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Finite element computation of discrete configurational forces in crystal plasticity

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ABSTRACT

In this contribution the theory of configurational forces is applied to a viscoplastic material model with plastic slip in the basal and prismatic slip systems of an hcp crystal structure. Thereby the derivation of the configurational force balance is related to a translational invariance of the underlying energetics. The computation of configurational forces in this dissipative media requires the computation of gradients of the internal variables. In the context of the finite element method, this usually requires a projection of integration point data to the global mesh nodes. Alternatively, the gradients can be computed using a rather unknown subelement technique. The numerical accuracy of the different methods is qualitatively and quantitatively analyzed from a configurational force point of view. In a final example, the influence of the crystal orientation and plastic slip in multiple slip systems on the loading of a mode I crack is discussed with the help of the computed configurational forces. Furthermore, the influence of hardening is considered in this scenario.

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1. Introduction

The theory of configurational forces has previously been used to compute driving forces on defects, see for example the review in Gross et al. (2003) and the literature cited in there. The application of configurational forces to fracture has been pursued in many publications, see for example Steinmann (2000), Steinmann et al. (2001), Mueller et al. (2002), Kolling et al. (2002), Näser et al. (2007), Miehe et al. (2007) and Gürses and Miehe (2009). The concept has also received attention in the computational mechanics community. Details on the implementation of configurational forces in the context of the finite element method can be found in Gürses and Miehe (2009), Mueller and Maugin (2002), Gross et al. (2002), Mueller et al. (2004), Thoutireddy and Ortiz (2004), Kolling and Mueller (2005) and Miehe and Gürses (2007). These works include *r*- and *h*-adaptive strategies, based on the numerical error indicated by configurational forces. The basics of the mainly elastic origin of the theory of configurational forces can be found in Kienzler and Herrmann (2000), Gurtin (2000) and Maugin (1993) and the recent publication (Maugin, 2010). These works pick up the ideas that where already addressed in the seminal works by Eshelby (1951) and Eshelby (1970).

The extension of the theory to inelastic processes, together with a numerical application of fracture mechanics, can be found in the contributions (Menzel et al., 2004; Nguyen et al., 2005; Näser et al., 2007; Simha et al., 2008). The results of the present investigation are in agreement with Menzel et al. (2004), Nguyen et al. (2005) and Näser et al. (2007). However, we will provide a different derivation of the configurational force balance in conjunction with a more detailed analysis of possible numerical strategies.

Micro- and ultra-precision machining are rapidly growing areas of research. At the micro level, cutting processes combine a high geometric variability with comparatively high material removal rate. In contrast to conventional cutting processes, effects such as the size ratio between the tool and the microstructure of the workpiece material need to be considered. Known material models from conventional cutting can be applied only up to a certain extent to the areas of micro and ultra-precision machining. These models usually do not take the anisotropic properties of the materials into account. These are, however, necessary to describe the surface morphology and its characteristic effects. A good example for this is the spring back effect as illustrated in Fig. 1.

In order to make the theory and its numerical implementation applicable to micro- and ultra-precision machining processes, fracture mechanical scenarios are analyzed. Besides the anisotropic elastic response, the plastic deformation in the individual slip systems must be considered. In a first approach attention is given

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to the hcp-crystal structure and a viscoplastic material model is used, that takes slip in the basal and prismatic slip systems into account. The individual slip system experiences hardening due to the slip in its own (self hardening) and other slip systems (latent hardening). For the sake of simplicity the hardening is considered to be linear. For a more elaborate material law of hcp-titanium including length scale effects the reader is referred to Dunne et al. (2007).

The main focus of the present investigation is to provide an algorithmic setting for the treatment of the configurational force balance. In this regard, different computational strategies are realized, compared and discussed. The intention of this investigation is not the exact modeling of the material response, but rather the configurational framework of crystal plasticity in conjunction with a proper numerical treatment, that is especially suited for inhomogeneous problems, as are encountered in micro cutting of polycrystalline materials. Furthermore, in a first step we focus on a small strain setting and stationary cracks (cuts). The extension of the theory to applications with large deformations is more or less straightforward.

2. Modeling in physical space – crystal plasticity

In the bulk the equilibrium condition is given by the relation

$$\mathrm{div}\boldsymbol{\sigma} + \boldsymbol{f} = \boldsymbol{0}, \tag{1}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor, $\boldsymbol{f}$ represents volume forces, and the divergence operator is denoted by div. In index notation for Cartesian coordinates the equilibrium condition (1) reads $\sigma_{ij,j} + f_i = 0$, where Einstein's summation convention over repeated indices is utilized. The kinematics in the small strain limit are governed by the following linear and symmetric relation between the infinitesimal strain tensor $\boldsymbol{\varepsilon}$ and the displacement $\boldsymbol{u}$:

$$\boldsymbol{\varepsilon} = \frac{1}{2}\left(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^{\mathrm{T}}\right). \tag{2}$$

The ∇ operator is used to indicate the gradient with respect to the spatial coordinates $\boldsymbol{x}$. The system of equations can be solved under appropriate boundary conditions, if the constitutive equations are provided. In the later application and the numerical examples, a crystal plastic behavior is considered, including viscoplastic effects with latent hardening. The stress response is given by Hooke's law:

$$\boldsymbol{\sigma} = \mathbb{C}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{p}}), \tag{3}$$

where $\mathbb{C}$ is the fourth order stiffness tensor and $\boldsymbol{\varepsilon}^{\mathrm{p}}$ represents the plastic strain. In a crystal plastic setting, the plastic strain is constructed from the slip $\gamma^{(k)}$ in the kth slip systems, via

$$\boldsymbol{\varepsilon}^{\mathrm{p}} = \sum_k \gamma^{(k)}\boldsymbol{P}^{(k)}, \quad \text{where} \quad \boldsymbol{P}^{(k)} = \frac{1}{2}\left(\boldsymbol{s}^{(k)} \otimes \boldsymbol{n}^{(k)} + \boldsymbol{n}^{(k)} \otimes \boldsymbol{s}^{(k)}\right). \tag{4}$$

In the above relation the projector $\boldsymbol{P}^{(k)}$ is formed by the slip direction $\boldsymbol{s}^{(k)}$ of, and the normal $\boldsymbol{n}^{(k)}$ to the kth slip system. The symbol $\otimes$ represents the dyadic product between two vectors. The projector is used to compute the Schmid stress (Schmid and Boas, 1941) in the kth slip system by the projection

$$\tau^{(k)} = \boldsymbol{P}^{(k)} : \boldsymbol{\sigma} = \boldsymbol{\sigma} : \boldsymbol{P}^{(k)}, \tag{5}$$

where : indicates the scalar product between two second order tensors. In this investigation, the crystal structure of hcp-titanium is considered. The first 3 slip systems are the basal slip systems, while slip systems 4 to 6 are the prismatic slip systems. The secondary pyramidal slip systems are not taken into account here. For a sketch of the crystal structure in conjunction with the considered slip systems, see Fig. 2.

In order to simulate the time dependent material response, evolution equations for the plastic slip $\gamma^{(k)}$ and the hardening of each slip system $\alpha^{(k)}$ have to be provided. The following set of evolution equations is proposed:

$$\dot{\gamma}^{(k)} = \frac{1}{\eta}\langle|\tau^{(k)}| - \tau_y^{(k)}\rangle \mathrm{sgn}(\tau^{(k)}), \tag{6}$$

$$\tau_y^{(k)} = \tau_0^{(k)} + \tau_h^{(k)}, \tag{7}$$

$$\tau_h^{(k)} = \sum_l H^{(kl)}\alpha^{(l)}, \tag{8}$$

$$\dot{\alpha}^{(k)} = |\dot{\gamma}^{(k)}|. \tag{9}$$

In the flow rule (6) the symbol $\langle\cdot\rangle$ represents the Macauley brackets, and η the viscosity, while in (7) $\tau_0^{(k)}$ is the initial yield stress in the kth slip system. The hardening is described in (8) by the hardening matrix $H^{(kl)}$, which allows for the consideration of latent hardening. This completes the material description. The model is still rather simple, but incorporates the important features, such as the crystal orientation, its influence on the evolution of the plastic deformation, and hardening.

The material law is implemented in a finite element scheme at integration (Gauß) point level. The time integration is done in an implicit manner by a Euler backwards scheme in conjunction with a predictor corrector method, as it is classically done in plasticity. The only subtlety that has to be considered is the changing number of slip systems identified as active in the predictor step, see e.g. Simo et al. (1988). As the implementation of the material law is not in the focus of this investigation, where we want to concentrate

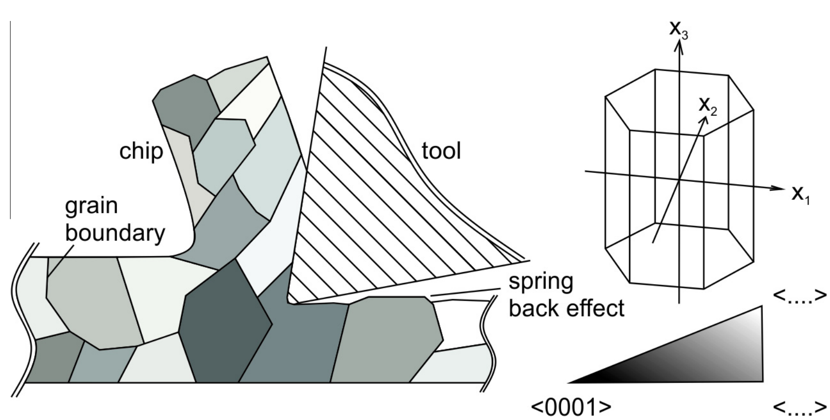

Fig. 1. Process conditions with respect to the microstructure of the workpiece in micro- and ultra-precision cutting.

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