\right)\right) \cdot \left(1 - \left(\frac{\bar{T} - T_0}{T_m - T_0}\right)^m\right) \cdot \left(A \cdot (\epsilon_{t+1} - \epsilon_t) + \frac{B}{n+1} \cdot (\epsilon_{t+1}^{n+1} - \epsilon_t^{n+1})\right) \tag{5}$$

with A, B, n, C, m and T_m as material constants, which were determined by the algorithm of Klocke et al. for quenched/tempered AISI 4140 [22]. $\dot{\epsilon}_0$ and T_0 are reference values for strain rate and temperature, while $\bar{\dot{\epsilon}}$ and $\bar{T}$ are average values for strain rate and temperature during a step from time instant t to $t + 1$. The grain size d was calculated by the interface energy de_a, which scales with the internal surface, which in return scales with d. Therefore, it can be solved for d. In [19] it is shown in detail that all the remaining terms in equation (2) can be expressed as functions of the specific heat capacity and were therefore available for calculation in a 2D FE model of orthogonal cutting. The FE process model is needed to calculate the distributions for strain, strain rate and temperature, which were also required to determine the Helmholtz free energy increment df according to equations (1) to (5). In total there are three conditions, which have to be fulfilled for the initiation of DRX: i) Helmholtz potential is decreasing ($df \leq 0$), ii) critical temperature is reached ($T \geq T_{crit}$), iii) critical stored mechanic energy is reached ($e_{me} \geq e_{crit}$). The FE process model itself was validated with respect to the cutting force components, chip geometry and temperature distributions [19]. The investigated material was quenched/tempered AISI 4140 (48 HRC). The orthogonal cutting test set-up as well as the interpretation of the cutting results were published earlier so that all details may be obtained from [23]. In the present work, the coated cemented carbide tools (WC-Co, CVD-MT Ti(C,N)+TiN+Al_2O_3) are considered. All investigated cutting conditions (undeformed chip thickness h = 0.05; 0.10; 0.20 mm, cutting speed v_c = 50, 100, 150 m/min) resulted in white layer formation.