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FEM-simulation of machining induced nanocrystalline surface layers in steel surfaces prepared for tribological applications

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ABSTRACT

A formation of nanocrystalline grains due to dynamic recrystallization within the workpiece surface layer (AISI4140) resulting from machining has proven to be suitable for obtaining improved tribological and fatigue behaviour. In the work presented an optimization of the machining process is carried out with cutting simulations using a continuous remeshing method and describing surface layer generation. The simulations describe the influence of process parameters and tool geometry on evolution of grain size distributions within the subsurface and affected depth after this thermo-mechanical processing. The validation is performed by experimental analyses based on cutting technology and focused ion beam technique.

1. Introduction

Nanocrystalline grains within the surface layers of metallic materials show beneficial properties such as combination of high strength and ductility [1] and considerably influence friction and wear characteristics [2]. The formation of these tribologically induced surface layers [3] can already start during manufacturing, by leading to a change of near-surface workpiece material [4,5]. In recent years severe plastic deformation [6] has established itself as a significant procedure for the production of ultrafine grains. These materials have an average grain size g_s of less than 1 μm after processing. The manufacturing processes, however, are focused on the production of nanocrystalline grains in bulk material rather than on a preconditioning of the surface layer [7]. The best-known are equal channel angular pressing [8], high pressure torsion [9] and accumulated roll bonding [10]. There are well-known surface treatments capable of generating nanocrystalline surface layers, e.g. deep rolling when a local shear force starts to act [11] or friction stir processing [12].

The development of a machining operation for generating a grain refinement underneath the workpiece surface by inducing severe plastic deformation within the surface layers can be carried out by modifying the process and geometry parameters of the cutting process [13–15]. Parameters that mainly influence plastic strain ε_{pl}, plastic strain rate $\dot{\varepsilon}_{pl}$ as well as process temperature T and therefore have to be taken into account are cutting edge radius r_β, depth of cut h and cutting velocity v_c [16]. Very high plastic shear strains ε_{pl} and plastic strain rates $\dot{\varepsilon}_{pl}$ lead to severe multiplication of dislocation density and finally to the generation of nanocrystalline grains within the workpiece surface layer. Furthermore, a process induced temperature T has to be generated during the machining process that enables these generated dislocations to form elongated subgrains [4].

In order to make an accurate prediction of the microstructural change within workpiece surface layers the plastic deformations and the temperature distributions should be known at first. Then the machining parameters should be related to the microstructural changes. The mechanisms that occur during the evolution of nanocrystalline grains within solid materials and surface layers are mostly described by model approaches based on dynamic recrystallization [17–20].

Thus, grain refinement has been predicted by modelling. However, the approaches do not consider the grain size formation as an evolution during the plastic deformation arising from cutting but as a result of post processing. Furthermore, the grain size distributions are mostly regarded as only one value and not as a distribution within the workpiece surface layer. Current microstructural simulation models are often not suitable for reflecting forming history, e.g. plastic strain rate $\dot{\varepsilon}_{pl}$ and temperature T as they are not described by an incremental approach concerning the processing time. This paper intends to overcome this by the development of an incremental formulation. Due to the implementation of an evolution formula to express recrystallization kinetics the grain size g_s is described as distribution within the surface layer after machining and agrees well with experimental results. Thus, the cutting simulation enables a preconditioning of the grain size changes. These results offer the potential for the aimed generation of nanocrystalline grain distributions with tribological optimized properties already during manufacturing, by choosing correct cutting parameters.

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2. Experimental

All experiments were carried out with indexable inserts made of the uncoated cemented carbide from the company Walter AG. The main cutting edge had a clearance angle α of 7°, a rake angle γ of $-7°$ and a wedge angle β of 90°. The broaching was performed at a numerically controlled broaching machine of the company Karl Klink GmbH in orthogonal cutting in order to allow for validation of the simulation. As the aimed application is turned bearings of crankshafts and their tribological optimization, the test samples were made of AISI4140 (the German steel 42CrMo4) in a state quenched and tempered at 450 °C. Variations of depth of cut h were performed in a range of 30–100 μm. The geometry of the tools was preconditioned with mean cutting edge radii r_β in a range of 30–150 μm by abrasive grinding with a drag finishing machine DF 4815 of the company OTEC GmbH. The cutting edge radii r_β were determined by a confocal light microscope of the company NanoFocus AG. Cutting velocities v_c in a range of 25–150 m/min were applied. In turning experiments not included here due to space limitations it could be shown that this strategy allows for good surface quality and tribological optimization. The evaluation of workpiece surfaces after machining was undertaken using a Focussed Ion Beam (FIB) system. The quantitative microstructural analysis was conducted with a linear intercept method by AxioVision Image Analysis Software from the company Carl Zeiss AG.

3. FE-simulation

3.1. Modelling of machining

The 2D-FE-modelling of the chip separation was realized by a self-developed continuous remeshing routine. Friction was considered based on the approach following coulomb law [21]. The model was built up with the commercial code ABAQUS/Standard consisting of a full coupled thermo-mechanical analysis and user defined subroutines to provide the simulation of grain formation. The initial workpiece geometry was modelled as a rectangular plane body with a length of 1000 μm and a height of 600 μm. The workpiece and the tool were meshed with 4-node bilinear displacement and temperature elements (CPE4T). The tool was defined as a rigid body and the heat transfer between the two partners were defined assuming perfect contact. Surface film conditions enabled heat transfer due to radiation. The workpiece material and the recrystallization kinetics were defined by a user subroutine [22]. The coefficient of friction was considered by Coulomb's law with $\mu = 0.35$ which showed good suitability in combination with the workpiece material and the chip separation [21].

To model the cutting induced grain size evolution within the workpiece surface layers resulting from machining, the behaviour of the machined material has to be described by an adequate material model. Therefore, a material model was used that has the ability to describe the orthogonal cutting process of AISI4140 and showed good agreement to experimental results [23]. The description of elastic-plastic material behaviour was carried out by an isotropic yield stress model according to Vöhringer and Voce with yield criterion following von Mises with athermal und thermal portion. The thermal fraction was based on the assumption of thermally activated dislocation movements. The athermal fraction was modelled by application of an extended Voce approach linked to a temperature dependency on the shear coefficient. The yield stress was thus analyzed in dependency of plastic strain rate $\dot{\varepsilon}_{pl}$, accumulated plastic strain ε_{pl} and temperature T. Using this model represents a difference to existing models, which often assume a pronounced overweight of thermal or athermal causes. The description of the plastic material behaviour and the recrystallization kinetics of the workpiece material AISI4140 were launched by the ABAQUS subroutine UHARD during modelling of machining.

3.2. Modelling of grain refinement

The Zener–Hollomon parameter Z

$$Z = \dot{\varepsilon}_{pl} \cdot \exp[Q \cdot (k_B \cdot N_A \cdot T)^{-1}] \tag{1}$$

that describes a dynamic recrystallization depending on plastic strain rate $\dot{\varepsilon}_{pl}$ and temperature T defines the recrystallized grain size g_r

$$g_r = K_1 \cdot Z^{K_2} \tag{2}$$

following the approaches of [17,18,24]. The activation energy Q for this material system was identified as 2.85 eV based on the Avogadro constant $N_A = 6.02 \times 10^{23}\ \mathrm{mol}^{-1}$ and the Boltzmann constant $k_B = 1.38 \times 10^{-23}\ \mathrm{J\,K}^{-1}$. The Zener–Hollomon constants K_1 and K_2 were adjusted to the material system by using a nonlinear regression analysis under the assumption of fully dynamically recrystallized volume fraction $x^{D(0\to1)}$ of 1. The Zener–Hollomon constants K_1 and K_2 were calculated as 85.715×10^4 and -0.269, respectively. At the beginning of the calibration procedure the knowledge reported in [25] was used because there values are presented which show a suitable description of the dynamic recrystallization theory for steels. $x^{D(0\to1)}$

$$X^{D(0\to1)} = 1 - \exp[-G \cdot (\varepsilon_{pl} - \varepsilon_{cr})^{K_3}] \tag{3}$$

is the fraction of material that has been recrystallized due to the accumulated plastic strain ε_{pl}. Thus, the grain size g_s after machining can be calculated in terms of a dynamically recrystallized volume fraction $x^{D(0\to1)}$ starting from not recrystallized grains changing to totally recrystallized subgrains by exceeding a defined accumulated plastic strain ε_{pl} with a formula from type Avrami following the approach of [19]. The velocity parameter G

$$G = K_4 \cdot (\varepsilon_{0,5}^{K_3})^{-1} \tag{4}$$

with the equivalent plastic strain $\varepsilon_{0,5}$

$$\varepsilon_{0,5} = K_5 \cdot (K_6 \cdot g_0^{0,5} \cdot Z^{K_7} - \varepsilon_{cr}) \tag{5}$$

thereby provides information about the dynamic recrystallization rate. The critical dynamic plastic strain ε_{cr}

$$\varepsilon_{cr} = K_8 \cdot g_0^{0,5} \cdot Z^{K_9} \tag{6}$$

must hereby be exceeded due to machining in dependency of the initial grain size g_0 and the Zener–Hollomon parameter Z to initiate a dynamic recrystallization. To adjust the dynamic recrystallized volume fraction $x^{D(0\to1)}$ to the existing nanocrystalline material system the following values for K_3–K_9 were detected, respectively: $K_3 = 2.500$, $K_4 = 0.6935$, $K_5 = 0.9710$, $K_6 = 0.0005$, $K_7 = 0.1482$, $K_8 = 0.0016$ and $K_9 = 0.0881$. The constants K_3–K_9 were therefore determined in a calibration phase. First a sensitivity analysis was carried out to understand the influence of the single constants on the grain size value, subsequently. Due to the implementation of an evolution formula to describe the recrystallization kinetics by a dynamically recrystallized volume fraction $x^{D(0\to1)}$ a minimum of grain size g_s

$$g_s = X^{D(0\to1)} \cdot g_r + (1 - X^{D(0\to1)}) \cdot g_0 \tag{7}$$

is gained after machining. Thus, an incremental formulation to analyze the microstructural change resulting from dynamic recrystallization is implemented.

For modelling of grain refinement cutting simulations and orthogonal cutting experiments were carried out with varying machining parameters. Thereby, a comparison between experimental resulting grain size g_s and numerical investigated accumulated plastic strain ε_{pl}, plastic strain rate $\dot{\varepsilon}_{pl}$ as wells as temperature T was carried out. For the experimental calculation of the grain size g_s average values from the profile line analyses were established. A large spectrum of the cutting