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A novel numerical framework for self-similarity in plasticity: Wedge indentation in single crystals

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Abstract

A novel numerical framework for analyzing self-similar problems in plasticity is developed and demonstrated. Self-similar problems of this kind include processes such as stationary cracks, void growth, indentation etc. The proposed technique offers a simple and efficient method for handling this class of complex problems by avoiding issues related to traditional Lagrangian procedures. Moreover, the proposed technique allows for focusing the mesh in the region of interest. In the present paper, the technique is exploited to analyze the well-known wedge indentation problem of an elastic-viscoplastic single crystal. However, the framework may be readily adapted to any constitutive law of interest. The main focus herein is the development of the self-similar framework, while the indentation study serves primarily as verification of the technique by comparing to existing numerical and analytical studies. In this study, the three most common metal crystal structures will be investi-

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gated, namely the face-centered cubic (FCC), body-centered cubic (BCC), and hexagonal close packed (HCP) crystal structures, where the stress and slip rate fields around the moving contact point singularity are presented. *Keywords:* Self-similarity, Crystal plasticity, Wedge indentation, Asymptotic fields

1 1. Introduction

Self-similarity exists in a broad range of elastic-plastic problems, where 2 history dependence precludes direct solution methods. Such problems include 3 geometrically self-similar indentation, as well as problems in void growth 4 and phase transformation. The analysis of such problems often relies on 5 cumbersome (traditional) Lagrangian procedures. But why not exploit the 6 self-similar nature of the solutions to such problems when developing the omputational framework? The first steps toward this were made in the 8 early works by Hill and Storåkers (1990); Bower et al. (1993); Storåkers and 9 Larsson (1994); Biwa and Storåkers (1995) where frameworks for the ex-10 ploitation of self-similarity in indentation problems were developed. Their 11 methods started from the well-known analogy between a flat punch and a 12 stationary crack so deformation induced by a non-flat indenter with rather 13 arbitrary axi-symmetric geometries, could be analyzed by cumulative superposition of stationary flat punch solutions, for elastic and power law creeping ¹⁶ solids. However, as discussed by Saito and Kysar (2011) and in more detail below, the proper analogy for a non-flat indenter is with a quasi-statically 17

propagating crack. Drugan and Rice (1984) and Drugan (1986) explained that for elastic-plastic materials that satisfy the maximum plastic work inequality, the asymptotic fields for stationary and quasistatically propagating cracks are different in both isotropic and anisotropic materials. Furthermore the asymptotic fields may change as a consequence of large rotations and deformations. Hence, care must be taken with such methods, especially for anisotropic materials.

In the present work, a general computational framework specialized for geometrically self-similar problems in elastic-plastic solids is developed. The framework does not, as the previously mentioned self-similar methods, rely on reference solutions nor is it restricted to specific material laws. As an example, the framework is applied to wedge indentation of elastic-plastic single crystals.

For more than three decades, investigations have shown both analytically 31 and numerically, that the material behaviour during indentation involves 32 complex elastic-plastic deformation with finite strains and rotations. The 33 early studies were closely related to crack growth which shares similarities 34 to the indentation problem. For example, the boundary value problem of a 35 stationary crack tip is analogous to that of a flat punch indentation. Likewise, 36 the boundary value problem of a quasi-statically closing crack is analogous to 37 that of a nearly-flat wedge indenter where the *contact point singularity* (e.g. 38 the point where the indenter loses contact with the surface as it impinges 39 into a material) moves quasistatically along the surface. 40

Analytical investigations of the asymptotic behaviour around a singular 41 point in the crack tip and wedge indentation fields have been conducted by 42 e.g. Drugan et al. (1982); Drugan and Rice (1984); Drugan (1986); Rice 43 (1987); Drugan (2001); Saito and Kysar (2011) based on an extension of slip 44 line theory that assumes a linear elastic, ideally plastic behavior (rather than 45 the rigid, ideally plastic behavior typically associated with slip line theory) 46 and also can account for the elastic and plastic anisotropy of the crystal me-47 chanical response. The governing partial differential equations are hyperbolic 48 so the analytical solution is obtained via the method of characteristics. As 49 consequence, the deforming domain is divided into sectors within which а 50 deformation is either elastic or is ideally plastic on a well-defined set of slip 51 systems. The sectors are separated by different types of discontinuities on 52 sector boundaries, depending on the specific problem at hand. 53

For indentation (or cracks), the asymptotic solutions near the contact 54 point (or crack tip) singularities consist of angular sectors centered at the 55 singular point. The stress state in both plastically and elastically deform-56 ing regions can be readily calculated. Special attention must be paid to the 57 boundaries between the angular sectors that consist of radial lines emanat-58 ing from the singular point. If the singular point is stationary the solutions 59 admit stress and velocity discontinuities across the radial sector boundaries. 60 However, singular points, and hence sector boundaries, that move quasistat-61 ically through elastic-plastic materials that obey the maximum plastic work 62 inequality have solutions that admit velocity discontinuities but not stress 63

discontinuities (Drugan and Rice, 1984; Drugan, 1986). Thus, the asymp-64 totic fields associated with stationary and quasistatically moving singulari-65 ties are quite different. Saito and Kysar (2011); Saito et al. (2012); Sarac 66 and Kysar (2017) showed that asymptotic fields for flat punches and nearly-67 flat wedge indenters have significant differences, with related experimental 68 analyses (Kysar et al., 2010; Sarac et al., 2016). These studies were heav-69 ily inspired by Rice (1987) and Kysar (2001a,b) where the differences with 70 regard to cracks were reported, with related experimental analyses of sta-71 tionary cracks (Bastawros and Kim, 2000; Crone and Shield, 2001) as well as 72 uasistatically growing cracks (Kysar, 2000; Kysar and Briant, 2002). Rice 73 et al. (1990) was among the first to confirm the distinct material behaviour 74 in the vicinity of both a stationary and quasi-static crack tip through nu-75 merical analysis, with other studies by Mesarovic and Kysar (1996); Kysar 76 (2001a,b). 77

Recently, Saito et al. (2012) conducted numerical studies of the wedge 78 indentation process confirming the analytical predictions by Saito and Kysar 79 (2011). However, these investigations (Rice et al., 1990; Saito et al., 2012) 80 are based on traditional incremental Lagrangian frameworks that suffer from 81 numerical difficulties such as developing contact interfaces as well as prob-82 lems with modelling a moving singularity due to the incremental procedure 83 (not to mention the problem of maintaining sufficient mesh resolution over 84 the span where the contact point moves). Obviously, such numerical issues 85 are undesired and compromise accuracy of results. Thus, the main goal of 86

the present study is to develop a general numerical framework specialized for 87 self-similar problems in plasticity that avoids the numerical issues of the tra-88 ditional procedures. In the following, self-similarity is referred to as a process 89 where the fields, such as stress and strain fields, do not change for an observer 90 continuously changing magnification of the view at a problem dependent rate. 91 For example, considering wedge indentation, the fields beneath the indenter 92 remain of identical shape, but change magnitude when the indenter impinges 93 deeper into the material. To verify the numerical procedure, results of wedge 94 indentation into the face-centered cubic (FCC) crystal structure will be com-95 pared to the analytical and numerical work of Saito and Kysar (2011) and 96 Saito et al. (2012). Additionally, in order to demonstrate the capability of 97 the developed framework, new results are presented for body-centered cubic 98 (BCC) and hexagonal close-packed (HCP) crystal structures and compared 99 to the analytical results in Saito and Kysar (2011). 100

The paper is divided into the following sections: The wedge indentation problem, analytical solutions, and material model are outlined in Section 2, self-similarity and the numerical framework are derived in Section 3, verification and results are presented in Section 4, and finally some concluding remarks are given in Section 5. Index notation, including Einstein's summation convention, is used throughout and the notation (`) signifies a time derivative.

¹⁰⁸ 2. Indentation with a nearly flat wedge indenter

Quasi-static wedge indentation is chosen as the benchmark problem for 109 the numerical framework developed as both analytical and numerical re-110 sults exist for comparison (Saito and Kysar, 2011; Saito et al., 2012). Saito 111 et al. (2012) considered indentation into a single metal crystal with a nearly 112 flat wedge indenter such that, ϕ , (cf. Fig. 1) approaches 0°. Here, friction 113 between the indenter and the material is neglected and an elastic, ideally 114 plastic single crystal with a very low critical resolved shear stress equal on 115 all slip systems is assumed (see model parameters in Table 1). The pro-116 posed numerical framework is not limited to such extreme conditions, but 117 this configuration ensures the conditions required for the analytical solutions 118 developed by Saito and Kysar (2011). Additionally, this set-up allows for a 119 two-dimensional (2D) plane strain analysis under a small strain assumption 120 by employing effective in-plane slip systems that combine deformation on 121 symmetric pairs of out-of-plane slip systems into an effective in-plane defor-122 mation. A detailed description and discussion of the effective slip systems 123 can be found in Section 2.2. 124

A detailed study of the analytical solutions can be found in Saito and Kysar (2011) based on the extension of slip line theory that assumes linear elastic and ideally plastic behavior. Here, the FCC, BCC, and HCP crystal structures are treated for the 2D plane strain case. Saito and Kysar (2011) derived an analytical solution for a moving contact point singularity based on the assumption that stress discontinuities cannot exist in the deformation

fields under these conditions (see Drugan and Rice, 1984). Following Rice 131 (1987), the analytical investigation by Saito and Kysar (2011) showed that 132 the asymptotic deformation fields consist of angular sectors centered at the 133 singular point; the angular sectors can deform either elastically or plasti-134 cally. The angular sectors are separated by radial rays emanating from the 135 singular point that coincide either with the slip direction or the slip plane 136 normal of the effective in-plane slip system. As described by Rice (1987), 137 if the radial ray coincides with a slip direction, dislocations operate in glide 138 shear along the ray and if the radial ray coincides with the slip plane normal 139 dislocations operate in kink-shear mode. If the contact point singularity is 140 stationary with respect to the crystal, the stress fields can admit stress jumps 141 across the radial rays. However, if the contact point singularity moves qua-142 sistatically relative to the crystal, the angular sectors and sector boundaries 143 move through the crystal as well. Under this condition, the stress fields do 144 not admit discontinuities across the radial sector boundaries, but velocity 145 discontinuities across the radial sector boundaries are allowed (Drugan and 146 Rice, 1984) 147

The solution by Saito and Kysar (2011) for the asymptotic fields associated with the contact point singularity of a nearly-flat wedge impinging into an FCC crystal is reproduced in Fig. 2a. The solution consists of four elastically deforming angular sectors separated by three plastically deforming radial rays. By adopting the slip systems in Table 2, it is seen that the glide shear is related to slip system (1) and (3), and the kink shear is related to slip system (2). The asymptotic solution for the BCC crystal is shown
in Fig. 2b, having only three sectors separated by two plastically deforming
rays (glide shear).

Saito and Kysar (2011) showed that the asymptotic solution for the stresses in the vicinity of the moving contact point singularity for the FCC and BCC crystals are described according to Eqs. (1)-(3) with $C_1 = \sqrt{3}/2$, $C_2 = \sqrt{3}$, and $C_3 = \sqrt{3}/2$ for FCC, and $C_1 = 3/4$, $C_2 = 3/2$, and $C_3 = 3/4$ for BCC.

$$\frac{\sigma_{11} - \sigma_{22}}{2\tau_0} = C_1 \sin(2\theta) \tag{1}$$

$$\frac{\sigma_{11} + \sigma_{22}}{2\tau_0} = C_2 \theta \tag{2}$$

$$\frac{\sigma_{12}}{\tau_0} = C_3[1 - \cos(2\theta)] \tag{3}$$

where σ_{ij} is the stress tensor, τ_0 is the critical resolved shear stress, and θ is the angle depicted in Fig. 2.

The analytical solutions of the stress field are presented in Figs. 7a and 159 9a for the FCC and BCC structures, respectively. The stress distribution is 160 plotted as a function of the angle θ with $\theta = 0$ at the undeformed surface 161 in front of the moving contact point and $\theta = -\pi$ at the indenter surface 162 going in a clockwise direction (see Fig. 2). Additionally, the analytical stress 163 trajectory and yield surface are presented in Figs. 7b and 9b for the FCC 164 and BCC structures, respectively. The yield surfaces are adopted directly 165 from Table 2 through Table 4 in Saito and Kysar (2011). The last crystal 166

structure of interest in this paper is the HCP structure. Saito and Kysar (2011) determined that the asymptotic solutions for the HCP crystal must include at least one plastic angular sector, unlike the FCC and BCC structures in which all angular sectors are elastic. Hence, an analytical solution of the stress field has not yet been derived for the HCP crystal (cf. Fig. 11b).

172 2.1. Material model

The plane strain study of indentation in single crystals is performed in a small strain setting. Thus, the total strain, ε_{ij} , is determined from the displacement, u_i , such that; $\varepsilon_{ij} = (u_{i,j} + u_{j,i})/2$ and furthermore the total strain is decomposed into the elastic part, ε_{ij}^e , and the plastic part, ε_{ij}^p ($\varepsilon_{ij} = \varepsilon_{ij}^e + \varepsilon_{ij}^p$). When the strain field (and its decomposition) are known, the stress field can be determined from the relationship; $\sigma_{ij} = \mathscr{L}_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}^p)$, where \mathscr{L}_{ijkl} is the elastic stiffness tensor.

To determine the plastic part of the total strains for a single crystal, a summation over all slip systems, α , is performed according to

$$\dot{\varepsilon}_{ij}^{p} = \sum_{\alpha} \dot{\gamma}^{(\alpha)} P_{ij}^{(\alpha)}, \quad P_{ij}^{(\alpha)} = \frac{1}{2} \left(s_{i}^{(\alpha)} m_{j}^{(\alpha)} + m_{i}^{(\alpha)} s_{j}^{(\alpha)} \right)$$
(4)

where $P_{ij}^{(\alpha)}$ is the Schmid tensor, $\dot{\gamma}^{(\alpha)}$ is the slip rate, and $s_i^{(\alpha)}$ and $m_i^{(\alpha)}$ are the unit vectors defining the slip direction and the slip plane normal, respectively (see Fig. 3). To determine the slip rate on each slip system, the following visco-plastic power law slip rate relation proposed by Hutchinson (1976) is

adopted

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \operatorname{sgn}\left(\tau^{(\alpha)}\right) \left(\frac{|\tau^{(\alpha)}|}{g^{(\alpha)}}\right)^{1/m}$$

where $\tau^{(\alpha)} = \sigma_{ij} m_i^{(\alpha)} s_j^{(\alpha)}$ is the resolved shear stress and $g^{(\alpha)}$ is the slip resistance. The slip resistance $g^{(\alpha)} = \tau_0^{(\alpha)}$ since only elastic, ideally plastic materials are considered in the present study.

The visco-plastic law in Eq. (5), implies that the rate-sensitivity of the material response increases for an increasing rate-sensitivity exponent, m, and vice versa, (N.B. The slip plane normal is denoted by unit vector m_i whereas the rate-sensitivity exponent is denoted by the scalar m). Thus, for $m \to 0$, the constitutive material model approaches the rate-independent material response.

For the self-similar indentation problem dimensional analysis dictates that the indentation solution is governed by the following parameters

$$\dot{\gamma}^{(\alpha)}\left(\frac{x_i}{a}\right) = F\left(\frac{\tau_0}{E}, \frac{\dot{a}}{a\dot{\gamma}_0}, \phi, m, \nu\right).$$
(6)

189 2.2. Effective slip systems

The reason for choosing a 2D plane stain model is mainly for verification purposes of comparing the results of the computations to the existing analytical solution, but also because many detailed experiments are conducted under nominally plane strain conditions in single crystals. However, the numerical framework in Section 3 can equally well be exploited for three-dimensional
(3D) boundary value problems.

To ensure 2D plane strain deformation of single crystals, it is necessary to 196 choose the plane of plane strain to coincide with a mirror symmetry plane in 197 the crystal (see e.g. Rice, 1987; Kysar et al., 2005; Niordson and Kysar, 2014). 198 Here, following Rice (1987), the $(\bar{1}01)$ plane is chosen as the mirror symmetry 199 plane for the plane strain deformation in the FCC and BCC crystals. The 200 specimen geometry and the external loading must also have mirror symmetry 201 about the crystallographic mirror plane. In that way the plastic slip systems 202 can be grouped into *mirrored pairs*; both members of a pair share the same 203 magnitude of resolved shear stress. Each of the two slip systems within a 204 mirrored pair will then activate with the same slip rate, assuming the critical 205 resolved shear stress is the same on both slip system. In this way the 12 206 slip systems from the FCC $\{111\}\langle 110\rangle$ family of slip systems reduces to 6 207 mirrored pairs of slip systems. For three of the mirrored pairs, the out-of-208 plane components of the plastic slip on one slip system will counteract that 209 of the other slip system within the pair. The other three mirrored pairs do 210 not have mutually canceling out-of-plane deformations, so the experiments 211 and analyses are performed under conditions of small scale yielding (Rice, 212 1968) so that the elastically deforming region surrounding the plastic zone 213 suppresses the out-of-plane deformation, and hence the activation, of these 214 other three mirrored pairs. 215

216

Based on the crystal structure (see Fig. 3), three mirrored pairs of slip

systems combine to form three effective plane strain slip systems in an FCC crystal, with each particular effective slip system denoted by α (the two underlying slip systems paired into the effective slip system are denoted αa and αb).

Referring to Fig. 3, effective slip system 1 has unit slip direction $s_i^{(1)}$ 221 oriented at an angle of $\theta_1 = \tan^{-1}(\sqrt{2}) \approx 54.7356^\circ$ relative to the specimen 222 x_1 -axis. Effective slip system 2 has unit slip direction $s_i^{(2)}$ oriented at an angle 223 of $\theta_2 = 0^\circ$ relative to the specimen x_1 -axis. Effective slip system 3 has unit 224 slip direction $s_i^{(3)}$ oriented at an angle of $\theta_3 = \pi - \tan^{-1}(\sqrt{2}) \approx 125.2644^{\circ}$ 225 relative to the specimen x_1 -axis. In the FCC crystal, effective slip systems 1 226 and 3 consist of a pair of coplanar slip systems whereas effective slip system 2 227 consists of a collinear pair of slip systems. In Kysar et al. (2005, 2010); Saito 228 and Kysar (2011), the mirror plane was chosen equivalently to be (110), but 229 the effective plane strain slip systems were oriented at the same respective 230 angles for the orientation used herein. 231

Now considering a BCC crystal with crystallographic orientation of the 232 specimen rotated by 90° relative to that of the FCC crystal, as illustrated 233 in Fig. 3. A BCC crystal has 24 different slip systems of type $\{1\overline{1}0\}\langle111\rangle$ 234 and $\{11\overline{2}\}/(111)$ (Hirth and Lothe, 1992). By choosing the $(\overline{1}01)$ plane as 235 the mirror symmetry plane for the plane strain deformation there are 12 236 237 mirrored pairs of slip system of which 6 pairs are capable of inducing a plane strain deformation state. One of the mirrored pairs consists of $(\overline{1}2\overline{1})[111]$ 238 and $(\bar{1}\bar{2}\bar{1})[1\bar{1}1]$. Since $s_i^{(\alpha)}$ and $m_i^{(\alpha)}$ for both slip systems lie within the $(\bar{1}01)$ 239

plane, both slip systems individually admit plane strain plastic deformation with $s_i^{(1)}$ oriented such that $\theta_1 = \tan^{-1}(\sqrt{2}) \approx 54.7356^\circ$ and $s_i^{(3)}$ oriented such that $\theta_3 = \pi - \tan^{-1}(\sqrt{2}) \approx 125.2644^\circ$ relative to the specimen x_1 -axis. Another mirrored pair of slip systems consists of $(101)[\bar{1}\bar{1}1]$ and $(101)[1\bar{1}\bar{1}]$, which when activated in tandem produce an effective plain strain plastic slip system oriented such that $\theta_2 = 0^\circ$.

The remaining four mirrored pairs can be activated in tandem to form four effective in-plane slip systems, two of which have $s_i^{(\alpha)}$ parallel to $s_i^{(1)}$ and the other two of which have $s_i^{(\alpha)}$ parallel to $s_i^{(3)}$. However, the resolved shear stresses on these slip systems are smaller than that of effective slip systems 1 and 3 so these have been neglected in this analysis.

Lastly, for the HCP crystal, effective slips systems are not required when 251 oriented such that the basal plane is the plane of deformation since three in-252 plane slip systems exist for this configuration. The method for determining 253 the effective slip systems are adopted from Rice (1987) and Niordson and 254 Kysar (2014). The individual crystallographic slip systems and the corre-255 sponding effective slip systems are summarized in Table 2 and the orientation 256 of the wedge indenter is shown in Fig. 3. The $s_i^{(\alpha)}$ and $m_i^{(\alpha)}$ of the individual 257 crystallographic slip systems, in general, have components in the out-of-plane 258 direction. In order to simplify the analytical and numerical analyses, (Rice, 259 1987) showed it convenient to treat each mirrored pairs of slip systems as 260 an effective in-plane slip system with unit effective in-plane unit slip direc-261 tion $S_i^{(\alpha)}$ and unit effective in-plane unit slip plane normal as $M_i^{(\alpha)}$. It is 262

then necessary to scale the values of the critical resolved shear stress and the
reference plastic strain rate for the effective slip systems.

To that end τ_0 and $\dot{\gamma}_0$ are defined as the critical resolved shear stress and reference plastic strain rate, respectively, on the individual crystallographic plastic slip systems. Then $S_i^{(\alpha)}$ is substituted for $s_i^{(\alpha)}$ and $M_i^{(\alpha)}$ is substituted for $m_i^{(\alpha)}$ in Eq. (4) when calculating the resolved shear stresses. Finally, the effective critical resolved shear stresses and the effective reference plastic strain rates are scaled, respectively, with dimensionless scaling parameters $\lambda^{(\alpha)}$ and $\beta^{(\alpha)}$ to calculate the effective critical resolved shear stress, $\tau_0^{(\alpha)}$, and the effective reference strain rate, $\dot{\gamma}_0^{(\alpha)}$ for each of the effective in-plane slip systems according to

$$\tau_0^{(\alpha)} = \lambda^{(\alpha)} \tau_0, \quad \text{and} \quad \dot{\gamma}_0^{(\alpha)} = \beta^{(\alpha)} \dot{\gamma}_0$$
(7)

where the values of $\lambda^{(\alpha)}$ and $\beta^{(\alpha)}$ for each effective slip system for FCC, BCC and HCP are listed in Table 2.

²⁶⁷ 3. Self-similarity and the numerical framework

268 3.1. Self-similar relation

In the context of plasticity, self-similarity may be defined as solutions to a boundary value problem where field quantities remain unchanged in shape, and only the spatial extent of the solution scales with time or deformation. Such solutions may be encountered in indentation, void growth, and station273 ary crack problems to name a few.

The governing equation to be derived in the following holds for any history dependent self-similar solution and as such can be exploited to address a wide range of problems. Here, considering indentation, self-similarity is obtained when the indentation rate, defined as $\dot{a}/a = \dot{c}$, is constant, where *a* is the half contact length (i.e. the distance from the center of the indentation to the contact point singularity) and \dot{a} the contact point velocity, as illustrated in Fig. 1.

Before the self-similar method is described further, two different coor-281 dinate systems applied in the derivation will be defined. The first is the 282 reference coordinate system, x_i , that describes the position of all material 283 points at time t = 0 and the second is the self-similar coordinate system 284 in which coordinates of material points change with time. The axes of the 285 self-similar coordinate system expand and stretch accordingly with the evo-286 lution of the self-similar field. There exists a family of self-similar coordinate 287 systems, all related by scaling factors, but a specific self-similar coordinate 288 system where the coordinates are normalized with the half contact length, a, 289 according to $\xi_i = x_i/a$ is employed here. Thus, the contact point singularity 290 is located at $\xi_i = (1, 0)$. 291

During indentation, self-similarity may be recognized by an observer who changes magnification in proportion to the indentation contact length, as this is the only characteristic length in the problem. Thus, any field quantity, f, must have the functional dependence $f(\xi_i)$. Under self-similar conditions, the only time dependence in the problem enters through the evolution of the characteristic length, *a*. Thus, the time rate of change of any field quantity in the self-similar coordinate system can be expressed through the following self-similar relation

$$\dot{f} = \frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial \xi_i} \frac{\partial \xi_i}{\partial t} = -\frac{\dot{a}}{a} \xi_i \frac{\partial f}{\partial \xi_i} = -\dot{c} \xi_i \frac{\partial f}{\partial \xi_i} \tag{8}$$

where \dot{c} can be viewed as the magnification rate.

This constitutes a relation between time varying and spatially varying quantities, enabling a numerical framework specialized for self-similar problems along the same lines as those first laid out by Dean and Hutchinson (1980) for steady-state problems where the stationary field translates.

To establish a better understanding of the self-similar problem, the self-297 similarly expanding field solution (constant magnification rate, \dot{c}) is analyzed 298 (see Fig. 1). By integrating $\dot{a}/a = \dot{c}$ with respect to time, t, an explicit re-299 lation between the half contact length, a_0 , at t = 0, and the current half 300 contact length, a, at time, t, can be obtained; $a = a_0 e^{\dot{c}t}$. From this relation, 301 it is seen that the contact length grows exponentially over time. Hence, it fol-302 lows that any length quantity related to the indentation process must evolve 303 exponentially in time as there are no further independent length quantities. 304 This is illustrated in Fig. 4, where the basis related to the reference coordi-305 nate system, x_i , is given by $(\underline{g}_1, \underline{g}_2)$ such that the contact point at time t = 0306 is located at $(a_0,0)$. As indentation progresses, the basis in a self-similar 307

coordinate system will be stretched according to $(\underline{G}_{1}^{(t)}, \underline{G}_{2}^{(t)}) = (\underline{g}_{1}, \underline{g}_{2})a_{0}e^{\dot{c}t}$, maintaining the contact point (singularity) at $\xi_{i} = (1, 0)$. It then follows from the relation between bases (or equivalently the relation for the exponentially increasing contact length) that a material point and its history in the indentation process can be tracked according to $\xi_{i} = (x_{i}/a_{0})e^{-\dot{c}t}$ in the self-similar coordinate system. The coordinates of a material point, x_{i} , in the self-similar coordinate system, ξ_{i} , therefore diminish with time.

With a suitable relation established between time derived and spatially 315 derived quantities, a numerical integration technique similar to that of Dean 316 and Hutchinson (1980) can be adopted. However, in contrast to the integra-317 tion lines from Dean and Hutchinson (1980), which represent the material 318 flow in a predefined direction, the integration technique here is based on 319 spatial integration along lines starting far away in the elastic region, going 320 towards the origin of the self-similar field (in this case the indenter tip), 321 carrying the history dependence of material points (see illustration of a inte-322 gration line in Fig. 1). As a consequence of the integration lines being located 323 radially around the indenter tip, it is convenient to express the self-similar 324 relation, Eq. (8), in a self-similar polar coordinate system with the origin 325 located at the tip of the indenter. The self-similar expression can thus be 326 expressed as $\dot{f} = -\dot{c}\rho\partial f/\partial\rho$ where ρ is defined as the radial distance to a 327 328 point on the integration line. This self-similar relation will be employed in the development of the numerical framework. 329

330 3.2. Numerical framework

The self-similar finite element model developed in the present study is a 331 novel approach to handle this class of problems, inspired by the early work 332 of Dean and Hutchinson (1980) for steady-state problems. The self-similar 333 condition established in Section 3.1 states that any time derived quantity, 334 f, in the constitutive model can be directly related to a spatial derivative 335 through the magnification rate, \dot{c} , according to the relation $\dot{f} \neq -\dot{c}\rho\partial f/\partial\rho$. 336 Thus, any quantity of interest at a given material point, ρ^* , can be evaluated 337 by integrating along a self-similar line, starting far away from the center 338 of the self-similarity (in this case indenter tip) in the elastic zone, ρ^0 , and 339 ending at the point of interest closer to the indenter tip, ρ^* (see integration 340 path in Fig. 1). The point of interest, ρ^* , will then contain the load history 341 of all points further away from the indenter tip. The self-similar integration 342 procedure is performed with a classical forward Euler integration scheme. 343

As in Dean and Hutchinson (1980), the displacement field, u_i , is determined from the conventional principle of virtual work (PWV) for a quasistatic self-similar problem

$$\int_{V} \mathscr{L}_{ijkl} \varepsilon_{kl} \delta \varepsilon_{ij} \mathrm{d}V = \int_{S} T_{i} \delta u_{i} \mathrm{d}S + \int_{V} \mathscr{L}_{ijkl} \varepsilon_{kl}^{p} \delta \varepsilon_{ij} \mathrm{d}V \tag{9}$$

where $T_i = \sigma_{ij}n_j$ is the surface traction with n_j denoting the unit outward normal vector, V is the volume, and S is the bounding surface. Using the finite element method, the PVW is discretized using a 2D 8-node isopara-

metric elements with reduced Gauss integration $(2 \times 2 \text{ Gauss points})$.

The procedure for obtaining the self-similar solution is very similar to the one suggested by Juul et al. (2017) for a single crystal visco-plastic steadystate model, however, the integration is now carried out along lines emanating from the center of the self-similar field. The pseudo-algorithm for the selfsimilar procedure is as follows (superscript n refers to the iterative step):

- 1. The plastic strains from the previous iteration, $\varepsilon_{ij}^{p(n-1)}$, are used to determine the current displacement field, $u_i^{(n)}$, from the PVW in Eq. (9) $\varepsilon_{ij}^{p(n-1)} = 0$ in the first iteration).
- The total strains, ε⁽ⁿ⁾_{ij}, are determined from the displacement field, u⁽ⁿ⁾_i.
 The slip on each slip system and the plastic strain field are determined by the self-similar integration procedure.
 - (a) First the spatial derivatives of the slip and total plastic strains are determined by applying the self-similar relation $(\partial f/\partial \rho = -\dot{f}/(\rho \dot{c}))$

$$\frac{\partial \gamma^{(\alpha)}}{\partial \rho} = -\frac{\dot{\gamma}_0^{(\alpha)}}{\rho \dot{c}} \operatorname{sgn}\left(\tau^{(\alpha)}\right) \left(\frac{|\tau^{(\alpha)}|}{g^{(\alpha)}}\right)^{1/m} \tag{10}$$

$$\frac{\partial \varepsilon_{ij}^p}{\partial \rho} = \sum_{\alpha} \frac{\partial \gamma^{(\alpha)}}{\partial \rho} P_{ij}^{(\alpha)} \tag{11}$$

(b) Secondly, the current slip $\gamma^{(\alpha)(n)}$ on each slip system and the current plastic strains, $\varepsilon_{ij}^{p(n)}$, are determined by performing the self-similar integration

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$$\gamma^{(\alpha)(n)} = \int_{\rho^0}^{\rho^*} \frac{\partial \gamma^{(\alpha)}}{\partial \rho} d\rho, \quad \text{and} \quad \varepsilon_{ij}^{p(n)} = \int_{\rho^0}^{\rho^*} \frac{\partial \varepsilon_{ij}^{(p)}}{\partial \rho} d\rho.$$
(12)

4. The current stresses $\sigma_{ij}^{(n)}$ are then determined by applying the elastic constitutive relation; $\sigma_{ij} = \mathscr{L}_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}^p)$.

5. Step 1 through 4 is repeated, continuously feeding the new plastic field
into the right hand side of Eq. (9), until convergence is obtained. Convergence is evaluated by comparing the displacement and stress field of
the current iteration with the previous iteration.

It is noticed that the numerical framework is an iterative procedure (in contrast to the traditional incremental procedures), directly bringing out the
self-similar state of the problem.

The stability of the self-similar framework is found to be very robust to various parameters, and even for very low rate-sensitivity exponents convergence will be obtained without any special approach to the problems. However, this version of the framework also relies on the modifications suggested by Niordson (2001) and Nielsen and Niordson (2012a), where substeps between the Gauss points are introduced in the spatial integration procedure which increases the stability of the framework.

381 4. Results

The established numerical framework for self-similar problems is applied to the wedge indentation process to validate the solution for the stress and slip rate fields around the moving contact point (see also Saito et al., 2012). The mesh is scaled around the contact point, such that the mesh is very fine in the vicinity of the contact point where a detailed view is desired, while the mesh is gradually coarser when moving away from the point of interest in order to save computational time (see illustration in Fig. 5).

389 4.1. Stress Fields

In this part, the stress distribution will be presented for the FCC, BCC, and HCP crystal structures as contour plots, angular variation around the moving contact point singularity, and as the stress trajectory in stress space. The contour plots are presented in the self-similar coordinate system, ξ_i , such that the contact point is always located at the coordinate $\xi_i = (1,0)$ (the contact point singularity).

Figure 6 presents contour plots of the stress components for the FCC crystal structure. According to Drugan and Rice (1984), stress discontinuities are not admissible across a quasi-statically moving surface in a plastically deforming material, which is also confirmed by the continuous stress distributions. Upon further inspection of the stresses, it is seen that some stress contour lines appear as rays emanating from the contact point. This is in accordance with the asymptotic solutions in Eqs. (1)-(3). Moreover, it is ⁴⁰³ noticed that the asymptotic solution breaks down some distance from the
⁴⁰⁴ contact point as the field is no longer independent of the radius from the
⁴⁰⁵ contact point.

To investigate the angular variation of the stresses around the contact 406 point, the stresses have been extracted along an arc around the contact point 407 using an inverse isoparametric mapping scheme. The extracted numerical 408 values (markers) are plotted together with the analytical solution (lines) in 409 Fig. 7. Here, the vertical lines represent the sector boundaries shown in 410 Fig. 2a. It is seen that there is a good agreement between the analytical 411 and numerical results both in terms of the angular development but also the 412 magnitude. Furthermore, it is seen that the stress components satisfy the 413 boundary conditions in terms of $\sigma_{12} = 0$ and $\sigma_{22} = 0$ at $\theta = 0$ (the free 414 undeformed surface) and $\sigma_{12} = 0$ at $\theta = -180^{\circ}$ (the frictionless indenter 415 surface). 416

Lastly, the stress trajectory is plotted in Fig. 7b, starting in the vicinity of 417 (0,0) which is at the free surface $(\theta = 0)$ going in clockwise direction ending 418 at the indenter surface. The elastic sectors (I-IV) are indicated on the stress 419 trajectory according to Fig. 2a. The stress trajectory shows that the stresses 420 start in an elastic region at the undeformed surface, then as $\theta \to -54.7^{\circ}$, the 421 stresses develop into a state where the trajectory touches the yield surface at 422 a point corresponding to a radial sector boundary undergoing glide shear (i.e. 423 a radial ray of plastically deforming material). Afterwards, the material again 424 becomes elastic until a second radial sector boundary (this time undergoing 425

kink shear) is encountered at $\theta = -90^{\circ}$ where the stresses just reach the yield surface and then become elastic again. At $\theta = -125.3^{\circ}$, the final radial sector boundary is encountered (glide shear) and the stress trajectory goes back to the initial point where the material behaviour is elastic. The fact that the material behaves elastically close to the indenter surface, indicates large stress triaxiality which is also confirmed by the stress component in Fig. 7a, where $\sigma_{11} = \sigma_{22}$ (Saito et al., 2012).

Figure 8 presents contour plots of the stresses for the BCC structure. 433 Comparing to the solution for FCC (Fig. 6) similar features are observed for 434 all stress components. Moreover, a similar asymptotic nature of the stresses 435 only being dependent on the angle in the immediate vicinity of the moving 436 contact point singularity is also valid. The stress components plotted along 437 an arc around the contact point is shown in Fig. 9a for the BCC crystal, along 438 with the analytical solutions from Eqs. (1)-(3). Again, the numerical solution 439 is seen to be in good agreement with the analytical solution. In addition, 440 the stress trajectory is presented in Fig. 9b for the BCC structure. Here, 441 recall that it is expected to see one sector less than for the FCC structure 442 as the analytical solution does not predict the existence of a radial sector 443 boundary at $\theta = -90^{\circ}$ (Saito and Kysar, 2011). Starting in the vicinity of 444 (0,0) and moving in the clockwise direction, the first radial sector boundary 445 446 (glide shear) is encountered. At the top horizontal line of the yield surface, it is noticed that the numerical solution is, in fact, close to the yield surface, 447 even though this should not be the case for the BCC structure. This can 448

⁴⁴⁹ be explained by the fact that a rate dependent model has been employed ⁴⁵⁰ in the numerical model which results in a sector boundary at $\theta = -90^{\circ}$ ⁴⁵¹ being activated because of the stress trajectory is very close to the yield ⁴⁵² surface (Saito and Kysar, 2011). By employing a rate independent model ⁴⁵³ in the framework this should be avoidable. Lastly, the second radial sector ⁴⁵⁴ boundary (also glide shear) is encountered and the material goes back to ⁴⁵⁵ being elastic approaching the initial state.

Finally, the HCP crystal is considered. The shape of the stress contours 456 for the HCP structure (Fig. 10) have minor differences in the details but are 457 overall similar to the stress contours for the FCC and BCC crystals. For 458 the HCP structure (Fig. 11), none of the asymptotic solutions considered 459 by Saito and Kysar (2011) were admissible, indicating the existence of at 460 least one angular plastic sector. The angular stress distribution in Fig. 11a 461 shows similarities to the FCC and BCC structure but the curves are less 462 smooth. Moreover, the numerical solution for the HCP structure still comply 463 with the boundary conditions in terms of $\sigma_{12} = 0$ and $\sigma_{22} = 0$ at $\theta =$ 46 0 (the free surface) and $\sigma_{12} = 0$ at $\theta = -180^{\circ}$ (the frictionless indenter 465 surface). The stress trajectory in Fig. 11b starts in the vicinity of (0, 0), and 466 moves in the clockwise direction. From the numerical solution, the trajectory 467 approaches the vertex in the upper left corner, then continue on the yield 468 surface, going towards the upper right vertex and subsequently towards the 469 vertex to the right of the starting point. This indicates that the material 470 behaves plastically within certain sectors as predicted by Saito and Kysar 471

472 (2011).

473 4.2. Slip rate fields

The slip rate for the FCC, BCC, and HCP crystal structure will be pre 474 sented in the following as contour plots near the moving contact point sin-475 gularity (the same normalization of the axes as for the stresses is used). The 476 main goal of this part is to bring forward the discontinuities expected in slip 477 rate. These discontinuities were not directly seen in the previous results of 478 the stress field since stress discontinuities are not admissible for a moving 479 contact point singularity (Drugan and Rice, 1984). It should be noticed that 480 the analytically proven discontinuities (Drugan and Rice, 1984; Rice, 1987; 481 Saito and Kysar, 2011) will appear as rays with a finite width in the field of 482 interest due to the rate dependent material model employed. 483

Figure 12 displays the normalized slip rate on the three effective slip sys-484 tems for the FCC structure as well as the total slip rate (the sum $\dot{\gamma}^{(tot)}$ = 485 $\sum^{\alpha} |\dot{\gamma}^{(\alpha)}|$). According to Fig. 2a, a glide shear discontinuity should be ob-486 served at $\theta = -125.3^{\circ}$ on slip system (1) which is also the case (Fig. 12a). 487 The numerical predictions also holds for the two other analytical prediction 488 by Saito and Kysar (2011) for slip system (2) which shows a kink shear ray 489 -90° (Fig. 12b) and lastly a glide shear ray on slip system (3) at at $\theta =$ 490 -54.7° (Fig. 12c). The glide shear ray in Fig. 12a is of particular inθ 491 492 terest as it is seen that the ray is reflected at the displacement symmetry boundary $(\xi_1 = 0)$, into a kink shear ray at $\theta = -125.3^{\circ}$. A better illus-493

tration of this is shown in Fig. 12d, where the sum of the slip rates on all 494 systems is presented. It is seen that the kink shear ray arising from slip 495 system (1) at point B is intersecting the kink shear ray on slip system (2)496 at point C. From a geometric point of view, these two rays should intersect 497 on a line of $\theta = -64.7^{\circ}$, which is confirmed by the numerical results. Upon 498 further inspection of the line OC, only slip system (1) contributes to plastic 499 deformation below the line of $\theta = -64.7^{\circ}$, whereas all slip systems contribute 500 to the deformation above the line. The observations for both the stress and 501 the slip rate fields are consistent with the results obtained by Saito et al. 502 (2012) for the FCC crystal. 503

In Fig. 13, the same results are presented for the BCC crystal structure. 504 Since the BCC structure has slip systems identical to the FCC crystal, the 505 same angles are observed (obviously, there is a change in the magnitudes, as 506 the effective parameters are different). For slip system (1) (Fig. 13a), the 507 glide shear ray is again observed at $\theta = -125.3^{\circ}$, and at $\theta = -54.7^{\circ}$ for 508 slip system (3) (Fig. 13c). Moreover, the contour plot in Fig. 13b shows a 509 kink shear ray at $\theta = -90^{\circ}$ similar to the one for the FCC structure, which 510 according to the analytical solution should not exist. This is ascribed to the 511 rate dependent model activating the kink shear due to the stress trajectory 512 being very close to the yield surface (see Fig. 9b). Additionally, a small 513 feature at approximately $\theta = -120^{\circ}$ in Fig. 13b is not part of the analytical 514 solution and its magnitude changes with the rate-sensitivity, m (the same 515 feature is in fact seen for the FCC crystal in Fig. 12b, however, it is much 516

⁵¹⁷ smaller). For the BCC crystal a kink shear ray is also seen to emanate from ⁵¹⁸ the displacement symmetry boundary (Fig. 13d) perpendicular to the glide ⁵¹⁹ shear ray in slip system (1), making this system solely responsible for the ⁵²⁰ plastic deformation below the OC line. Furthermore, it is also here observed ⁵²¹ that a kink shear ray, is reflected of the displacement symmetry boundary, ⁵²² and that it intersects the kink shear ray on slip system (2) on a $\theta = -64.7^{\circ}$ ⁵²³ line in accordance with the geometrical expectation.

Lastly, the slip rate fields are presented for the HCP structure (Fig. 14) 524 which deviate slightly from the FCC and BCC structures due to the difference 525 in slip systems. Even though an analytical solution was not established for 526 the HCP crystal, it is clear that the discontinuities coincide with the slip 527 systems, where slip system (1) creates a glide shear ray at $\theta = -120^{\circ}$, a kink 528 shear ray is formed on slip system (2) at $\theta = -90^{\circ}$, and finally another glide 529 shear ray is formed at $\theta = -60^{\circ}$ on slip system (3). Besides the discontinuities 530 related to the slip systems, an additional feature is observed in Fig. 14c at 531 approximately $\theta = -80^{\circ}$. Similarly to the unexpected feature in Fig. 13b, 532 this feature is expected to be an artifact of the rate dependency. As for 533 the FCC and BCC crystal structures, a kink shear ray for slip system (1) 534 reflects of the displacement symmetry boundary, however, it is much less 535 pronounced for the HCP crystal. This kink shear ray should intersect the 536 kink shear ray that emanates from slip system (2) at an angle of $\theta = -67^{\circ}$ 537 (based on geometrical observations), however, the intersection is only vaguely 538 observable from Fig. 14d. 539

540 5. Concluding remarks

A novel numerical framework for self-similar problems in plasticity has been developed. The framework is specialized to this class of problems and eliminates a number of issues encountered when employing traditional Lagrangian procedures. Moreover, the framework readily enables focusing the mesh for high resolution of field solutions in the regions of interest.

Main focus in the presented work is on the development and verification 546 of the self-similar framework. The verification is conducted by applying the 547 newly developed framework to wedge indentation in a 2D small strain setting 548 for single crystal plasticity, where both analytical (Saito and Kysar, 2011) and 549 numerical (Saito et al., 2012) results exist for comparison. The framework, 550 however, is general and holds for any self-similar problem in plasticity (also 551 in 3D and with appropriate extensions for finite strains). The key findings 552 are: 553

• The stress distribution in the vicinity of the contact point singularity corresponds to the analytical predictions by Saito and Kysar (2011) both qualitatively and quantitatively for the FCC and BCC crystal structure. Furthermore, the stress field for FCC is similar to the numerical results of Saito et al. (2012) showing the same qualitative features.

560 561 • Numerical simulation indeed reveals discontinuities in the slip rate corresponding to the predictions of Saito and Kysar (2011). Based on the

analytical results both glide shear and kink shear sector boundaries exist for the FCC structure and this gives rise to three discontinuity lines
emanating from the contact point singularity. The sector boundaries
readily fall out by applying the new numerical framework.

• For the HCP crystal structure, an analytical expression was not con-566 structed as the asymptotic solutions by Saito and Kysar (2011) were 567 not admissible, implying that at least one plastic sector exists (only 568 elastic sectors exist for FCC and BCC). The numerical results for the 569 HCP crystal confirmed the existence of such sectors by having part 570 of the stress trajectory remaining on the yield surface. Furthermore, 571 both glide shear and kink shear discontinuities are predicted by the 572 numerical model for the HCP crystal. 573

For the BCC crystal, only glide shear discontinuities should exist according to analytical solutions, giving two sector boundaries. However, the numerical solutions also predict a third sector boundary corresponding to a kink shear discontinuity. The authors believe that this has to do with the rate dependent material model for which the kink shear discontinuity appears because the stress trajectory is very close to the yield surface.

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Figure 1: Wedge indentation in a rate dependent single crystal. Inside the self-similar history dependent domain (SS domain) the developed numerical framework is applied, whereas outside this domain, the material is treated as being linear elastic.



Figure 2: Sector structure for asymptotic fields beneath the contact point singularity (a) with kink shear sector boundary (FCC) and (b) without kink shear sector boundary (BCC) (Saito and Kysar, 2011). The parameter $\alpha = 54.7^{\circ}$ for both the FCC and BCC crystal structures.



Figure 3: Crystallographic orientation of the specimen relative to the wedge indenter, and the effective slip systems for the FCC, BCC, and HCP crystal structures, respectively.



Figure 4: Development of self-similarity through time in (a) the reference coordinates with the basis vectors $(\underline{g}_1, \underline{g}_2)$, and in (b) the self-similar coordinate system with the stretched basis vectors $(\underline{G}_1^{(t)}, \underline{G}_2^{(t)})$.



Figure 5: Right hand side of the domain used for numerical simulations. The dashed arrows indicate the direction of gradually increasing element size. The boundary of the domain is sufficiently far away from the contact point to have negligible influence on the results (the boundary is clamped).



Figure 6: Stress distribution around the right hand side contact point, $\xi_i = (1, 0)$, in FCC crystal for the stress components (a) σ_{11}/τ_0 , (b) σ_{22}/τ_0 and (c) σ_{12}/τ_0 .



Figure 7: Stress distribution for FCC around the right hand side contact point projected as (a) angular distribution, and (b) stress trajectory with the thick line representing the yield surface. The lines represent the analytical solution while the markers indicate the numerical results.



Figure 8: Stress distribution around the right hand side contact point, $\xi_i = (1, 0)$, in BCC crystal for the stress components (a) σ_{11}/τ_0 , (b) σ_{22}/τ_0 and (c) σ_{12}/τ_0 .



Figure 9: Stress distribution for BCC around the right hand side contact point projected as (a) angular distribution, and (b) stress trajectory with the thick line representing the yield surface. The lines represent the analytical solution while the markers indicate the numerical results.



Figure 10: Stress distribution around the right hand side contact point, $\xi_i = (1,0)$, in HCP crystal for the stress components (a) σ_{11}/τ_0 , (b) σ_{22}/τ_0 and (c) σ_{12}/τ_0 .



Figure 11: Stress distribution for HCP around the right hand side contact point projected as (a) angular distribution, and (b) stress trajectory with the thick line representing the yield surface. Here, only the numerical solution is presented.



Figure 12: Slip rate around the right hand side contact point, $\xi_i = (1,0)$, in FCC crystal for the slip systems (a) $|\dot{\gamma}^{(1)}|/\dot{c}$, (b) $|\dot{\gamma}^{(2)}|/\dot{c}$, (c) $|\dot{\gamma}^{(3)}|/\dot{c}$, and (d) $\dot{\gamma}^{(\text{tot})}/\dot{c}$ $(\dot{\gamma}^{(\text{tot})} = \sum^{\alpha} |\dot{\gamma}^{(\alpha)}|)$.



Figure 13: Slip rate around the right hand side contact point, $\xi_i = (1,0)$, in BCC crystal for the slip systems (a) $|\dot{\gamma}^{(1)}|/\dot{c}$, (b) $|\dot{\gamma}^{(2)}|/\dot{c}$, (c) $|\dot{\gamma}^{(3)}|/\dot{c}$, and (d) $\dot{\gamma}^{(\text{tot})}/\dot{c}$ $(\dot{\gamma}^{(\text{tot})} = \sum^{\alpha} |\dot{\gamma}^{(\alpha)}|)$.



Figure 14: Slip rate around the right hand side contact point, $\xi_i = (1,0)$, in HCP crystal for the slip systems (a) $|\dot{\gamma}^{(1)}|/\dot{c}$, (b) $|\dot{\gamma}^{(2)}|/\dot{c}$, (c) $|\dot{\gamma}^{(3)}|/\dot{c}$, and (d) $\dot{\gamma}^{(\text{tot})}/\dot{c}$ $(\dot{\gamma}^{(\text{tot})} = \sum^{\alpha} |\dot{\gamma}^{(\alpha)}|)$.

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736	1	Model parameters
737	2	Effective slip systems for plane strain model
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Parameter	Significance	Value
τ_0/E	Yield strain	$\sim 1e^{-5}$
ν	Poisson ratio	0.3
m	Strain rate-sensitivity exponent	0.02
$\dot{\gamma}_0$	Reference slip rate	$0.001 s^{-1}$
\dot{c}	Magnification rate	$0.1 s^{-1}$
ϕ	Indenter angle	0.038°
	Table 1: Model parameters.	

Effective slip system no.	(1)	(2)	(3)
	FCC		
Angle to $[101]$ in $(\overline{1}01)$ plane	54.7°	0°	-54.7°
Crystallographic slip system (a)	$(111)[1\bar{1}0]$	$(11\bar{1})[101]$	$(\bar{1}1\bar{1})[0\bar{1}\bar{1}]$
Crystallographic slip system (b)	$(111)[0\bar{1}1]$	$(\bar{1}11)[101]$	$(\bar{1}1\bar{1})[\bar{1}\bar{1}0]$
(αa) (αa) (αb) (αb)			
$\beta^{(\alpha)} = \frac{s_i^{(\alpha)} m_j^{(\alpha)} + s_i^{(\alpha)} m_j^{(\alpha)}}{s^{(\alpha)} m^{(\alpha)}}$	$\sqrt{3}$	$\frac{2}{\sqrt{3}}$	$\sqrt{3}$
$\lambda^{(\alpha)} = rac{ au^{(\alpha)}}{ au^{(\alpha a)}} = rac{ au^{(\alpha)}}{ au^{(\alpha b)}}$	$\frac{2}{\sqrt{3}}$	$\sqrt{3}$	$\frac{2}{\sqrt{3}}$
	BCC	(
Angle to $[010]$ in $(\overline{1}01)$ plane $[^{\circ}]$	54.7°	0°	-54.7°
Crystallographic slip system (a)	$(\bar{1}\bar{2}\bar{1})[1\bar{1}1]$	$(101)[\bar{1}\bar{1}1]$	$(\bar{1}2\bar{1})[111]$
Crystallographic slip system (b)	-	$(101)[1\bar{1}\bar{1}]$	-
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$\beta^{(\alpha)} = \frac{s_i^{(\alpha a)} m_j^{(\alpha a)} + s_i^{(\alpha b)} m_j^{(\alpha b)}}{\alpha}$	1	$\frac{2}{\sqrt{2}}$	1
s_i^{i} , m_j^{i} ,		V 3	
$\lambda^{(lpha)} = rac{ au^{(lpha)}}{ au^{(lpha a)}} = rac{ au^{(lpha)}}{ au^{(lpha b)}}$	1	$\sqrt{3}$	1
	HCP		
Angle to $[11\overline{2}0]$ in (0001) plane $[^{\circ}]$	60°	0°	-60°
Crystallographic slip system (a)	$(10\bar{1}0)[1\bar{2}10]$	$(1\bar{1}00)[\bar{1}\bar{1}20]$	$(01\bar{1}0)[2\bar{1}\bar{1}0]$
Crystallographic slip system (b)	-	-	-
(αa) (αa) (αb) (αb)			
$\beta^{(\alpha)} = \frac{s_i^{(\alpha)} m_j^{(\alpha)} + s_i^{(\alpha)} m_j^{(\alpha)}}{s_i^{(\alpha)} m_j^{(\alpha)}}$	1	1	1
$s_i \cdot m_j$			
$\lambda^{(\alpha)} = \frac{\tau^{(\alpha)}}{\tau^{(\alpha)}} = \frac{\tau^{(\alpha)}}{\tau^{(\alpha)}}$	1	1	1
$\tau^{(\alpha a)}$ $\tau^{(\alpha b)}$	±	*	±

 Table 2: Effective slip systems for plane strain model.

P.C.