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Published in:
Archive of Applied Mechanics

Link to article, DOI:
[10.1007/s00419-019-01567-4](https://doi.org/10.1007/s00419-019-01567-4)

Publication date:
2019

Document Version
Peer reviewed version

[Link back to DTU Orbit](#)

Citation (APA):
Juul, K. J., El-Naaman, S. A., Nielsen, K. L., & Niordson, C. F. (2019). A steady-state modeling framework incorporating the Kuroda–Tvergaard model: demonstrated on single crystal crack growth. *Archive of Applied Mechanics*, 89(10), 2133–2145 . <https://doi.org/10.1007/s00419-019-01567-4>

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A steady-state modeling framework incorporating the Kuroda-Tvergaard model: Demonstrated on single crystal crack growth

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Received: date / Accepted: date

Abstract A new modeling framework for analyzing steady-state elastic-viscoplastic single crystal problems at micron scale is presented. The model takes as offset the higher order gradient plasticity theory by Kuroda and Tvergaard [Kuroda and Tvergaard, 2006. Studies of scale dependent crystal viscoplasticity models. J. Mech. Phys. Solids. 54, pp. 1789-1810], and it is strongly inspired by an existing steady-state framework for conventional elastic-viscoplastic materials. Details on the modeling framework are laid out, and the numerical challenges and stability issues are discussed. Subsequently, the modeling framework is demonstrated on Mode I steady-state crack growth in HCP single crystals, where the impact of size effects on the active plastic zone that surrounds the crack tip is investigated. The focus is on the plastic zone shape and size, as well as its influence on the macroscopic fracture toughness. In this way, the chosen benchmark problem for the new modeling framework serves as an extension to the conventional study of the corresponding problem without size effects presented in Juul et al. [Juul et al., 2017. Steady-State Crack Growth in Single Crystals under Mode I Loading. J. Mech. Phys. Solids. 101, pp. 209-222]. The tendency is that the plastic zone is smeared out (seen as less distinct features) when increasing the material rate-sensitivity. This is in-line with already published work in the literature. It is shown that the size-effect has a limited effect on the qualitative features of the plastic zone, whereas it clearly suppresses the magnitude of the features due to the added gradient hardening effect. Moreover, the hardening effect tends to lower the shielding ratio, and hence a key result is that single crystal materials appear less crack resistant than conventional studies suggest at the micron scale.

Keywords Rate sensitivity · Quasi-static crack growth · Size effects · Crystal plasticity · Back stress

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1 Introduction

Steady-state modeling techniques that readily take into account history dependent behavior has recently received renewed attention for its wide range of application. Such techniques were originally developed by Dean and Hutchinson [4] and Parks et al. [20] for classical steady-state crack growth in rate-independent materials. The basic idea behind the method is the observation that near tip field quantities remain unchanged to an observer traveling with the crack tip. Ever since this framework has been used extensively and developed further to a large range of steady-state problems. Recently, Juul et al. [12] extended the steady-state modeling of isotropic materials to include a conventional rate-sensitive crystal plasticity theory. The framework efficiently extracts highly detailed fields near a propagating crack tip, and it applies to any plane strain crystal configuration. In their study, a comprehensive investigation of the near tip plastic zone size and shape, as well as the corresponding crack tip shielding was conducted. For example, the characteristics of the plastic zones for FCC, BCC, and HCP crystal structures were presented and compared to existing literature when possible (Rice [22], Rice et al. [23]).

Juul et al. [12] focused on conventional crystal plasticity, but the requirement for more sophisticated constitutive laws that includes size effects has motivated the present work. The effect of interest is, here, the additional hardening related to plastic strain gradients - or, in other words, hardening related to the presence of geometrically necessary dislocations (GNDs) when dealing with steady-state problems. The effect of GNDs on steadily growing cracks obtained through size effects and viscous behavior has primarily been limited to isotropic plasticity. Among the steady-state studies of isotropic gradient plasticity is Wei and Hutchinson [26] and Wei et al. [28], investigating the tractions ahead of the crack tip, crack opening profiles, and the shielding ratio for different length parameters and plasticity models. These studies showed that the tractions in the immediate vicinity of the tip increased significantly due to the suppression of plasticity also causing the shielding ratio to drop. Wei and Hutchinson [27] also investigated the influence of interface models, underlying the conditions for which the models best represent the physics. All of the previous studies relied on rate-independent formulations whereas the study by Nielsen et al. [18] employs a rate-dependent strain gradient plasticity model. This study investigates the shielding ratio and tractions along the crack face as well but also presents a method to determine the rate-independent response with a rate-dependent model. The study showed that the gradient effects in the rate-dependent model have a similar tendency to increase tractions as well as the crack tip shielding ratios.

The model by Kuroda and Tvergaard [14] treats size-effects in single crystals, and it has formed the basis for many traditional (non steady-state) investigations. The theory takes conventional viscoplasticity as offset and allows size effects to enter the material response through a so-called “back stress” which is a result of the internal stress fields arising from gradients in the GND field. The size effects enter the constitutive laws through a length parameter which is introduced for dimensional consistency and requires calibration to experimental observations. Furthermore, this higher order theory directly allows for boundaries impenetrable to dislocations to be enforced as constraints on the evolution of GNDs, governed by a separate partial differential equation.

As discussed by many authors (e.g. in Gurtin [9] Evers et al. [7], Bayley et al. [2], El-Naaman et al. [6, 5], Husser and Bargmann [10]), the back stress can be interpreted as a long range internal stress field that evolves with spatial gradients of the geometrically necessary dislocation (GND) density. However, by increasing the length parameter, or diminishing size, the back stress plays an increasing role. Unfortunately, traditional models have also shown that this model might lead to numerical stability issues that are strongly tied to the viscoplastic relation. In particular, a strong non-linearity arises when pushing parameters toward the rate-independent limit.

In the present study, the classical Mode I crack growth problem is chosen as a benchmark since results exist for both conventional isotropic and crystal plasticity models. The objective is to extend the steady-state framework into the size dependent single crystal plasticity theory by Kuroda and Tvergaard [14]. Thus, the present work aims to extend the existing modeling capabilities and focuses on creating a new numerical procedure that lends itself to future studies of single crystal behavior at the micron scale. This work serves two purposes where the primary goal is to develop and demonstrate the new gradient enhanced single crystal steady-state model and secondly, to extend the analysis of steady-state crack growth in conventional rate-sensitive single crystal materials presented in Juul et al. [12] to illustrate the effect of size in single crystals.

The paper is divided into the following sections: The gradient enhanced material model and the numerical formulation are presented in Sections 2 and 3, the boundary value problem is restated in Section 4, results are presented in Section 5 and, lastly, concluding remarks are stated in Section 6.

2 Plasticity Theory

Throughout the paper, index notation, including Einstein's summation convention, is used and the notation $(\dot{})$ denotes a time derivative.

2.1 Rate-sensitive material model

A small strain formulation (2D plane strain) is employed and the total strain; $\varepsilon_{ij} = (u_{i,j} + u_{j,i})/2$, can thereby be decomposed into an elastic part, ε_{ij}^e , and a plastic part, ε_{ij}^p , such that; $\varepsilon_{ij} = \varepsilon_{ij}^e + \varepsilon_{ij}^p$. Subsequently, the stress field can be determined from the elastic relationship; $\sigma_{ij} = \mathcal{L}_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}^p)$, where $\mathcal{L}_{ijkl}$ is the elastic stiffness tensor.

In the adopted crystal plasticity framework, the plastic strain rate components are determined by the sum of slip contributions from each slip system, (α) , according to

$$\dot{\varepsilon}_{ij}^p = \sum_{\alpha} \dot{\gamma}^{(\alpha)} P_{ij}^{(\alpha)} \quad \text{with} \quad P_{ij}^{(\alpha)} = \frac{1}{2} \left(s_i^{(\alpha)} m_j^{(\alpha)} + m_i^{(\alpha)} s_j^{(\alpha)} \right) \quad (1)$$

where $P_{ij}^{(\alpha)}$ is the Schmid orientation tensor, $\dot{\gamma}^{(\alpha)}$ is the slip rate, and $s_i^{(\alpha)}$ and $m_i^{(\alpha)}$ are unit vectors pointing in the slip direction and the direction of the slip plane normal, respectively (see Fig. 1). The slip rate relation for $\dot{\gamma}^{(\alpha)}$ is based

on the model suggested by Hutchinson [11], but here incorporating a back stress, $\tau_b^{(\alpha)}$, to allow length scale effects entering the existing relation (see e.g. Groma [8], Yefimov et al. [30], Evers et al. [7], Bayley et al. [2]). The back stress can be related directly to the gradients of the GND density, impeding slip at non-uniform pile-ups of GNDs (see Section 2.3). Based on this concept, the driving force behind dislocation motion is the effective resolved shear stress, $\tau_{eff}^{(\alpha)} = \tau^{(\alpha)} - \tau_b^{(\alpha)}$ (see Evers et al. [7]) giving the modified slip rate relation

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \text{sgn} \left(\tau^{(\alpha)} - \tau_b^{(\alpha)} \right) \left(\frac{|\tau^{(\alpha)} - \tau_b^{(\alpha)}|}{g^{(\alpha)}} \right)^{1/m} \quad (2)$$

where $\dot{\gamma}_0$ is the reference slip rate, $\tau^{(\alpha)} = \sigma_{ij} m_i^{(\alpha)} s_j^{(\alpha)}$ is the resolved shear stress, and $g^{(\alpha)}$ is the slip resistance. For simplicity, the slip resistance, $g^{(\alpha)}$, is taken to follow the power law relation; $g^{(\alpha)} = \tau_0 (1 + |\gamma_{acc}^{(\alpha)}| G / \tau_0)^N$, where G is the shear modulus and $\gamma_{acc}^{(\alpha)}$ is the accumulated slip. From the slip resistance it is noticed that only self-hardening of the slip systems is considered (latent hardening is neglected for simplicity).

The slip rate relation in Eq. (2), gives rise to a rate sensitive material response, which is controlled by the rate sensitivity exponent, m . In the limit, this rate sensitive material model will approach the rate independent response for $m \rightarrow 0$.

2.2 Strain Gradient Plasticity

The field of higher order gradient plasticity theories can be divided into two; 1) being the work conjugate type, and 2) the non-work conjugate type. The present study is based on the non-work conjugate theory proposed by Kuroda and Tvergaard [14,15], which is an extension of conventional crystal plasticity. The non-work conjugate type theories are characterized by not employing higher order stresses as work conjugate to the strain gradients. Hence, the non-work conjugate formulation is based on the conventional equilibrium equation, $\sigma_{ij,j} = 0$ (in absence of body forces). This formulation provides an additional (separate) partial differential equation that describes the evolution of the GND density in relation to the slip gradients;

$$\frac{1}{b} \gamma_{,i}^{(\alpha)} s_i^{(\alpha)} + \rho_G^{(\alpha)} = 0. \quad (3)$$

Here, b is the length of the Burgers vector, and $\rho_G^{(\alpha)}$ is the GND density on the individual slip systems (Ashby [1]). Equation (3) accounts only for edge dislocations, as the present study is in 2D. Rewriting Eq. (3) in weak form yields

$$\frac{1}{b} \int_V \delta \rho_{,i} s_i^{(\alpha)} \gamma^{(\alpha)} dV = \frac{1}{b} \int_S \delta \rho \chi^{(\alpha)} dS + \int_V \delta \rho \rho_G^{(\alpha)} dV, \quad \chi^{(\alpha)} \equiv \gamma^{(\alpha)} n_i s_i^{(\alpha)} \quad (4)$$

where $\delta \rho$ is a virtual GND density and n_i is the unit outward normal vector.

Regarding non-conventional boundary conditions, a hard interface, i.e. an interface impenetrable for dislocation, corresponds to; $\chi^{(\alpha)} \equiv \gamma^{(\alpha)} n_i s_i^{(\alpha)} = 0$, whereas a free boundary, allowing dislocation to exit though the boundary is enforced as; $\rho_G^{(\alpha)} = 0$. A detailed discussion of the GND boundary conditions and their physical interpretation can be found in Kuroda and Tvergaard [15].

2.3 Back Stress

The back stress dependency on the gradients is an essential choice in the non-work conjugate type theories as it directly influences the viscous slip rate and thereby the resolved shear stress on the individual slip systems (see Eq. (2)). One can interpret the back stress as a long range internal stress field (back stress) due to the evolving spatial gradients in the GND densities. The long range internal stress field is argued to impede the movement of dislocations in the gradient direction, which gives rise to a kinematic hardening behavior (see e.g. El-Naaman et al. [6] for various back stress models).

The present study is based on a thermodynamically consistent formulation adopted from El-Naaman et al. [6], where the back stress is assumed to be given as the divergence of the vector-valued higher order stress, $\xi_i^{(\alpha)}$. That is

$$\tau_b^{(\alpha)} \equiv -\xi_{i,i}^{(\alpha)}, \quad (5)$$

with ξ_i being the so-called micro-stress derived from the plastic contribution to the free energy, $\psi_G^{(\alpha)}$, as

$$\xi_i^{(\alpha)} = \frac{\partial \psi_G^{(\alpha)}}{\partial \gamma_{,i}^{(\alpha)}}. \quad (6)$$

The free energy potential is chosen to have the quadratic form (a more general set of expressions can be found in e.g. El-Naaman et al. [6])

$$\psi_G^{(\alpha)} = \frac{1}{2} \tau_0 L^2 |\gamma_{,i}^{(\alpha)} s_i^{(\alpha)}|^2, \quad (7)$$

where L is an energetic length parameter, required to ensure dimensional consistency. An immediate consequence of the quadratic nature of the defect energy is that the back stress becomes linear in the second order slip gradient, such that

$$\tau_b^{(\alpha)} = -\tau_0 L^2 \gamma_{,ki}^{(\alpha)} s_i^{(\alpha)} s_k^{(\alpha)} \quad (8)$$

Expressed in terms of the GND densities, the back stress can be written as

$$\tau_b^{(\alpha)} = \tau_0 b L^2 \rho_{G(e),i}^{(\alpha)} s_i^{(\alpha)}. \quad (9)$$

which shows that it has a linear dependency on the GND density gradient. Thus, a uniform field of GNDs will not give rise to any internal long range stress fields.

3 Steady-State Framework

The framework, developed by Dean and Hutchinson [4] and Parks et al. [20], is employed to create a new steady-state framework that includes the strain gradient crystal plasticity model by Kuroda and Tvergaard, inspired by the work of Nielsen et al. [18] and Nielsen and Niordson [17]. Dean and Hutchinson [4] originally defined steady-state for a growing crack as the condition where the field quantities, in the vicinity of the crack tip, remain constant relative to an observer traveling with the crack tip. Thus, any time derived quantity, $\dot{f}$, can be

related to the corresponding spatial derivative in the direction of material movement (along so-called streamlines) according to $\dot{f} = -\dot{a}\partial f/\partial x$, with $\dot{a}$ being the constant crack speed. This important transformation of a time derived quantity into a spatial quantity allows any incremental quantity at a given material point, (x_1^*, x_2^*) , to be evaluated by integrating along a streamline, starting upstream (x_1^0, x_2^0) of the crack tip and ending at the point of interest, (x_1^*, x_2^*) , downstream (see e.g. Juul et al. [13]). Thus, the point of interest contains the history of all upstream material points on the streamline. The streamline integration procedure is only required in regions where history dependent variables evolve. Thus, the integration is only performed in the region surrounding the crack tip and the crack faces, where elastic-plastic behavior takes place. This is illustrated by the strip of height $2H$ in Fig. 2.

The cornerstone of the new steady-state framework, incorporating the Kuroda and Tvergaard material model, is to determine the displacement field, u_i , from the conventional principle of virtual work for the quasi-static problems;

$$\int_V \mathcal{L}_{ijkl} \varepsilon_{kl} \delta \varepsilon_{ij} dV = \int_S T_i \delta u_i dS + \int_V \mathcal{L}_{ijkl} \varepsilon_{kl}^p \delta \varepsilon_{ij} dV, \quad (10)$$

where $T_i = \sigma_{ij} n_j$ is the surface traction and n_j is the unit outward normal vector. The gradient effect enters through the back stress which is determined by solving the GND density equation. The solution scheme runs in a staggered approach, where the back stress is based on the slip field determined in the previous iteration. The systems of equations for the two field quantities completely decouples (see Section 2.2), and the only exchange of data between the two systems is the feeding of the back stress, $\tau_b^{(\alpha)}$, into the calculation of the displacement field, and the subsequent feeding of slip, $\gamma^{(\alpha)}$, into the calculation of the back stress field.

The pseudo algorithm for the steady-state framework, including the gradient enhanced model, is identical to the procedure for the conventional model in Juul et al. [12], except for the added step three, where the back stress is determined (n is the current iterative step), and the use of the effective resolved shear stress in 4a:

1. The plastic strain from the previous iteration, $\varepsilon_{ij}^{p(n-1)}$ is used to determine the displacement field, $u_i^{(n)}$, from the virtual work principle in Eq. (10) (the iterative procedure is initiated with an elastic step i.e. $\gamma^{(\alpha)} = 0$).
2. The total strain, $\varepsilon_{ij}^{(n)}$ is determined from the displacement field.
3. The back stress, $\tau_b^{(\alpha)}$ is determined from Eq. (9) based on the value of the total slip $\gamma^{(\alpha)(n-1)}$ from the previous iteration (in the first iteration the GND density is zero, $\rho_{G(e)}^{(\alpha)} = 0$ i.e. the back stress is zero, $\tau_b^{(\alpha)} = 0$).
4. The slip and plastic strain field are determined by the streamline integration procedure:
 - (a) First the spatial derivative of the slip on the individual systems and plastic strains are determined by utilizing the steady-state relation, $\partial f/\partial x =$

$-\dot{f}/\dot{a}$:

$$\frac{\partial \gamma^{(\alpha)}}{\partial x} = -\frac{\dot{\gamma}_0}{\dot{a}} \operatorname{sgn}(\tau^{(\alpha)} - \tau_b^{(\alpha)}) \left(\frac{|\tau^{(\alpha)} - \tau_b^{(\alpha)}|}{g^{(\alpha)}} \right)^{1/m} \quad (11)$$

$$\frac{\partial \varepsilon_{ij}^p}{\partial x} = \sum_{\alpha} \frac{\partial \gamma^{(\alpha)}}{\partial x} P_{ij}^{(\alpha)} \quad (12)$$

- (b) Secondly the current total slip $\gamma^{(\alpha)(n)}$ and the total current plastic strain $\varepsilon_{ij}^{p(n)}$ is determined through streamline integration:

$$\gamma^{(\alpha)(n)} = \int_{x_0}^{x^*} \frac{\partial \gamma^{(\alpha)}}{\partial x} dx, \quad \text{and} \quad \varepsilon_{ij}^{(p)(n)} = \int_{x_0}^{x^*} \frac{\partial \varepsilon_{ij}^{(p)}}{\partial x} dx \quad (13)$$

The integration is performed numerically by employing a classical forward Euler scheme.

5. The current stress field $\sigma_{ij}^{(n)}$ is then updated using the elastic relationship, $\sigma_{ij} = \mathcal{L}_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}^p)$.
6. Step 1 through 5 is repeated until the displacement, slip, and stress fields have converged. Convergence is evaluated by requiring a sufficiently small iterative change in the individual solution vectors according to: $\|\kappa^{(n)} - \kappa^{(n-1)}\| / \|\kappa^{(n)}\| < 10^{-6}$, where κ represents the displacement, slip, and stress fields, respectively.

The displacement field discretization is based on a quadratic 8-node isoparametric element and the GND field discretization is based on a linear 4-node isoparametric element according to the procedure in e.g. Nielsen and Niordson [17], El-Naaman et al. [6], Juul et al. [13]. Reduced Gauss integration (2×2 Gauss points) is employed for the 8-node element, while full Gauss integration (2×2 Gauss points) is used for the 4-node elements.

4 Benchmark problem - Mode I crack growth

The problem investigated concerns the effect of strain gradients related to crack growth in HCP single crystals. The goal of the study is to investigate the relation between the fracture energy at the macroscopic scale and that on the microscopic scale by determining how the so-called crack tip shielding (J_{ss}/J_{tip}) is affected when diminishing size (increasing material length parameter).

The investigation of the shielding ratio relies on the SSV-model proposed by Suo et al. [25], where the primary assumption is that the crack tip does not emit any dislocations. From this requirement it directly follows that the free path between dislocations must be significantly larger than the lattice constant, rendering the possibility for crack tip blunting, as a result of already existing dislocations, minor. The crack tip will, therefore, remain sharp and propagate by atomic separation or cleavage. This material behavior is modeled by embedding the crack in an elastic strip of height $2D$ (see Fig. 2), such that linear elastic fracture mechanics theory can be used to evaluate the energy release (using the J-integral, see e.g. Shih et al. [24]) and thereby the crack tip shield ratio J_{ss}/J_{tip} . Applying the J-integral, the fracture criteria for the propagating crack will be; $J_{tip} = \Gamma_{tip}$,

where Γ_{tip} is the critical energy required for the crack to advance while J_{ss} is the remotely applied energy release rate (see e.g. Wei and Hutchinson [27] for details on the model limitations). The height of the elastic strip, referred to as the SSV-domain, can be used as either a fitting parameter (see Suo et al. [25]) or it can be estimated from dislocation theory (see e.g. Beltz et al. [3], Lipkin et al. [16]). In the following, this dimension will be treated as a variable in a parametric study.

The present version of the SSV-model differs slightly from the original set-up as additional requirements must be enforced in terms of higher order boundary conditions that are needed in the Kuroda-Tvergaard model. The higher order boundary conditions are here related to the GND density at the boundary of the SSV-domain. Essentially a micro free boundary, allowing for dislocations to exit the elastic-plastic domain, is enforced. This type of boundary conditions is chosen to phenomenologically represent that dislocations may exit through the crack face, even though an elastic strip exists in between the crack face and the elastic-plastic domain. This assumption is expected to comply with the assumptions in the SSV-model as the dislocations entering the SSV-domain are unlikely to cause major blunting of the crack tip, i.e. the crack will continue to grow by atomic separation. It should also be mentioned that the study of the plastic zones (where the SSV-domain is absent) is conducted under identical conditions (crack faces being micro free). In both studies, the outer boundary is micro hard, blocking dislocations (however since the outer boundary is far away from the crack tip plastic zone, this condition has negligible influence).

The crack growth problem is similar to that considered by Juul et al. [12] and studied in a conventional crystal plasticity setup. However, for simplicity only the hexagonal closed packed (HCP) structure is considered as this will eliminate the need for invoking effective slip systems accounting for out-of-plane slip on the crystallographic slip systems (see e.g. Niordson and Kysar [19], Juul et al. [12]).

A sharp Mode I 2D plane strain crack grows under steady-state conditions at constant velocity $\dot{a}$ (see Fig. 2). The problem is treated quasi-statically (effects of inertia are neglected) and assumes small scale yielding. On the outer boundary of the domain, a Mode I far-field condition is applied (illustrated in Fig. 2) following the elastic solution (see e.g. Williams [29]), such that

$$\sigma_{ij} = \frac{K_I}{\sqrt{2\pi r}} f_{ij}(\theta) \quad (14)$$

where r and θ are polar coordinates with respect to the crack tip, $f_{ij}(\theta)$ are the dimensionless Mode I functions, and K_I is the stress intensity factor.

The material parameters and model setup are adopted from Wei and Hutchinson [27], with the addition of the length parameter controlling the size-effects. A dimensional analysis states that the shielding ratio, J_{ss}/J_{tip} , at steady-state must have the functional form

$$\frac{J_{ss}}{J_{tip}} = F\left(\frac{\dot{a}}{R_0\dot{\gamma}_0}, \frac{R_0}{D}, \frac{L}{R_0}, \frac{\tau_0}{G}, N, m, \nu\right) \quad (15)$$

where the quantity $\zeta = \dot{a}/(R_0\dot{\gamma}_0)$ represents the dimensionless velocity, R_0 is a reference plastic zone size parameter given by; $R_0 = (K_0/\tau_0)^2$, with $K_0 = \sqrt{E\Gamma_{tip}/(1-\nu^2)}$, and $G = E/(2(1+\nu))$ is the shear modulus. The dimensional dependency in Eq. (15) outlines the key parameters of interest.

The near tip active plastic zone in the elastic-viscoplastic model is visualized by adopting the absolute value of the accumulated slip rate (also employed in Rice et al. [23])

$$\dot{A} = \sum_{\alpha} |\dot{\gamma}^{(\alpha)}|. \quad (16)$$

To obtain a quantity comparable across large velocity spans, the absolute sum of slip on all systems is normalized slightly different compared to Rice et al. [23]. Normalization of Eq. (16) follows Juul et al. [12], where the quantity $\zeta \dot{\gamma}_0 \tau_0 / G$ is used to obtain non-dimensionality taking the crack propagation velocity into account.

The finite element mesh contains 102400 elements and it is gradually scaled in both the x_1 - and x_2 -directions, to provide a highly refined mesh in the vicinity of the crack tip. Approximately 19000 of the 102400 elements are within the region enclosing the plastic zone in order to provide a detailed solution. The remaining material properties used for the analysis are listed in Tab. 1.

5 Results

5.1 Near Tip Active Plastic Zones

The characteristics of the near tip plastic zone for a quasi-static crack growing either in FCC or BCC crystals, with perfectly plastic material behavior ($N = 0$), have been investigated by Rice [22] and Rice et al. [23] using both analytical and numerical models in a conventional set-up (no size effects). Even though results for HCP crystals are not treated in Rice [22], the present results are heavily inspired by Rice's analysis and it is assumed that the velocity discontinuities under similar conditions, will arise close to the crack tip in HCP crystals. Hence, angular sectors with distinct material behaviour near the crack tip are expected. However, it is worth to notice that the velocity discontinuities will, in fact, be bands of finite width due to the viscoplastic material model adopted in the present theory. For the study of velocity discontinuities, a low rate-sensitivity exponent, m , is enforced in order to approximate the rate-independent response and thereby be in line with the conditions for the early analytical studies by Rice [22]. Furthermore, it should also be emphasized that for this part of the study, the SSV-domain is absent ($D = 0$) allowing for elastic-plastic behavior in the entire domain, complying with the assumptions by Rice [22].

To give a better feeling for the effect of size, the active plastic zones are first presented with and without size effects in Figs. 3 and 4. The results display the zones for different rate-sensitivity, m , and a fixed growth velocity $\zeta = 500$ (recall that; $\zeta = \dot{a}/(R_0 \dot{\gamma}_0)$).

Numerical stability allows only a rather limited increase in the length parameter. However, comparing Figs. 3a and 3b (low rate sensitivity) it is seen that the overall characteristics are the same with and without size effects, while closer inspection reveals that the plastic zone is slightly smaller in the case including size effects. This is expected as the size effects increase material hardening, thereby suppressing plasticity. Especially when inspecting the elastic sectors between features (B) and (C), and (C) and (D) it is seen that the plastic zones are smaller

(wider elastic regions). The direction of velocity discontinuities are unaffected by the size-effect, however, their sharpness and length are increased when accounting for the material length parameter. Furthermore, it is observed that they are either parallel or perpendicular to the slip systems for both size scales considered as Rice [22] demonstrates for FCC and BCC crystals).

5.2 Crack Tip Shielding Ratio

The slightly modified SSV-model presented in Section 4 is now introduced to identify the influence of size effects on the shielding ratio (related to material toughness). The study is performed at two different crack propagation velocities which will be referred to as fast and slow crack growth, respectively. These terms relate to the dimensionless crack velocity, ζ , being either $\zeta = 500$ (fast) or $\zeta = 10$ (slow) (recall that; $\zeta = \dot{a}/(R_0\dot{\gamma}_0)$). Note that the fast growing crack is considered not to be in a range where dynamic effects are important and thus, the effect of inertia is negligible (quasi-static crack growth).

First, the crack tip shielding ratio as a function of the SSV-domain height is investigated for different rate-sensitivities and material length scale parameters. Figure 5a and 5b presents the shielding ratio for a slow and a fast growing crack, respectively. At both velocities, it is observed that the shielding ratio is increasing when the thickness of the SSV-domain decreases ($R_0/D \rightarrow \infty$). This is expected due to the increasing amount of plasticity (more energy dissipated) in the vicinity of the crack tip when the height of the SSV-domain (elastic strip) diminishes. Comparing the individual graphs, for either velocity, it is revealed that the crack tip shielding ratio is decreasing when the material length parameter is increased. This can be explained by the increasing resistance to plastic deformation originating from the hardening effect caused by the GNDs (less dissipation of energy). This is also consistent with the previous effect seen on the plastic zone which becomes slightly smaller when accounting for size effects. In addition, the effect of size is found to be less pronounced when the rate-sensitivity is increased (also discussed previously).

It is noted from Fig. 5 that the crack tip shielding ratio for the fast and slow growing cracks displays some interesting characteristics (first discussed by Nielsen et al. [18]). For the slow crack (Fig. 5a), the shielding ratio is increasing in a monotonic manner with increasing rate-sensitivity, while the opposite is observed for the fast growing crack (Fig. 5b), i.e. the crack tip shielding ratio monotonically decreases with increasing rate-sensitivity. A direct consequence of this behavior is the existence of a specific velocity (termed the characteristic velocity), at which the crack tip shielding ratio becomes independent of the rate-sensitivity and thus reveal the rate-independent solution. The existence of this specific velocity is related to the rate dependency introduced through Eq. (2), and it is a result of the stress build-up or relaxation occurring depending on the velocity. At high velocities, the plastic material deformation is restricted (less dissipation), leading to a stress build-up in the material and a lower shielding effect. At low velocities, the material more easily deforms plastically (relaxation takes place), resulting in more energy dissipation and a larger shielding effect is observed. Therefore, there must exist a crossing between these two scenarios at an intermediate velocity referred

to as the characteristic velocity (see also Nielsen et al. [18], Nielsen and Niordson [17]).

To illustrate the phenomenon of a characteristic velocity, the uniquely defined intersection of the curves is investigated in Fig. 6 (for fixed height of the SSV-domain, R_0/D , and hardening exponent, N), where the shielding ratio is shown as a function of the crack propagation velocity, $\zeta = \dot{a}/(R_0\dot{\gamma}_0)$. The intersection of curves (defining the characteristic velocity) are marked by arrows, and it establishes a point at which the crack tip shielding is independent of the rate-sensitivity, m , despite the fact that the plastic zone can be different and that it depends on rate-sensitivity at this specific velocity. What is intriguing is the fact that the Kuroda-Tvergaard model is not formulated in a rate-independent version, but the results presented may still be interpreted as the rate-independent limit, although the numerical calculation for $m \rightarrow 0$ is unstable and essentially out of reach (see also discussion in El-Naaman et al. [5]). Thus, the existence of the characteristic velocity establishes a possibility of future studies of rate-independent results by the Kuroda and Tvergaard model.

Comparing the characteristic velocity for different length parameters, it is observed that an increasing length parameter tends to shift towards a higher characteristic velocity. This is expected and it is tied to the length parameter introducing a hardening effect (see also the discussion related to plastic zones in Figs. 3 and 4). When the resistance to plastic deformation increases, the point at which the process changes from being dominated by relaxation to stress build-up (the characteristic velocity) will occur at a higher velocity. This is also noticed in Juul et al. [12], where the characteristic velocity increases for an increase in conventional strain hardening. Another interesting observation is the evolution of the crack tip shielding ratio as function of velocity for the results with and without size effects. As the velocity increases, the difference becomes smaller (especially for high rate-sensitivity).

6 Concluding Remarks

The plastic zone and corresponding shielding ratio of quasi-static crack growth have been studied. Crack growth at a constant velocity is modeled in a steady-state framework directly bringing out the state of interest. The present work serves as a higher order extension of the work by Juul et al. [12], and presents a steady-state framework which incorporates size effects in elastic-viscoplastic material model.

During the study of size effects in single crystals with the developed framework, numerical stability issues were encountered. The stability issues with the Kuroda-Tvergaard model, known from traditional Lagrangian frameworks, that arise when introducing a back-stress into the slip rate relation was also experienced in the present steady-state framework. This means that it is difficult to increase the length scale parameter to a level where the size effects were strongly pronounced, even when introducing a relaxation method (inspired by Peirce et al. [21] and Nielsen et al. [18]) to stabilize the numerical framework. In spite of the moderately pronounced size effects, it was still possible to obtain conclusive results and determine the effect of size for steadily growing cracks in a single crystal.

Similarly to Juul et al. [12], bands of intense slip reveal themselves in the slip rate field, dividing the plastic zones into sectors as predicted by Rice [22], and

these have a direct influence on the macroscopic fracture toughness of the material. A detailed investigation of the macroscopic fracture toughness is performed by applying the SSV model. This study revealed the size effects to play an important role when studying the macroscopic fracture toughness of a single crystal. The main focus of this study is on the influence of size effects and rate-sensitivity for materials with an HCP crystal structure, and the following is concluded:

- The numerical simulation of the HCP crystal revealed bands of intense slip in the slip rate field. An increasing rate sensitivity leads to an increase in the plastic zone size, but at the same time also a smearing effect giving a less distinct view of the features surrounding the crack tip. The size effect does not influence the characteristics of the plastic zone, however, it does affect the magnitude. By increasing the length parameter, and thereby the significance of size effects, the plastic zone becomes smaller due to the hardening effect caused by the GNDs, however, the effect is much less pronounced for a high rate sensitivity.
- In accordance with the influence of the size effects on the plastic zones, the macroscopic fracture toughness is also affected. When the material length parameter is increased, the macroscopic fracture toughness decreases as the plastic zone shrinks and less energy is dissipated through plastic deformation due to the hardening effect. Studies of high (low) crack propagation velocities revealed that an increasing rate sensitivity leads to a monotonically decreasing (increasing) macroscopic fracture toughness. This suggests that a characteristic velocity exists which corresponds to the rate independent material response. The existence of a characteristic velocity is in accordance with the findings of e.g. Nielsen and Niordson [17], Juul et al. [12], El-Naaman et al. [5].
- The behavior of either monotonic increase or decrease leads to an identification of a characteristic velocity at which the macroscopic toughness becomes independent of the rate sensitivity i.e. the macroscopic toughness corresponding to the rate independent material response. The hardening effect originating from the plastic strain gradient tends to increase the characteristic velocity and at the same time decrease the shielding ratio. In addition, it was observed that the influence of the gradient effects becomes less pronounced for materials with high rate sensitivity. This provides a useful method to study the rate-independent response, especially for gradient enhanced models that only exists in rate dependent formulations.

During the present investigation, the Kuroda and Tvergaard model was found to be very sensitive to the slip rate provided by the conventional part of the program. Generally, when a back stress of approximately 60% of the critically resolved shear stress was reached, the solution started to diverge rendering solution impossible within the present framework. Similar problems are also experienced with this type of model for traditional Lagrangian frameworks (El-Naaman et al. [6,5]) and the steady-state framework inherits similar stability issues.

Acknowledgements The work is financially supported by The Danish Council for Independent Research in the project “New Advances in Steady-State Engineering Techniques”, grant DFF-4184-00122.

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(a)

(b)

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Table 1: Mechanical Properties, recall that; $R_0 = (K_0/\tau_0)^2$, with $K_0 = \sqrt{E\Gamma_{tip}/(1-\nu^2)}$.

Parameter	Significance	Value
τ_0/G	Yield strain	0.001
ν	Poisson's ratio	0.30
b	Burgers vector	0.286 nm
N	Hardening exponent	0-0.15
m	Rate sensitivity	0.01-0.1
L/R_0	Energetic length parameter	0.0 – 0.015
$\dot{\gamma}_0$	Reference strain rate	0.002
Γ_{tip}	Near tip fracture energy	1 J/m ²