

An integration scheme for elastoplastic rate-independent single crystals based on Maier's minimum principle

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Abstract

A novel formulation to determine the incremental crystallographic slip in a rate-independent elastoplastic single crystal subjected to mixed traction and velocity boundary conditions is proposed. Slip is governed by Schmid's law. The present formulation is based on a theorem due to Maier [Meccanica (1968), 3;121–130], which amounts to a statement of the principle of maximum dissipation. It reduces the present problem to one of non-negative quadratic programming. The quadratic program is solved using the non-negative least squares algorithm due to Lawson and Hanson, which has mathematically guaranteed convergence properties. The incremental elastoplastic formulation is used to simulate tensile, and simple shear deformation of copper crystals symmetrically oriented for multi-slip. The predicted mechanical and microstructural responses compare well with the experimental measurements, and computational results reported in the literature. A computer implementation of the present method is found to be about an order of magnitude faster than a previous formulation based on the unregularised Schmid's law.

Keywords: Crystal plasticity; Elastoplastic behaviour; Computational methods for plasticity; Optimisation; Non-smooth response

1 Introduction

In a number of metallic materials, plastic deformation is accommodated by crystallographic slip within grains. Crystallographic slip can be described by two types of laws: rate-independent and rate-dependent. According to the rate-independent Schmid's law [1], slip cannot activate in a crystallographic slip system when the resolved shear stress therein, τ , is smaller than a critical value, called the critical resolved shear stress, τ_c . The earliest models of slip [2–6] were rate-independent models, which did not assume an explicit relation between the slip rate, $\dot{\gamma}$, and τ ;

plastic power minimisation was invoked to determine the slip rates in slip systems wherein $\tau = \tau_c$.

The simplest form of the $\dot{\gamma}$ - τ relationship in a rate-dependent viscoplastic material is due to Pierce et al. [7]. They took $\dot{\gamma} \sim (\tau/\tau_c)^{1/m}$, with $m = \partial \ln \tau / \partial \ln \dot{\gamma}$ termed the rate-sensitivity. For coarse-grained copper at room temperature, $1/m \approx 140$, and increases with decreasing grain size [8]. Based on physical, and mathematical considerations, a number of $\dot{\gamma}$ - τ forms have since been proposed in the literature: e.g., $\dot{\gamma} \sim \langle (\tau/\tau_c)^{1/m} - 1 \rangle$ [9], $\dot{\gamma} \sim \langle (\tau - \tau_c)/K \rangle^n$ [10], where $\langle \cdot \rangle$ denote Macaulay brackets. The predictive capabilities of

some of these forms has been studied by Busso and Cailletaud [11].

Rate-independent, and rate-dependent laws have both been used in the literature to predict characteristics such as spontaneous banding [12–14], damage evolution [15, 16], and for the prediction of the mechanical response, and microstructural evolution under imposed complex strain paths [10, 17–19]. Despite receiving continuous development over many decades, algorithmic challenges remain in the implementation of these laws within plasticity models [20, 21].

Efficiently determining which slip-systems activate within a time step remains a challenge in models incorporating the rate-independent law. Two types of approaches have been adopted to address it. In the first approach, heuristic algorithms have been proposed to determine the set of active slip systems [9, 22–25]. These algorithms are heuristic in that they do not guarantee convergence to the correct solution within a finite number of iterations. The approach proposed by Schmidt-Baldassari [26] avoids the heuristic determination of the active set of slip-systems. His augmented Lagrangian formulation leads to a non-linear optimisation problem. This approach is also used by Petryk and Kurska [27, 28] in implementing their work increment minimisation strategy. Ben Bettaieb et al. [29] proposed exploring the combinatorial possibilities of active slip systems. However, solution approaches based on nonlinear optimisation, or combinatorial exploration are computationally much more demanding than the heuristic ones [21]. The second approach is based on the geometrical understanding that the yield surface has a closed convex polyhedral shape in stress space, with each slip system contributing a hyperface, and that the difficulty of identifying the active slip system occurs at the corners of this polyhedron, where multiple faces meet. At the corners, the normal to the polyhedral surface becomes non-unique. Therefore, the second approach rounds-out the corners, i.e., regularises the yield surface, and thereby ensures a unique normal, e.g., Arminjon [30], Gambin [31], Akpama et al. [32], and Mánik et al. [33]. A comprehensive review of these and other regularisation techniques, as applied to rate-independent materials can be found in Mánik and Holmedal [34], and Mánik et al. [33].

Likewise, amongst the models incorporating the rate-dependent law, solving the non-linear systems of equations for the stress state using the experimentally measured value of the rate-sensitivity is computationally expensive. It is common in the literature to assume a larger value of rate-sensitivity than the measured one for computational efficiency [21], although it may physically be more accurate to model the constitutive law as rate-independent in this circumstance.

In the limit of small rate-sensitivity, $m \downarrow 0$, the predictions from models that incorporate the rate-dependent law must approach those assuming the rate-independent one. However, the approach to this limit is slow. Therefore, the predictions of the rate-dependent law for small but practicable m , and that of the rate-independent law may diverge [20]. The rate-dependent law necessarily leads to predictions that vary continuously with the initial conditions. For example, in a simulation of plastic deformation, if the initial lattice orientation of a crystal or grain were slightly varied, only commensurately slight differences would appear in its predicted final orientation, or the mechanical response. On the other hand, using the rate-independent law, predictions that vary abruptly with the initial conditions are possible. A stark example is the Taylor ambiguity [34], which refers to the non-uniqueness of slip-rates that satisfy all the boundary, and constitutive conditions. Non-unique slip-rates can result in non-unique predicted stress-strain response, non-unique lattice rotations, and hence, non-unique final texture. It is emphasised that the abrupt change in response that results from the rate-independent law is physically justified, and experimentally realised [35, 36]. However, it is troublesome when it appears in numerical simulations. This justifies the further study of the numerical treatment of the rate-independent law.

Lin [37] performed the first analysis of rate-independent elastoplastic single crystals. He recognised that elastoplastic analysis went beyond rigid-plastic analysis in that it allowed the determination of the sequence of slip system activation. While Lin [37] described the criteria that must be satisfied for the activation of subsequent slip systems, he did not give a procedure to find them amongst the many combinatorial possibilities. Cuitiño and Ortiz [9] and Borja and

Wren [22] proposed algorithms for this latter task. These, and subsequent works, due to Anand and Kothari [23], Schröder and Miehe [24], Knockaert et al. [38], Miehe and Schröder [39], McGinty and McDowell [25], Zamiri and Pourboghraat [40], and Ben Bettaieb et al. [29] have been reviewed by Akpama et al. [32]. In their review, the latter authors have divided the proposed algorithms into two groups: return mapping algorithms, and ultimate algorithms, and have compared the two strategies through numerical simulations. A recent algorithm, due to Nijhuis et al. [41], traces the hypersurfaces of the yield surface corresponding to the slip systems until it reaches the point of intersection of all the active hypersurfaces.

The solution methodologies in the works described above enforce the consistency condition [42] at the end of each time step in the simulation. Another strategy adopted in the literature is based on the maximum dissipation theorem of plasticity [40, 43–46]. In this approach, the problem of determining the slip increments over a time-step is expressed as a problem of maximising the plastic dissipation, subject to the constraints given by Schmid’s law. Since Schmid’s law is expressed in terms of non-smooth inequality constraints, Zamiri and Pourboghraat [40] replace it with a single smooth constraint of logarithmic-exponential form. On the one hand, this strategy makes the constraint equation differentiable, and thereby reduces the computational effort required to solve the optimisation problem. On the other hand, it amounts to regularising the yield surface by rounding out its corners. It thereby artificially forces a continuous response upon the rate-independent problem, pushing it toward the characteristic behaviour of the rate-dependent model. Scheunemann et al. [43, 44], Niehüser and Mosler [45], Perdahcioğlu [46] used the interior point method with a logarithmic barrier function to smooth the constitutive constraint. Again, the use of the barrier function amounts to smoothing the yield surface, with the consequence of forcing an artificially continuous response. In the literature, in order to minimise such smoothing, the coefficient of the barrier function in the Lagrangian is either taken to be very small upfront [46], or decreased with progressing iterations [43–45, 47], so that the predicted slip is approximately equal to the physical slip. However, as shown by Prüger

and Kiefer [21], even small errors in the slip increments can produce sizeable errors in the predicted hardening, and thereby adversely affect the subsequently predicted response, particularly with anisotropic hardening.

An integration scheme that determines the slip increments over a time step without resorting to smoothing Schmid’s law is presently proposed. Smoothing is avoided not only by not regularising the inequalities representing Schmid’s law, but also by avoiding the use of numerical techniques that amount to such regularisation. The problem of determining the slip increments over a time-step is represented as a quadratic optimisation problem, subject to simple non-negativity constraints. Because of its simple structure, the solution of the present problem is more direct than that of general non-linear optimisation problem: It is solvable non-heuristically by modifying an efficient classical algorithm, due to Lawson and Hanson [48], with mathematically guaranteed convergence properties.

The development in Sec. 2 below follows that of Maier [49], proposed for a structural engineering problem. As in Maier’s work, the present treatment accommodates the imposition of mixed traction, and velocity boundary conditions. While the hardening of the slip systems is assumed to be isotropic and linear over a time-step, the optimisation problem is solved in the lattice orientation at the end of the time step. The present method is thus semi-implicit in the sense of McGinty and McDowell [25].

The present method can predict abruptly varying response over the space of initial conditions. In order to demonstrate this property, uniaxial tensile tests under multislip conditions are simulated. It is shown in Sec. 3 that the present model is able to describe qualitatively different responses arising from slight differences in the initial orientations of crystals. The physical validity of these predictions is verified by demonstrating good agreement with the results of the single crystal experiments of Franciosi and co-workers in copper.

Prüger and Kiefer [21] have quantified the computational effort associated with two rate-independent and two rate-dependent formulations. They found that the rate-independent formulations execute more than twice as fast as the rate-dependent ones featuring the physical value of rate sensitivity. One of their rate-independent

formulations, the augmented Lagrangian method of Schmidt-Baldassari [26], does not regularise Schmid's law, while the other nonlinear complementarity function formulation does. It will be shown that computer execution of the present formulation is about ten times faster than that of the augmented Lagrangian formulation, and about the same as the nonlinear complementarity formulation.

2 Elastoplastic model of the crystal

Consider a single crystal in a homogeneous state of stress and deformation in the time interval $t \in (t_0, t_0 + \Delta t)$, $\Delta t > 0$. Following the standard approach in crystal plasticity modelling [33], two coordinate systems are introduced: (i) The global (G) Cartesian coordinate system $\mathbf{e}_1\text{-}\mathbf{e}_2\text{-}\mathbf{e}_3$, in which the imposed stress and/or deformation increment components are prescribed; and (ii) The Cartesian coordinate system, (C), which rotates with the crystal lattice, wherein the constitutive response of the crystal is described. Let the orthonormal tensor $\mathbf{\Omega}(t)$ denote the orientation of the crystal coordinate system with respect to the global coordinate system. Then, the components of an arbitrary 1-tensor $\mathbf{v}$ in the global (G) and crystal (C) coordinate systems, denoted $v_i^{(G)}$, and $v_i^{(C)}$, respectively, obey the transformation law

$$v_i^{(C)} = \Omega_{ij}(t)v_j^{(G)}, \text{ or } v_i^{(G)} = \Omega_{ji}(t)v_j^{(C)}. \quad (1)$$

Here and elsewhere, summation over repeated Latin subscript indices is implied. Likewise, the components of an arbitrary 2-tensor $\mathbf{A}$ transform following:

$$\begin{aligned} A_{ij}^{(C)} &= \Omega_{ik}(t)\Omega_{jl}(t)A_{kl}^{(G)}, \text{ or,} \\ A_{ij}^{(G)} &= \Omega_{ki}(t)\Omega_{lj}(t)A_{kl}^{(C)}. \end{aligned} \quad (2)$$

2.1 Mixed boundary conditions

Crystal deformation is prescribed by imposing a complementary set of components of the symmetric Cauchy stress tensor $\bar{\sigma}_{ij}(t = t_0 + \Delta t)$, and the velocity gradient, $\bar{L}_{ij}(t)$, on the crystal at time $t = t_0 + \Delta t$:

$$\sigma_{ij}^{(G)}(t_0 + \Delta t) = \sigma_{ji}^{(G)}(t_0 + \Delta t) = \bar{\sigma}_{ij} = \bar{\sigma}_{ji}, \quad (3)$$

for $ij \in \mathcal{S}$, and

$$L_{ij}^{(G)}(t_0 + \Delta t) = \bar{L}_{ij}, \text{ and } L_{ji}^{(G)}(t_0 + \Delta t) = \bar{L}_{ji}, \quad (4)$$

for $ij \in \mathcal{L}$.

The subscript sets, $\mathcal{S}$, and $\mathcal{L}$ in Eqs. (3), and (4) are disjoint and span the Cartesian components: $\mathcal{S} \cup \mathcal{L} = \{11, 22, 33, 23, 32, 13, 31, 12, 21\}$. Also, if $ij \in \mathcal{S}$, $ji \in \mathcal{S}$, and if $ij \in \mathcal{L}$, $ji \in \mathcal{L}$. In general, $\bar{L}_{ij}$, and $\bar{L}_{ji}$ may be unequal.

Using Eq. (2), Eqs. (3), and (4) can be expressed in terms of the stress and velocity gradients in the (C) system as

$$\Omega_{ki}(t_0 + \Delta t)\Omega_{lj}(t_0 + \Delta t)\sigma_{kl}^{(C)}(t_0 + \Delta t) = \bar{\sigma}_{ij}, \quad (5)$$

for $ij \in \mathcal{S}$, and

$$\Omega_{ki}(t_0 + \Delta t)\Omega_{lj}(t_0 + \Delta t)L_{kl}^{(C)}(t_0 + \Delta t) = \bar{L}_{ij}, \quad (6)$$

for $ij \in \mathcal{L}$, respectively. $\mathbf{\Omega}(t_0 + \Delta t)$ is not known a priori. Its iterative determination starting from the initial estimate $\mathbf{\Omega}(t_0 + \Delta t) \approx \mathbf{\Omega}(t_0)$ will be described in Sec. 2.10 below. Until then, it is assumed that an estimate of $\mathbf{\Omega}(t_0 + \Delta t)$ is available.

Let $\mathbf{D} = (\mathbf{L} + \mathbf{L}^T)/2$, and $\mathbf{W} = (\mathbf{L} - \mathbf{L}^T)/2$ be the homogeneous rate of deformation, and spin tensors, respectively. Let

$$\begin{aligned} \bar{D}_{ij} &= (\bar{L}_{ij} + \bar{L}_{ji})/2, \\ \bar{W}_{ij} &= (\bar{L}_{ij} - \bar{L}_{ji})/2, \\ \bar{D}_{ij}^{(C)} &= (\bar{L}_{ij}^{(C)} + \bar{L}_{ji}^{(C)})/2, \text{ and} \\ \bar{W}_{ij}^{(C)} &= (\bar{L}_{ij}^{(C)} - \bar{L}_{ji}^{(C)})/2. \end{aligned} \quad (7)$$

Adding and subtracting the transpose of each of the equations in Eqs. (5), and (6) to themselves, using the symmetry of $\bar{\sigma}_{ij}$, $\sigma_{ij}^{(C)}$, $\bar{D}_{ij}$ and $D_{ij}^{(C)}$, the skew-symmetry of $\bar{W}_{ij}$, and $W_{ij}^{(C)}$, and expressing the results in terms of Eq. (7) gives

$$\Omega_{ki}(t_0 + \Delta t)\Omega_{lj}(t_0 + \Delta t)\sigma_{kl}^{(C)}(t_0 + \Delta t) = \bar{\sigma}_{ij}, \quad (8)$$

for $ij \in \mathcal{S}$,

$$\Omega_{ki}(t_0 + \Delta t)\Omega_{lj}(t_0 + \Delta t)D_{kl}^{(C)}(t_0 + \Delta t) = \bar{D}_{ij}, \quad (9)$$

for $ij \in \mathcal{L}$, and

$$\Omega_{ki}(t_0 + \Delta t)\Omega_{lj}(t_0 + \Delta t)W_{kl}^{(C)}(t_0 + \Delta t) = \bar{W}_{ij}, \quad (10)$$

for $ij \in \mathcal{L}$. Given $\sigma_{ij}^{(C)}(t_0)$, $\Omega(t_0)$, other microstructural variables at the beginning of the time step, and the boundary conditions, Eqs. (8)–(10), it is sought to determine $\sigma_{ij}^{(C)}(t_0 + \Delta t)$, $\Omega(t_0 + \Delta t)$, etc., at the end of the time step.

2.2 The elastic response

The present work follows Maier [49], which presents a small deformation formulation. It differs from the formulation of Schröder and Miehe [24], and Scheunemann et al. [43] in that it allows the mixed imposition of strain increment components and stress components on the crystal.

$\mathbf{D}$ is decomposed additively into elastic and plastic parts:

$$\mathbf{D} = \mathbf{D}^e + \mathbf{D}^p. \quad (11)$$

Assuming that the material response is purely elastic, i.e., $\mathbf{D}^p = \mathbf{0}$, it is presently sought to solve Eqs. (8), and (9) for $\sigma_{ij}^{(C)}$. The elastic strain increment over the time interval $(t_0, t_0 + \Delta t)$ is $\mathbf{D}^e \Delta t$. The linear elastic constitutive law expressed in the crystal frame (C) is recalled [50, Chap. 7]:

$$\sigma_{ij}^{(C)}(t_0 + \Delta t) - \sigma_{ij}^{(C)}(t_0) = \mathbb{C}_{ijkl}^{(C)} D_{kl}^{e,(C)} \Delta t, \quad (12)$$

where $\mathbb{C}^{(C)}$ represents the material-dependent rank-4 stiffness tensor of the crystal, expressed in the crystal's coordinate frame.

Substituting Eq. (12) into Eq. (8), and recognising that $\mathbf{D} = \mathbf{D}^e$ in Eq. (9) yields the six equations:

$$\Omega_{ki}(t_0 + \Delta t)\Omega_{lj}(t_0 + \Delta t)\mathbb{C}_{klmn}^{(C)} D_{mn}^{e,(C)} = \frac{\bar{\sigma}_{ij} - \bar{\sigma}_{ij}^0}{\Delta t}, \quad (13)$$

for $ij \in \mathcal{S}$, and

$$\Omega_{mi}(t_0 + \Delta t)\Omega_{nj}(t_0 + \Delta t)D_{mn}^{e,(C)} = \bar{D}_{ij}, \quad (14)$$

for $ij \in \mathcal{L}$. Here,

$$\bar{\sigma}_{ij}^0 = \Omega_{ki}(t_0 + \Delta t)\Omega_{lj}(t_0 + \Delta t)\sigma_{kl}^{(C)}(t_0) \quad (15)$$

denotes the stress at time t_0 co-rotated with the lattice to time $t_0 + \Delta t$. Of the 9 equations in Eqs. (13), and (14), 6 equations, say, those corresponding to $i \geq j$, are independent.

The six unknown components of the symmetric tensor, $D_{mn}^{e,(C)}(t_0 + \Delta t)$, $mn \in \mathcal{S} \cup \mathcal{L}$, can be determined by solving Eq. (13), and Eq. (14) for given $\Omega(t_0 + \Delta t)$. Substituting $D_{mn}^{e,(C)}(t_0 + \Delta t)$ into Eq. (12) yields the Cauchy stress components. To indicate that these stress components are the outcome of an elastic calculation, they are denoted $\sigma_{ij}^{e,(C)}(t_0 + \Delta t)$:

$$\sigma_{ij}^{e,(C)}(t_0 + \Delta t) := \sigma_{ij}^{(C)}(t_0) + \mathbb{C}_{ijkl}^{(C)} D_{kl}^{e,(C)} \Delta t. \quad (16)$$

2.3 The plastic eigenstrain problem

Let a plastic eigenstrain [51], $D_{i^*j^*}^{p,(C)} \Delta t$, prescribed in the crystal frame, (C) , be imposed upon the crystal. Let the imposed eigenstrain be symmetric: $D_{i^*j^*}^{p,(C)} = D_{j^*i^*}^{p,(C)}$. The self-stress developed in the crystal due to this eigenstrain is to be determined.

To this end, consider the 4-tensor, whose components in the (C) coordinate frame are given by

$$\hat{D}_{ij^{i^*j^*}}^{p,(C)} = \begin{cases} 1, & \text{if } i^* = j^*, \text{ and } i^*j^* = ij, \\ 1/2, & \text{if } i^* \neq j^*, \text{ and } i^*j^* = ij, \\ 1/2, & \text{if } i^* \neq j^*, \text{ and } i^*j^* = ji, \\ 0, & \text{otherwise.} \end{cases} \quad (17)$$

For example, taking $i^* = j^* = 1$,

$$\hat{D}_{ij^{11}}^{p,(C)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (18)$$

and taking $i^* = 1$, and $j^* = 2$, or $i^* = 2$, and $j^* = 1$,

$$\hat{D}_{ij^{12}}^{p,(C)} = \hat{D}_{ij^{21}}^{p,(C)} = \begin{pmatrix} 0 & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (19)$$

$\hat{D}_{ij^{i^*j^*}}^{p,(C)}$ can be thus regarded as the basis matrix corresponding to the i^*j^* , and j^*i^* -components of the matrix representation of $\mathbf{D}_{ij}^{p,(C)}$ in the (C) coordinate frame. It is easily verified that superposition of the individual components regenerates

$D_{ij}^{p,(C)}$, i.e.,

$$D_{ij}^{p,(C)} \Delta t = \hat{D}_{ij1^*j^*}^{p,(C)} D_{1^*j^*}^{p,(C)} \Delta t, \quad (20)$$

with summation implied over the repeated 1^* , and j^* indices.

The self-stresses due to $\hat{D}_{ij1^*j^*}^{p,(C)} \Delta t$ for fixed $1^*j^* \in \mathcal{S} \cup \mathcal{L}$ is first determined. The boundary conditions of the self-stress problem are obtained by setting $\bar{\sigma}_{ij} = 0$, for $ij \in \mathcal{S}$, and $\bar{D}_{ij} = 0$, for $ij \in \mathcal{L}$, in Eqs. (8), and (9). Let $\hat{D}_{ij1^*j^*}^{e,(C)} \Delta t$ be the elastic strain developed, so that the rate of deformation is given by Eq. (11) as:

$$D_{ij1^*j^*}^{(C)} = D_{ij1^*j^*}^{e,(C)} + \hat{D}_{ij1^*j^*}^{p,(C)}. \quad (21)$$

Using Eq. (12), Eq. (8) becomes

$$\Omega_{ki}(t_0 + \Delta t) \Omega_{lj}(t_0 + \Delta t) \mathbb{C}_{klmn}^{(C)} D_{mni^*j^*}^{e,(C)} = 0, \quad (22)$$

for $ij \in \mathcal{S}$, and Eq. (9) becomes

$$\begin{aligned} \Omega_{mi}(t_0 + \Delta t) \Omega_{nj}(t_0 + \Delta t) D_{mni^*j^*}^{e,(C)} = \\ - \Omega_{mi}(t_0 + \Delta t) \Omega_{nj}(t_0 + \Delta t) \hat{D}_{mni^*j^*}^{p,(C)}, \end{aligned} \quad (23)$$

for $ij \in \mathcal{L}$, for fixed 1^*j^* . Again, these equations can be solved for the six unknowns, $D_{mni^*j^*}^{e,(C)}$. Substituting $D_{mni^*j^*}^{e,(C)}$ into Eq. (12) then yields the self-stress components, which are denoted

$$Z_{ij1^*j^*}^{(C)} := \mathbb{C}_{ijkl}^{(C)} D_{khi^*j^*}^{e,(C)}. \quad (24)$$

$Z_{ij1^*j^*}^{(C)} \Delta t$, the self-stress developed in the crystal due to the plastic strain, $\hat{D}_{ij1^*j^*}^{p,(C)} \Delta t$, is thus an influence coefficient. The self-stress $\sigma_{ij}^{p,(C)}$ developed in response to the plastic eigenstrain, $D_{kl}^{p,(C)}$, can be obtained by superposing the individual plastic strain components weighted by their influence coefficients, following Eq. (20):

$$\sigma_{ij}^{p,(C)} := Z_{ijkl}^{(C)} D_{kl}^{p,(C)} \Delta t. \quad (25)$$

The superscript p in $\sigma_{ij}^{p,(C)}$ identifies these stress components as being engendered by plastic eigenstrains.

The special case that $\mathcal{S} = \emptyset$, which implies that all the components of plastic strain increment

are imposed, will of interest in the sequel. Then, Eq. (22) vanishes, and Eq. (23) becomes

$$D_{mni^*j^*}^{e,(C)} = -\hat{D}_{mni^*j^*}^{p,(C)}, \quad (26)$$

for all 1^*j^* . Substituting Eq. (26) into Eq. (24) then gives

$$\begin{aligned} Z_{ij1^*j^*}^{(C)} &= -\mathbb{C}_{ijmn}^{(C)} \hat{D}_{mni^*j^*}^{p,(C)} \\ &= -\mathbb{C}_{ij1^*j^*}^{(C)}, \end{aligned} \quad (27)$$

where Eq. (17), and the minor symmetry of $\mathbb{C}_{ijmn}^{(C)}$ are used to obtain the second equality.

Consider the crystal upon which the mixed boundary conditions, Eqs. (8), and (9), are imposed, and which develops known plastic strain components $D_{ij}^{p,(C)} \Delta t$ over the time step. By the principle of linear elastic superposition, the stress components developed therein are

$$\sigma_{ij}^{(C)}(t_0 + \Delta t) = \sigma_{ij}^{e,(C)}(t_0 + \Delta t) + \sigma_{ij}^{p,(C)}. \quad (28)$$

Expanding the right side using Eqs. (16), and (25) yields:

$$\begin{aligned} \sigma_{ij}^{(C)}(t_0 + \Delta t) &= \sigma_{ij}^{(C)}(t_0) + \\ &\quad \mathbb{C}_{ijkl}^{(C)} D_{kl}^{e,(C)} \Delta t + Z_{ijkl}^{(C)} D_{kl}^{p,(C)} \Delta t. \end{aligned} \quad (29)$$

2.4 The rate-independent plastic crystal

Let the crystal under consideration possess S slip systems that shear by the mechanism of slip. Let $\mathbf{b}^s$, and $\mathbf{n}^s$ denote the slip direction, and slip plane normal vectors corresponding to slip system $s \in \{1, 2, \dots, S\}$. The components $b_i^{s,(C)}$, and $n_i^{s,(C)}$, of these vectors in the crystal coordinate system are material-dependent constants. The components of the Schmid tensor associated with slip system s in the crystal coordinate system are

$$m_{ij}^{s,(C)} = (b_i^{s,(C)} n_j^{s,(C)} + n_i^{s,(C)} b_j^{s,(C)})/2. \quad (30)$$

Slip systems s_1 and s_2 with oppositely signed Schmid tensors, $\mathbf{m}^{s_1} = -\mathbf{m}^{s_2}$, are considered distinct in the present treatment. They correspond to oppositely signed slip, and are denoted

$$s_1 = \check{s}_2, \text{ and } s_2 = \check{s}_1. \quad (31)$$

Oppositely signed slip systems will feature together in the hardening law, discussed in Sec. 2.5 below.

For example, in an fcc crystal deforming by $\{111\}\langle 110\rangle$ slip, $S = 24$, counting the positive and negative senses of each physical slip system as distinct. Suppose slip systems $1 = \check{2}$, and $2 = \check{1}$ refer to opposite senses of slip in, say, the $(111)[\bar{1}\bar{1}0]$ slip system. Slip in either slip system will affect the dislocation density in both of them, as will be shown below.

Let $\gamma^s(t) > 0$ be the accumulated slip in the slip system s at time t . They determine the plastic strain increment over the time interval $(t_0, t_0 + \Delta t)$ as

$$D_{ij}^{p,(C)} \Delta t = \sum_{s=1}^S (\gamma^s(t_0 + \Delta t) - \gamma^s(t_0)) m_{ij}^{s,(C)}. \quad (32)$$

Each slip system is associated with a critical resolved shear stress (CRSS), $\tau^s(t)$. Schmid's law [1] states that slip system s can activate only if the resolved shear stress (RSS), $\sigma_{ij}^{(C)}(t) m_{ij}^{s,(C)}$, therein equals its CRSS:

$$\frac{d\gamma^s}{dt}(t) \begin{cases} \geq 0, & \text{if } \sigma_{ij}^{(C)}(t) m_{ij}^{s,(C)} = \tau^s(t), \text{ and} \\ = 0, & \text{if } \sigma_{ij}^{(C)}(t) m_{ij}^{s,(C)} < \tau^s(t), \end{cases} \quad (33)$$

for $t \in (t_0, t_0 + \Delta t)$. Suppose the stress state 'progresses regularly' in the sense of Maier [49], i.e., if for some $t^* \geq t_0$, $\sigma_{ij}^{(C)}(t^*) m_{ij}^{s,(C)} = \tau^s(t^*)$, then $\sigma_{ij}^{(C)}(t) m_{ij}^{s,(C)} = \tau^s(t)$, for all $t \in (t^*, t_0 + \Delta t)$. Then, Eq. (33) can be expressed in terms of differences:

$$\gamma^s(t_0 + \Delta t) - \gamma^s(t_0) \begin{cases} \geq 0, & \text{if } \sigma_{ij}^{(C)}(t_0 + \Delta t) m_{ij}^{s,(C)} = \tau^s(t_0 + \Delta t), \text{ and} \\ = 0, & \text{if } \sigma_{ij}^{(C)}(t_0 + \Delta t) m_{ij}^{s,(C)} < \tau^s(t_0 + \Delta t). \end{cases} \quad (34)$$

The slip increment, $\gamma^s(t_0 + \Delta t) - \gamma^s(t_0)$, need not accumulate uniformly throughout the time step; slipping may initiate at any intermediate time, t^* , within the time step, $(t_0, t_0 + \Delta t)$.

2.5 The Cuitiño-Ortiz hardening law

A number of hardening laws have been proposed in the literature to describe the evolution of the CRSS, $\tau^{(s)}$ with slip. The Cuitiño and Ortiz [9]

model is adopted presently. In this model, slip systems can slip in either sense, positive or negative, whereas the present slip systems have a unique sense (Eq. (31)). The hardening evolution given by Cuitiño and Ortiz [9] is slightly modified below in order to reflect this difference.

First, the dislocation density ρ^s in slip system s is taken to evolve with slip, γ^s , following:

$$\frac{d\rho^s}{dt}(t) = \frac{1}{b\Lambda} \frac{d(\gamma^s + \gamma^{\check{s}})}{dt}(t) - f\rho^s \frac{d(\gamma^s + \gamma^{\check{s}})}{dt}(t), \quad (35)$$

where, Λ denotes the mean free path of a dislocation, b denotes the Burger's vector, and f determines the rate of dynamic recovery. If Λ were assumed constant, Eq. (35) is solvable in closed form:

$$\rho^s(t) = \rho_{\text{sat}} \left[1 - \left(1 - \frac{\rho_0}{\rho_{\text{sat}}} \right) \exp \left(- \frac{\gamma^s(t) + \gamma^{\check{s}}(t)}{\gamma_{\text{sat}}} \right) \right], \quad (36)$$

with ρ_{sat} , ρ_0 , and γ_{sat} being regarded as material parameters. It is clear that $\rho^s = \rho^{\check{s}}$. Dislocation motion engenders point obstacles, whose number density in slip system s is taken to be

$$n^s(t) = \frac{1}{2} \sum_{s'=1}^S a^{ss'} \rho^{s'}(t). \quad (37)$$

The characteristic slip, shear stress, and plastic modulus of slip system s are defined as:

$$\gamma_c^s = \frac{b\rho^s}{2\sqrt{n^s}}, \quad \tau_c^s = \alpha\mu b\sqrt{\pi n^s}, \quad h_c^s = \frac{\tau_c^s}{\gamma_c^s}, \quad (38)$$

respectively. In Eq. (38), the material parameter, b is the magnitude of the Burger's vector, α the dislocation interaction parameter, and μ the linear elastic shear modulus. In terms of these variables, Cuitiño and Ortiz [9] give the hardening rate of slip system s

$$\frac{d\tau^s}{dt} = \sum_{s'=1}^S H^{ss'} \frac{d\gamma^{s'}}{dt} \quad (39)$$

as:

$$H^{ss'} = h_c^s \left(\frac{\tau^s}{\tau_c^s} \right)^3 \left\{ \cosh \left[\left(\frac{\tau_c^s}{\tau^s} \right)^2 \right] - 1 \right\}, \quad (40)$$

if $s = s'$, or $s = \check{s}'$, and zero otherwise. According to Eq. (40), $H^{ss'}$ monotonically decreases with the CRSS, τ^s . The decreasing function displays a sharp knee at $\tau^s \approx \tau_c^s$. The decrease is rapid for $\tau^s < \tau_c^s$ and slower for $\tau^s > \tau_c^s$.

In the Cuitiño and Ortiz [9] model, Eq. (38) relates the obstacle density, n^s , to the characteristic shear stress, τ_c^s . This contrasts with the widely used (extended) Taylor relation, wherein it is assumed that the CRSS, $\tau^s \sim \sqrt{n^s}$ [52]. Also, in the Cuitiño and Ortiz [9] model, the CRSS, τ^s evolves only in the active slip systems according to Eq. (39). Latent hardening is accounted for by increasing τ_c^s , which can be visualised as sliding the knee of the hardening curve forward. On the other hand, in models based on the extended Taylor relation, the CRSS, τ^s , evolves in all the slip systems, both active and latent.

The initial CRSS at $\gamma^s = 0$ for all slip systems is denoted τ_0 . $H^{ss'}(t)$ given by Eq. (40) varies non-linearly with time, $t \in (t_0, t_0 + \Delta t)$. If this variation were neglected, and if it were assumed that $H^{ss'}(t) \approx H^{ss'}(t_0)$, for $t \in (t_0, t_0 + \Delta t)$, Eq. (39) can be integrated to obtain

$$\tau^s(t_0 + \Delta t) = \tau^s(t_0) + \sum_{s'=1}^S H^{ss'}(t_0)(\gamma^s(t_0 + \Delta t) - \gamma^s(t_0)). \quad (41)$$

The numerical condition for neglecting the variation of $H^{ss'}(t)$ will be given in Sec. 2.8.

Let the slip systems associated with the rows and columns of $H^{ss'}$ be numbered $\{s_1, \check{s}_1, s_2, \check{s}_2, \dots, s_{S/2}, \check{s}_{S/2}\}$. Then, the $H^{ss'}$ matrix given by Eq. (40) has a block diagonal structure, with $S/2$, 2×2 blocks, arranged along its diagonal. The four elements in each 2×2 block will be equal, and positive. $H^{ss'}$ will thus be positive semi-definite, with $S/2$ zero eigenvalues, and $S/2$ positive eigenvalues. The positive semi-definiteness of $H^{ss'}$ is an essential pre-requisite for the algorithm to be developed presently.

In a number of hardening models, either based on the extended Taylor relation, or otherwise (e.g., Pierce et al. [7]) the $H^{ss'}$ matrix will not, in general, be positive semi-definite [53]. Such hardening models are therefore incompatible with the present algorithm.

2.6 Equivalent quadratic program

Following Maier [49], consider the quadratic optimisation problem

$$\min_{\Delta\gamma^s \geq 0} \sum_{s=1}^S \sum_{s'=1}^S \frac{1}{2} E^{ss'} \Delta\gamma^{s'} \Delta\gamma^s + \sum_{s=1}^S f^s \Delta\gamma^s, \quad (42)$$

where

$$\begin{aligned} E^{ss'} &= H^{ss'} - m_{ij}^{s,(C)} Z_{ijkl}^{(C)} m_{kl}^{s',(C)}, \\ f^s &= \tau^s(t_0) - \sigma_{ij}^{e,(C)}(t_0 + \Delta t) m_{ij}^{s,(C)}, \text{ and} \\ \Delta\gamma^s &= \gamma^s(t_0 + \Delta t) - \gamma^s(t_0). \end{aligned} \quad (43)$$

The Karush-Kuhn-Tucker critical conditions for the minimisation problem, Eq. (42), are

$$\sum_{s'=1}^S E^{ss'} \Delta\gamma^{s'} + f^s \begin{cases} = 0, & \text{if } \Delta\gamma^s > 0, \text{ and} \\ \geq 0, & \text{if } \Delta\gamma^s = 0. \end{cases} \quad (44)$$

Now,

$$\begin{aligned} \sum_{s'=1}^S E^{ss'} \Delta\gamma^{s'} + f^s &= \tau^s(t_0) + \sum_{s'=1}^S H^{ss'} \Delta\gamma^{s'} \\ &\quad - m_{ij}^{s,(C)} \left(\sigma_{ij}^{e,(C)}(t_0 + \Delta t) + Z_{ijkl}^{(C)} \sum_{s'=1}^S \Delta\gamma^{s'} m_{kl}^{s',(C)} \right). \end{aligned} \quad (45)$$

Using Eq. (41), the sum of the first two terms on the right side are seen to be $\tau^s(t_0 + \Delta t)$. Recognising from Eqs. (43), and (32) that

$$D_{kl}^{p,(C)} = \sum_{s'=1}^S \Delta\gamma^{s'} m_{kl}^{s',(C)}, \quad (46)$$

and using Eqs. (29), and (41), it is found that

$$\sum_{s'=1}^S E^{ss'} \Delta\gamma^{s'} + f^s = \tau^s(t_0 + \Delta t) - m_{ij}^{s,(C)} \sigma_{ij}^{(C)}(t_0 + \Delta t). \quad (47)$$

Eq. (44) thus becomes:

$$\begin{aligned} &\tau^s(t_0 + \Delta t) - m_{ij}^{s,(C)} \sigma_{ij}^{(C)}(t_0 + \Delta t) \\ &\begin{cases} = 0, & \text{if } \Delta\gamma^s > 0, \text{ and} \\ \geq 0, & \text{if } \Delta\gamma^s = 0, \end{cases} \end{aligned} \quad (48)$$

which coincides with Eq. (34). As originally observed by Maier [49], this shows that the problem of satisfying Schmid's law, Eq. (34), can be exactly recast as minimising the quadratic objective function in Eq. (42).

The quadratic objective function, Eq. (42), is convex and possesses a unique solution if $E^{ss'}$ is symmetric and positive definite. Maier [49] has shown that the part $-m_{ij}^{s,(C)} Z_{ijkl}^{(C)} m_{kl}^{s',(C)}$ is indeed symmetric and positive definite. Thus, if $H^{ss'}$ were also symmetric and positive definite, a unique solution is guaranteed, as the sum of two symmetric positive definite matrices is also symmetric positive definite. This was shown in the setting of single crystals by Mandel [54], and Hill and Rice [55].

Consider the special case $\mathcal{S} = \emptyset$, wherein all the components of the strain increment are imposed over a step. Then, using Eq. (27), the first equation in Eq. (43) becomes:

$$E^{ss'} = H^{ss'} + \mathbb{C}_{ijkl}^{(C)} m_{ij}^{s,(C)} m_{kl}^{s',(C)}. \quad (49)$$

With this $E^{ss'}$ the minimisation problem, Eq. (42), becomes identical to that in Zamiri and Pourboghraat [40], and Scheunemann et al. [43], who derive it from the principle of maximum dissipation. Thus, physically, Eq. (42) represents a statement of the principle of maximum dissipation.

2.7 Algorithmic solution

Algorithm 1 describes the solution for the $n \times 1$ column-vector $\{x\}$ of the non-negative quadratic program:

$$\min_{\{x\} \geq \{0\}} \frac{1}{2} [x]^T [E] [x] + [x]^T [f], \quad (50)$$

where $[E]$ is a given $n \times n$ symmetric positive definite matrix, and $[f]$ a given $n \times 1$ column vector, subject to the non-negativity constraints:

$$x_j \geq 0, \quad j \in \{1, 2, \dots, n\}. \quad (51)$$

Assume temporarily that the set of indices $\mathcal{P} \subseteq \{1, 2, \dots, n\}$ for which

$$x_j > 0, \quad j \in \mathcal{P}, \text{ and} \quad (52)$$

$$x_j = 0, \quad j \in \mathcal{Z} = \{1, 2, \dots, n\} - \mathcal{P},$$

is known. Let $[E_{\mathcal{P}\mathcal{P}}]$, $\{f_{\mathcal{P}}\}$, and $\{x_{\mathcal{P}}\}$ denote the $\mathcal{P}$ -slices of $[E]$, $\{f\}$, and $\{x\}$, respectively. That is, if $\mathcal{P}_i$ denotes the i -th element of $\mathcal{P}$, the ij -th element of $[E_{\mathcal{P}\mathcal{P}}]$ is $E_{\mathcal{P}_i \mathcal{P}_j}$, and the i -th element of $[f_{\mathcal{P}}]$, and $[x_{\mathcal{P}}]$ are $f_{\mathcal{P}_i}$, and $x_{\mathcal{P}_i}$, respectively. Then Eq. (50) becomes the unconstrained minimisation

$$\min_{x_{\mathcal{P}}} \frac{1}{2} [x_{\mathcal{P}}]^T [E_{\mathcal{P}\mathcal{P}}] [x_{\mathcal{P}}] + [x_{\mathcal{P}}]^T [f_{\mathcal{P}}], \quad (53)$$

which can be solved by setting the gradient of the objective function with respect to $[x_{\mathcal{P}}]$ in Eq. (53) to zero, yielding

$$[E_{\mathcal{P}\mathcal{P}}] [x_{\mathcal{P}}] = -[f_{\mathcal{P}}]. \quad (54)$$

In practise, $\mathcal{P}$ is not known *a priori*. Eq. (54) is used to determine the incremental slip at each stage of its iterative construction.

Algorithm 1 is substantially similar to the NNLS algorithm proposed by Lawson and Hanson [48, p. 161]. An implementation of Algorithm 1, named **pqpnonneg**, due to J. Hajek, and B. Denney, is available as a part of the open-source matrix analysis software, **octave** [56]. Much of the logical effort in Algorithm 1 goes into determining the set of active slip-systems, $\mathcal{P}$, which is updated in each pass through the while-loop, beginning in step 4. The computational effort is concentrated in step 7, which implements Eq. (54), and in steps 3 and 15, wherein the gradient is evaluated. The test, which determines whether the current $\mathcal{P}$ is correct, appears in step 4 of the pseudo code. For symmetric positive definite $[E]$, the convergence of the algorithm is mathematically guaranteed [48]. The heuristic algorithms mentioned in Sec. 1 do not come with convergence guarantees.

An important feature of Algorithm 1 is the absence of any numerical tolerances. Numerical tolerances in this algorithm would have the undesirable effect of smoothing the yield surface during computation. Their absence ensures that sharp corners of the yield surface are treated exactly.

Another aspect of Algorithm 1 is the absence of any Jacobian computations. This is in contrast to the computational approaches noted in Sec. 1, wherein numerous Jacobian matrices must be computed during iterative solution. This aspect

Algorithm 1 Algorithm to solve the quadratic programming problem, Eqs. (50), and (51).

```

1: procedure NNQP( $E, f$ )
2:   Set  $\mathcal{P} \leftarrow \emptyset$ , and  $\mathcal{Z} \leftarrow \{1, 2, \dots, n\}$ , and  $x_j \leftarrow 0, \forall j \in \mathcal{Z}$ .
3:   Compute the gradient of the cost function:  $w \leftarrow Ex + f$ .
4:   while  $\mathcal{Z} \neq \emptyset$  and  $\min_{j \in \mathcal{Z}} w_j < 0$  do
5:     Find an index  $t \in \mathcal{Z}$  such that  $w_t = \min_{j \in \mathcal{Z}} w_j$ .
6:     Move the index  $t$  from  $\mathcal{Z}$  to  $\mathcal{P}$ :  $\mathcal{P} \leftarrow \mathcal{P} \cup \{t\}$ ,  $\mathcal{Z} \leftarrow \mathcal{Z} - \{t\}$ .
7:     Solve  $E_{\mathcal{P}\mathcal{P}} z_{\mathcal{P}} = -f_{\mathcal{P}}$ . Set  $z_{\mathcal{Z}} \leftarrow 0$ .
8:     if  $z_j > 0$  for all  $j \in \mathcal{P}$  then
9:       Set  $x \leftarrow z$ .
10:    else
11:      Find an index  $q \in \mathcal{P}$  such that  $\frac{x_q}{x_q - z_q} = \min_{\substack{z_j \leq 0, \\ j \in \mathcal{P}}} \frac{x_j}{x_j - z_j}$ .
12:      Set  $\alpha = x_q / (x_q - z_q)$ .
13:      Set  $x \leftarrow x + \alpha(z - x)$ .
14:      Move all indices  $j \in \mathcal{P}$  for which  $x_j = 0$  from  $\mathcal{P}$  to  $\mathcal{Z}$ .
15:      Compute the gradient of the cost function:  $w \leftarrow Ex + f$ .
16:  return  $x$ .
```

makes the present approach simpler, and computationally much faster. Other practically realised computational advantages will be noted at the end of Sec. 3.1.1.

2.8 Time stepping

The quadratic program, Eqs. (42), and (43), assumes constant hardening, $H^{ss'}$, within a time step. This assumption is inconsistent with Eq. (40), which describes the nonlinear variation of the hardening rate, $H^{ss'}(t)$, with accumulated slip, $\gamma^s(t)$. It is sought to address this inconsistency by adaptively selecting sufficiently small time steps within each of which $H^{ss'}(t)$ is approximately constant.

Let ΔT be a prescribed basic time step [57], and let $\varepsilon_{\text{hard}}$ be a prescribed tolerance for the relative hardening within a time step. The actual time step,

$$\Delta t = \frac{\Delta T}{2^n}, \quad (55)$$

is taken to correspond to the smallest $n \in \{0, 1, \dots\}$, such that the relative hardening within the Δt time step is bounded, i.e.,

$$|H^{ss}(t + \Delta t) - H^{ss}(t)| \leq \varepsilon_{\text{hard}} \frac{(H^{ss}(t + \Delta t) + H^{ss}(t))}{2}, \text{ where,} \quad (56)$$

for all activated slip systems s that satisfy $\gamma^s(t + \Delta t) > \gamma^s(t)$ in that step. If Eq. (56) is satisfied, Eq. (41) is applied to evolve the CRSS in time.

The condition of constant $H^{ss'}(t)$ over a time step can be approximated by decreasing ΔT , or $\varepsilon_{\text{hard}}$, or both. While any of these approaches should lead to convergence of the predicted mechanical response of the crystal, the computational effort associated with each approach may be significantly different. On the one hand, if for fixed ΔT , $\varepsilon_{\text{hard}}$ were decreased, a number of time step cut-backs, corresponding to larger n in Eq. (55), will occur in the parts of the simulation wherein the hardening varies rapidly. On the other hand, if for fixed $\varepsilon_{\text{hard}}$, ΔT were decreased sufficiently, greater computational effort will be expended even when the variation in the hardening is small. The computational cost associated with each of these approaches will be quantitatively discussed, and optimised, in Sec. 3.1.2.

2.9 Lattice rotation

Neglecting elastic spin, the total spin $\bar{W}_{ij}^{(C)}$ in Eq. (10) can be decomposed into plastic, and lattice spin components [33]:

$$\bar{W}_{ij}^{(C)} = W_{ij}^{\text{p},(C)} + W_{ij}^{\text{lat},(C)}, \quad (57)$$

$$W_{ij}^{\text{p},(C)} \Delta t = \sum_{s=1}^S \Delta \gamma^s \left(\frac{b_i^{s,(C)} n_j^{s,(C)} - b_j^{s,(C)} n_i^{s,(C)}}{2} \right). \quad (58)$$

Thus, the lattice spin is

$$W_{ij}^{\text{lat},(C)} \Delta t = \bar{W}_{ij}^{(C)} \Delta t - W_{ij}^{\text{P},(C)} \Delta t, \quad (59)$$

which can be used to evolve the lattice orientation following Perdahcioğlu [46] as

$$\Omega_{ij}(t_0 + \Delta t) = \exp\left(W_{ij}^{\text{lat},(C)} \Delta t\right) \Omega_{ij}(t_0). \quad (60)$$

2.10 Semi-implicit iterations

As noted below Eq. (6), the calculation of the slip increments, $\Delta\gamma^s$, assumes that $\Omega_{ij}(t_0 + \Delta t)$ is known. However, Eqs. (59) and (60) show that $\Omega_{ij}(t_0 + \Delta t)$ is determined by $\Delta\gamma^s$. This cyclic dependence can be resolved using the semi-implicit iterations of McGinty and McDowell [25], over the counter, k . Initially, it is assumed that $\Omega_{ij}^{(k=0)}(t_0 + \Delta t) = \Omega_{ij}(t_0)$. For $k \geq 1$, taking $\Omega_{ij}(t_0 + \Delta t) = \Omega_{ij}^{(k-1)}(t_0 + \Delta t)$ in Eqs. (5), and (6), slip increments $\Delta\gamma^{s,(k)}$, and the corresponding lattice orientation at the end of the time step $\Omega_{ij}^{(k)}(t_0 + \Delta t)$ are determined. The iterations are stopped when the norm of the relative difference between the slip increments computed in successive iterations becomes sufficiently small, presently 0.1%. The adequacy of this tolerance has been verified by ensuring that no change in the predicted mechanical response occurs even when it is decreased by a factor of 100.

3 Results

3.1 Uniaxial tension

3.1.1 Mechanical

In a uniaxial multislip test, a single crystal is loaded along a crystallographic axis of high symmetry. Although many slip systems should be equally loaded in this condition, and activate slip, surprisingly few slip systems are found to activate in experiments. The inevitable alignment error between the tensile axis and the symmetric crystallographic axis in the experiment, and microstructural evolution that promotes deviation away from the symmetrical response are thought to be responsible for this behaviour [9].

Parameter	Reference	Value
$\mathbb{C}_{1111}^{(C)}$	Eq. (12)	168.4 GPa
$\mathbb{C}_{1122}^{(C)}$	Eq. (12)	121.4 GPa
$\mathbb{C}_{2323}^{(C)}$	Eq. (12)	75.4 GPa
γ_{sat}	Eq. (36)	$1.1 \cdot 10^{-3}$
ρ_0	Eq. (36)	10^9m^{-2}
ρ_{sat}	Eq. (36)	$4 \cdot 10^{13} \text{m}^{-2}$
τ_0	Sec. 2.5	2.5 MPa
α	Eq. (37)	0.3
μ	Eq. (37)	56.4 GPa
b	Eq. (37)	2.56 Å
$a_{ss} = a_s$	Eq. (37)	$4.9 \cdot 10^{-4}$
a_{CP}/a_s	Eq. (37)	5.3
a_{CD}/a_s	Eq. (37)	24.5
a_{HL}/a_s	Eq. (37)	18.5
a_{GJ}/a_s	Eq. (37)	16.5
a_{LC}/a_s	Eq. (37)	50.4
ΔT	Eq. (55)	$1 \cdot 10^{-3}$
$\varepsilon_{\text{hard}}$	Eq. (56)	1

Table 1: Material, and computational parameters used to fit the copper single crystal data of Franciosi [35].

Multislip represents a difficult test case for numerical models. It calls for qualitatively different predictions of the mechanical, and microstructural response of crystals with similar initial lattice orientations. In other words, it is required to predict a rapidly varying response as a function of the initial lattice orientation. This may be possible with the present model, and computational methodology as they do not involve smoothing or regularisation. This motivates comparing the present predictions with the experimental observations obtained from the multislip tests of Franciosi and co-workers reported in the literature.

Franciosi and Zaoui [58, 59] and Franciosi [35] performed quasistatic uniaxial tension experiments on copper single crystals at 200K oriented for multislip. They also performed micrographic observations of the specimen surfaces in order to determine the number of activated slip planes. They noted considerable specimen-to-specimen variation in the stress-strain response of nominally identically oriented specimen. They found that the stress-strain curve of some crystals had a positive curvature, while that of others were negative. They termed them ‘SG’-type (single glide) and ‘P’-type (parabolic), respectively.

It is proposed to simulate the uniaxial tension of one ‘SG’-type, and one ‘P’-type orientation, corresponding to the tensile axis being

parallel to the $\langle 011 \rangle$, and $\langle 001 \rangle$ crystallographic directions, respectively. The model single crystal specimen are subjected to uniaxial tension along the x_1 direction of the x_1 - x_2 - x_3 coordinate system. In this setting, the prescribed values in Eqs. (3), and (4) are $\bar{\sigma}_{ij} = 0$, for $ij \in \mathcal{S} = \{22, 33, 23, 32, 13, 31, 12, 21\}$, and $\bar{L}_{ij} = 1$, for $ij \in \mathcal{L} = \{11\}$. Plastic deformation is taken to occur by the activation of $\{111\}\langle 110 \rangle$ slip systems in the crystal.

Simulations are performed beginning with two lattice orientations, termed ‘ideal’, and ‘perturbed’, for each nominal orientation. The ‘ideal’ orientation refers to the condition of exact coincidence of the symmetric crystallographic direction with the tensile axis, x_1 . Franciosi and Zaoui [58] noted that the lattice orientations of their single crystal specimen deviated by up to 2° from the symmetric crystallographic orientations. To mimic this deviation, the lattice orientation of the ‘perturbed’ model crystal is rotated about an axis in the x_2 - x_3 plane by 2° . The rotation axis is selected such that the RSS developed in one of the most loaded slip systems is maximised. The mechanical responses of the ideal and perturbed crystals are expected to bound the experimentally obtained mechanical response.

The hardening model due to Cuitiño and Ortiz [9] has been summarised in Sec. 2.5. Model parameters are fit so that the predicted mechanical response of the perturbed model grains captures the lower bound of the experimental stress-strain curves. The fitting of the model parameters is guided by experiments. First, the dislocation density measurements of Hordon and Averbach [60], and Livingston [61] in copper single crystals is used to approximate the values of ρ_0 , and ρ_{sat} . τ_0 is taken from Franciosi and Zaoui [59]. Following Franciosi and Zaoui [59], the parameters $a^{ss'}$ appearing in Eq. (37) are assigned distinct values based on the type of interaction (self (S), coplanar (CP), co-directional (CD), Hirth lock (HL), glissile junction (GJ), and Lomer-Cottrell (LC)) between the dislocations of slip systems s , and s' . Single slip was reported to occur in the initial part of the stress-strain curve of the experimental $\langle 011 \rangle$ crystal [59]. Temporarily assigning large values to the other $a^{ss'}$ coefficients, the value of a_S is determined such that the initial part of the $\langle 011 \rangle$ stress-strain curve is fit. Then, retaining the large values assigned to the other $a^{ss'}$ coefficients,

the value of a_{CP} alone is gradually decreased to capture the slope increase in the latter part of the $\langle 011 \rangle$ stress-strain curve. Simultaneously, γ_{sat} is adjusted to control the transition from single slip to coplanar slip. With the values of the aforementioned parameters frozen, attention is then shifted to the $\langle 001 \rangle$ crystal. The parameters a_{CD} , a_{HL} , a_{GJ} , and a_{LC} are gradually decreased, and their effect on the predicted $\langle 001 \rangle$ stress-strain curve is noted. It is ensured that the decrease in these parameters does not alter the predicted $\langle 001 \rangle$ stress-strain curve. It is found that if slip systems interacting through Lomer-Cottrell (LC) locking were allowed to simultaneously activate, the shape of the predicted stress-strain curve differs qualitatively from the experimental one. Accordingly, a_{LC} is assigned a high value. By trial and error, the other three parameters, a_{CD} , a_{HL} , and a_{GJ} are determined to fit the experimental $\langle 001 \rangle$ curve. The model parameters so obtained are listed in Table 1.

The $a^{ss'}$ coefficients in Table 1 differ from those of Kubin et al. [62] and Madec and Kubin [63] by several orders of magnitude. This is because the physical meaning of $a^{ss'}$ differ between these works. Presently, $\sum_{s'} a^{ss'} \rho^{s'}$ determine the characteristic stress, τ_c^s according to Eq. (38). In Kubin et al. [62] and Madec and Kubin [63], $\sum_{s'} a^{ss'} \rho^{s'}$ directly determines the critical resolved shear stress, τ^s . The present $a^{ss'}$ coefficients are, however, comparable to those in Cuitiño and Ortiz [9]. The present a_{SH} , and a_{CP} are nearly equal to those in Cuitiño and Ortiz [9]. The present $a_{\text{LC}}/a_{\text{SH}}$ has the greatest value of all coefficient ratios, also as in Cuitiño and Ortiz [9]. Cuitiño and Ortiz [9] assumed that $a_{\text{CP}} = a_{\text{CD}} = a_{\text{HL}}$. This equality is presently relaxed, as it is not borne out by dislocation dynamics studies [62]. The fitted values of a_{CP} , a_{CD} , and a_{HL} , obtained presently are clearly disparate.

Presently, uniaxial tension is simulated to a strain of 0.16, as in the experiments. The values of the computational parameters, viz., the basic time step, ΔT , and the relative hardening tolerance, $\varepsilon_{\text{hard}}$, are also given in Table 1. Their determination will be described in Sec. 3.1.2.

Fig. 1 compares the present predictions of the stress-strain curves assuming both ideal and perturbed initial orientations, with the experimental ones measured by Franciosi [35]. The predictions

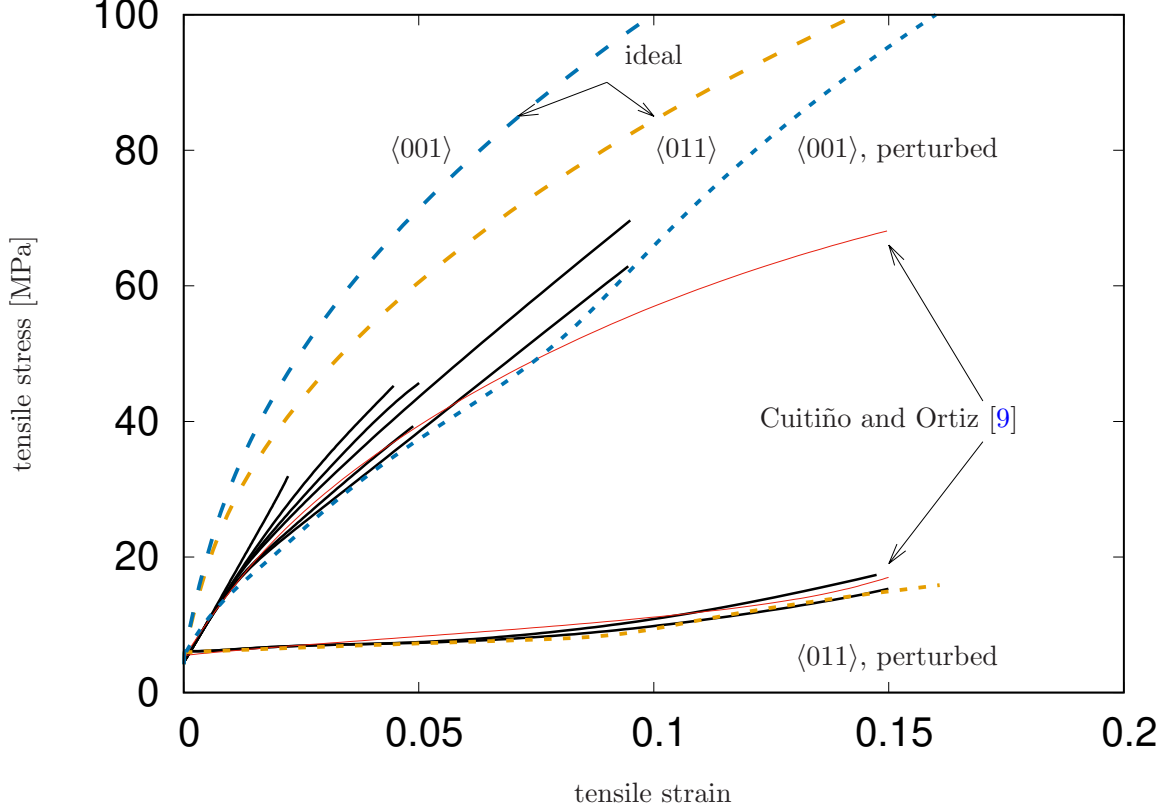


Fig. 1: Comparison of the single crystal stress-strain curves predicted (dashed lines) presently with the experimental curves (black solid lines) of Franciosi [35] for Cu at 200K. The predictions assuming the ideal, and 2° perturbed initial orientations bound the experimental ones from above and below, respectively. The red solid lines are the predictions of Cuitiño and Ortiz [9].

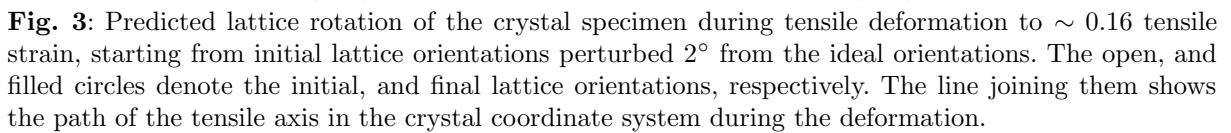
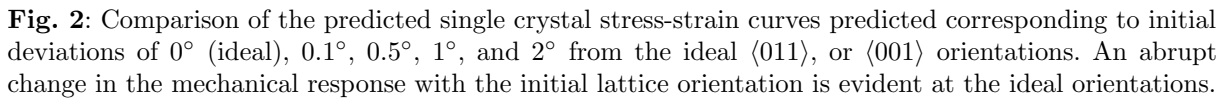
for the ideal, and perturbed initial orientations of both crystals bound the experimental curves from above, and below, respectively. The fit lower bounds are tight, while the upper bounds are not. The predictions of Cuitiño and Ortiz [9] are also reproduced in Fig. 1. It is seen that the present predictions better capture the continued hardening trend of the $\langle 001 \rangle$ crystal.

Fig. 2 shows the stress-strain curves predicted for various misorientations of the initial model crystal from the ideal orientation. The predicted stress-strain curve corresponding to a misorientation as small as 0.1° qualitatively resembles that of the 2° misoriented crystal. Thus, the predicted mechanical response changes abruptly, with small changes in the initial orientation near the ideal orientations. In experimental specimen, some misalignment between the high symmetry crystallographic directions, $\langle 011 \rangle$, and $\langle 001 \rangle$, and the

tensile axis, is inevitable. This appears to underlie the significant difference between the predicted mechanical response of the ideal orientations, and the experimental data in Fig. 1.

The lattice orientation of ideal crystals remains constant with tensile strain. The predicted lattice evolution in the perturbed the crystals up to 0.16 strain is shown in a stereographically projected inverse pole figure in Fig. 3. The lattice of the perturbed $\langle 011 \rangle$ crystal rotates away from the ideal orientation. The lattice of the perturbed $\langle 001 \rangle$ rotates approximately toward the ideal $\langle 001 \rangle$, but does not stop after reaching it. It continues rotating with the same sense past the ideal $\langle 001 \rangle$ orientation.

The predicted evolution of the slip system-level characteristics, viz., accumulated slip, γ^s , CRSS, τ^s , hardening, $H^{ss'}$, and dislocation density, ρ^s , in the ideal and perturbed $\langle 011 \rangle$ and $\langle 111 \rangle$ crystals



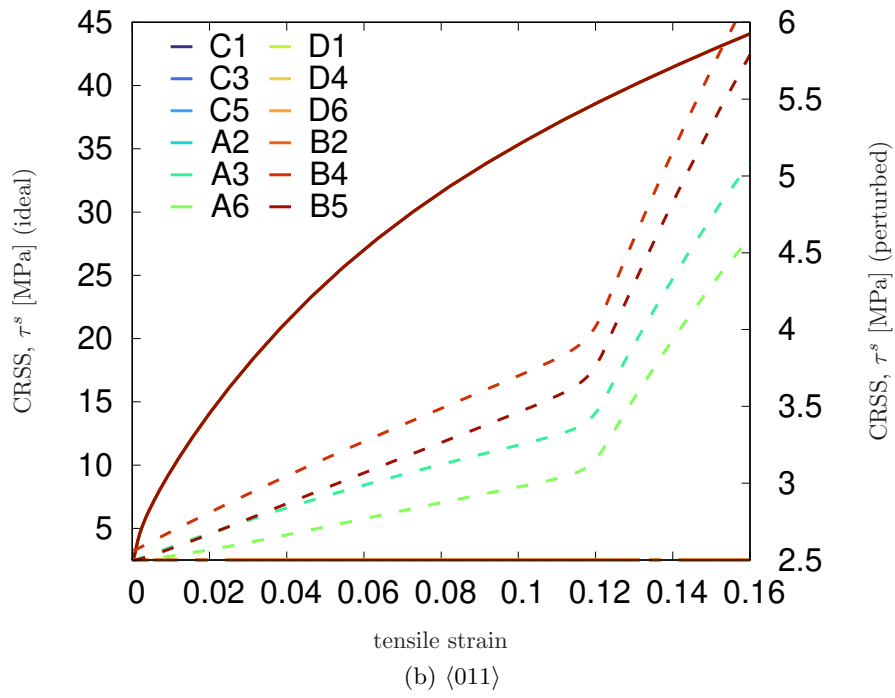
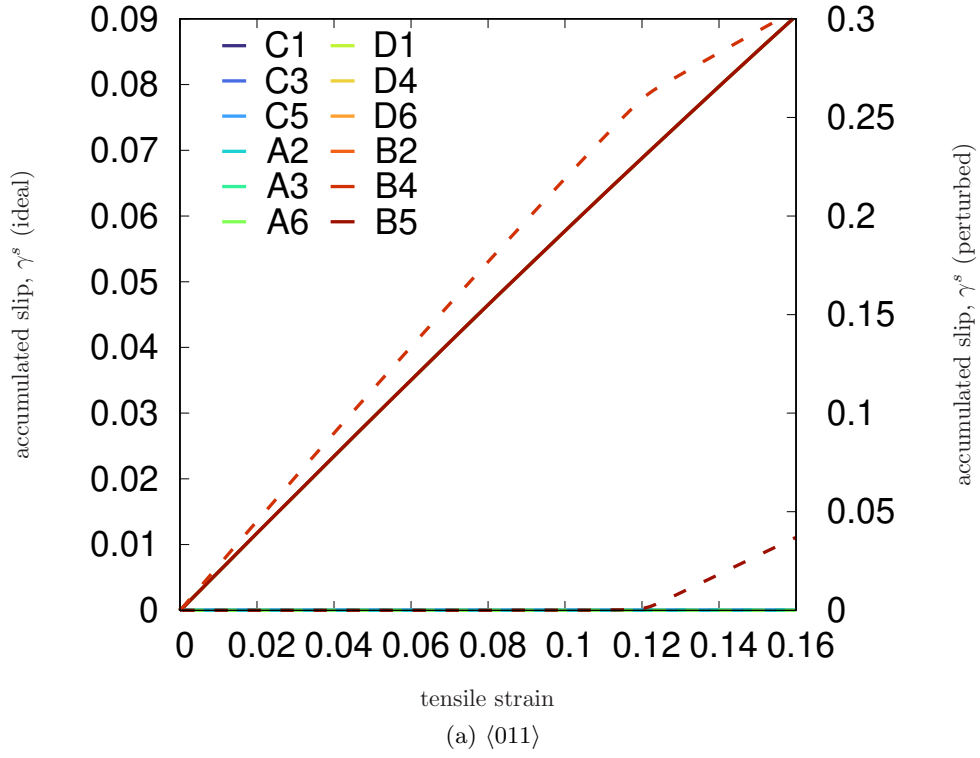
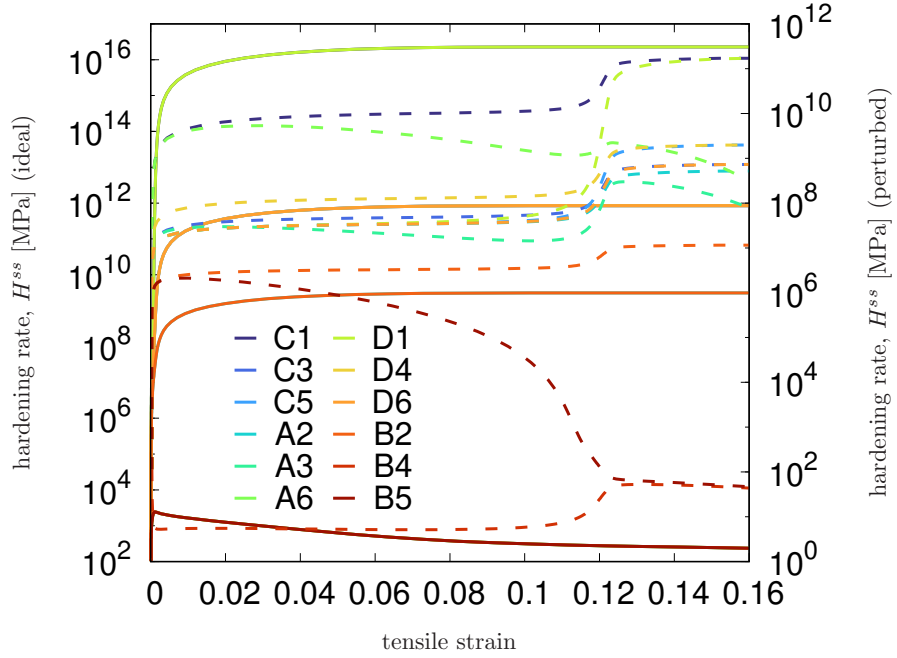
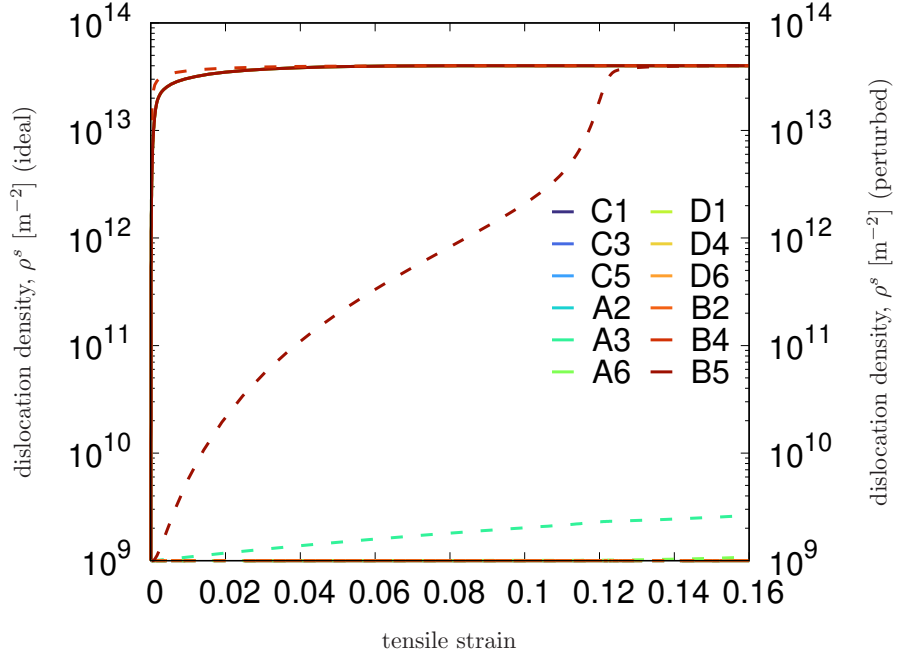


Fig. 4: Evolution with uniaxial tensile strain of the (a) accumulated slip, γ^s , and (b) CRSS, τ^s , in all the slip systems of the ideal (solid lines, left vertical axis) and 2° perturbed (dashed lines, right vertical axis) $\langle 011 \rangle$ crystal.



(a) $\langle 011 \rangle$



(b) $\langle 011 \rangle$

Fig. 5: Evolution with uniaxial tensile strain of the (a) hardening rate, $H^{ss'}$, and the (b) dislocation density, ρ^s , in all the slip systems of the ideal (solid lines, left vertical axis) and 2° perturbed (dashed lines, right vertical axis) $\langle 011 \rangle$ crystal.

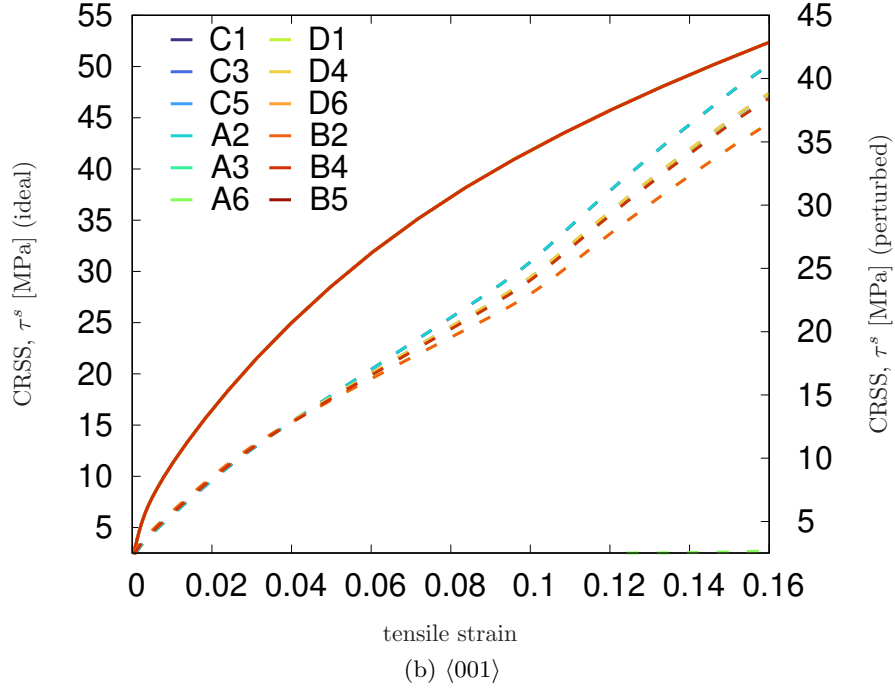
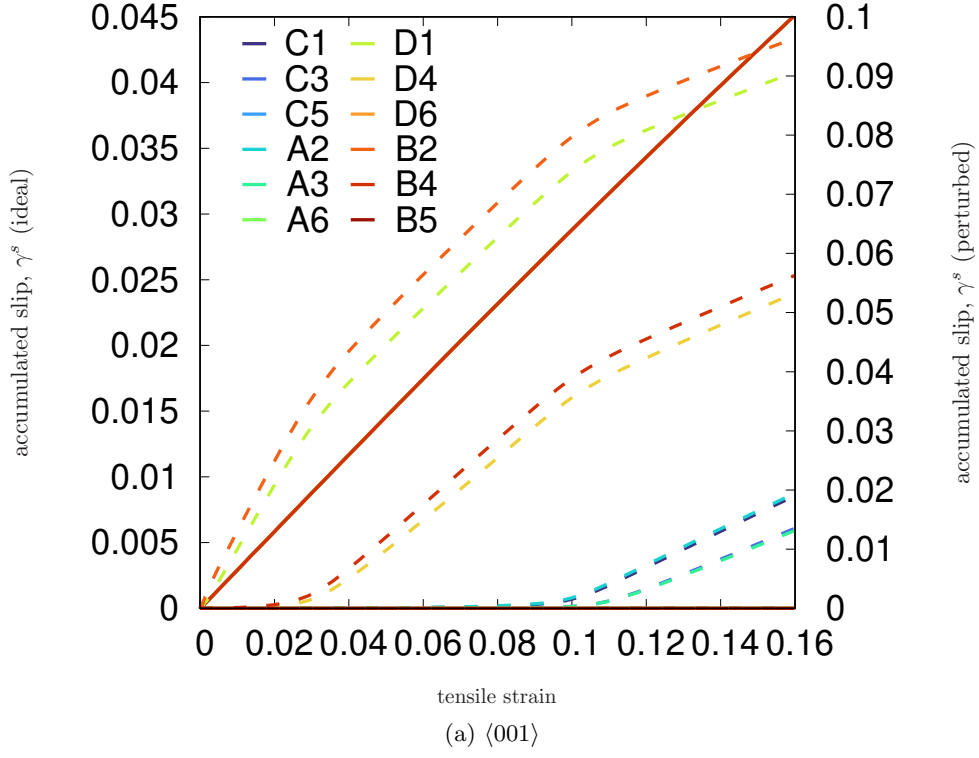


Fig. 6: Evolution with uniaxial tensile strain of the (a, b) accumulated slip, γ^s , (c, d) CRSS, τ^s , and (e, f) dislocation density, ρ^s , in all the slip systems of the (a, c, e) ideal and (b, d, f) perturbed $\langle 001 \rangle$ crystal.

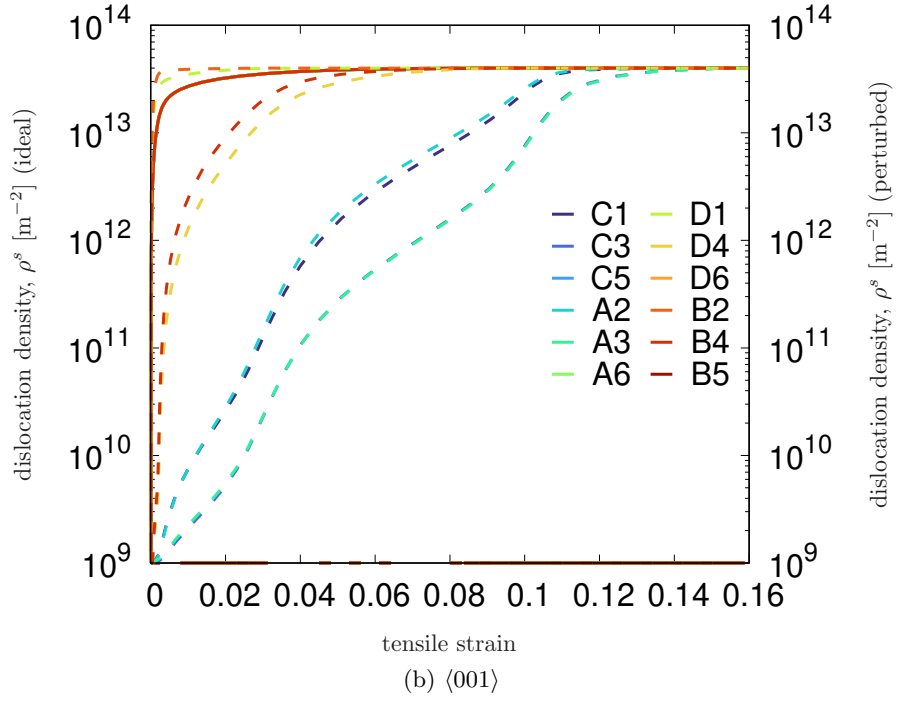
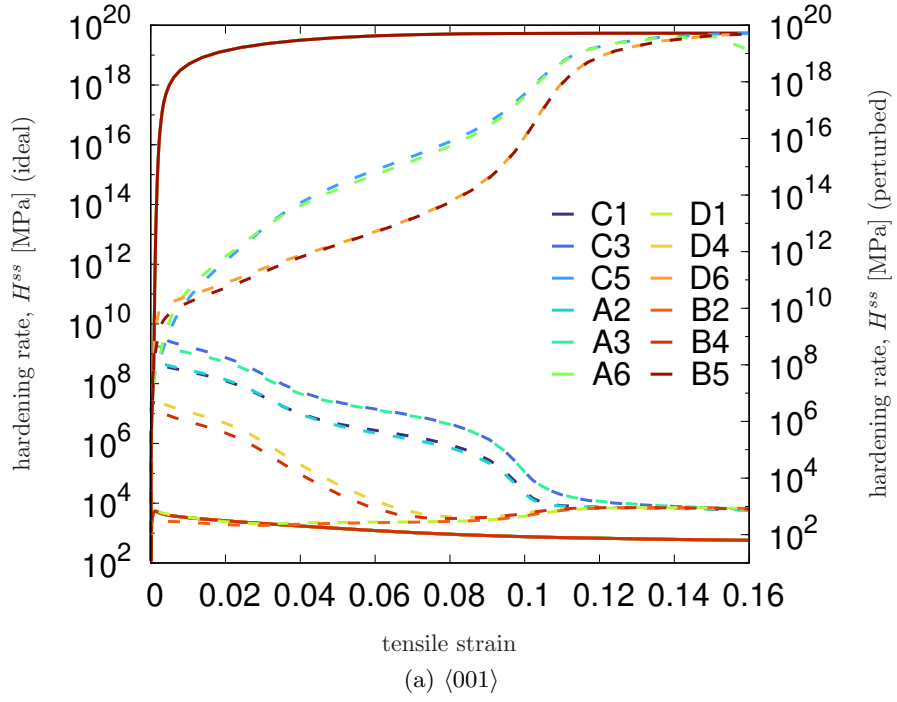


Fig. 7: Evolution with uniaxial tensile strain of the (a, b) accumulated slip, γ^s , (c, d) CRSS, τ^s , and (e, f) dislocation density, ρ^s , in all the slip systems of the (a, c, e) ideal and (b, d, f) perturbed $\langle 001 \rangle$ crystal.

are shown in Figs. 4, and 5, and Figs. 6, and 7, respectively. Slip systems are identified according to the Schmid and Boas [1] notation for fcc crystals. In these figures, solid, and dashed lines indicate responses of the ideal, and perturbed initial orientations, respectively. Also, although slip systems s , and $\bar{s}$ with opposite senses are treated distinctly in the model, they are represented together in these figures.

Fig. 4a shows that 4 slip systems in the ideal $\langle 011 \rangle$ crystal activate uniformly throughout the deformation. On account of the strong latent hardening interactions in the model, $a^{ss'}$, they harden each other substantially, as shown in Fig. 4b. As only activated slip systems can harden, the other slip systems retain their initial CRSS, τ_0 . However, as shown in Fig. 5a, the 4 active slip systems cause a huge increase in the latent hardening rates, H^{ss} , of the inactive ($\gamma^s = 0$) slip systems. The H^{ss} of the active slip systems, however, decreases with progressing deformation. Finally, Fig. 5b shows that the dislocation density increases rapidly to saturation in the activated slip systems. However, since dislocation density can increase only in the active slip systems, in all the inactive slip systems, $\rho^s = \rho_0$. The foregoing observations apply also to the ideal $\langle 001 \rangle$ crystal, shown in Figs. 6, and 7, with the only change that 8 slip systems activate therein.

Slip accumulation in the perturbed $\langle 011 \rangle$ crystal, shown in Fig. 4a is considered next. One slip system, B4, is clearly dominant. Its coplanar slip system, B5, starts contributing considerable slip only beyond about 0.12 tensile strain; at 0.12 tensile strain, the accumulated slip in B5 is only 1×10^{-3} , which is approximately equal to γ_{sat} . The observation of appreciable slip in only one slip system in the initial part of the deformation, extending to a pair of coplanar slip systems, agrees with the experimental observation of Franciosi and Zaoui [59, Table 1]. Even though the total slip in B5 is much smaller than that in B4, the predicted dislocation density in B5 is sizeable at a tensile strain of 0.12. This is because the dislocation density is governed by the exponential relationship, Eq. (36). For $\gamma^s/\gamma_{\text{sat}} \approx 1$, Eq. (36) gives $\rho^s \approx \rho_{\text{sat}}(1 - 1/e)$. The exponential relationship itself has been validated experimentally in copper by Hordon and Averbach [60, Fig. 7].

Although not evident in Fig. 4a, in the perturbed $\langle 011 \rangle$ crystal also, 4 slip systems are altogether activated. The slip activity in three of these slip systems is small, but adequate to increase τ^s , and ρ^s as seen in Fig. 4b, and Fig. 5b, respectively, and to decrease H^{ss} , as seen in Fig. 5a. Because of the dominance of one slip system, B4, τ^s in the perturbed $\langle 011 \rangle$ crystal is smaller than that in the ideal one, as seen in Fig. 4b. This explains the much softer stress-strain response of the perturbed $\langle 011 \rangle$ crystal in Fig. 1. The upward bend of the SG-type stress-strain curve of this crystal coincides with the strain at which significant slipping begins in the B5 slip system. Therefore, the bend can be attributed to the large τ_c in the B5 slip system due to latent hardening from slip activity in B4.

Turning next to the perturbed $\langle 001 \rangle$ crystal, Fig. 6a shows the evolution of slip activity in this crystal as dashed lines. The B2, and A3 slip systems activate initially, followed by B4, and D4 at a small tensile strain. Unlike the perturbed $\langle 011 \rangle$ crystal, slip is thus distributed over non-coplanar slip systems. Franciosi and Zaoui [59, Table 1] noted the activation of 2–4 non-coplanar slip systems at 0.1 tensile strain in two distinct $\{111\}$ planes. The present observation of slip distributed over 3 $\{111\}$ plane does not exactly agree with their observation. Franciosi and Zaoui [59] however, note an uncertainty on account of clamping effects in their experiments, which causes spatial variation in slip activation in then specimen.

Although prominent slip is predicted in only 4 slip systems of the perturbed $\langle 001 \rangle$ crystal, Fig. 6b shows that the CRSS evolves comparably in the 8 slip systems that were equally activated in the ideal $\langle 001 \rangle$ crystal. Likewise, Fig. 7a shows the H^{ss} in these slip systems decreasing, and Fig. 7b shows the ρ^s therein increasing. This shows that 8 slip systems are activated in the perturbed $\langle 001 \rangle$ crystal, many of them but slightly.

The rapid variation of the mechanical response with initial orientation, noted in Fig. 2, is produced by qualitatively different slip activity in the slip systems. The set of active slip systems itself remains the same in both the ideal and perturbed crystals; only the quantum of slip differs. It is important to capture all the slip increments, $\Delta\gamma^s$, both large, and small, accurately, in order to predict the large variation observed in Fig. 2. For, as seen in Figs. 4b, and 6b, even minuscule slip

in a slip system produces a considerable CRSS increase therein, which, in turn, affects the course of slip activity during further deformation. This predicted response arises because the hardening rate of activated slip systems that were hitherto latent is very steep, according to the Cuitiño and Ortiz [9] model. This model feature purposed to capture the reloading response observed in the latent hardening experiments of Franciosi and Zaoui [58].

The condition used to define slip activation is clearly of great importance in determining the slip increments over a time step. Conditions that invoke rate-dependence, viscosity, or non-linear complementary functions round the corners of the yield surface. They smear slip activity, and thereby make it more equitably distributed amongst the activated slip systems, to a greater or lesser extent [21]. This artificially pushes the predicted mechanical response toward that of the ideal orientation. Algorithmic approaches, such as the interior point method, also amount to rounding the corners.

The present formulation retains Schmid’s law in its non-smooth form. Thus, it does not smear slip increments. The non-smoothness may be expected to affect the numerical stability of the integration scheme. However, Fig. 2 shows no numerical instability: The predicted mechanical responses vary systematically with initial orientation, and smoothly with imposed deformation. The observed numerical stability arises from the well-posedness of the quadratic program. The diagonal form of the hardening matrix (Eq. (40)), and large values of H^{ss} (Figs. 5a, and 7a) ensure a unique numerically unambiguous solution to the quadratic program, Eq. (42). It will be shown later in Sec. 3.2 that under shear loading also, hardening has the effect of stabilising the predicted mechanical response.

Explicit uniaxial tensile simulations of symmetric crystals produce non-unique solutions for the slip increments. This is called the Taylor ambiguity [34]. In order to suppress the Taylor ambiguity, numerous works in the literature e.g., Anand and Kothari [23], Schröder and Miede [24], McGinty and McDowell [25], Delannay et al. [64], and Mánik and Holmedal [34], propose that of all the non-unique solutions to the rate-independent

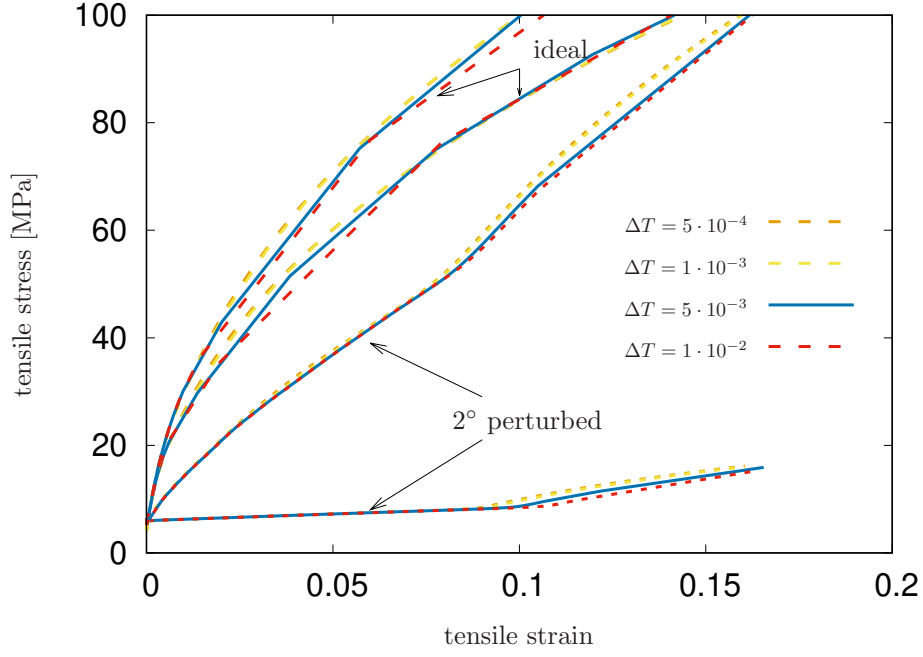
problem, the one that minimises the sum of the squares of the slip rates, $\sum_{s=1}^S (\Delta\gamma^s)^2$ is optimal.

Explicit simulations of the present ideal crystals will be affected by the issue of Taylor ambiguity. However, the present simulations of the ideal crystals (solid lines in Figs. 4, and 6) converge to a unique solution, which automatically satisfies the minimum-sum-of-squares criterion noted above. Also, the present simulations of the ideal $\langle 001 \rangle$ crystal evidently have no difficulty predicting slip activity in more than 5 slip systems. The hardening matrix, $H^{ss'}$, with positive block diagonal entries is responsible for these desirable features. The simulation becomes numerically unstable if $H^{ss'} \equiv 0$, for all s , and s' , corresponding to a perfectly plastic material.

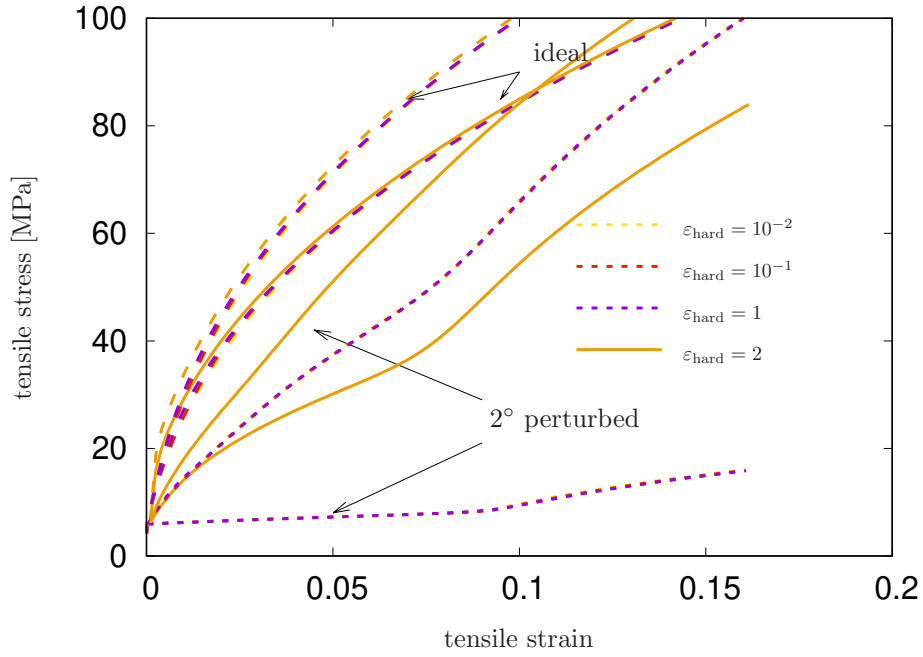
A pair of computational observations from the present simulations are noteworthy. First, Algorithm 1 allows the addition and deletion of slip systems to and from the active set. However, practically, it is found that slip systems once added to the active set are seldom deleted, suggesting that the algorithmic strategy is very efficient. Second, the convergence of Algorithm 1 is guaranteed only for a positive definite quadratic coefficient matrix, $E^{ss'}$ in Eq. (42). The hardening matrix, $H^{ss'}$ makes the dominant contribution to the coefficient matrix. $H^{ss'}$ is positive semi-definite, as noted in Sec. 2.5. Even so, rapid convergence is always observed in Algorithm 1. In order to understand this desirable behaviour, it is observed that the algorithm never manipulates the full $E^{ss'}$ matrix. Instead, it operates on the matrix slice, $[E_{\mathcal{P}\mathcal{P}}]$, in Eq. (53). Since $\mathcal{P}$ never contains both the positive s and negative $\check{s}$ senses of a slip system, the matrix slice is always a diagonal matrix with positive diagonal entries, and hence positive-definite. Thus, although matrix $E^{ss'}$ is not positive definite, its operational part, $[E_{\mathcal{P}\mathcal{P}}]$ is.

3.1.2 Computational

As noted in Sec. 2.8, the approximation of constant hardening, $H^{ss'}$, over a time step can be better realised by reducing the basic time step, ΔT , or the relative hardening tolerance, $\varepsilon_{\text{hard}}$, or both. Amongst these possibilities, it remains to determine a computationally efficient approach. To this end, Fig. 8a shows the convergence of the predicted response with a fixed $\varepsilon_{\text{hard}} = 10^{-2}$, and



(a) fixed $\varepsilon = 10^{-2}$



(b) fixed $\Delta T = 10^{-3}$

Fig. 8: Two approaches to obtaining convergence of the predicted stress-strain curve: (a) by decreasing ΔT , for fixed $\varepsilon_{\text{hard}} = 10^{-2}$, and (b) by decreasing $\varepsilon_{\text{hard}}$, for fixed $\Delta T = 10^{-3}$. Convergence occurs in both (a) and (b), at $\Delta T = 10^{-3}$, and $\varepsilon_{\text{hard}} = 1$, respectively. In both (a), and (b), a solid line is the drawn for the key value just before convergence.

Table 2: Computational time required for uniaxial tensile simulations of crystals initially perturbed 2° from the ideal $\langle 001 \rangle$ orientation.

$\varepsilon_{\text{hard}} = 10^{-2}$			$\Delta T = 10^{-3}$		
ΔT	Computational time (in seconds)	steps	$\varepsilon_{\text{hard}}$	Computational time (in seconds)	steps
$1 \cdot 10^{-2}$	77	1656	2	2	151
$5 \cdot 10^{-3}$	71	1662	1	2	156
$1 \cdot 10^{-3}$	56	1619	10^{-1}	5	251
$5 \cdot 10^{-4}$	51	1708	10^{-2}	56	1619

decreasing ΔT . Contrarily, Fig. 8b shows the convergence of the predicted response with a fixed $\Delta T = 10^{-3}$, and decreasing $\varepsilon_{\text{hard}}$. The mechanical response is seen to converge for $\Delta T \leq 10^{-3}$ in Fig. 8a, and for $\varepsilon_{\text{hard}} = 1$ in Fig. 8b.

The computational time required for each of these simulations of the 2° perturbed $\langle 001 \rangle$ crystal is tabulated in Table 2. The converged solution that corresponds to the least computational time is obtained for $\Delta T = 10^{-3}$, and $\varepsilon_{\text{hard}} = 1$. These computational parameters are listed in Table 1, and used throughout Sec. 3.1.1.

3.2 Simple shear

In the uniaxial tension of Sec. 3.1.1, only a single deformation constraint, L_{11} is imposed. In order to demonstrate the present methodology in the scenario of a fully constrained multislip deformation, simple shear to large strains of initially symmetrically oriented crystals is simulated. This problem was studied by Bertram and Kraska [65], and by Prüger and Kiefer [21], who simulated the simple shear deformation of two crystals (001)[100], and (013)[100]. In this designation, the crystallographic plane, and direction correspond to the shear plane, and the shear direction, respectively.

In the setting of fully constrained simple shear, the prescribed values in the right side of Eqs. (3), and (4) become $\bar{L}_{ij} = 1$, for $ij = \{12\}$, and $\bar{L}_{ij} = 0$, for $ij = \{11, 22, 33, 23, 32, 13, 31, 21\}$. Thus, $\mathcal{L} = \{11, 22, 33, 23, 32, 13, 31, 12, 21\}$, and $\mathcal{S} = \emptyset$. The present simulations are performed assuming the same hardening as in Sec. 3.1. In contrast, the simulations of Bertram and Kraska [65], and Prüger and Kiefer [21], assumed no hardening.

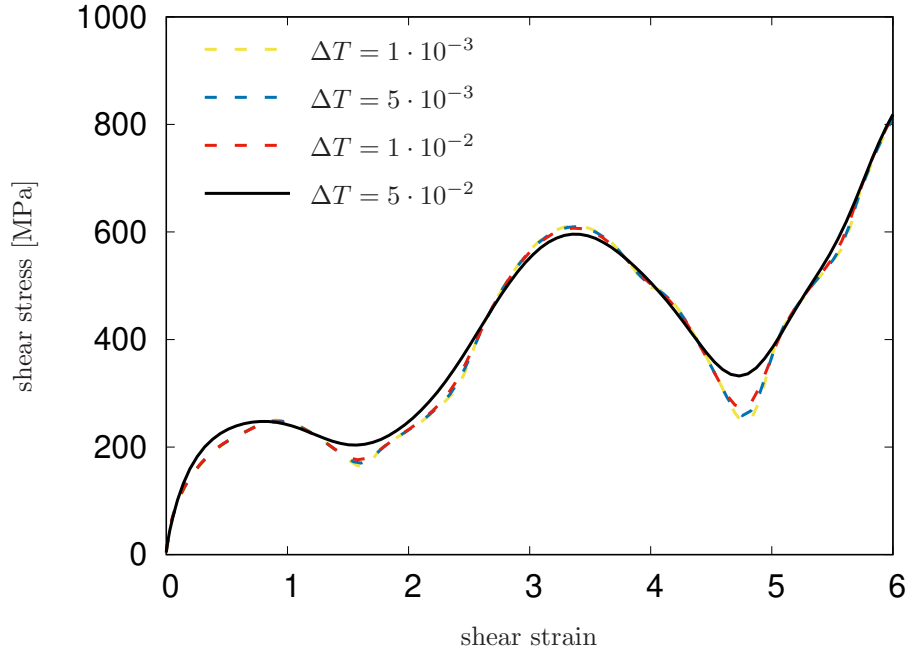
By way of a convergence study, the stress-strain response in simple shear of the (001)[100], and (013)[100] crystals is predicted assuming $\varepsilon_{\text{hard}} = 1$, as in Sec. 3.1. Fig. 9 shows the predicted

stress-strain curves obtained. Converged stress-strain response is obtained for $\Delta T \leq 10^{-2}$. This value is greater than the basic time step obtained in Sec. 3.1.2. The following results therefore are predicted assuming $\varepsilon_{\text{hard}} = 1$, and $\Delta T = 10^{-2}$.

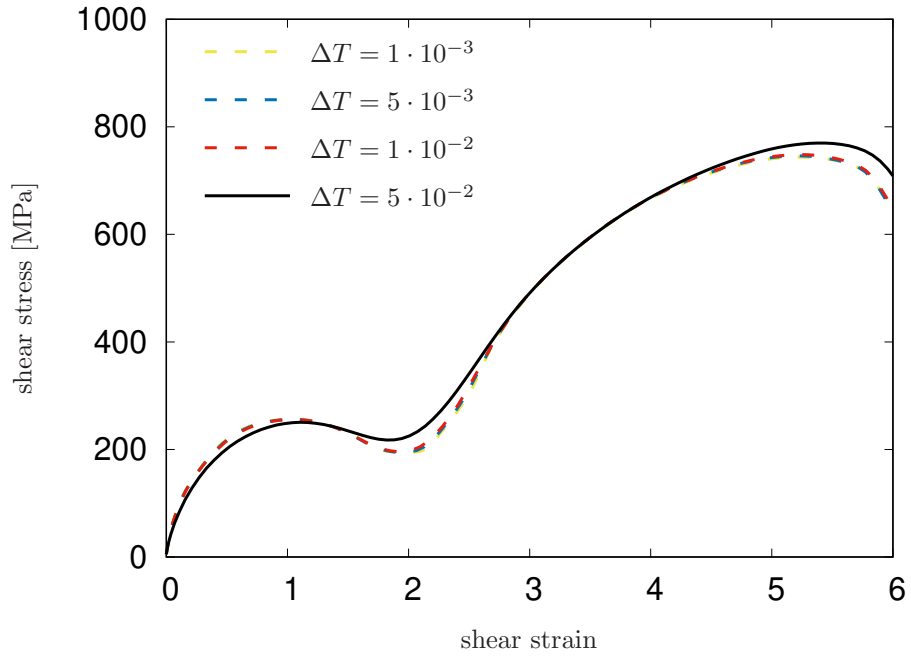
The predicted stress-strain response of the ideal and 2° perturbed crystals is shown in Fig. 9. The ideal and perturbed single crystals exhibit similar responses that do not diverge from each other. This is contrary to an observation of [21]. They noted the sensitivity of the stress-strain response of their (013)[100] crystal to small orientation perturbations. Since the present model crystal hardens, while that of Prüger and Kiefer [21] does not, it is inferred that hardening stabilises the mechanical response.

The slip evolution with shear strain in all the slip systems of the (001)[100], and the (013)[100] crystals is shown in Fig. 11. The response corresponding to both the ideal and perturbed crystals are shown, using solid, and dashed lines, respectively. Slip accumulation in the ideal (001)[100] crystal, shown in Fig. 11a coincides with that obtained by Prüger and Kiefer [21], despite the difference in hardening. Slip activation in this crystal is thus entirely determined by the kinematics of the deformation.

However, slip accumulation in the ideal and perturbed (013)[100] crystals are quite different from that obtained by Prüger and Kiefer [21]. In particular, in Fig. 11b, co-directional systems C1, and D1 dominate the other slip systems starting at a shear strain of about 3 in the present hardening simulations. The dominance only occurs a shear strain of ~ 5 in the non-hardening simulation of Prüger and Kiefer [21]. The corresponding CRSS evolution with shear strain in all the slip systems of the (001)[100], and the (013)[100] crystals is shown in Fig. 12.



(a) initial orientation: (001)[100]



(b) initial orientation: (013)[100]

Fig. 9: Predicted stress-strain curves of the ideal (a) (001)[110], and (b) (013)[001] crystals, assuming $\varepsilon_{\text{hard}} = 1$. In both (a), and (b), a solid line is drawn for the unconverged curve corresponding to $\Delta T = 5 \cdot 10^{-2}$.

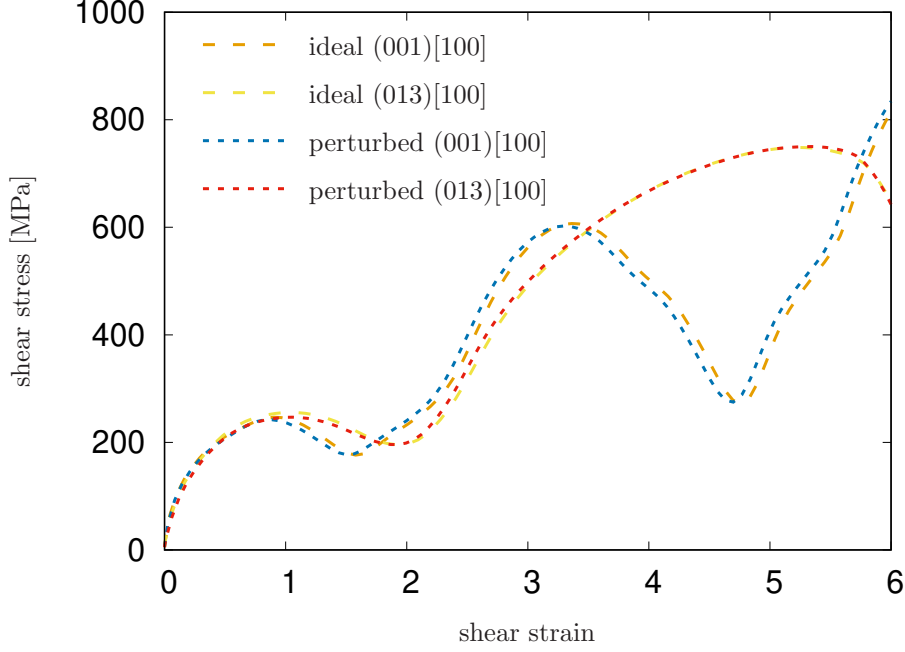


Fig. 10: Comparison of the predicted mechanical response of the ideal and 2° -perturbed (001)[100], and (013)[100] crystals. The mechanical response of the perturbed crystal does not deviate from that of the ideal crystal.

Table 3: Computational time required for the simple shear simulations to shear strain 6.0 in the crystals with initial orientation (001)[100], and (013)[100].

(001)[100]			(013)[100]		
ΔT	Computation time (in seconds)	steps	ΔT	Computation time (in seconds)	steps
$5 \cdot 10^{-2}$	3	132	$5 \cdot 10^{-2}$	3	149
$1 \cdot 10^{-2}$	8	611	$1 \cdot 10^{-2}$	8	634
$5 \cdot 10^{-3}$	14	1211	$5 \cdot 10^{-3}$	14	1241
$1 \cdot 10^{-3}$	64	6007	$1 \cdot 10^{-3}$	64	6113

The present formulation is implemented in `octave` [56], and run on a desktop computer with one Intel i9 14900 processor with a maximum clock speed of 5.8GHz. The computational (wall) time associated with the finite shear simulations of the ideal (001)[100], and (013)[100] crystals is given in Table 3. The perturbed crystal simulations take similar times, and therefore, are not listed. Convergence is achieved for $\Delta T \leq 10^{-2}$. The $\Delta T = 10^{-2}$ simulations take 8 seconds to run.

Prüger and Kiefer [21] have listed computational times for the same simple shear simulations corresponding to various formulations. Of them,

the rate-independent augmented Lagrangian formulation [26] does not regularise the yield surface, and is thus comparable to the present formulation. Prüger and Kiefer [21] list 118 seconds as its running time. Their nonlinear complementary function formulation, which regularises the yield surface, takes 22 seconds to run. Both the rate-dependent formulations in their study, with physically realistic rate-sensitivity values, have much longer run times.

As shown in Table 3, the converged present simulations corresponding to $\Delta T = 10^{-2}$ take 8s to run. Even accounting for the present CPU clock speed advantage, this is about 10 times

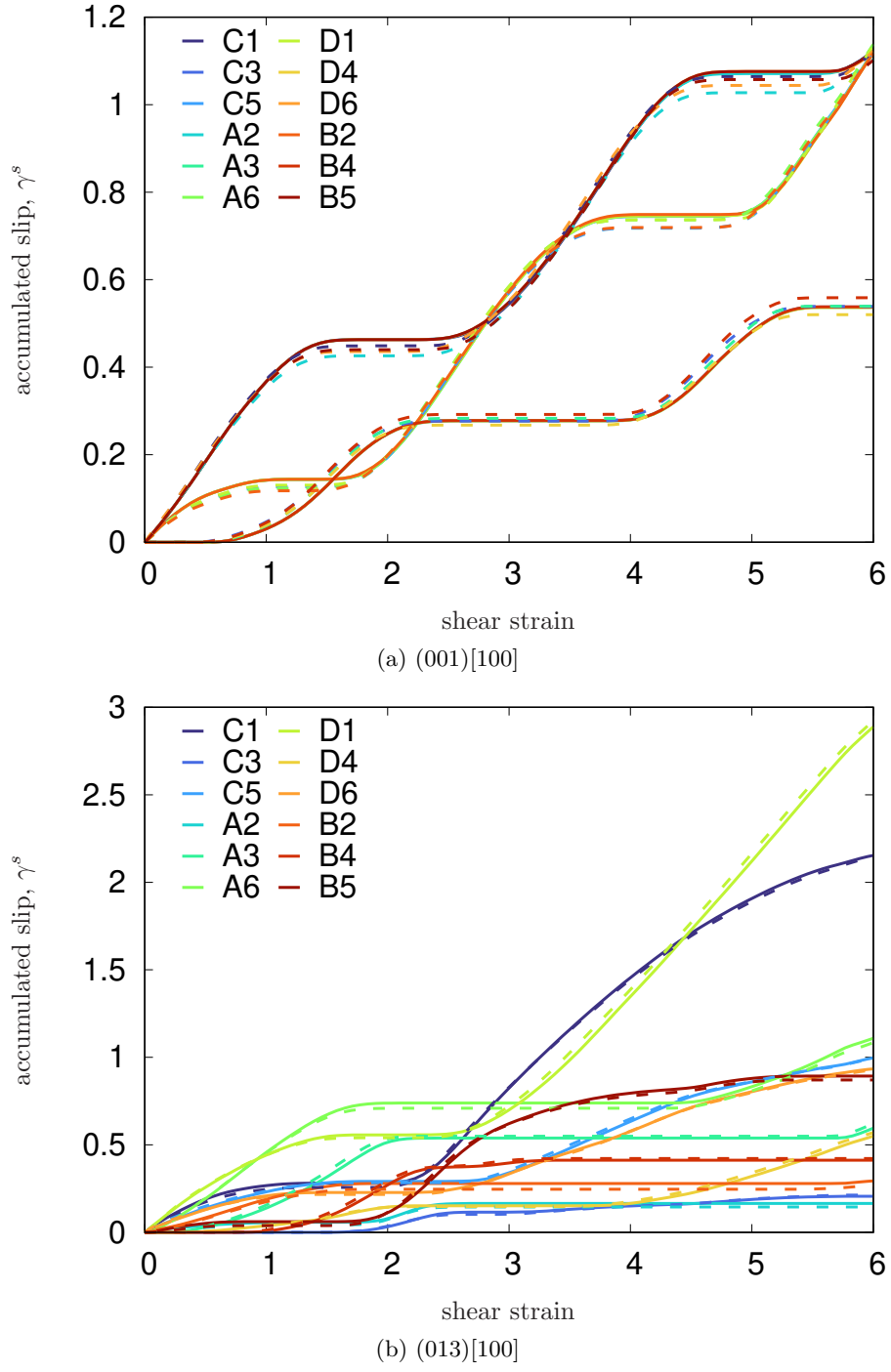
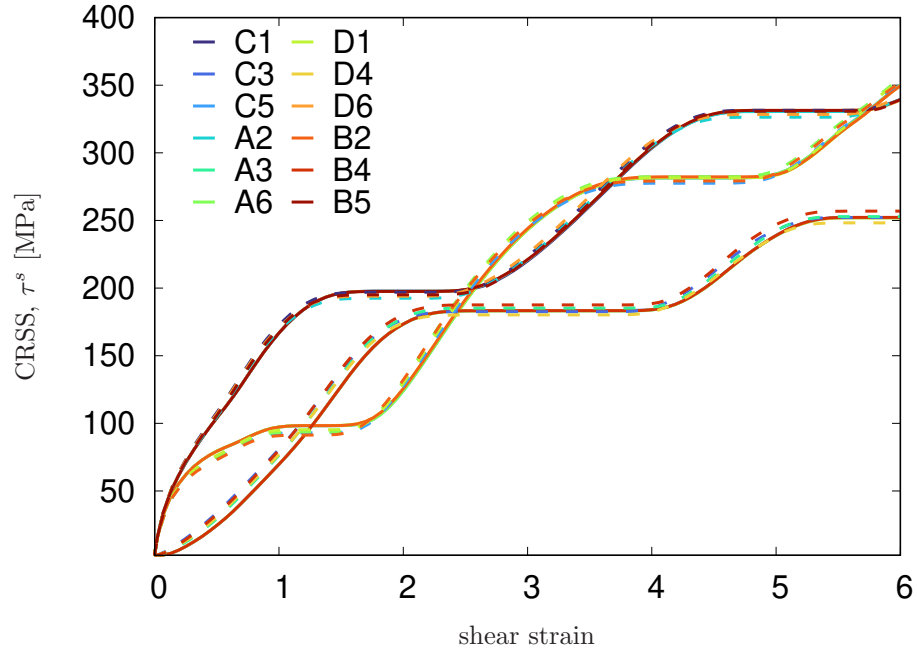
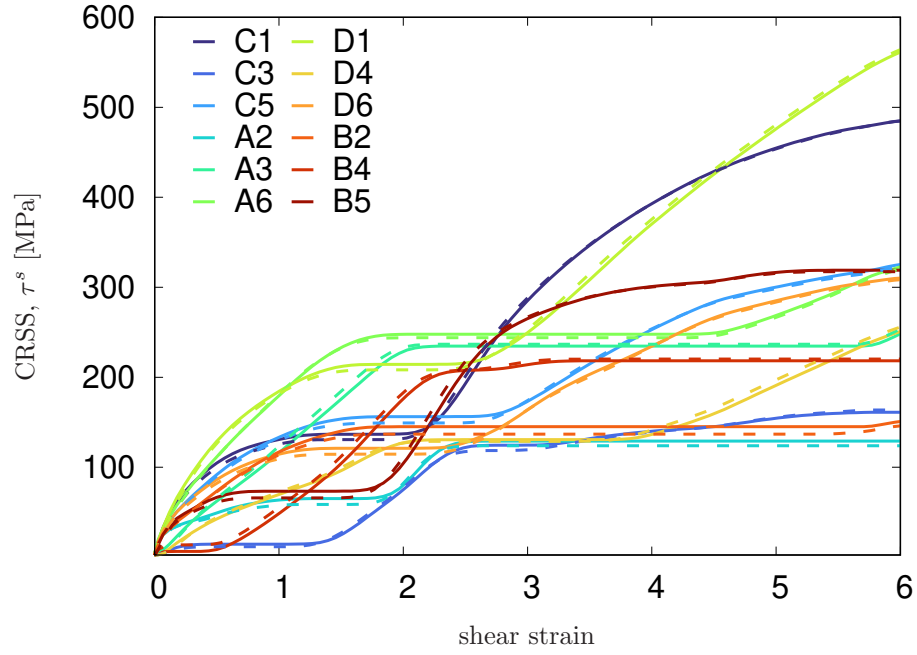


Fig. 11: Evolution with shear strain of the accumulated slip, γ^s , in all the slip systems of the ideal (solid lines) and perturbed (dashed lines) (a) (001)[100], and (b) (013)[100] crystals.



(a) (001)[100]



(b) (013)[100]

Fig. 12: Evolution with shear strain of the CRSS, τ^s , in all the slip systems of the ideal (solid lines) and perturbed (dashed lines) (a) (001)[100], and (b) (013)[100] crystals.

faster than the 118 seconds run time of the augmented Lagrangian formulation. The run time of the present simulations is similar to that of the nonlinear complementary function formulation. It must also be noted that the present simulations incorporate hardening, while the simulations of Prüger and Kiefer [21] do not. Adding hardening to the latter will increase the number of iterations for achieving convergence, and hence, run time. The factor of 10 enhancement in computational efficiency, noted above for the present formulation, is thus an underestimate.

4 Discussion

In the setting of incremental small-deformation plasticity, the present work has developed a robust computational scheme to uniquely determine the slip increments in a crystalline material point subjected to mixed boundary conditions. The scheme is based on a theorem of Maier [49], and is, as such, subject to its assumptions.

The first assumption is that the hardening-rate of each slip system is positive, and proportional to its slip-rate. This condition is satisfied by the Cuitiño and Ortiz [9] model, and indeed, this consideration motivated its adoption in the present work. In the Cuitiño and Ortiz [9] model, the hardening matrix is positive semi-definite. A number of hardening models proposed in the literature, however, may result in hardening matrices without this favourable character. They are incompatible with the present formulation and computational approach, as the quadratic program then loses convexity, and therefore, does not possess a unique solution. Mariano [66] has proved a dual form of Maier’s theorem featuring internal variables that control hardening, and extended the theorem to non-Cauchy solids. However, his developments do not directly address the restriction noted above.

The present small deformation formulation requires small time steps. Finite deformation formulations overcome this restriction; they permit arbitrarily large time steps. A number of continuum finite deformation formulations for elastoplastic deformations, developed in the literature, have been critically reviewed by Xiao et al. [67]. They have discussed the pros and cons of each formulation, from both mathematical and physical perspectives. They show that an Eulerian formulation with logarithmic rates can provide a

mathematically rigorous, and physically accessible formulation of continuum elastoplasticity. An extensive literature on finite deformation formulations of crystal plasticity also exists. In, e.g., the algorithms of Miehe et al. [68], and Schmidt-Baldassari [26], slip increments over a finite time step are determined iteratively while accounting for the attendant non-linear hardening.

The second restriction in the present methodology comes from the assumption of a constant hardening rate within a step. This restriction precludes the application of the present quadratic program based algorithmic scheme to finite elastoplastic deformation, wherein, in general, non-linear hardness evolution over a large time step must be accounted for.

In recent works, Ryś et al. [14] and Scherer [69], have predicted spatially inhomogeneous deformation leading to substructure formation (banding), in crystal plasticity finite element simulations of single crystals, subjected to macroscopically homogeneous deformation. In these studies, inhomogeneous deformation is triggered even in nominally perfect initial single crystals by numerical perturbations introduced during computation. These perturbations lead different material points in the simulation domain to follow diverging paths through hardening, and lattice orientation spaces. This is found true for both rate-independent or rate-dependent responses. In these works, the hardening matrix, $H^{ss'}$, is indefinite, a feature regarded as the cause of banding predictions.

However, Mahesh [70] predicted deformation and shear banding in favourably oriented copper single crystals, modeled as rigid-plastic rate-dependent domains. His predictions captured the experimental evolution of the orientation of the band interface, and lattice rotation of the matrix and band. Importantly, these predictions assumed the Cuitiño and Ortiz [9] hardening model, which yields a positive semi-definite hardening matrix. This shows that positivity of the hardening matrix does not preclude banding predictions. In fact, given the strong sensitivity of the present single material point predictions to initial conditions in Fig. 2, but not in Fig. 10, one may expect the present methodology to reveal interesting dependence of the banding response on initial conditions, and loading, if embedded in larger scale spatial models. Such a study of banding will be taken up in future work.

5 Conclusions

An integration-scheme that determines the incremental slip in all the slip systems of an elastic-rate independent plastic single crystal over a finite deformation step has been presently proposed. It accommodates arbitrary mixed boundary conditions imposed upon the crystal, comprised of imposed traction, and imposed incremental displacements. By appealing to Maier's minimisation theorem, which in the present case is a statement of the theorem of maximum dissipation, the present methodology reduces the mechanics problem to one of quadratic programming over the space of non-negative variables.

The key novel feature of the present formulation is that it introduces no smoothing or regularisation, particularly in the law governing slip-activation. It therefore predicts dramatically different mechanical and microstructural responses of the simulated single crystals starting from nearly the same initial conditions. This capability is demonstrated by applying the present methodology to simulate multislip tests in uniaxial tension. The predictions so obtained are shown to be physically realistic by confirming their agreement with experimental observations reported in the literature. Even so, the present formulation is at least an order of magnitude more computationally efficient than the existing augmented Lagrangian formulation, which also does not regularise the yield surface.

Two significant limitations are associated with the present formulation. The assumption of a constant hardening rate within each time step is intrinsic to the method, and limits the size of the time steps in the simulations. Also, the solution of the quadratic programming problem requires a positive definite hardening matrix. The present formulation is numerically unstable when applied to perfectly plastic materials, and fails for slip-softening materials.

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Declarations

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