A multiplicative finite strain crystal plasticity formulation based on additive elastic corrector rates: Theory and numerical implementation

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Abstract

The purpose of continuum plasticity models is to efficiently predict the behavior of structures beyond their elastic limits. The purpose of multiscale materials science models, among them crystal plasticity models, is to understand the material behavior and design the material for a given target. The current successful continuum hyperelastoplastic models are based on the multiplicative decomposition from crystal plasticity, but significant differences in the computational frameworks of both approaches remain, making comparisons not straightforward.

In previous works we have presented a theory for multiplicative continuum elastoplasticity which solved many long-standing issues, preserving the appealing structure of additive infinitesimal Wilkins algorithms. In this work we extend the theory to crystal plasticity. We show that the new formulation for crystal plasticity is parallel and comparable to continuum plasticity, preserving the attractive aspects of the framework: (1) simplicity of the kinematics reaching a parallelism with the infinitesimal framework; (2) possibility of very large elastic strains and unrestricted type of hyperelastic behavior; (3) immediate plain backward-Euler algorithmic implementation of the continuum theory avoiding algorithmically motivated exponential mappings, yet preserving isochoric flow; (4) absence of Mandel-type stresses in the formulation; (5) objectiveness and weak-invariance by construction due to the use of flow rules in terms of elastic corrector rates. We compare the results of our crystal plasticity formulation with the classical formulation from Kalidindi and Anand based on quadratic strains and an exponential mapping update of the plastic deformation gradient.

Keywords: Crystal plasticity, hyperelasticity, elastic rate correctors

1. Introduction

Plastic deformation is an intrinsic part of the processing and behavior of metals and alloys, which involve permanent macroscopic changes to the geometrical shape of components and structures under different loading types \cite{1,2}. The analysis of this deformation process is performed today mostly through finite elements \cite{5}. In general, the elastoplastic deformation processes and their numerical simulation are substantially more complicated than the deformation processes in which only elastic deformations (even when large) are present. Attending to the purpose of the analysis, the level of

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detail pursued in describing the physical process is a balance between accuracy in describing that physical process and the needed resources. There are two main approaches to model this behavior: one based on the continuum theory of plasticity [1, 4] (common for engineering structures design) and the other based on multiscale strategies, among them crystal plasticity [5] (common in materials science and materials design).

Frequently, advances in the continuum theory of plasticity came from numerical difficulties and inconsistencies found in the numerical implementation of the theory. For example, hyperelasticity is now established as the standard approach in continuum elastoplasticity [6, 4]. It has been popularized in plasticity due to the complexity of algorithms that incremental objectivity posed in the formulation; e.g. the Hughes-Winget [7] and Rolph-Bathe [8] algorithms, still available today in many codes to deal with some anisotropic models. The bypass to these difficulties came from the proper consideration of the state variables and the fulfillment of the physical requirement of path independency of the elastic contribution [9, 10] (i.e. exact integrability by fulfilling Bernstein’s conditions [11, 12]). Furthermore, the widely accepted way to obtain the elastic state variables is currently the use of the Kröner-Lee [13, 14] multiplicative decomposition, motivated in crystal plasticity [15, 16, 6] (the concepts behind where introduced previously by Bilby et al [17]). The conceptual superiority of the multiplicative decomposition promoted different formulations which preserved that decomposition in the derivation of the elastic variables, even for anisotropy and cyclic hardening (e.g. [9, 18, 19, 20, among others). This superiority is manifest by the preservation of ellipticity properties [21] and of weak-invariance [22, 23, 24] during plastic flow (so unhardened results do not depend on the arbitrary reference configuration), apart from the clear and well-known physical motivation. Indeed, multiplicative decompositions and hyperelastic schemes are also important in kinematic (energetic) hardening to avoid spurious dissipation obtaining stable loops, see e.g. Figs. 4–9 and 19 in [25]. However, Green ansatzes and plastic metrics are frequently used to obtain the elastic strains (state variable for hyperelasticity) in complex models, when the multiplicative decomposition poses mathematical/algorithmic difficulties in traditional formulations based on the classical plastic flow evolution equations (e.g. [26, 27, 28, 29, 30, 31], among many others).

The exchange of concepts between crystal plasticity and continuum plasticity continued with the pursuit of simplicity in the computational algorithms, for which the additive structure of infinitesimal plasticity and of the Wilkins radial return algorithm [32] seem optimal. For example, the works of Weber and Anand [33] and Eterović and Bathe [34] in continuum plasticity, brought the possibility of additive algorithms at finite strains in terms of logarithmic strains preserving the multiplicative decomposition, thereafter followed by many other authors for the isotropic case [35, 36, 37], and extended to the anisotropic elastoplastic case [20]. That was possible due to the use of the exponential mapping in the algorithmic implementation, which furthermore preserved the volume during plastic flow in a natural way. Indeed, this conservation was not fulfilled by initial formulations which used flow rules based on the Lie derivative of the elastic Finger tensor—e.g. Eq. (9.2.16) in [38]; see pp. 385-386 in [39]. The exponential mapping has been thereafter passed to crystal plasticity formulations [40], although not the use of logarithmic strains. The preservation of the additive structure of algorithms for infinitesimal strains required small or moderate elastic strains when using the multiplicative decomposition [20], both in the continuum plasticity and in the crystal plasticity formulations [41]. Note that this condition applies also to trial elastic states, so, in addition, small steps must be used. In crystal plasticity, since quadratic strains are employed, small elastic strains are often assumed to simplify the algorithms. Remarkably, the exponential mapping has been introduced and used as an algorithmic artifact (or ad-hoc algorithmic alternative to the standard backward-Euler algorithm, despite being motivated in the solution of the differential equation), not as part of the continuum theory; and as such has been extended to crystal plasticity; see e.g. Sec. 46 in [39], and how the mapping is introduced in references [20, 33, 54, 37], among many others.

Departing from the initial works of Ewing and Rosenhain [42, 43] and Taylor and Elam [44, 45],
polycrystalline plasticity was developed \cite{46, 47, 48} and was adapted into the framework of large-strain continuum mechanics by Rice and Hill \cite{49, 50}. Further works extended the framework considering both rate-independent and rate-dependent plasticity \cite{51, 52, 53, 54, 55, 49, 50, 51, 52}. Elaborate hardening laws were then proposed in other works, e.g. isotropic in \cite{56, 57}, kinematic in \cite{58, 59}, for creep in \cite{60, 61}, and cyclic softening in \cite{62}. Physics-based models rely on the microscopic physical mechanisms of plastic deformation, e.g. dislocation densities (considered as internal microstructural state variable), grain size and shape, second fractions, precipitate morphology, etc. The dislocation density is considered as the most important variable, and therefore, it is also treated in many works \cite{63, 64, 65, 66, 67, 68, 69, 70}. Hence, whereas continuum plasticity and crystal plasticity share most ingredients, there are specific constitutive equations for crystal plasticity mainly related to hardening tied to dislocations density. Indeed, crystal plasticity theory may be considered a homogenization of the dislocation theory \cite{71, 72}, where the Burgers vector is \( \mathbf{b} = l_{RVE} \gamma \mathbf{s} \), for a Representative Volume Element of dimension \( l_{RVE} \) in the plane direction \( \mathbf{m} \), and \( \gamma \) is the continuum equivalent slip in direction \( \mathbf{s} \). Kinematics of crystal plasticity is of utmost importance in the modelling of both phenomenological and physics-based micromechanical plastic flow.

Noteworthy, there are many constitutive laws for the slip rates and the evolution of the internal variables, but few works pay attention to the development of rigorous numerical implicit implementations directly derived from kinematics of a continuum theory. As happened in continuum plasticity, they may unveil a better treatment of both aspects (theory and algorithm). The initial implicit approaches for rate-dependent formulations, including efficient and well-posed integration, have been reviewed by Cuitiño and Ortiz \cite{73}. The derivation of a general return-mapping scheme for rate-independent single crystal models has been proposed by Borja and Wren \cite{74} for the infinitesimal theory and by Kalidindi and Anand \cite{75}, and Miehe \cite{76, 40} for finite strains, in which the mentioned exponential mapping has been proposed in the crystal plasticity context. Currently, one of the better established frameworks in materials science is the one of Kalidindi and Anand \cite{75}. However, whereas some ingredients of the crystal plasticity theory and its numerical implementation are well established, other ingredients differ in the literature, which bring different approximations to simplify either the theoretical or the numerical treatments. For example, Jaumann rate based formulations are still common (e.g. \cite{77, 78, 79, 80, 81}), despite the mentioned issues regarding integrability. Other works use quadratic stored energies along the second Piola Kirchhoff stress in the intermediate configuration (e.g. \cite{82, 83, 84}, among others), the Mandel stress (e.g. \cite{85, 86}), or any other stress tensor under the restriction that elastic strains are small. Whereas this usually holds in metals, the formulations lack generality. Interestingly, the logarithmic strains advocated for continuum plasticity \cite{87, 88} and employed with the exponential mapping \cite{33, 34, 35}, are seldom used in crystal plasticity. Of course, if elastic strains are considered small, a further simplification is to consider a small strains framework from the outset, as still employed in many recent works (e.g. \cite{89, 90}). Indeed, as shown below, this option is also close to a large strains framework if plastic spin is also considered.

In summary, crystal plasticity and continuum plasticity share most of the ingredients, and in the pursuit of sound, simple and computationally efficient formulations, developments in one framework have been passed to the other framework. However, the acceptance of a general fully satisfactory formulation applicable to both frameworks has still not been achieved. In view of the above comments, the main aspects that such formulation must take into account are: (1) both elastic and kinematic hardening behavior must be exactly integrable (hyperelastic) and general (unrestricted in form); (2) the continuum theory and the integration algorithm must be objective, preserve ellipticity properties of elastic energies and be weak-invariant, which is facilitated if (3) the elastic state variables come from the multiplicative decomposition and the plastic flow equation is insensitive to the reference configuration; (4) an implicit computational algorithm must be conceptually simple, when possible (5) mimicking the additive structure of the infinitesimal framework; (6) the formulation should not be restricted to small elastic strains, elastic isotropy, or have any similar limitation; and (6) both
continuum plasticity and crystal plasticity formulations should be parallel, except for specific particularities given by the physics considered in each approach, like specific flow mechanisms or specific crystal elastic anisotropy.

Recently we have presented a novel approach to deal with multiplicative flow kinematics based on elastic strain corrector rates [91]. Motivated in finite strain anisotropic non-equilibrium viscoelasticity [92, 93], the approach is based on conventional flow rules directly written in terms of these rates, consistently derived from thermodynamics, the dissipation equation, and the chain rule. Whereas a parallelism is found between these continuum corrector rates and the algorithmic strain corrector, the former is defined as a continuum rate immediately derived from the chain rule. The plastic flow evolution equation is written directly in terms of this rate instead of the rate of a plastic measure. The plastic gradient only plays a mapping role when applicable. We have shown that the continuum theory may be written, in a completely equivalent manner, in terms of any stress-strain conjugate pair [91], and have shown that for the fully isotropic case it particularizes to the framework based on the Lie derivative of the elastic Finger tensor [15, 16], but written in a conventional way. However, when using logarithmic strains, the plain backward-Euler integration algorithm reduces to an additive structure identical to that of infinitesimal plasticity [94]. It does so keeping the multiplicative decomposition of the deformation gradient, allowing for arbitrarily large elastic strains, allowing for any isotropic or anisotropic stored energy, and not needing any approximation for an exponential mapping (which is not explicitly present since we employ a plain backward-Euler approximation). Moreover, the plastic spin is completely uncoupled, so no assumption on it is needed for computing the symmetric part in the continuum plasticity model. We have extended this approach to model cyclic plasticity at finite strains without explicitly employing the backstress concept [95], and thereafter developed the (to the authors’ knowledge) first plane stress projected algorithm employing the multiplicative decomposition [96].

The purpose of this work is to extend this novel approach also to crystal plasticity, showing that a parallel structure to continuum plasticity is attained, preserving the above-mentioned properties. In particular, the formulation is not restricted to infinitesimal elastic strains or elastic isotropy, the exponential mapping is not explicitly employed, and the integration algorithm has an additive structure similar to the infinitesimal counterpart. To facilitate comparisons, we summarize in the next section a typical framework employed in crystal plasticity, namely, the Kalidindi-Anand formulation, in which we also introduce our notation. Thereafter, in the following sections we introduce the continuum formulation of our proposal and the implicit integration algorithm, including the algorithmic tangent. We finish with some examples comparing numerical results from both approaches and conclusions.

2. Summary of the conventional crystal plasticity formulation

A large amount of crystal plasticity models used in materials science and their numerical implementations are based on the Kalidindi-Anand framework [75] (see also [97, 98]), or variations of this approach. The Kalidindi-Anand framework is developed using Green-Lagrange strains in the intermediate configuration and their associated second Piola-Kirchhoff stresses.

Using the notation of our previous works and e.g. [3, 4, 99], we denote the deformation gradient $\mathbf{X}$ from time $t = 0$ to time $t$ as $\mathbf{X}_t$. The Kröner-Lee multiplicative decomposition of the deformation gradient in elastic (plus rigid body rotations) and plastic part is

$$\mathbf{X}_t = \mathbf{X}_e \mathbf{X}_p$$

so

$$\mathbf{X}_e = \mathbf{X}_t \mathbf{X}_p^{-1}$$

and the plastic velocity gradient in the intermediate configuration by $\dot{\mathbf{X}}_p$ is denoted by $\dot{\mathbf{X}}_p$. Assuming $\mathcal{G}$ possible glide mechanisms (e.g. 12 in a FCC crystal), from the work of
intermediate configuration, it seems logical to define a Schmidt stress $\kappa_g$ (direct transformation between them). However, since the plane and direction are orthonormal in the intermediate configuration, it can be defined in any configuration and using any stress measure, because there is a constant, as $\gamma_g$ is the glide amount of the crystal plane $m_g$ (e.g. 4 planes in a FCC crystal) in direction $s_g$ (one of the 3 directions per plane in the FCC crystal), and $s_g \cdot m_g = 0$ and $|s_g| = |m_g| = 1$ in the intermediate configuration. Introduced by Weber and Anand in the context of continuum mechanics, and by Kalidindi and Anand in the context of crystal plasticity; most current models use an algorithmic (exponential map) update motivated in the solution of the differential equation $X_p X_p^{-1} = l_p$ for $l_p$ constant, as

$$t + \Delta t \begin{pmatrix} \dot{X}_p \\ 0 \end{pmatrix} = t + \Delta t \begin{pmatrix} X_p \end{pmatrix}_0 = \exp(t + \Delta t \mathbf{I}_p \Delta t) \begin{pmatrix} I \\ 0 \end{pmatrix} X_p \simeq \begin{pmatrix} I + t + \Delta t \mathbf{I}_p \Delta t \end{pmatrix}_0 X_p$$

where the last approximation used, e.g. by Eterović and Bathe [34] (see also [75]), holds for small steps ($\|t + \Delta t \mathbf{I}_p \Delta t\| << 1$); a condition which in any case should be used for accuracy reasons. For computing the stresses from a hyperelastic relation we need the elastic state variables, which in these plasticity models (as a difference with the continuum isotropic ones which use logarithmic strains), is the right elastic Cauchy-Green deformation tensor (or alternatively the Finger tensor). This tensor is obtained from Eqs. (1), (3) as

$$t + \Delta t \begin{pmatrix} C_e \end{pmatrix} = t + \Delta t \begin{pmatrix} X_e^T \end{pmatrix}_0 X_e \simeq \begin{pmatrix} I - t + \Delta t \begin{pmatrix} \mathbf{I} \end{pmatrix}_p \Delta t \end{pmatrix} tr \begin{pmatrix} C_e \end{pmatrix} \begin{pmatrix} I - t + \Delta t \mathbf{I}_p \Delta t \end{pmatrix} \begin{pmatrix} \mathbf{I} \end{pmatrix}_0 X_p$$

with $tr X_e := t + \Delta t \begin{pmatrix} \mathbf{I} \end{pmatrix}_0 X_e t + \Delta t X_e^{-1}$ defined as the trial elastic deformation gradient and $tr C_e := tr X_e^T tr \begin{pmatrix} \mathbf{I} \end{pmatrix}_0 X_e$ defined as the trial right Cauchy-Green deformation tensor. Note that all these definitions are performed in an algorithmic setting, just as a specific integration framework, without a direct link to a continuum theory. A further approximation often used to simplify some algorithm settings is to neglect once more higher order terms with the condition that elastic (including trial elastic) strains are small, so

$$t + \Delta t \begin{pmatrix} C_e \end{pmatrix} \simeq \begin{pmatrix} C_e \end{pmatrix} - \begin{pmatrix} \mathbf{I} \end{pmatrix}_e \begin{pmatrix} t \end{pmatrix} \begin{pmatrix} \mathbf{I} \end{pmatrix}_0 X_p \begin{pmatrix} t \end{pmatrix} + \begin{pmatrix} t \end{pmatrix} \begin{pmatrix} \mathbf{I} \end{pmatrix}_0 X_p \begin{pmatrix} t \end{pmatrix}$$

The elastic Green-Lagrange strains in the intermediate configuration (pull-back of the Almansi strains by $t + \Delta t X_e$) are obtained immediately from this tensor as—we reserve the symbol $E$ for logarithmic strains

$$t + \Delta t \begin{pmatrix} A_e \end{pmatrix} := \frac{1}{2} (t + \Delta t \begin{pmatrix} C_e \end{pmatrix} - \begin{pmatrix} \mathbf{I} \end{pmatrix}_0 X_p \begin{pmatrix} t \end{pmatrix})$$

The hyperelastic relation in these models is restricted to quadratic forms of the type $\Psi(A_e, \ldots) = \frac{1}{2} A_e : \mathbb{C}^e : A_e$, where by the ellipsis we indicate crystal symmetry group information contained in the tensor of constants $\mathbb{C}^e$. Then, the second Piola-Kirchhoff stress tensor in the intermediate configuration is (evaluated at the trial or at the final state)

$$t + \Delta t \begin{pmatrix} s | e \end{pmatrix} = \mathbb{C}^e : t + \Delta t \begin{pmatrix} A_e \end{pmatrix} \text{ and } tr \begin{pmatrix} s | e \end{pmatrix} = \mathbb{C}^e : tr \begin{pmatrix} A_e \end{pmatrix}$$

The next important issue is the computation of the Schmid resolved stress for each mechanism. Obviously, it can be defined in any configuration and using any stress measure, because there is a direct transformation between them. However, since the plane and direction are orthonormal in the intermediate configuration, it seems logical to define a Schmidt stress $\bar{\kappa}_g$ as the work conjugate to
the slip rate \( \dot{\gamma}_g \), so the dissipated power, using the classical expression in terms of the *unsymmetric* Mandel stress tensor \( \Xi := C_e S^{\text{e}} \) and the plastic velocity gradient \( l_p \), is —e.g. cf. Eq. (42) in [95] —

\[
D_g = \Xi : l_{pg} = \frac{s_g \cdot C_e S^{\text{e}}}{\tilde{r}_g} m_g := \tilde{r}_g \dot{\gamma}_g
\]  

(7)

Note that \( s_g \cdot C_e S^{\text{e}} \cdot m_g \neq m_g \cdot C_e S^{\text{e}} \cdot s_g \) because the Mandel stress tensor is unsymmetric \((\Xi \neq \Xi^T)\), but it is the work conjugate of \( l_p \) in the dissipation equation. However, given the elusive interpretation of \( \Xi \), some approximations are often employed considering that elastic strains are typically infinitesimal, e.g.

\[
s_g \cdot C_e S^{\text{e}} \cdot m_g \simeq s_g \cdot S^{\text{e}} \cdot m_g \simeq s_g \cdot \tau_R \cdot m_g \simeq s_g \cdot \sigma_R \cdot m_g
\]  

(8)

where \( \tau_R \) are the rotated Kirchhoff stresses and \( \sigma_R \) are the rotated Cauchy stresses, i.e. \( \sigma_R = R_e^T \sigma R_e \), where \( \sigma \) are the Cauchy stresses and \( R_e \) are the rotations from the polar decomposition of the elastic deformation tensor: \( X_e = R_e U_e \), with \( U_e = +\sqrt{C_e} \) being the right stretch tensor. The specific algorithm depends on the authors, and whether it is semi-implicit, fully implicit, rate-dependent or rate-independent. However, a typical scheme from the finite element displacements field \( u(x) \) at the integration point of a finite element is (of course an iteration loop is needed for implicit schemes)

\[
t^{+\Delta t}_0 u \rightarrow t^{+\Delta t}_0 X \rightarrow tr X_e \rightarrow tr \tilde{r}_g \rightarrow \Delta \dot{\gamma}_g \rightarrow \Delta l_p \rightarrow t^{+\Delta t}_0 X_p^{-1} \rightarrow \{ t^{+\Delta t}_0 X_e, t^{+\Delta t}_0 A_e t^{+\Delta t} S^{\text{e}} \}
\]  

(9)

with \( t^{+\Delta t}_0 X = d^{t^{+\Delta t}} x/d^{t^0} x \) and \( t^{+\Delta t}_0 x = x^0 + t^{+\Delta t}_0 u \) are the updated coordinates. Note that this is an *algorithmic* implementation of the plastic dissipative process given by the specific form of the dissipation equation

\[
D = \Xi : l_p \simeq \sum_{g=1}^{G} \Xi : l_{pg} = \sum_{g=1}^{G} D_g \geq 0
\]  

(10)

The purpose of the present formulation is to depart from a more convenient form of the dissipation equation, avoiding many of the algorithmic approximations and arriving to an algorithmic implementation which is a direct application of the plain Backward-Euler scheme to the continuum theory. Furthermore, as in the continuum plasticity framework, the algorithm will have the structure of a small strains algorithm, to which explicit kinematic mappings are applied for the large strain case.

3. Proposed framework: Continuum formulation

3.1. Kinematics of plastic deformation: trial and corrector rates. Mapping tensors

The external power \( P \) may be split into a conservative part \( \bar{\psi} \) and a dissipative part \( D \) as

\[
P = \bar{\psi} + D
\]  

(11)

In order to take natural advantage of this split, in our formulation we consider the elastic gradient \( X_e \) as an internal *variable of state* which defines the intermediate stress-free local (incompatible) configuration, meaning that only the current value is relevant to the state of the solid. On the contrary, the plastic part \( X_p \) is an internal variable which is *not* a variable of state, meaning that its history is relevant to the current state of the solid. The variable of state \( X_e \), considered as *dependent*, may be written in terms of the *independent* (driving) variables \( X \) and \( X_p \) as \( X_e (X, X_p) \). Note that by definition if \( \dot{X}_p = 0 \), then \( l_p = 0 \) and the dissipation \( D = 0 \) (regardless of the value of \( P = \bar{\psi} \));
and if $\dot{X} = 0$, then the velocity gradient vanishes and the power $\mathcal{P} = 0$ (regardless of the value of $\mathcal{D} = -\dot{\psi}$), Then, by immediate use of the chain rule, the rate is

$$
\dot{X}_e (X, X_p) = \left. \frac{\partial X_e}{\partial X} \right|_{\dot{X}_p = 0} : \dot{X} + \left. \frac{\partial X_e}{\partial X_p} \right|_{\dot{X} = 0} : \dot{X}_p =: \text{tr} \dot{X}_e + \text{ct} \dot{X}_e
$$

(12)

where the first addend $\text{tr} \dot{X}_e$ represents the partial continuum rate of $X_e$ when the plastic flow (dissipation) is frozen (hence we name trial rate for similarity with the algorithmic concept). The second addend $\text{ct} \dot{X}_e$ represents the partial derivative of $X_e$ when the external deformation (i.e. $X$) is frozen, so no external power input takes place and there is just an internal evolution dissipating stored energy. These concepts are typically employed in predictor-corrector algorithms of computational plasticity, but we remark herein that we are still dealing with the continuum formulation; they are just the partial derivatives when considering the explicit dependencies in $X_e (X, X_p)$. In other words, they represent at every instant the conservative and dissipative fractions in $\dot{X}_e$.

These concepts may be applied to all kinematic quantities. For example, the spatial velocity gradient can be written as

$$
l = \ddot{X} X^{-1} = \dot{X}_e X_e^{-1} + X_e \left( \dot{X}_p X_p^{-1} \right) X_e^{-1} = l_c + X_e l_p X_e^{-1} = l_c + \left( X_e \odot X_e^{-T} \right) : l_p
$$

(13)

so the two contributions to the elastic velocity gradient $l_e (l, l_p)$ are

$$
l_e = l - \left( X_e \odot X_e^{-T} \right) : l_p
$$

(14)

with $[Y \odot Z]_{ijkl} = Y_{ik} Z_{jl}$. Then, we can define a purely geometric mapping tensor from the elastic deformation gradient as $M_e^{d} = - \left( X_e \odot X_e^{-T} \right)$, so —see details on this type of formalism in continuum mechanics in [100].

$$
l_e (l, l_p) = l + M_e^{d} \left|_{l=0} \right. : l_p = l_c |_{l_p = 0} + l_e |_{l=0} =: \text{tr} l_e + \text{ct} l_e
$$

(15)

where $\text{tr} (\bullet)$ and $\text{ct} (\bullet)$ refer again to trial (i.e. the rate with $\dot{X}_p = l_p = 0$) and corrector (i.e. the rate with $\dot{X} = l = 0$) contributions. The tensor $M_e^{d} |_{l=0}$ performs the push-forward of the plastic velocity gradient $l_p := \dot{X}_p X_p^{-1}$, lying in the intermediate configuration, to the spatial one where $l_c$ and $l$ live (so they can be added). The symmetric (deformation rate) and skew-symmetric (spin) parts are, respectively

$$
d_e (d, l_p) = d - \text{sym} \left( X_e l_p X_e^{-1} \right) =: \text{tr} d_e + \text{ct} d_e
$$

(16)

$$
w_e (w, l_p) = w - \text{skw} \left( X_e l_p X_e^{-1} \right) =: \text{tr} w_e + \text{ct} w_e
$$

(17)

with, for example

$$
\text{tr} d_e = M_e^{d} \left|_{d_p = 0} \right. : d = \mathbb{I}^S : d = d
$$

(18)

where $\mathbb{I}^S$ is the fully symmetric identity tensor ($M_e^{d} \left|_{d_p = 0} \right. = \mathbb{I}^S$ because both $\text{tr} d_e$ and $d$ lie in the same, spatial, configuration); and

$$
\text{ct} d_e = M_e^{d} \left|_{d_p = 0} \right. : l_p = - \frac{1}{2} \left( X_e \odot X_e^{-T} + X_e^{-T} \odot X_e \right) : l_p = - \text{sym} \left( X_e l_p X_e^{-1} \right)
$$

(19)

with $[Y \boxtimes Z]_{ijkl} = Y_{il} Z_{jk}$.
Quadratic (Green-Lagrange) strains are obtained directly from the deformation gradients, and they are usual in finite element programs to build the geometrical stiffness matrices, so they will be also important in establishing links between our framework and the typical finite element programs. Consider the Green-Lagrange strains obtained from the corresponding deformation gradients as

\[ A = \frac{1}{2} (X^T X - I), \quad A_e = \frac{1}{2} (X_e^T X_e - I), \quad A_p = \frac{1}{2} (X_p^T X_p - I) \]  

(20)

Obviously \( A \neq A_e + A_p \) because they lie in different configurations: \( A \) and \( A_p \) live in the reference, undeformed configuration, whereas \( A_e \) lives in the intermediate configuration. However, since \( X_e = X X_p^{-1} \), it is straightforward to verify that

\[ A_e (A, X_p) = \frac{1}{2} (X_e^T X_e - I) = X_p^{-T} (A - A_p) X_p^{-1} = X_p^{-T} \odot X_p^{-T} : (A - A_p) \]  

(21)

where the possibility of the operation \( (A - A_p) \) results from the fact that they lie in the same, undeformed configuration. However, \( A_e \) lies in the intermediate configuration, so the mapping tensor \( X_p^{-T} \odot X_p^{-T} \) performs the proper push-forward operation. On the other hand, from the dependencies \( A_e (A, X_p) \) which have been explicitly obtained in Eq. (21), by use of the chain rule, the rate \( \dot{A}_e \) may be written as

\[ \dot{A}_e = \frac{\partial A_e}{\partial A} \bigg|_{X_e=0} : \dot{A} + \frac{\partial A_e}{\partial X_p} \bigg|_{A=\dot{X}=0} : \dot{X}_p \]  

(22)

\[ = \dot{A}_e \bigg|_{\dot{X}_p=0} + \dot{A}_e \bigg|_{A=\dot{X}=0} = \text{tr} \dot{A}_e + \text{ct} \dot{A}_e \]  

(23)

so identifying terms we find an interesting meaning for the previous mapping tensor (known at any given instant from the multiplicative decomposition) which will be used below

\[ \frac{\partial A_e (A, X_p)}{\partial A} \bigg|_{X_e=0} = X_p^{-T} \odot X_p^{-T} \equiv \mathbf{M}_{\dot{A}} \bigg|_{\dot{X}_p=0} \]  

(24)

Note that this tensor maps the rate \( \dot{A} \) in the material configuration to the trial elastic one in the intermediate configuration \( \text{tr} \dot{A}_e \) if we use \( \dot{X}_p \).

3.2. Stress power, work-conjugacy, and logarithmic strains framework

The stress-strain work-conjugate measures for the formulation may be chosen arbitrarily, because there is a one-to-one relation between them that makes the stress power invariant to such choice (refer to [100] for relations and equivalences between measures, and to [91] for full physical equivalence of the elastoplastic formulations if properly transformed). For instance, the stress power per reference volume \( P \) may be written in any of the following equivalent forms, among others

\[ P = J \sigma : d = \tau : d = S : \dot{A} = T : \dot{E} \]  

(25)

where \( \tau \) is the spatial Kirchhoff stress tensor and \( J = \det(X) \). The tensor \( E = \ln U \) is the logarithmic strain tensor in the reference configuration, \( \dot{E} \) is its rate, \( U \) is the right stretch tensor and \( T \) is the generalized Kirchhoff stress tensor, which is the work conjugate of \( E \) in the most general anisotropic case (see details and proof in [91]). To grasp a physical meaning for this tensor we note that in the case of elastic isotropy (regardless of strains being large) \( T = \tau_R \) (rotated Kirchhoff stresses), an equality which holds in any case for diagonal terms. In anisotropy, or moderately large strains \( T \simeq \text{sym}(\Xi) \). The relation between \( A \) and \( E \) is simple when using the spectral decomposition

\[ A = \sum_{i=1}^{3} \frac{1}{2} (\lambda_i^2 - 1) n_i \otimes n_i \quad \text{and} \quad E = \sum_{i=1}^{3} \ln \lambda_i n_i \otimes n_i \]  

(26)
Then we can relate them through the fourth order mapping tensor

\[
E = M^E_A : A \quad \text{with} \quad M^E_A = \sum_{i=1}^{3} \frac{2 \ln \lambda_i}{\lambda_i^2 - 1} M_i \otimes M_i
\]  

(27)

where \( \lambda_i \) are the principal stretches, \( n_i \) are the material principal directions of deformation, \( M_i := n_i \otimes n_i \) and \( M^E_A \) is the corresponding mapping tensor. Then, the rates are also related in a similar way through mapping tensors

\[
\dot{E} = M^E_A : \dot{A} \quad \text{or} \quad \dot{A} = M^A_E : \dot{E}
\]  

(28)

with the invertible mapping tensor, defined from the current deformation state \[100\]

\[
M^E_A = \frac{dE}{dA} = \left( M^A_E \right)^{-1} = \sum_{i=1}^{3} \frac{1}{\lambda_i^2} M_i \otimes M_i + \sum_{i=1}^{3} \sum_{j \neq i} \frac{2 \ln (\lambda_j/\lambda_i)}{\lambda_j^2 - \lambda_i^2} M_{ij} \otimes M_{ij}
\]  

(29)

where \( M_{ij} = \frac{1}{3} (n_i \otimes n_j + n_j \otimes n_i) \). Equivalent one-to-one relations apply between \( \dot{E}_c \) and \( \dot{A}_c \) by simply changing the total principal stretches and their directions by the principal elastic ones. Then, it is apparent that similar relations to those given by Eqs. (22) and (23) apply also to logarithmic strains with the dependencies \( E_c(E, X_p) \). Applying the mappings and comparing with the rate relations from the chain rule

\[
\dot{E}_c = \left[ M^E_{A_e} : \frac{\partial A_e}{\partial A} \bigg|_{X_p=0} : M^A_E \right] : \dot{E} + \left[ M^E_{A_e} : \frac{\partial A_e}{\partial X_p} \bigg|_{X=0} \right] : \dot{X}_p
\]  

(30)

\[
= \frac{\partial E_c}{\partial E} \bigg|_{X_p=0} : \dot{E} + \frac{\partial E_c}{\partial X_p} \bigg|_{X=0} : \dot{X}_p
\]  

(31)

\[
= \dot{E}_c \bigg|_{X_p=0} + \dot{E}_c \bigg|_{X=0} = tr \dot{E}_c + ct \dot{E}_c
\]  

(32)

so we have the same split of the rate of the elastic logarithmic rate tensor in a conservative (“trial”) part and a dissipative (“corrector”) one. The specific properties of logarithmic strains will be exploited below.

If there is a one-to-one mapping between elastic strain measures, we can define the stored energy in terms of any strain measure, for example in terms of logarithmic strains. A classical approach in metal plasticity uses quadratic energies in terms of logarithmic strains; see e.g. \[87\], \[88\], \[101\]. Then, we write the energy as \( \Psi(E_c, ...) \). Applying the mappings and comparing with the rate relations from the chain rule

\[
\dot{T} = \dot{\Psi} + \dot{D} = \frac{d\Psi}{dE_c} : \dot{E}_c + D = \frac{d\Psi}{dE_c} : (tr \dot{E}_c + ct \dot{E}_c) + D
\]  

(33)

Thus, following standard Coleman arguments \[107\], we consider two cases. In the first one the internal evolution is frozen (i.e. conservative with \( \dot{X}_p = ct \dot{E}_c = 0 \) and \( D = 0 \)), which gives

\[
\dot{T} = \left. \frac{\partial \Psi(E_c(E, X_p))}{\partial E} \right|_{X_p=0} : \dot{E} = \left. \frac{d\Psi}{dE_c} : \frac{\partial E_c(E, X_p)}{\partial E} \right|_{X_p=0} : \dot{E}
\]  

(34)
Since this equation must hold for all \( \dot{E} \), we have

\[
T = \left. \frac{\partial \Psi(E_c(E, X_p))}{\partial E} \right|_{\dot{X}_p=0} = T^{\text{ic}} : \left. \frac{\partial E_c}{\partial E} \right|_{\dot{X}_p=0} =: T^{\text{ic}} : M^{tr}_{E_c} \tag{35}
\]

where \( T^{\text{ic}} := d\Psi/dE_c \) is the generalized Kirchhoff stress in the intermediate configuration (derived from the stored energy), \( T \) is the generalized Kirchhoff stress tensor in the material configuration and \( M^{tr}_{E_c} := \partial E_c/\partial E \big|_{\dot{X}_p=0} \) is a geometric mapping tensor converting the energy-derived stress \( T^{\text{ic}} \) to the one obtained from equilibrium \( T \). In the second case, the external power is frozen \( (\dot{X} = \dot{E} = 0) \), so Eq. (33) results in—cf. Eq. (10)

\[
\mathcal{D} = -T^{\text{ic}} : ct \dot{E}_c \geq 0 \tag{36}
\]

This expression is identical to that obtained for anisotropic continuum elastoplasticity using elastic corrector rates, see [91][94], and also identical to that obtained for anisotropic finite nonlinear (non-equilibrium) viscoelasticity based on the Sidoroff multiplicative decomposition [92]. We remark that there is no approximation in Eq. (36) and that both \( T^{\text{ic}} \) and \( ct \dot{E}_c \) are symmetric tensors—cf. Eq. (10).

3.3. Plastic flow: kinematic relations from crystal slip rates

Consider several consecutive steps (one may think of each step involving just one sliding mechanism)

\[
t + \Delta t X_p = t + \Delta t X_p^t t - \Delta t X_p^t \Delta t X_p^t \tag{37}
\]

and the polar decompositions

\[
t + \Delta t R_p t + \Delta t U_p^t t - \Delta t R_p^t t - \Delta t U_p^t \Delta t R_p^t \Delta t U_p^t \tag{38}
\]

Obviously

\[
t + \Delta t R_p \neq t + \Delta t R_p^t t - \Delta t R_p^t \Delta t R_p \text{ and } t + \Delta t U_p \neq t + \Delta t U_p^t t - \Delta t U_p^t \Delta t U_p^t \tag{39}
\]

so from a constitutive standpoint \( U_p \) and \( R_p \) are meaningless [108] because a rotation would be changed in character to stretch (and vice-versa) in subsequent steps, changing the nature of past deformations/dissipation. Hence, the decomposition for \( X_p \) is meaningful only for incremental infinitesimal steps (or equivalently in rate form as \( \dot{l}_p = \dot{d}_p + \dot{w}_p \)). Indeed, the order in which the incremental \( X_p \) takes place is important in plastic gradients.

Consider on the contrary successive corrections to the elastic deformation gradient, i.e.

\[
t + \Delta t X_p^t = t + \Delta t X_p^{ct} X_e^{(n)} \cdots t + \Delta t X_p^{ct} X_e^{(1)} \tag{40}
\]

In this case, the polar decomposition \( t + \Delta t X_p^t = t + \Delta t R_e t + \Delta t U_e \) is meaningful, because elastic deformations are path independent (function of state). This observation, which is also connected to the property of weak-invariance [23][22] because the plastic reference is not present, is relevant when considering several slip systems [102]. Hence, we can determine \( U_e \) (which is all needed to compute the stresses) and \( R_e \), from which \( X_e \) follows.

For simplicity consider for now a unique slip system, which plane is \( m \) and which direction is \( s \), both in the reference and intermediate (isoclinic) configurations. We assume that the plastic deformation gradient does not change the crystal directions. Since \( s \perp m \), consider also the cartesian system of
representation defined by the slip direction and slip plane \( # \equiv \{ s, m, s \times m \} \). If a slip \( \gamma(t) \) takes place in this slip mechanism, from a reference configuration \( \tau \), the plastic deformation gradient is

\[
^t\tau X_p = I + \gamma(t)s \otimes m = \begin{bmatrix} 1 & \gamma(t) \\ \gamma(t) & 1 \end{bmatrix} \quad \text{and} \quad ^t\tau X_p^{-1} = I - \gamma(t)s \otimes m \tag{41}
\]

where by \([\bullet]_#\) we imply matrix representation in the system \( # \). Since in the intermediate configuration \( \dot{s} = \dot{m} = 0 \), its rate is

\[
^t\dot{X}_p = \dot{\gamma} s \otimes m = \begin{bmatrix} 0 & \dot{\gamma}(t) \\ 0 & 0 \end{bmatrix} \quad \text{#} \tag{42}
\]

Then, using Eqs. (41) and (42), it is immediate to check that

\[
^t l_p = ^t\dot{X}_p \dot{X}_p^{-1} = [\gamma s \otimes m][I - \gamma s \otimes m] = \begin{bmatrix} 0 & \dot{\gamma}(t) \\ 0 & 0 \end{bmatrix} \quad \equiv ^t\dot{X}_p \tag{43}
\]

so \(^t l_p\) is independent of the referential state at \( \tau \), i.e. of \( X_p \), a property known as weak-invariance \([23, 22]\). Thus, the reference configuration \(^t\tau X_p\) is irrelevant in \( l_p \), since it can be changed to any \( \tau \in [0, t] \) without changing the value of \( l_p \).

Now consider the internal corrector phase during which the external flow is frozen, i.e. \( \dot{X} = 0 \), and \( \dot{X}_e \big|_{\tau = 0} = c_\tau \dot{X}_e \). Consider the incremental step, where we have simultaneously \(^t t + \Delta t \tau X = ^t t + \Delta t X = ^t t + \Delta t X_p\) and \(^t t + \Delta t \tau X = ^t t + \Delta t X = ^t t + \Delta t X_p\)

\[
^t t + \Delta t X = ^t t + \Delta t X_e \quad ^t t + \Delta t X_p = ^t t \dot{X}_e \quad ^t t + \Delta t X_p^{-1} = ^t t \dot{X}_p \tag{44}
\]

so \(^c t X_e \quad ^t t + \Delta t X_p = I \) results in the following expression, always valid

\[
^c t \dot{X}_e \quad ^t t + \Delta t X_p + ^c t X_e \quad ^t t + \Delta t X_p = 0 \Rightarrow ^t t + \Delta t \dot{X}_p \quad ^t t + \Delta t X_p^{-1} = - ^c t X_e^{-1} \dot{X}_e \tag{45}
\]

Note that we can change \( t \) by a reference state \( \tau \) and \( t + \Delta t \) by \( t \) as long as the corrector gradient corresponds to that from \( \tau \) to \( t \).

Now consider the correction of a single glide mechanism from \( \tau \) to \( t \)

\[
^c t X_e = I - \gamma s \otimes m = \begin{bmatrix} 1 & -\gamma(t) \\ 0 & 1 \end{bmatrix} = X_e^{-1} \quad \text{and} \quad ^c t \dot{X}_e = \begin{bmatrix} 0 & -\dot{\gamma}(t) \\ 0 & 0 \end{bmatrix} \quad \equiv \dot{X}_e \tag{46}
\]

Then, for each mechanism

\[
-^c t \dot{l}_e := ^c t X_e^{-1} \dot{X}_e = -^c t \dot{I}_e = -^c t \dot{X}_e \quad ^c t X_e^{-1} = \begin{bmatrix} 0 & \dot{\gamma}(t) \\ 0 & 0 \end{bmatrix} \quad \equiv -^c \dot{X}_e = ^t \dot{X}_e \equiv ^t l_p \tag{47}
\]

Therefore, for a given glide mechanism, the corrector rate of the elastic deformation gradient is minus the rate of the plastic deformation gradient, and both are independent of the respective deformation gradients (i.e. of the reference configuration respect to which they are computed).
However, consider now two glide mechanisms occurring simultaneously. For simplicity we consider the typical 2D think model in which $s_1 \otimes m_1 = s \otimes m$ and $s_2 \otimes m_2 = m \otimes s$. Consider the exponential mapping so we can write the incremental gradient from $t$ to $t + \Delta t$, depending on the order, as different possibilities, for example

$$\exp(\Delta t \tilde{\gamma}_1^p s \otimes m) \exp(\Delta t \tilde{\gamma}_2^p m \otimes s) \neq \exp(\Delta t \tilde{\gamma}_2^p m \otimes s) \exp(\Delta t \tilde{\gamma}_1^p s \otimes m)$$

(48)

Indeed, note that in the first two cases, the reference configuration for the following substep has been changed. Hence, in $l_p$ the order of the slip in the mechanisms is important because it affects the reference configuration. Moreover, if we use the typical approximation

$$t + \Delta t X_p = \exp(\Delta t l_p) \simeq I + \Delta t l_p = I + \Delta t \tilde{\gamma}_i^p s \otimes m + \Delta t \tilde{\gamma}_i^p s \otimes m$$

(50)

then, in general, for this approximation $\det(t + \Delta t X_p) \neq 1$, so $t + \Delta t X_p = \exp(\Delta t l_p) \simeq I + \Delta t l_p$ results in non-isochoric flow when multiple slip mechanisms are involved.

Despite the findings in Eq. (17), when multiple mechanisms are involved, the following ansatzes result in different approximations for large deformations (refer to discussion around Eqs. (6), (7) and (13) and Fig. 8 in [109]):

$$l_p = \dot{X}_p X_p^{-1} = \sum_{g=1}^{G} \gamma_g s_g \otimes m_g \text{ or } \dot{\epsilon}_c = c^t \dot{X}_e c^t X_e^{-1} = -\sum_{g=1}^{G} \gamma_g s_g \otimes m_g \simeq c^t \dot{\epsilon}_c = c^t X_e^{-1} c^t \dot{X}_e$$

(51)

![Figure 1: Decomposition of the plastic rate in deformation rate and rotation rate. The final intermediate configuration is isoclinic.](image)

Note that for small steps, where $c^t X_e \simeq I$ we can write $c^t \dot{X}_e \simeq c^t \dot{\epsilon}_c \simeq c^t \dot{\epsilon}_c$. The relation of $c^t \dot{\epsilon}_c$ and $c^t \dot{\epsilon}_c$ with $\dot{\epsilon}_c$ is given by $X_e = \text{tr} X_e c^t X_e$ and $\dot{X}_e = \text{tr} \dot{X}_e c^t X_e + \text{tr} X_e c^t \dot{X}_e$ as—see also Eq. (13) and note that $l = \text{tr} \dot{l}_e$

$$\dot{l}_e = \dot{X}_e X_e^{-1} = \text{tr} \dot{l}_e + c^t \dot{l}_e = \text{tr} \dot{l}_e + X_e c^t \dot{l}_e X_e^{-1} = \text{tr} \dot{X}_e \text{tr} X_e^{-1} + \text{tr} X_e c^t \dot{X}_e c^t X_e^{-1} \text{tr} X_e^{-1}$$

(52)

$$= \text{tr} \dot{l}_e + \text{tr} X_e c^t \dot{l}_e \text{ tr} X_e^{-1}$$

(53)

The configurations are shown in Fig. 2. In view of this equation, and going back to the discussion in Eq. (21) on the addition for objects in the same configuration, we note that in incremental formulations, the addition of subsequent slips in $l_p$ takes place in different configurations (away from the reference configuration by a different amount given by the updated $X_p$, whereas the additions in $c^t \dot{l}_e$ take place in the same frozen configuration, away from the spatial configuration by the fixed
amount during the whole step given by $\tr X_e$ (namely they are the partial internal evolution rate with $\dot{X} = 0$, i.e. $l_i \big|_{\dot{X} = 0}$)

Considering again a single mechanism, we can take the current intermediate configuration as reference configuration and the following infinitesimal strain and rotation rates over that configuration

$$c^t \dot{\epsilon}_e = -\dot{\gamma} \text{sym} (s \otimes m) =: -\dot{\gamma} s \otimes m = \begin{bmatrix} 0 & -\frac{1}{2} \dot{\gamma} & 0 \\ -\frac{1}{2} \dot{\gamma} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$ \hfill (54)

$$c^t \omega_e \equiv c^t W_e = -\dot{\gamma} \skw (s \otimes m) =: -\dot{\gamma} s \otimes m = \begin{bmatrix} 0 & -\frac{1}{2} \dot{\gamma} & 0 \\ \frac{1}{2} \dot{\gamma} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$ \hfill (55)

Remarkably, because $s \otimes m$ is constant (recall that the intermediate configuration remains always isoclinic and $s \perp m$), these deformation rates take always place in the same principal directions, at $45^\circ$; i.e.

$$c^t \dot{\epsilon}_e = -\dot{\gamma} s \otimes m = -\frac{1}{2} \dot{\gamma} n_1 \otimes n_1 + \frac{1}{2} \dot{\gamma} n_2 \otimes n_2$$ \hfill (56)

where $n_1 = 1/\sqrt{2} (s + m)$ and $n_2 = 1/\sqrt{2} (-s + m)$ are the principal directions, see Figure 1. In this case it can be shown that logarithmic strains are the integral of infinitesimal strains; i.e. the rate of logarithmic strains, the rate of the infinitesimal strains, and the deformation rate in the intermediate configuration, are the same (see details and interpretation in [110])

$$\text{sym} \left( c^t \tilde{I}_e \right) \equiv c^t \dot{E}_e \equiv c^t \dot{\epsilon}_e = -\dot{\gamma} s \otimes m$$ \hfill (57)

so we arrive at the following corrector identities, holding in crystal plasticity without approximation

$$c^t \tilde{I}_e \equiv c^t \dot{X}_e = c^t \dot{E}_e + c^t W_e = -\dot{\gamma} s \otimes m - \dot{\gamma} s \otimes m$$ \hfill (58)

Then, the rate of the elastic deformation gradient is, without approximation

$$\dot{X}_e = \tr \dot{X}_e + c^t \dot{X}_e$$

$$= \tr \dot{X}_e + c^t \dot{E}_e + c^t W_e$$

$$= \tr \dot{X}_e - \dot{\gamma} s \otimes m - \dot{\gamma} s \otimes m$$ \hfill (59)
Note that once \( ct \dot{E}_e = -\gamma s \otimes \dot{m} \) is given, we also have immediately \( ct W_e = -\gamma s \otimes \dot{m} \); it is the requirement to enforce that the intermediate configuration is isoclinic. In a crystal there are several \( g = 1, \ldots, G \) glide mechanisms, and we consider

\[
ct \dot{E}_e = - \sum_{g=1}^{G} \dot{\gamma}_g s_g \otimes m_g = \sum_{g=1}^{G} \left( c t \dot{E}_{eg} + c t W_{eg} \right) = c t \dot{E}_e + c t W_e \tag{60}
\]

The resolved shear stress in the intermediate configuration is defined by the dissipation power in Eq. \(36\) and the condition of being work-conjugate of \( \dot{\gamma}_g \) so \( D_g = \tau_{\gamma_g}^{\text{cr}} \gamma_g \) with

\[
\tau_{\gamma_g}^{\text{cr}} := s_g \cdot T^{\text{cr}} m_g = (s_g \otimes m_g) : T^{\text{cr}} \equiv s_g \otimes m_g : T^{\text{cr}} \equiv T^{\text{cr}} : s_g \otimes m_g \tag{61}
\]

where the last identities hold because of the symmetry of \( T^{\text{cr}} \). If the glide strain rate is \( \dot{\gamma}_g \), obviously when the mechanism is not activated, we have \( \dot{\gamma}_g = 0 \), and when the mechanism is activated, we have \( \dot{\gamma}_g \neq 0 \) (\( \dot{\gamma}_g > 0 \) if the forward and backward slip directions are considered as two mechanisms). The elastic corrector rates for each mechanism is written as:

\[
ct \dot{E}_{eg} = -\dot{\gamma}_g s_g \otimes m_g = -\dot{\gamma}_g N_g^{s} \tag{62}
\]

\[
ct W_{eg} = -\dot{\gamma}_g s_g \otimes w \otimes m_g = -\dot{\gamma}_g N_g^{w} \tag{63}
\]

with the definitions for convenience of notation: \( N_g^{s} := s_g \otimes m_g \) and \( N_g^{w} := s_g \otimes w \otimes m_g \). The rate of the elastic strains is

\[
\dot{E}_e = t^r \dot{E}_e + c t \dot{E}_e = t^r \dot{E}_e - \sum_{g=1}^{G} \dot{\gamma}_g s_g \otimes m_g \tag{64}
\]

As seen below, a simple backward-Euler update is

\[
t^+ \Delta t_0 E_e = t^r E_e + \Delta c t E_e = t^r E_e - \sum_{g=1}^{G} \Delta \gamma_g s_g \otimes m_g \tag{65}
\]

where the order in the addition is irrelevant, no exponential mapping is employed, and the flow is fully isochoric because \( \text{trace}(\Delta c t E_e) = 0 \). Of course, once \( t^+ \Delta t_0 E_e \) is known, the elastic stretch tensor is immediately computed as indicated in Eq. \(92\) and the rotation as indicated in Eq. \(93\) below—recall the arguments around Eq. \(40\). Note that the plastic gradient is not involved explicitly in our formulation (except of course for mappings if a Total Lagrangean Finite Element formulation is used), so the idea behind of weak-invariance is followed.

4. Continuum elastoplastic tangent and comparison with infinitesimal plasticity

The algorithm is written in a more efficient and clean way when using matrix notation by stacking all the mechanisms in a vector, and the continuum elastoplastic matrix is better appreciated in this format. Let \( N^s_a \) be the Mandel pseudovector notation of the symmetric Schmid tensor \( N^s_a \), and let \( \mathbf{N} = [N^s_1, N^s_2, \ldots N^s_A] \) (dimension \( 6 \times A \)) be the collection of the active ones, \( a = 1, \ldots, A \in \mathcal{A} \), where \( \mathcal{A} \) is the active set. The active slip systems are those such that the Schmid stress \( \tau_{\gamma_g}^{\text{cr}} \) is greater than the resolved critical stress (CRSS) \( \tau_{\gamma_g}^{\text{cr}} \) for the given slip system, i.e.

\[
f_g = |\tau_{\gamma_g}^{\text{cr}}| - \tau_{\gamma_g}^{\text{cr}} \geq 0 \quad \text{with } \tau_{\gamma_g}^{\text{cr}} := N^s_g : T^{\text{cr}} \tag{66}
\]
In rate-dependent plasticity, the inequality is chosen, and the absolute value may be omitted if we considered signed directions (24 mechanisms in FCC). Using Mandel notation also for the elastic strain rate \( \dot{\mathbf{E}}_e \) (dimension 6 \( \times \) 1), we have

\[
\dot{\mathbf{E}}_e = \text{tr} \dot{\mathbf{E}}_e + \mathbf{c}^t \dot{\mathbf{E}}_e = \text{tr} \dot{\mathbf{E}}_e - \mathbf{N} \dot{\mathbf{r}}
\]  

(67)

where \( \dot{\mathbf{r}} = [\dot{\gamma}_1, ..., \dot{\gamma}_A]^T \) (dimension \( A \times 1 \)). The rate of the stress tensor is

\[
\dot{\mathbf{T}}^{\text{ec}} = \frac{\partial^2 \Psi(E, ...)}{\partial E_c \partial E_c} \ : \ \dot{\mathbf{E}}_e =: \mathbf{A}^{\text{ec}} : \dot{\mathbf{E}}_e
\]  

(68)

where \( \mathbf{A}^{\text{ec}} \) is the elastic tangent (not necessarily constant, although typically assumed constant in metal plasticity [87, 88]). This equation may be written again in Mandel matrix notation as \( \dot{\mathbf{T}}^{\text{ec}} = \mathbf{A}^{\text{ec}} : \dot{\mathbf{E}}_e \)

so

\[
\dot{\mathbf{T}}^{\text{ec}} = \mathbf{A}^{\text{ec}}(\text{tr} \dot{\mathbf{E}}_e - \mathbf{N} \dot{\mathbf{r}})
\]  

(69)

To perform simple intuitive comparisons with the classical infinitesimal theory of plasticity, consider rate independent plasticity (we do not discuss about the uniqueness of the solution; see e.g. [98, 111, 112]). In this case, the rates are given by the condition that \( f_\beta = 0 \). Considering the vector of active conditions as \( \mathbf{F} = [f_1, ..., f_A]^T \), we require \( \dot{\mathbf{r}} = 0 \). Since \( \mathbf{N} \) remains constant, this implies

\[
\dot{\mathbf{r}} = \mathbf{N}^T \mathbf{A}^{\text{ec}} \text{tr} \dot{\mathbf{E}}_e - \mathbf{N}^T \mathbf{A}^{\text{ec}} \mathbf{N} \dot{\mathbf{r}} = 0
\]  

(70)

so

\[
\dot{\mathbf{r}} = \mathbf{N}^T \mathbf{A}^{\text{ec}} \text{tr} \dot{\mathbf{E}}_e - \mathbf{N}^T \mathbf{A}^{\text{ec}} \mathbf{N} \dot{\mathbf{r}} = 0
\]  

(71)

This Equation may be compared to that of classical (unhardened) infinitesimal continuum plasticity, e.g. Eq. (2.2.18) of [6], Eq. (6.64) of [37] and Eq. (3.97) of [112], among others, showing identical form despite being a finite strain crystal plasticity model, unrestricted in the magnitude or anisotropy of elastic and plastic responses. Of course, inside this framework hardening may be equally considered. As well-known, the solution of the system of equations may not be unique in the inviscid case, and several solutions have been proposed as Moore-Penrose solutions, work minimization [113] or the ultimate algorithm [98, 114, 74, 112]; however the examples below will be performed with rate-dependent plasticity, as usual in materials science, so we do not elaborate further. The tangent may be obtained also as in small strains continuum plasticity, namely substituting Eq. (70) into Eq. (69)

\[
\dot{\mathbf{T}}^{\text{ec}} = [\mathbf{A}^{\text{ec}} - \mathbf{A}^{\text{ec}} \mathbf{N} (\mathbf{N}^T \mathbf{A}^{\text{ec}} \mathbf{N})^{-1} \mathbf{N} \mathbf{N}^T \mathbf{A}^{\text{ec}}] \text{tr} \dot{\mathbf{E}}_e =: \mathbf{A}_{\text{ecp}}^{\text{ec}} : \text{tr} \dot{\mathbf{E}}_e
\]  

(72)

Except for the obvious matrix form (because it includes all active systems simultaneously), note that the expression for \( \mathbf{A}_{\text{ecp}}^{\text{ec}} \) is the same as that of the continuum elastoplastic tangent for infinitesimal continuum elastoplasticity, cf. Eq. (2.2.22) of [6], Eq. (6.67) of [37] or Eq. (3.98) of [112]. Indeed, it is also the same layout as that obtained for continuum finite strain elastoplasticity using this same framework; see Eq. (59) in [34]. The tensors \( \dot{\mathbf{T}}^{\text{ec}} \) and \( \text{tr} \dot{\mathbf{E}}_e \) live in the isoclinic configuration for logarithmic strains. The tensor \( \mathbf{A}_{\text{ecp}}^{\text{ec}} \) relating both rates is the main block of the elastoplastic formulation because any other constitutive tensor between any other stress/strain couple in any configuration is obtained from this one using explicit geometrical mappings. For example, a natural elastoplastic tangent may be \( \mathbf{A}_{\text{p}}^{\text{ecp}} \) such that \( \mathbf{T} = \mathbf{A}_{\text{p}}^{\text{ecp}} : \dot{\mathbf{E}}_e \), relating the generalized Kirchhoff stress tensor in the reference configuration with the logarithmic strain rate in that configuration. In this case, the rate of Eq. (35) may be used

\[
\dot{\mathbf{T}} = \dot{\mathbf{T}}^{\text{ec}} : \mathbf{M}^{\text{tr}} \dot{\mathbf{E}}_e + \dot{\mathbf{T}}^{\text{ec}} : \mathbf{M}^{\text{tr}} \dot{\mathbf{E}}_e
\]  

(73)
\[ M_E E_e = \frac{d}{dt} \left( \frac{\partial E_e}{\partial E} \right) \]

is the derivative of the mapping between both configurations in the logarithmic space; it is elaborate but the term can be neglected (see details in [91, 94]). Equation (73) contains two terms. The first term relates the rates \( \dot{T} |_e \) and \( \dot{T} \) in the intermediate and the reference configuration when these configurations are frozen. The second term in Eq. (73) contains the influence of the continuously evolving configurations in the mapping tensor when the plastic deformation gradient is fixed. However, from a practical side, in numerical implementations it is customary to develop the algorithm in a frozen intermediate configuration; a setting that is similar in nature to updated Lagrangean finite element formulations. Hence, we take

\[ \dot{T} = \dot{T} |_e : M_E E_e = tr \dot{E}_e : A_{ep} : M_E E_e \]

If, for example, we wish the tangent such that \( \dot{S} = C_{ep} : \dot{A} \), we just have to employ the proper mapping tensors [100]. We deal more in detail below for the actual elastoplastic tangent for the specific Total Lagrangean finite element formulation.

5. Incremental computational formulation for rate-dependent plasticity

Since most algorithms and simulations of crystal plasticity in materials science employ rate-dependent formulations, we develop here the specific algorithm for this case and compare results in Section 7 with published results employing an equivalent classical crystal plasticity formulation.

The computational algorithm integrates in two phases the trial rate and the corrector rate. The first phase “integrates” the trial rate, i.e. the partial derivatives for \( \dot{X}_p = 0 \). The second phase integrates the internal evolution by the corrector phase, i.e. the partial derivatives with \( \dot{X}_p = 0 \).

5.1. Trial elastic state

Since the first part of the integration process “integrates” the partial derivatives with \( \dot{X}_p = 0 \), this is a purely conservative (hyperelastic) phase. Therefore, since the result is path-independent we do not need to perform the integration, we just compute the final state at the end of this substep, which is characterized by the elastic gradient

\[ tr X_e = t + \Delta t \frac{t_0 X_e}{t_0 X_e} \]

from which the trial elastic logarithmic strain and the trial stress are immediately obtained

\[ tr E_e = \frac{1}{2} \ln (tr X_e^T tr X_e) \quad \text{and} \quad tr T^{(e)} = \frac{d\Psi (tr E_e)}{dtr E_e} \]

where \( tr \Psi := \Psi (tr E_e) \) is the trial elastic strain energy. Note that \( tr E_e \) is not the total integral of \( tr \dot{E}_e \) from \( t = 0 \) (which we do not need to perform). Instead, taking reference at time \( t \), conceptually it would be

\[ tr E_e = \dot{E}_e + \int_t^{t + \Delta t} tr \dot{E}_e d\tau \]

However, as mentioned, Eq. (78) gives \( tr E_e \) without any approximation. Both \( tr E_e \) and \( tr T^{(e)} \) tensors live in the trial elastic configuration defined by \( tr X_e^{-1} \) from the spatial one at time \( t \) or by \( t_0 X_p \) from the material one. The objective of the second phase of the stress integration algorithm below is to obtain \( tr X_e \) and the related stress \( tr T^{(e)} \) upon knowledge of \( tr E_e \), which is kept fixed during the second substep.
5.2. Example of rate-sensitive (viscous-type) constitutive equations

The presented framework may be used both in rate-independent and rate-dependent plasticity. To demonstrate an application we develop an integration algorithm comparable to the typical rate-dependent plasticity, e.g. Ch. 6 in [5].

For the shear rate function of each glide mechanism we choose the well-known phenomenological power law proposed by Hutchinson (Eq. (2.4) in [115], see also Eq. (2.17) in [116] and the similar Eq. (23) in [117]) motivated in the continuum mechanics power law for creep

\[
\dot{\gamma}_g(\tau^e_{cg}, \tau^e_{cg}) = \dot{\gamma}_0 \left( \frac{\tau^e_{cg}}{\tau^e_{cg}} \right)^{1/m} \text{sgn}(\tau^e_{cg})
\]

(80)

where \( \dot{\gamma}_0 \) is a material parameter, a reference shear rate that is related to the loading velocity, \( \tau^e_{cg} \) is the hardened critical resolved shear stress of slip system \( g \), and \( m \) is the rate sensitivity exponent (often \( N := 1/m \) is used in the literature). We also assume that the critical resolved shear stress hardens due to dislocation pile-up and other related effects, following the phenomenological relation — e.g. Eq. (18) in [109]

\[
\dot{\tau}^e_{cj}(\dot{\gamma}_j, \tau^e_{cj}, j = 1, \ldots, G) = \sum_{j=1}^{G} h_{gj} H^j \left| \dot{\gamma}_j \right| \left( 1 - \frac{\tau^e_{cj}}{\tau^e_{sj}} \right)^\alpha
\]

(81)

The hardening rate of the critical resolved shear stress of each mechanism accounts for the contribution of all the mechanisms; it has an isotropic hardening form. \( \tau^e_{cj} \) is the current critical resolved shear stress of slip system \( j \), \( h_{gj} \) is the lateral, latent hardening parameter/ratio (typically \( h_{gj} \in [1, 1.4] \), with 1 for coplanar and 1.4 otherwise; and \( h_{gj} = 1 \), see e.g. discussion in Sec. 3.2 of [118]), and \( H^j \) is the hardening modulus. The parameter \( \tau^e_{sj} \) is the saturated critical resolved shear stress for slip system \( j \) and \( \alpha \) is the hardening exponent.

5.3. Plastic correction. Example: system of equations for viscous-type plasticity

There are several ways to build an iterative algorithm to solve the previous equations in an implicit way. The scheme is the same as in infinitesimal continuum plasticity with the obvious exception of the flow direction given by the crystal slip mechanisms and the specific rate-dependent formulae employed. We choose \( E_e \) and \( \tau^e_{cg} (g = 1, \ldots, G) \) as the variables and the following \( 6 + G \) residues as nonlinear equations to solve. Classical plain Newton-Raphson iterations are used to solve the system equations. Using again Serif fonts to denote the Mandel vector/matrix notation, the residuals enforcing a standard backward-Euler integration scheme are (the first set is a rate-dependent counterpart of the typical yield conditions)

\[
t^{+\Delta t} R_g := \Delta \tau^e_{cg} - \Delta t^{+\Delta t} \dot{\tau}^e_{cg} \rightarrow 0, \quad i = 1, \ldots, G
\]

(82)

\[
t^{+\Delta t} R_E := t^{+\Delta t} E_e - t^e E_e + \sum_{g=1}^{G} \Delta \gamma_g N^e_g \rightarrow 0
\]

(83)
The residual vector is \( R = [R_1, \ldots, R_G, R_t^T]^T \) with dimension \( G + 6 \). The tangent with dimension \((G + 6) \times (G + 6)\) for step \( t + \Delta t \) is:

\[
[d^{t+\Delta t} R]_k^{[k]} = \begin{bmatrix}
\frac{d^{t+\Delta t} R_{t}^{[k]}}{d^{t+\Delta t} r_{c_1}^{e}} & \ldots & \frac{d^{t+\Delta t} R_{t}^{[k]}}{d^{t+\Delta t} r_{c_G}^{e}} \\
\vdots & \ddots & \vdots \\
\frac{d^{t+\Delta t} R_{G}^{[k]}}{d^{t+\Delta t} r_{c_1}^{e}} & \ldots & \frac{d^{t+\Delta t} R_{G}^{[k]}}{d^{t+\Delta t} r_{c_G}^{e}}
\end{bmatrix}
\]

with \( V = [r_{c_1}^{e}, \ldots, r_{c_G}^{e}, E_t]^T \) being the iterative variables. Taking for simplicity in the exposition a constant elastic behavior \( dT_e^c/dE_e = A^e \rightarrow A_e^c \), the terms of the tangent, in tensor notation, are obtained from Eqs. (82), (83) as —we omit the time and iteration indices for brevity

\[
\frac{\partial R_E}{\partial E_e} = \mathbb{I} + \Delta t \sum_{g=1}^{G} N^g \otimes \frac{\partial \gamma_g}{\partial T_e^c} : A_e^c
\]

\[
\frac{\partial R_g}{\partial E_e} = -\Delta t \sum_{j=1}^{G} \frac{\partial r_{c_g}^{e}}{\partial \gamma_j} \frac{\partial \gamma_j}{\partial T_e^c} : A_e^c
\]

and

\[
\frac{\partial R_{E}}{\partial r_{c_g}^{e}} = N^g \Delta t \frac{\partial \gamma_j}{\partial r_{c_g}^{e}}
\]

\[
\frac{\partial R_d}{\partial r_{c_g}^{e}} = \delta_{gj} - \Delta t \left[ \frac{\partial r_{c_g}^{e}}{\partial T_e^c} + \frac{\partial r_{c_g}^{e}}{\partial \gamma_j} \right]
\]

which terms follow immediately from Eqs. (80) and Eq. (81), and \( \delta_{gj} \) is the Kronecker delta. During the iterations, once \( t^{+\Delta t} E_e \) and \( t^{+\Delta t} r_{c_g}^{e} \) \( (g = 1, \ldots, G) \) are known, the generalized Kirchhoff stress \( t^{+\Delta t} T_e^c \) is known and used from the hyperelasticity expression

\[
t^{+\Delta t} T_e^c = \frac{d\Psi}{d^{t^{+\Delta t} T_0} E_e} \frac{d^{t^{+\Delta t} T_0} E_e}{d^{t^{+\Delta t} T_0} E_e}
\]

and the shear rates from Eq. (80) in backward-Euler form:

\[
t^{+\Delta t} \gamma_g = \gamma_0 \left( \frac{t^{+\Delta t} T_e^c \cdot N^g}{t^{+\Delta t} r_{c_g}^{e}} \right)^{1/m} \text{sgn}(t^{+\Delta t} T_e^c \cdot N^g)
\]

so the solutions for all \( \Delta \gamma_g = \Delta t \cdot t^{+\Delta t} \gamma_g \) are also known.

If the finite element program is running in infinitesimal strains mode (i.e. a small strains formulation is pursued), the rest of the operations are omitted; we simply accept \( T_e^c \leftrightarrow \sigma \) and \( E_e \leftrightarrow \epsilon_e \) and \( \Delta t W_e \leftrightarrow \Delta \omega_e \). For a large strains formulation, for the next step it is necessary to update the elastic deformation gradient, which may be updated using the polar decomposition, because it is a state variable (path independent)

\[
t^{+\Delta t}_0 X_e = \text{tr} X_e \in A \cdot X_e = t^{+\Delta t}_0 R_e \cdot t^{+\Delta t}_0 U_e
\]

18
Since the update should be consistent with the final computed value of $t^+\Delta t^0 E_e$, we have

$$t^+\Delta t^0 U_e = \exp (t^+\Delta t^0 E_e)$$

(92)

and we take

$$t^+\Delta t^0 R_e = tr R_e \exp (\Delta t \mathcal{S} w)$$

(93)

with

$$\Delta t \mathcal{S} w = - \sum_{g=1}^{G} \Delta \gamma_g N_g^w$$

(94)

Once the iterative solution is obtained, a last step is to perform the mappings to the stress-strain couple used by the finite element program. In total Lagrangean formulations it is typical that this stress-strain couple is made by the second Piola Kirchhoff stress tensor $\mathbf{S}$ and the Green-Lagrange strains $\mathbf{A}$ in the reference (initial, undeformed) configuration [3]. This operation is non-iterative and employs just purely geometrical mappings [190].

5.4. Geometric postprocessor

With the final strains $t^+\Delta t^0 E_e$, the generalized Kirchhoff stresses in the converged configuration are

$$t^+\Delta t \mathcal{T} = \frac{d\Psi}{d\mathcal{T}} E_e$$

(95)

By work conjugacy, the stresses in the trial configuration (with $\mathbf{X}_p = 0$) are obtained from $\mathbf{T}^e_c$ : $\mathbf{E}_e = \mathbf{T}^{(tr)} : \mathbf{E}_e$, so

$$t^+\Delta t \mathbf{T}^{(tr)} = \left. \frac{\partial \Psi}{\partial \mathbf{T}^{(tr)} E_e} \right|_{\mathbf{X}_p = 0} = \left. \frac{d\Psi}{d\mathbf{T}^{(tr)} E_e} \right|_{\mathbf{X}_p = 0} \mathbf{T}^e_c$$

(96)

where, if the steps are small or loading proportional for large steps, we can consider $\mathbf{M}^E_{e} \mathbf{X}_p = 0 \approx \mathbf{I}^e$. Indeed, no distinction has been performed above between both configurations in the case of logarithmic strains and related stresses. Note that the stresses $t^+\Delta t \mathbf{T}^{(tr)} \neq t^+\Delta t \mathcal{T}$, whereas $t^+\Delta t \mathbf{T}^e = d\mathbf{T}^e / d\mathbf{T}^{(tr)} E_e$ are the trial stresses (independent of any plastic flow, corresponding to the trial strains $t^e E_e$) whereas the former $t^+\Delta t \mathcal{T} = \partial t^+\Delta t \mathcal{T} / \partial \mathbf{T}^{(tr)} E_e \left|_{\mathbf{X}_p = 0} \right.$ are the final elastic stresses $t^+\Delta t \mathbf{T}^e$ (corresponding to $t^+\Delta t E_e$, which depends on the plastic flow) mapped geometrically to the trial configuration. In general $t^e \mathbf{T}^e$ will be very different from $t^+\Delta t \mathcal{T}$ (they correspond to different strains) but $t^+\Delta t \mathbf{T}^{(tr)}$ will be similar or equal to $t^+\Delta t \mathcal{T}$ (they correspond to the same strains, but lie slightly different configurations); they are coincident in the case of proportional loading or with infinitesimal steps, because in such cases $\partial \mathbf{T}^e / \partial \mathbf{T}^{(tr)} E_e \left|_{\mathbf{X}_p = 0} \right. \approx \mathbf{I}^e$.

The purpose of employing the stresses $t^+\Delta t \mathbf{T}^{(tr)}$ is to use the trial configuration and simpler mapping tensors to arrive at the second Piola-Kirchhoff stress tensor in the reference configuration. Consider the following expression immediate from work-conjugacy and the chain rule

$$t^+\Delta t \mathbf{S}^{(tr)} = t^+\Delta t \mathbf{T}^{(tr)} : \frac{d\mathbf{T}^{(tr)} E_e}{d\mathbf{T}^{(tr)} A_e}$$

(97)

where $d\mathbf{T}^{(tr)} E_e / d\mathbf{T}^{(tr)} A_e$ is a mapping tensor obtained immediately from the stretches and principal directions of the trial state, see [190] and Eq. (29). Then, the reference second Piola-Kirchhoff stress used in total Lagrangean formulations is --see Eq. (21)

$$t^+\Delta t \mathbf{S} = t^+\Delta t \mathbf{S}^{(tr)} : \frac{d\mathbf{T}^{(tr)} A_e}{d\mathbf{T}^{(tr)} A_e} = t^+\Delta t \mathbf{S}^{(tr)} : (\mathbf{X}_p^{-1} \mathbf{T}^{-1} \otimes \mathbf{X}_p^{-1})$$

(98)
5.5. Comparison of frameworks

In Table 1 we compare both frameworks with relation to the main variables involved, steps and algorithmic approximations.

6. Consistent elastoplastic tangent moduli

In order to preserve the asymptotic quadratic convergence of Newton schemes, a consistent linearization of the stress integration algorithm is needed. As in the continuum case, we develop the basic tensor using logarithmic stress and strain measures in the trial configuration, which is the configuration in which all the stress integration takes place. This is due to the fact that the global integration algorithm just changes the displacements and, hence, gives at each global iteration a modified trial elastic gradient \( \dot{\mathbf{X}}_e \) for the element integration point. Then, for performing the output of the material subroutine, the tensor may be mapped to any other configuration or stress-strain couple, typically second Piola-Kirchhoff stresses and Green-Lagrange strains in the material configuration used in Total Lagrangean finite element formulations.

6.1. Kinematics

The basic tangent relating the stress change for that change is

\[
\dot{\mathbf{X}}_{e, t+\Delta t}^{\text{tr}} = \frac{d^t + \Delta^t \mathbf{T}\big|^{\text{tr}}}{d^t \mathbf{E}_e} \left( \frac{d^t + \Delta^t \mathbf{T}|^e}{d^t \mathbf{E}_e} \right) = (t + \Delta^t) \mathbf{A}_{e, t+\Delta t}^{\text{tr}} = \frac{d^t + \Delta^t \mathbf{E}_e}{d^t \mathbf{E}_e}
\]

which, recalling the arguments in Eq. (96), may be approximated by

\[
t^+\Delta t |_{\mathbf{A}_{e, t+\Delta t}}^{\text{tr}} = \frac{d^t + \Delta^t \mathbf{T}\big|^{\text{tr}}}{d^t \mathbf{E}_e} \left( \frac{d^t + \Delta^t \mathbf{T}|^e}{d^t \mathbf{E}_e} \right) = \frac{d^t + \Delta^t \mathbf{E}_e}{d^t \mathbf{E}_e} \approx \frac{d^t + \Delta^t \mathbf{E}_e}{d^t \mathbf{E}_e} = (t + \Delta^t) |_{\mathbf{A}_{e, t+\Delta t}}^{\text{tr}} = \frac{d^t + \Delta^t \mathbf{E}_e}{d^t \mathbf{E}_e}
\]

where \( t^+\Delta t |_{\mathbf{A}_{e, t+\Delta t}}^{\text{tr}} \) is the elasticity tensor (in terms of \( \mathbf{T}\big|^e \) and \( \mathbf{E}_e \)), evaluated at \( t + \Delta t \), but assumed constant in the examples. The tensor \( \frac{d^t + \Delta^t \mathbf{E}_e}{d^t \mathbf{E}_e} \) is the total derivative, result of the integration algorithm, and relates the trial elastic strain \( \mathbf{tr}\mathbf{E}_e \) with the final one \( t^+\Delta^t \mathbf{E}_e \). This relation is given by the residue function Eq. (83), which in tensor format is

\[
t^+\Delta t \mathbf{R}_e := t^+\Delta^t \mathbf{E}_e - t^r \mathbf{E}_e + \sum_{g=1}^{G} \Delta \gamma_g \mathbf{N}_g^s = 0
\]

so

\[
\frac{d^t + \Delta^t \mathbf{E}_e}{d^t \mathbf{E}_e} = I^s + \sum_{g=1}^{G} \mathbf{N}_g^s \otimes \frac{d\Delta \gamma_g}{d^t \mathbf{E}_e}
\]

The total derivative \( \frac{d\Delta \gamma_g}{d^t \mathbf{E}_e} \), depends on the specific model and desired algorithm (semi-implicit or fully implicit).

6.2. Example: viscous-type hardening equations

At the convergence step, for each glide mechanism \( g \), the backward-Euler approximation gives \( \Delta \gamma_g = \Delta t^+\Delta^t \gamma_g \), so

\[
\frac{d\Delta \gamma_g}{d^t \mathbf{E}_e} = \Delta t \frac{d^t + \Delta^t \gamma_g}{d^t \mathbf{E}_e}
\]
| Variable / step | Classical framework | Proposed formulation |
|----------------|---------------------|---------------------|
| Multiplicative decomposition | $X = X_c X_p$ | $X = X_c X_p$ |
| Integrated gradient | $X_p^{-1}$ (path dependent gradient) | $X_c$ (path independent gradient) |
| Plastic dissipation | $\mathcal{D} = \mathcal{E} : l_p = \sum_{g=1}^{G} \bar{\mathcal{G}}_{g}^p \dot{\gamma}_g$ | $\mathcal{D} = -T^e : \dot{\mathcal{E}}_e = \sum_{g=1}^{G} \bar{\mathcal{G}}_{g}^e \dot{\gamma}_g$ |
| Strain selection | Green-Lagrange (int. configuration): $X_e = XX_p^{-1} \rightarrow A_e = \frac{1}{2}(X_e^T X_e - I)$ | Logarithmic strains (int. config.): $E_e = \frac{1}{2} \ln(X_e^T X_e)$ |
| Stress conjugate | 2nd PK for energy and Mandel for dissipation: $\mathcal{E} = C_e S^e$ with $S^e = d\Psi / dA_e$ | Generalized Kirchhoff (symmetric) for both energy and dissipation $T^e = d\Psi / dE_e$ |
| Flow rule | Plastic velocity gradient $l_p = \sum_{g=1}^{G} \dot{\gamma}_g s_g \otimes m_g$ | Elastic velocity corrector gradient $\dot{t} \mathcal{I}_e = -\sum_{g=1}^{G} \dot{\gamma}_g s_g \otimes m_g = \dot{t} \dot{\mathcal{E}}_e + \dot{t} W_e$ |
| Resolved stress | $\bar{\mathcal{G}}_{g} = s_g \cdot C_e S^e \cdot m_g$ | $\bar{\mathcal{G}}_{g} = \dot{t} \mathcal{E}_e$ |
| Trial state | Just algorithmically motivated | From chain rule in $dX_e(X, X_p)/dt$ |
| Iterations result | $\forall g, \Delta \dot{\gamma}_g \rightarrow \Delta t \dot{t} \mathcal{I}_e \Rightarrow \Delta t \dot{\mathcal{E}}_e, \Delta t \dot{t} W_e$ | $\forall g, \Delta \dot{\gamma}_g \rightarrow \Delta t \dot{t} \mathcal{I}_e \Rightarrow \Delta t \dot{\mathcal{E}}_e, \Delta t \dot{t} W_e$ |
| Update | Exponential mapping of $l_p = \dot{X}_p X_p^{-1}$ $t+\Delta t X_0 = \frac{1}{2}(t+\Delta t X^{t+\Delta t} X^{-1} - I)$ | Additive rates from chain rule |
| Basic stress | $t+\Delta t S^e = d\Psi / dX_0 A_e$ | $t+\Delta t S^e / dX_0 = t+\Delta t E_e$ |
| Basic tangent | $t+\Delta t C_{ep}^e = d\Psi / dX_0 A_e$ | $t+\Delta t C_{ep}^e = d\Psi / dX_0 A_e$ |
| Mappings for TL | $t+\Delta t S^e \rightarrow t+\Delta t S$ | $t+\Delta t S^e \rightarrow t+\Delta t S$ |
| FE formulation | $t+\Delta t \bar{C}_{ep} \rightarrow t+\Delta t \bar{C}_{ep}$ | $t+\Delta t \bar{C}_{ep} \rightarrow t+\Delta t \bar{C}_{ep}$ |

Table 1: Comparison of crystal plasticity frameworks
To use Eqs. (80) and (81), we perform a change of variables to the one used therein by applying the chain rule—the sum is due to latent hardening in Eq. (81); an approximation may be obtained accounting only for self-hardening terms

\[
\frac{d\Delta \gamma_g}{dt} = \Delta t \left[ \frac{\partial^{t+\Delta t \gamma_g} \gamma^{t+\Delta t \gamma_g} C_e^{t+\Delta t \gamma_g}}{\partial^{t+\Delta t \gamma_g} T_e} \frac{d t^{t+\Delta t \gamma_g}}{d t^{t+\Delta t \gamma_g} E_e} + \frac{\partial^{t+\Delta t \gamma_g} \Delta t^{t+\Delta t \gamma_g} C_e^{t+\Delta t \gamma_g}}{\partial^{t+\Delta t \gamma_g} T_e} \frac{\Delta t^{t+\Delta t \gamma_g}}{d t^{t+\Delta t \gamma_g} E_e} \right] : \frac{d t^{t+\Delta t \gamma_g}}{d t^{t+\Delta t \gamma_g} E_e}
\]  

(104)

where \( \partial^{t+\Delta t \gamma_g} T_e = N^g \) and \( d t^{t+\Delta t \gamma_g} E_e = A^g \) (both constants), and \( \partial^{t+\Delta t \gamma_g} T_e = \partial^{t+\Delta t \gamma_g} E_e = A^g \) are scalar values obtained immediately from Eq. (81). The remaining term still to compute may be neglected in the tangent because it results in terms of the order of \((\Delta t)^2\). If included, a system of equations must be solved because it includes effects of cross-hardening; other option is to include only the self-hardening term. The term is

\[
\frac{\partial^{t+\Delta t \gamma_g} C_e^{t+\Delta t \gamma_g}}{\partial^{t+\Delta t \gamma_g} E_e} = \sum_{j=1}^{G} \frac{\partial^{t+\Delta t \gamma_g}}{\partial^{t+\Delta t \gamma_g} E_e} \frac{d t^{t+\Delta t \gamma_g}}{d t^{t+\Delta t \gamma_g} E_e} + \Delta t \frac{\partial^{t+\Delta t \gamma_g} C_e^{t+\Delta t \gamma_g}}{\partial^{t+\Delta t \gamma_g} E_e} \frac{\partial^{t+\Delta t \gamma_g}}{d t^{t+\Delta t \gamma_g} E_e}
\]  

(105)

where again the last term is of higher order. This is a system of equations with may be solved in matrix format to obtain all \( d\Delta \gamma_g/dtr E_e \). These may be substituted in Eq. (102), and thereafter the result in Eq. (100) to obtain \( t_{+\Delta t} A_{ep}^{tr} \).

6.3. Final mappings

Once the elastoplastic tangent in the trial intermediate configuration is known, it can be mapped into the reference configuration to the desired format, see, e.g. [92], [93], [94]. In particular, for total Lagrangean formulations we map the tangent to the usual material second Piola-Kirchhoff stress and Green-Lagrange strains, following the path

\[
t_{+\Delta t} A_{ep}^{tr} = \frac{d t_{+\Delta t} T_e^{tr}}{d t_{+\Delta t} E_e} \rightarrow t_{+\Delta t} C_{ep}^{tr} = \frac{d t_{+\Delta t} S_e^{tr}}{d t_{+\Delta t} A_e} \rightarrow t_{+\Delta t} C_{ep} = \frac{d t_{+\Delta t} S}{d t_{+\Delta t} A}
\]  

(106)

where the first mapping performs the conversion to quadratic measures and the second one transforms the tensor from the intermediate to the reference configuration.

7. Numerical examples

The purpose of the examples in this section is (1) to show that the formulation may be implemented successfully in an implicit finite element code and (2) to compare results from our proposal with a classical formulation. To this end, we demonstrate three finite element examples of single crystals (so differences may not be attributed to polycrystal issues or the specific RVE).

7.1. Uniaxial compression of a cylinder made of FCC single crystal

To compare the current framework with the classical formulation, we selected an example from [97]. We performed the computations with both frameworks and also compared our results to the results reported therein. The material is the face-centered (FCC) single crystal copper. For this type of crystal, there are 12 slip systems. As in Ref. [97], the loading direction is along the (011) direction of the crystal and along the \( X_3 \) (axial) direction of the specimen. The relation between the crystal
orientation and the specimen coordinate system is shown in Fig. 3. The parameters of the material are summarized in Table 2. Since \( \kappa_g \simeq \tau_g^e \) and \( \gamma_p \simeq \gamma_g \) and elastic strains are infinitesimal, we have used the same parameters for both models.

For the finite element analysis, the exact specimen dimensions, crystal orientation, loading direction as well as loading speed are prescribed. The finite element model is meshed into 40 elements, as in [97]. To run the example with the current framework, we used our in-house finite element code Dulcinea (already employed in other works of the group, e.g. [94, 93, 104, 119]). For the purpose of comparison, simulations with the conventional framework is performed with the commercial FE code Abaqus, using user subroutines employed and validated in other works, e.g. [120, 66, 67, 65].

To facilitate comparisons eliminating possible differences due to the specific element formulation, with the current framework in Dulcinea we used an element equivalent to Abaqus’ C3D20R: a quadratic brick element with 20 nodes and 8 integration points which does not suffer volumetric locking. Possible hourglass modes are not propagable. As shown in Fig. 3, the 20 nodes element would degenerate to the prism geometry because of the nature of the mesh. With the conventional framework in Abaqus, our simulations are run with the element type C3D20R and in Ref. [97] they used element C3D6, to which results from them we also compare.

If the material is isotropic, after the deformation, in both the simulated result and the experimental result [97], the dimension of the cylinder in \( x_2 \)-direction does not change, only the dimension in \( x_1 \)-direction changes. A comparison of the simulated deformed shapes by the current framework and the conventional framework in Kalidindi and Anand is shown in Fig. 3b. It is seen that differences are small.

### Table 2: Material parameters used for the copper single crystal

| Constant | Value | Constant | Value |
|----------|-------|----------|-------|
| \( C_{11} = A_{11} \) | 170 GPa | \( h_{gg} \) | [1.4, 1] |
| \( C_{12} = A_{12} \) | 124 GPa | \( H_g \) | 250 MPa |
| \( C_{44} = A_{44} \) | 75 GPa | \( \alpha \) | 2.5 |
| \( \dot{\gamma}_0 \) | 0.001 s\(^{-1}\) | \( \tau_{cg}^e \) | 16 MPa |
| \( m \) | 0.012 | \( \tau_{cg} \) | 190 MPa |
During the loading process, there is no rotation of the crystals, and the stress condition inside the cylinder is completely homogeneous. The simulated stress-strain curve by the current framework and by the framework of Kalidindi and Anand from Fig. 2 of Ref. [97] is given in Fig. 4. As it can be seen, the curves obtained with both frameworks are very similar, but differ slightly, specially at large strains, when using the same element type. The reason behind this difference at large strains may be due to the issues explained in Sec. 3.3 when the additive approximation in $\tilde{l}_e$ may differ from that in $lt$. It may also be attributable to the approximation performed for the exponential mapping in the multiplicative decomposition in the classical framework. In our framework the exponential function is evaluated using the spectral decomposition of the elastic deformations.

![Simple compression on [011]](image)

Figure 4: Simulated stress-strain curve of the current and the conventional frameworks with different element types, together with the simulated result in Fig. 2 of Ref. [97].

7.2. Simple shear test

The simple shear test has been frequently used to check the consistency of large strain formulations and of the stress-integration algorithm ([121] [23]). Therefore, we also selected this example to validate our proposed framework. The material parameters of the single aluminum crystal from Ref. [97] are used and summarized in Table 2. For the example, since deformations are homogeneous, any finite element may be employed (e.g. an 8-node brick). Displacements have been imposed via penalization. The shear stress-strain curves obtained from both frameworks are represented in Fig. 5. It can be seen that the results are similar for both frameworks, although there is again a small difference when strains become very large. As expected, fast global convergence is obtained, even though the important presence of rotation in this test (see Table [3]).

7.3. Drawing of a thin circular flange

This well-known example is a simplification for deep drawing of a cup ([111] [20]). The purpose is to simulate the deformation of the outer part of a circular sheet in the first phase of deep drawing process without using the contact elements. This simulation can be used to study the anisotropic elastoplasticity of the material, and the deformed shape reflects the earring condition in deep drawing.

A radial displacement up to 75mm is applied to the inner circle of the flange. The nodal forces of two nodes are recorded during the loading. The geometric shape, the loading condition and the
Figure 5: Shear stress-strain curve of the current and the conventional frameworks

Table 3: Simple shear test: global equilibrium convergence values at steps 50, 200, 400, 600

| Iteration | Residual norm | Energy norm |
|-----------|---------------|-------------|
|           | Step 50       | Step 200    | Step 400 | Step 600 | Step 50 | Step150 | Step 250 | Step 350 |
| (1)       | $1.982E+02$   | $2.193E+02$ | $2.705E+02$ | $4.002E+02$ | $1.585E+00$ | $1.754E+00$ | $2.154E+00$ | $3.125E+00$ |
| (2)       | $2.366E+01$   | $1.472E+01$ | $1.051E+01$ | $4.377E+01$ | $2.236E-07$ | $7.738E-08$ | $2.999E-08$ | $3.211E-07$ |
| (3)       | $1.422E-06$   | $1.355E-07$ | $5.151E-07$ | $1.743E-06$ | $8.082E-22$ | $6.485E-24$ | $7.201E-23$ | $5.089E-22$ |
locations of the two nodes are shown in Fig. 6. To avoid buckling, the vertical displacement of the flange is fully supported in one side and a vanishing rotation of the inner rim around the vertical axis is prescribed.

Figure 6: Drawing of a thin circular flange: (a) finite element model; (b) geometric dimensions

![Graphs showing nodal forces vs displacement for different crystal directions.](image)

(a) crystal direction: $x \rightarrow (1, 0, 0); z \rightarrow (0, 0, 1)$

(b) crystal direction: $x \rightarrow (1, 1, 0); z \rightarrow (0, 0, 1)$

(c) crystal direction: $x \rightarrow (0, 1, 1); z \rightarrow (1, 0, 0)$

Figure 7: Comparison of nodal forces at point A and B

This example is used to compare the results obtained by the current framework with those from the conventional framework. Since the problem is nearly under plane stress conditions, supported in one side, the simulations have been performed with Abaqus standard elements C3D8 (fully integrated 8-node bricks) and Dulcinea’s equivalent elements. Band-plot checks have been performed to discard any relevant locking phenomena [3]. Both models have 1536 elements. In the direction of the thickness, one layer of elements is used.

The purpose of this example is to compare both frameworks, so we have employed the material parameters shown in [2]. The material parameters of the single crystal Al from [37] are used, except for
Figure 8: Von Mises stress contour for three crystal orientations with the conventional framework performed in Abaqus

Figure 9: Von Mises stress contour for three crystal orientations with the proposed model performed in Dulcinea
To show the different deformed shapes due to different crystal orientations, the example has been computed with three single crystal orientations:

(a) Euler angles (0, 0, 0), whose crystal direction ⟨001⟩ aligns with the axial direction z of the flange, and the crystal direction ⟨100⟩ aligns with the x axial of the specimen coordinate system.

(b) Euler angles (45°, 0, 0), whose crystal direction ⟨001⟩ aligns with the axial direction of the flange, and crystal direction ⟨110⟩ aligns with the x axial of the specimen coordinate system

(c) Euler angles (180°, 45°, 180°), whose crystal direction ⟨011⟩ aligns with the axial direction of the flange, and crystal direction ⟨100⟩ aligns with the x axial of the specimen coordinate system.

If the material were isotropic, the outer rim of the flange would stay as a regular circle during the loading, but because of the crystallography of the FCC crystal, the outer rim shows different “wave” forms depending on different crystal orientations and loading directions, which is the same phenomenon as earring in deep drawing of an anisotropic (rolled) sheet metal. For all the three crystal orientations, the deformed shapes are shown in Figs. 8 and 9 along von Mises stresses. It is seen again that only small differences are observed. The nodal forces of two nodes in the top surface marked in Fig. 6 are obtained with both frameworks and plotted in Fig. 7 for all three crystal orientations. It is seen once more that, as expected and in line with the previous results, both frameworks give very similar results, but differ slightly as plastic deformations increase substantially.

All the simulations are done with total loading time set as 1 s, and with a fixed step size employing plain Newton-Raphson iterations. In Table 4, we list the global convergence iteration values of several typical steps for the simulation with initial crystal Euler angles (0, 0, 0). It is shown that the convergence is asymptotically quadratic as expected from Newton iterations, and the desirable residue is typically reached in 4 steps.

8. Conclusions

In this paper, we present a new framework for crystal plasticity based on elastic corrector rates, motivated in a similar successful formulation for continuum anisotropic hyperelasto-plasticity at large strains. The formulation uses the Kröner-Lee multiplicative decomposition, but does not need an explicit, algorithmically motivated, exponential mapping. Instead, the use of logarithmic strains result in an additive structure parallel to the classical continuum and algorithmic formulation of

| Iteration | Residual norm | Energy norm |
|-----------|---------------|-------------|
|           | Step 50       | Step 150    | Step 250    | Step 350    |
| (1)       | 1.189E+06     | 1.227E+06   | 1.241E+06   | 1.257E+06   |
| (2)       | 6.785E+03     | 5.185E+03   | 4.272E+03   | 3.784E+03   |
| (3)       | 1.641E+01     | 5.417E+00   | 2.335E+00   | 1.238E+00   |
| (4)       | 2.040E-01     | 3.079E-02   | 8.899E-03   | 9.737E-03   |

| Iteration | Step 50       | Step 150    | Step 250    | Step 350    |
|-----------|---------------|-------------|-------------|-------------|
| (1)       | 2.057E+06     | 2.123E+06   | 2.145E+06   | 2.168E+06   |
| (2)       | 4.741E+01     | 3.162E+01   | 2.071E+01   | 1.538E+01   |
| (3)       | 2.150E-03     | 2.058E-04   | 3.504E-05   | 8.734E-06   |
| (4)       | 3.357E-07     | 5.729E-09   | 2.952E-10   | 2.858E-11   |

Table 4: Global equilibrium convergence values at steps 50, 150, 150, 350 of the finite element simulation

the sensitivity exponent $m$ which has been $m = 0.1$ to reduce the computational time of the examples.
infinitesimal plasticity. Noteworthy, the integration is fully performed in terms of elastic variables instead of plastic ones. The formulation is also fully comparable to our continuum framework, with the natural exception of using the specific flow conditions for crystal plasticity. As in the continuum formulation, the unsymmetric Mandel stress plays no role in the formulation; any hyperelastic (e.g. nonquadratic, anisotropic) stored energy may be employed; the flow rule is conventional; a plain backward-Euler algorithm preserves volume during plastic flow; both the continuum and algorithmic formulation are parallel to that of infinitesimal plasticity and only explicit purely kinematic tensors transform the working stress-strain couple (logarithmic strains and generalized Kirchhoff stresses) to any desired one (e.g. Green-Lagrange strains and second Piola-Kirchhoff stresses). Hence, now two fully equivalent sound and robust frameworks for continuum and crystal plasticity are available, and may facilitate comparisons between simulations using both approaches.

We have performed comparisons with the classical crystal plasticity approach (Kalidindi-Anand algorithm). For the comparisons performed, as expected, we have observed only some differences when the plastic deformations are significantly large. We attribute those differences to the different approximations employed in adding simultaneous slips and in the exponential mapping.

We have also developed a fully implicit integration algorithm, consistently linearized, based on a plain backward-Euler algorithm. It is observed that, as expected, asymptotic quadratic convergence is obtained in both the local and global (equilibrium) iterations.

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