Beaver documentation

Details of the crystal plasticity model and implementation

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Contents

1 Introduction

This document describes the crystal plasticity model (see Sec. 2, with more theoretical details available in [1]), numerical implementation (see Sec. 3, with more technical details available in [2]) and derivation of material tangent stiffness (see Sec. 5), which has all been implemented in the FORTRAN subroutine `Beaver/src/main/hypela2.f` for MARC/MENTAT. Necessary definitions for notations and operations, and a few useful tensorial relations are summarized in the Appendix. In order to get familiar with the solution procedure and quickly test new features, an implementation based on MATLAB is provided in `Beaver/examples/Matlab_CP/main.m`, although this version is already slightly outdated.

2 Crystal plasticity model

2.1 Kinematics

Based on the microstructural elasto-(visco)plastic description of crystallographic slip, the deformation gradient tensor is multiplicatively split into the elastic and plastic parts (marked by the subscripts "e" and "p", respectively), reading

$$\boldsymbol{F} = \boldsymbol{F}_{\mathrm{e}} \cdot \boldsymbol{F}_{\mathrm{p}}. \tag{1}$$

Due to the rate-dependency, the velocity gradient tensor $\boldsymbol{L} = \dot{\boldsymbol{F}} \cdot \boldsymbol{F}^{-1}$ is introduced and decomposed as

$$\boldsymbol{L} = \boldsymbol{L}_{\mathrm{e}} + \boldsymbol{F}_{\mathrm{e}} \cdot \boldsymbol{L}_{\mathrm{p}} \cdot \boldsymbol{F}_{\mathrm{e}}^{-1}, \tag{2}$$

with the elastic and plastic parts separately defined by $\boldsymbol{L}_{\mathrm{e}} = \dot{\boldsymbol{F}}_{\mathrm{e}} \cdot \boldsymbol{F}_{\mathrm{e}}^{-1}$ and $\boldsymbol{L}_{\mathrm{p}} = \dot{\boldsymbol{F}}_{\mathrm{p}} \cdot \boldsymbol{F}_{\mathrm{p}}^{-1}$.

Moreover, $\boldsymbol{L}_{\mathrm{p}}$ for the plastic deformation by crystallographic slip is correlated to each initial slip direction $\vec{s}_0^{\alpha}$ and slip plane normal $\vec{n}_0^{\alpha}$, $\alpha = 1, 2, 3, \ldots, N_{\mathrm{s}}$, reading

$$\boldsymbol{L}_{\mathrm{p}} = \sum_{\alpha=1}^{N_{\mathrm{s}}} \dot{\gamma}^{\alpha} \boldsymbol{P}_0^{\alpha}, \tag{3}$$

with the (non-symmetric) Schmid tensor in the reference configuration defined by $\boldsymbol{P}_0^{\alpha} = \vec{s}_0^{\alpha} \vec{n}_0^{\alpha}$. Here N_{s} denotes the total number of slip systems and $\dot{\gamma}^{\alpha}$ the slip rate of slip system α.

2.2 Constitutive relations

With the constitutive relations, the material behaviour of a crystal is described, which consists of an elastic and a plastic part.

2.2.1 Elasticity

It is assumed that the elastic response of a crystal is relatively small, such that the elastic part of the response may be described by a linear relation as

$$\boldsymbol{S}_{\mathrm{e}} = {}^4\mathbb{C} : \boldsymbol{E}_{\mathrm{e}}, \tag{4}$$

where ${}^4\mathbb{C}$ denotes the 4th-order elasticity tensor,

$$\boldsymbol{S}_{\mathrm{e}} = \boldsymbol{F}_{\mathrm{p}} \cdot \boldsymbol{S} \cdot \boldsymbol{F}_{\mathrm{p}}^{\mathrm{T}} \tag{5}$$

is the (symmetric) elastic 2nd Piola-Kirchhoff stress tensor. Furthermore,

$$\boldsymbol{E}_{\mathrm{e}} = \frac{1}{2}(\boldsymbol{C}_{\mathrm{e}} - \boldsymbol{I}) \tag{6}$$

is the (symmetric) elastic Green-Lagrange strain tensor with

$$\boldsymbol{C}_{\mathrm{e}} = \boldsymbol{F}_{\mathrm{e}}^{\mathrm{T}} \cdot \boldsymbol{F}_{\mathrm{e}} \tag{7}$$

the (symmetric) elastic right Cauchy-Green deformation tensor (more details can be found in [3, 4]).

2.2.2 Plasticity

The plastic deformation is governed by the resolved shear stress on each slip system

$$\tau^\alpha = \boldsymbol{S}_\mathrm{e} \cdot \boldsymbol{C}_\mathrm{e} : \boldsymbol{P}_0^\alpha. \tag{8}$$

The visco-plastic relation between shear rate and resolved shear stress on each slip system is described by a power law, reading

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left(\frac{|\tau^\alpha|}{s^\alpha}\right)^{\frac{1}{m}} \mathrm{sign}(\tau^\alpha), \tag{9}$$

where s^α is the shear resistance, $\dot{\gamma}_0$ denotes the reference slip rate, and m the strain-rate sensitivity. The latter two are (fixed) material parameters. In order to incorporate hardening in the model, an evolution equation for s^α is defined by

$$\dot{s}^\alpha = \sum_{\beta=1}^{N_\mathrm{s}} h^{\alpha\beta} |\dot{\gamma}^\beta|. \tag{10}$$

Notice that the slip resistance s^α may increase due to hardening of the slip system α itself (self hardening), as well as due to hardening by other systems β (latent hardening). Many different choices can be made for the hardening modulus $h^{\alpha\beta}$, including

$$h^{\alpha\beta} = h_0 \left(1 - \frac{s^\alpha}{s_\infty}\right)^a \left(q + (1-q)\delta^{\alpha\beta}\right). \tag{11}$$

Here h_0 denotes the reference hardening modulus, s_∞ the extreme shear resistance, q the latent-hardening ratio, a the shape factor. These are (fixed) material parameters as well. Furthermore, $\delta^{\alpha\beta}$ denotes the Kronecker delta. In Beaver, also other slip resistance evolution equations can be chosen.

3 Numerical implementation

3.1 Problem definition

The total deformation gradient $\boldsymbol{F}$ is given and known at the beginning of each new time step. Unless stated differently, all quantities are assumed to be defined at the next (unknown) time step t_{n+1} (so e.g. $\boldsymbol{F} \equiv \boldsymbol{F}(t_{\mathrm{n}+1})$). All other quantities are updated according the equations above. One may select the assembled slip rate column $\underset{\sim}{\dot{\gamma}}$ as the direct variable to solve by starting from eqs. (3), (1), (4), (8) to (9) and thus a closed-loop chain relation is established, reading

$$\begin{aligned} &\underset{\sim}{\dot{\gamma}} \rightarrow \boldsymbol{L}_\mathrm{p} = \boldsymbol{L}_\mathrm{p}(\underset{\sim}{\dot{\gamma}}) \rightarrow \boldsymbol{F}_\mathrm{p} = \boldsymbol{F}_\mathrm{p}(\underset{\sim}{\dot{\gamma}}) \rightarrow \boldsymbol{F}_\mathrm{e} = \boldsymbol{F}_\mathrm{e}(\underset{\sim}{\dot{\gamma}}) \\ &\quad \rightarrow \boldsymbol{C}_\mathrm{e} = \boldsymbol{C}_\mathrm{e}(\Delta\underset{\sim}{\gamma}) \rightarrow \boldsymbol{S}_\mathrm{e} = \boldsymbol{S}_\mathrm{e}(\underset{\sim}{\dot{\gamma}}) \rightarrow \underset{\sim}{\tau} = \underset{\sim}{\tau}(\underset{\sim}{\dot{\gamma}}) \rightarrow \underset{\sim}{\dot{\gamma}}, \end{aligned} \tag{12}$$

which yields a straightforward nonlinear equation $\underset{\sim}{r}(\underset{\sim}{\dot{\gamma}}) = \underset{\sim}{0}$ to be solved, where r denotes the residual and should vanish at the balance state.

Due to the discrete time increment in practice, $\boldsymbol{F}_\mathrm{p}$ cannot be calculated directly from the slip rate $\underset{\sim}{\dot{\gamma}}$. To solve this issue, $\boldsymbol{L}_\mathrm{p}$ is often assumed to be constant during an increment from time t_n to t_{n+1} such that

$$\boldsymbol{F}_\mathrm{p} = \tilde{\boldsymbol{F}}_{\mathrm{p_{inc}}} \cdot \boldsymbol{F}_\mathrm{p}(t_n), \tag{13}$$

with the increment factor given by

$$\tilde{\boldsymbol{F}}_{\mathrm{p_{inc}}} = (\det(\boldsymbol{F}_{\mathrm{p_{inc}}}))^{-1/3} \boldsymbol{F}_{\mathrm{p_{inc}}} = J_{\mathrm{p_{inc}}}^{-\frac{1}{3}} \boldsymbol{F}_{\mathrm{p_{inc}}}, \tag{14a}$$

$$\boldsymbol{F}_{\mathrm{p_{inc}}} = \exp\left(\int_{t_n}^{t_{n+1}} \boldsymbol{L}_\mathrm{p} dt\right) = \exp(\boldsymbol{M}) \approx \left(\boldsymbol{I} - \frac{1}{2}\boldsymbol{M}\right)^{-1} \cdot \left(\boldsymbol{I} + \frac{1}{2}\boldsymbol{M}\right), \tag{14b}$$

where an alternative variable to $\boldsymbol{L}_\mathrm{p}$, the deformation gradient increment tensor is defined as

$$\boldsymbol{M} = \Delta t \boldsymbol{L}_\mathrm{p} = \sum_{\alpha=1}^{N_\mathrm{s}} \Delta\gamma^\alpha \boldsymbol{P}_0^\alpha. \tag{15}$$

Here $J_{\mathrm{p_{inc}}}$ is the determinant for correcting the volume deviation from unity and the Padé approximation is employed in eq. (14b) for a small $\Delta t \boldsymbol{L}_\mathrm{p}$.

Clearly, the slip increment of each slip system $\Delta\gamma^\alpha$ is introduced as an extra variable above. In order to approximately correlate $\Delta\gamma^\alpha$ to $\dot{\gamma}^\alpha$, many differential formats are possible and a trapezoidal format is currently selected, reading

$$\Delta\gamma^\alpha = \frac{\Delta t}{2}\left(\dot{\gamma}^\alpha(t_n) + \dot{\gamma}^\alpha\right). \tag{16}$$

Among various simulations with different imposed strain rates, the order of magnitude of the slip rate $\dot{\gamma}^\alpha$ may vary a lot. To circumvent the numerical issues related to this observation (complicated convergence tolerances and numerical accurateness), the choice has been made to take $\Delta\underset{\sim}{\gamma}$ as a direct variable to solve. At present, a new closed-loop chain relation is formulated, by starting from eqs. (15), (13), (1), (4), (8), (9) to (16), reading

$$\begin{aligned} \Delta\underset{\sim}{\gamma} &\rightarrow \boldsymbol{M} = \boldsymbol{M}(\Delta\underset{\sim}{\gamma}) \rightarrow \boldsymbol{F}_\mathrm{p} = \boldsymbol{F}_\mathrm{p}(\Delta\underset{\sim}{\gamma}) \rightarrow \boldsymbol{F}_\mathrm{e} = \boldsymbol{F}_\mathrm{e}(\Delta\underset{\sim}{\gamma}) \rightarrow \boldsymbol{C}_\mathrm{e} = \boldsymbol{C}_\mathrm{e}(\Delta\underset{\sim}{\gamma}) \\ &\rightarrow \boldsymbol{S}_\mathrm{e} = \boldsymbol{S}_\mathrm{e}(\Delta\underset{\sim}{\gamma}) \rightarrow \underset{\sim}{\tau} = \underset{\sim}{\tau}(\Delta\underset{\sim}{\gamma}) \rightarrow \dot{\underset{\sim}{\gamma}} = \dot{\underset{\sim}{\gamma}}(\Delta\underset{\sim}{\gamma}) \rightarrow \Delta\underset{\sim}{\gamma}, \end{aligned} \tag{17}$$

which implies a nonlinear equation $\underset{\sim}{r}(\Delta\underset{\sim}{\gamma}) = \underset{\sim}{0}$ to be solved. Once $\Delta\underset{\sim}{\gamma}$ is computed, other quantities can be updated accordingly as well. The latter solution procedure is implemented in the Marc/Mentat subroutines.

3.2 Residual

Column $\underset{\sim}{r}$ consists of components r^α. Based on the choice of the solution procedure (eq. (17)), the residual $\underset{\sim}{r}$ is defined by substituting eq. (16) in eq. (9) as

$$r^\alpha = \Delta\gamma^\alpha - \frac{\Delta t}{2}\left(\dot{\gamma}^\alpha(t_n) + \dot{\gamma}_0\left(\frac{|\tau^\alpha|}{s^\alpha}\right)^{1/m}\mathrm{sign}(\tau^\alpha)\right). \tag{18}$$

3.3 Linearization

The Newton-Raphson iteration method is adopted to solve $\underset{\sim}{r}(\Delta\underset{\sim}{\gamma}) = \underset{\sim}{0}$, which is linearized as

$$\underset{\sim}{r}_i + \underline{K}_i(\Delta\underset{\sim}{\gamma}_{i+1} - \Delta\underset{\sim}{\gamma}_i) = \underset{\sim}{0}, \tag{19}$$

at the iteration step i (omitted in the below), where the system Jacobian matrix $\underline{K}$ is defined by

$$\underline{K} = \frac{\partial \underset{\sim}{r}}{\partial \Delta\underset{\sim}{\gamma}}, \tag{20}$$

with the elements $(\underline{K})^{\alpha\beta} = \frac{\partial r^\alpha}{\partial \Delta\gamma^\beta}$.

4 System Jacobian matrix

In order to get the explicit form of eq. (20), the variational form of the residual is considered, which indicated with the symbol δ:

$$\begin{aligned}
\delta r^\alpha &= \delta\Delta\gamma^\alpha - \frac{\Delta t}{2}\delta\left(\dot{\gamma}_0\left(\frac{|\tau^\alpha|}{s^\alpha}\right)^{1/m}\operatorname{sign}(\tau^\alpha)\right) \\
&= \delta\Delta\gamma^\alpha - b^\alpha\delta\left(\frac{|\tau^\alpha|}{s^\alpha}\right)\operatorname{sign}(\tau^\alpha) \\
&= \delta\Delta\gamma^\alpha - b^\alpha\left(\frac{1}{s^\alpha}\delta|\tau^\alpha| - \frac{|\tau^\alpha|}{(s^\alpha)^2}\delta s^\alpha\right)\operatorname{sign}(\tau^\alpha) \\
&= \delta\Delta\gamma^\alpha - b^\alpha(s^\alpha\delta\tau^\alpha - \tau^\alpha\delta s^\alpha), \qquad (21)
\end{aligned}$$

with

$$b^\alpha = \frac{\Delta t}{2}\frac{1}{(s^\alpha)^2}\frac{\dot{\gamma}_0}{m}\left(\frac{|\tau^\alpha|}{s^\alpha}\right)^{1/m-1}. \qquad (22)$$

Here, the relation $\operatorname{sign}(\tau^\alpha)|\tau^\alpha| = \tau^\alpha$ has been employed. Then substituting eq. (21) to (20) and applying the chain rule imply

$$\underline{K} = \underline{I} + \frac{\partial \underset{\sim}{r}}{\partial \underset{\sim}{\tau}}\frac{\partial \underset{\sim}{\tau}}{\partial \Delta\underset{\sim}{\gamma}} + \frac{\partial \underset{\sim}{r}}{\partial \underset{\sim}{s}}\frac{\partial \underset{\sim}{s}}{\partial \Delta\underset{\sim}{\gamma}}, \qquad (23)$$

with

$$(\underline{I})^{\alpha\beta} = \delta^{\alpha\beta} \qquad (24)$$

$$\left(\frac{\partial \underset{\sim}{r}}{\partial \underset{\sim}{\tau}}\right)^{\alpha\beta} = \frac{\partial r^\alpha}{\partial \tau^\beta} = -\delta^{\alpha\beta}b^\beta s^\beta \qquad (25)$$

$$\left(\frac{\partial \underset{\sim}{r}}{\partial \underset{\sim}{s}}\right)^{\alpha\beta} = \frac{\partial r^\alpha}{\partial s^\beta} = \delta^{\alpha\beta}b^\beta\tau^\beta. \qquad (26)$$

The elements $\left(\frac{\partial \underset{\sim}{\tau}}{\partial \Delta\underset{\sim}{\gamma}}\right)^{\alpha\beta}$ and $\left(\frac{\partial \underset{\sim}{s}}{\partial \Delta\underset{\sim}{\gamma}}\right)^{\alpha\beta}$ are still unknown but can be determined in a straightforward manner, as will be shown in the following subsections.

4.1 Slip resistance w.r.t slip increment

Equation (10) is rewritten in the variational and incremental form, reading

$$\delta s^\alpha = \delta\Delta s^\alpha = \sum_{\beta=1}^{N_s} h^{\alpha\beta}\operatorname{sign}(\Delta\gamma^\beta)\delta\Delta\gamma^\beta. \qquad (27)$$

Equation (27) immediately implies

$$\left(\frac{\partial \underset{\sim}{s}}{\partial \Delta\underset{\sim}{\gamma}}\right)^{\alpha\beta} = \frac{\partial s^\alpha}{\partial \Delta\gamma^\beta} = h^{\alpha\beta}\operatorname{sign}(\Delta\gamma^\beta). \qquad (28)$$

4.2 Resolved shear stress w.r.t slip increment

The closed-loop chain relation given by eq. (17), can be used to split $\left(\frac{\partial \underset{\sim}{\tau}}{\partial \Delta \underset{\sim}{\gamma}}\right)^{\alpha\beta}$ as

$$\left(\frac{\partial \underset{\sim}{\tau}}{\partial \Delta \underset{\sim}{\gamma}}\right)^{\alpha\beta} = \frac{\partial \tau^{\alpha}}{\partial \Delta \gamma^{\beta}} = \underbrace{\frac{\partial \tau^{\alpha}}{\partial \boldsymbol{S}_{\mathrm{e}}^{\mathrm{T}}}}_{4.2.6} : \underbrace{\frac{\partial \boldsymbol{S}_{\mathrm{e}}}{\partial \boldsymbol{C}_{\mathrm{e}}^{\mathrm{T}}}}_{4.2.5} : \underbrace{\frac{\partial \boldsymbol{C}_{\mathrm{e}}}{\partial \boldsymbol{F}_{\mathrm{e}}^{\mathrm{T}}}}_{4.2.4} : \underbrace{\frac{\partial \boldsymbol{F}_{\mathrm{e}}}{\partial \boldsymbol{F}_{\mathrm{p}}^{\mathrm{T}}}}_{4.2.3} : \underbrace{\frac{\partial \boldsymbol{F}_{\mathrm{p}}}{\partial \boldsymbol{M}^{\mathrm{T}}}}_{4.2.2} : \underbrace{\frac{\partial \boldsymbol{M}}{\partial \Delta \gamma^{\beta}}}_{4.2.1} . \tag{29}$$

Various intermediate terms will be separately derived (from right to left) using eqs. (15), (13), (1), (4) and (8). The number indicated below each derivative in eq. (29) refers to the corresponding section below, in which the derivative will be derived.

4.2.1 Deformation gradient increment w.r.t. slip increment

The variational form of eq. (15) can be expressed as

$$\delta \boldsymbol{M} = \delta \left(\sum_{\alpha=1}^{N_{\mathrm{s}}} \Delta\gamma^{\alpha} \boldsymbol{P}_0^{\alpha} \right) = \sum_{\alpha=1}^{N_{\mathrm{s}}} \boldsymbol{P}_0^{\alpha} \delta \Delta \gamma^{\alpha}, \tag{30}$$

which implies

$$\left(\frac{\partial \boldsymbol{M}}{\partial \Delta \underset{\sim}{\gamma}}\right)^{\beta} = \frac{\partial \boldsymbol{M}}{\partial \Delta \gamma^{\beta}} = \boldsymbol{P}_0^{\beta}. \tag{31}$$

4.2.2 Plastic deformation gradient w.r.t. deformation gradient increment

The variational form of eq. (13) can be expressed as

$$\begin{aligned} \delta \boldsymbol{F}_{\mathrm{p}} &= \delta \tilde{\boldsymbol{F}}_{\mathrm{p_{inc}}} \cdot \boldsymbol{F}_{\mathrm{p}}(t_n) \\ &= \left({}^4\mathbb{I}^{\mathrm{RT}} \cdot \boldsymbol{F}_{\mathrm{p}}^{\mathrm{T}}(t_n) \right) : {}^4\mathbb{I}^{\mathrm{RT}} : \delta \tilde{\boldsymbol{F}}_{\mathrm{p_{inc}}}. \end{aligned} \tag{32}$$

Next, the variational form of eq. (14a) can be expressed as

$$\begin{aligned} \delta \tilde{\boldsymbol{F}}_{\mathrm{p_{inc}}} &= \delta \left(J_{\mathrm{p_{inc}}}^{-1/3} \right) \boldsymbol{F}_{\mathrm{p_{inc}}} + J_{\mathrm{p_{inc}}}^{-1/3} \delta \boldsymbol{F}_{\mathrm{p_{inc}}} \\ &= -\frac{1}{3} J_{\mathrm{p_{inc}}}^{-4/3} \boldsymbol{F}_{\mathrm{p_{inc}}} \delta J_{\mathrm{p_{inc}}} + J_{\mathrm{p_{inc}}}^{-1/3} \delta \boldsymbol{F}_{\mathrm{p_{inc}}}, \end{aligned} \tag{33}$$

with

$$\begin{aligned} \delta J_{\mathrm{p_{inc}}} &= \det(\boldsymbol{F}_{\mathrm{p_{inc}}} + \delta \boldsymbol{F}_{\mathrm{p_{inc}}}) - J_{\mathrm{p_{inc}}} \\ &= \det\left((\boldsymbol{I} + \delta \boldsymbol{F}_{\mathrm{p_{inc}}} \cdot \boldsymbol{F}_{\mathrm{p_{inc}}}^{-1}) - 1 \right) J_{\mathrm{p_{inc}}} \\ &\approx \operatorname{tr}(\delta \boldsymbol{F}_{\mathrm{p_{inc}}} \cdot \boldsymbol{F}_{\mathrm{p_{inc}}}^{-1}) J_{\mathrm{p_{inc}}} \\ &= J_{\mathrm{p_{inc}}} \boldsymbol{F}_{\mathrm{p_{inc}}}^{-1} : \delta \boldsymbol{F}_{\mathrm{p_{inc}}}, \end{aligned} \tag{34}$$

where the relations $\det(\boldsymbol{A}\cdot\boldsymbol{B}) = \det(\boldsymbol{A})\det(\boldsymbol{B})$, $\det(\boldsymbol{I}+\delta\boldsymbol{A}) \approx 1 + \operatorname{tr}(\delta\boldsymbol{A})$ and $\operatorname{tr}(\boldsymbol{A}\cdot\boldsymbol{B}) = \boldsymbol{A}:\boldsymbol{B}$ (also see Appendix) have been employed. Substituting eq. (34) to (33) yields

$$\begin{aligned} \delta \tilde{\boldsymbol{F}}_{\mathrm{p_{inc}}} &= -\frac{1}{3} J_{\mathrm{p_{inc}}}^{-1/3} \boldsymbol{F}_{\mathrm{p_{inc}}} \boldsymbol{F}_{\mathrm{p_{inc}}}^{-1} : \delta \boldsymbol{F}_{\mathrm{p_{inc}}} + J_{\mathrm{p_{inc}}}^{-1/3}\, {}^4\mathbb{I} : \delta \boldsymbol{F}_{\mathrm{p_{inc}}} \\ &= J_{\mathrm{p_{inc}}}^{-1/3} \left({}^4\mathbb{I} - \frac{1}{3} \boldsymbol{F}_{\mathrm{p_{inc}}} \boldsymbol{F}_{\mathrm{p_{inc}}}^{-1} \right) : \delta \boldsymbol{F}_{\mathrm{p_{inc}}}. \end{aligned} \tag{35}$$

Furthermore, the variational form of eq. (14b) can be expressed as

$$\delta \boldsymbol{F}_{\text{Pinc}} = \delta \left(\boldsymbol{I} - \frac{1}{2}\boldsymbol{M} \right)^{-1} \cdot \left(\boldsymbol{I} + \frac{1}{2}\boldsymbol{M} \right) + \left(\boldsymbol{I} - \frac{1}{2}\boldsymbol{M} \right)^{-1} \cdot \delta \left(\boldsymbol{I} + \frac{1}{2}\boldsymbol{M} \right), \tag{36}$$

with

$$\delta \left(\boldsymbol{I} + \frac{1}{2}\boldsymbol{M} \right) = \frac{1}{2}\delta \boldsymbol{M}, \tag{37a}$$

$$\delta \left(\boldsymbol{I} - \frac{1}{2}\boldsymbol{M} \right)^{-1} = \frac{1}{2} \left(\boldsymbol{I} - \frac{1}{2}\boldsymbol{M} \right)^{-1} \cdot \delta \boldsymbol{M} \cdot \left(\boldsymbol{I} - \frac{1}{2}\boldsymbol{M} \right)^{-1}. \tag{37b}$$

Substituting eqs. (14b) and (37) to (36) gives

$$\begin{aligned}
\delta \boldsymbol{F}_{\text{Pinc}} &= \frac{1}{2} \left(\boldsymbol{I} - \frac{1}{2}\boldsymbol{M} \right)^{-1} \cdot \delta \boldsymbol{M} \cdot \left(\boldsymbol{I} - \frac{1}{2}\boldsymbol{M} \right)^{-1} \cdot \left(\boldsymbol{I} + \frac{1}{2}\boldsymbol{M} \right) + \left(\boldsymbol{I} - \frac{1}{2}\boldsymbol{M} \right)^{-1} \cdot \frac{1}{2}\delta \boldsymbol{M} \\
&\approx \frac{1}{2} \left(\boldsymbol{I} - \frac{1}{2}\boldsymbol{M} \right)^{-1} \cdot \delta \boldsymbol{M} \cdot (\boldsymbol{F}_{\text{Pinc}} + \boldsymbol{I}) \\
&= \frac{1}{2} \left(\boldsymbol{I} - \frac{1}{2}\boldsymbol{M} \right)^{-1} \cdot \left({}^4\mathbb{I}^{\text{RT}} \cdot \left(\boldsymbol{F}^{\text{T}}_{\text{Pinc}} + \boldsymbol{I} \right) \right) : {}^4\mathbb{I}^{\text{RT}} : \delta \boldsymbol{M},
\end{aligned} \tag{38}$$

where the relations ${}^4\mathbb{I}^{\text{RT}} : \boldsymbol{A} = \boldsymbol{A}^{\text{T}}$ and ${}^4\mathbb{A} : (\boldsymbol{B} \cdot \boldsymbol{C}) = ({}^4\mathbb{A} \cdot \boldsymbol{B}) : \boldsymbol{C}$ (also see Appendix) have been employed. Now collecting eqs. (32), (35) and (38) implies

$$\frac{\partial \boldsymbol{F}_{\text{p}}}{\partial \boldsymbol{M}^{\text{T}}} = \frac{\partial \boldsymbol{F}_{\text{p}}}{\partial \tilde{\boldsymbol{F}}^{\text{T}}_{\text{Pinc}}} : \frac{\partial \tilde{\boldsymbol{F}}_{\text{Pinc}}}{\partial \boldsymbol{F}^{\text{T}}_{\text{Pinc}}} : \frac{\partial \boldsymbol{F}_{\text{Pinc}}}{\partial \boldsymbol{M}^{\text{T}}} \tag{39}$$

with

$$\frac{\partial \boldsymbol{F}_{\text{p}}}{\partial \tilde{\boldsymbol{F}}^{\text{T}}_{\text{Pinc}}} = \left({}^4\mathbb{I}^{\text{RT}} \cdot \boldsymbol{F}^{\text{T}}_{\text{p}}(t_n) \right) : {}^4\mathbb{I}^{\text{RT}}, \tag{40a}$$

$$\frac{\partial \tilde{\boldsymbol{F}}_{\text{Pinc}}}{\partial \boldsymbol{F}^{\text{T}}_{\text{Pinc}}} = J^{-1/3}_{\text{Pinc}} \left({}^4\mathbb{I} - \frac{1}{3}\boldsymbol{F}_{\text{Pinc}} \boldsymbol{F}^{-1}_{\text{Pinc}} \right), \tag{40b}$$

$$\frac{\partial \boldsymbol{F}_{\text{Pinc}}}{\partial \boldsymbol{M}^{\text{T}}} = \frac{1}{2} \left(\boldsymbol{I} - \frac{1}{2}\boldsymbol{M} \right)^{-1} \cdot \left({}^4\mathbb{I}^{\text{RT}} \cdot \left(\boldsymbol{F}^{\text{T}}_{\text{Pinc}} + \boldsymbol{I} \right) \right) : {}^4\mathbb{I}^{\text{RT}}. \tag{40c}$$

4.2.3 Elastic deformation gradient w.r.t. plastic deformation gradient

The variational form of eq. (1) can be expressed as

$$\begin{aligned}
\delta \boldsymbol{F}_{\text{e}} &= \delta(\boldsymbol{F} \cdot \boldsymbol{F}^{-1}_{\text{p}}) \\
&= \delta \boldsymbol{F} \cdot \boldsymbol{F}^{-1}_{\text{p}} + \boldsymbol{F} \cdot \delta \boldsymbol{F}^{-1}_{\text{p}} \\
&= ({}^4\mathbb{I}^{\text{RT}} \cdot \boldsymbol{F}^{-\text{T}}_{\text{p}}) : \delta \boldsymbol{F}^{\text{T}} + \boldsymbol{F} \cdot \delta \boldsymbol{F}^{-1}_{\text{p}} \\
&= ({}^4\mathbb{I}^{\text{RT}} \cdot \boldsymbol{F}^{-\text{T}}_{\text{p}}) : {}^4\mathbb{I}^{\text{RT}} : \delta \boldsymbol{F} - \boldsymbol{F} \cdot \boldsymbol{F}^{-1}_{\text{p}} \cdot \delta \boldsymbol{F}_{\text{p}} \cdot \boldsymbol{F}^{-1}_{\text{p}} \\
&= ({}^4\mathbb{I}^{\text{RT}} \cdot \boldsymbol{F}^{-\text{T}}_{\text{p}}) : {}^4\mathbb{I}^{\text{RT}} : \delta \boldsymbol{F} - \boldsymbol{F}_{\text{e}} \cdot ({}^4\mathbb{I}^{\text{RT}} \cdot \boldsymbol{F}^{-\text{T}}_{\text{p}}) : {}^4\mathbb{I}^{\text{RT}} : \delta \boldsymbol{F}_{\text{p}},
\end{aligned} \tag{41}$$

where the relations ${}^4\mathbb{I}^{\text{RT}} : \boldsymbol{A} = \boldsymbol{A}^{\text{T}}$, ${}^4\mathbb{A} : (\boldsymbol{B} \cdot \boldsymbol{C}) = ({}^4\mathbb{A} \cdot \boldsymbol{B}) : \boldsymbol{C}$ and $\delta \boldsymbol{I} = \boldsymbol{A} \cdot \delta \boldsymbol{A}^{-1} + \delta \boldsymbol{A} \cdot \boldsymbol{A}^{-1} = \boldsymbol{0}$ (also see Appendix) have been employed. The expression is simplified as follows

$$\delta \boldsymbol{F}_{\text{e}} = {}^4\mathbb{G} : \delta \boldsymbol{F} - \boldsymbol{F}_{\text{e}} \cdot {}^4\mathbb{G} : \delta \boldsymbol{F}_{\text{p}}, \tag{42}$$

with

$$ {}^4\mathbb{G} = ({}^4\mathbb{I}^{\mathrm{RT}} \cdot \boldsymbol{F}_{\mathrm{p}}^{-\mathrm{T}}) : {}^4\mathbb{I}^{\mathrm{RT}} \tag{43} $$

Since $\boldsymbol{F}$ is prescribed, equation (42) immediately implies

$$ \boxed{\frac{\partial \boldsymbol{F}_{\mathrm{e}}}{\partial \boldsymbol{F}_{\mathrm{p}}^{\mathrm{T}}} = -\boldsymbol{F}_{\mathrm{e}} \cdot {}^4\mathbb{G}.} \tag{44} $$

4.2.4 Elastic strain w.r.t. elastic deformation gradient

The variational form of eq. (7) can be expressed as

$$ \begin{aligned} \delta \boldsymbol{C}_{\mathrm{e}} &= \delta(\boldsymbol{F}_{\mathrm{e}}^{\mathrm{T}} \cdot \boldsymbol{F}_{\mathrm{e}}) \\ &= \delta \boldsymbol{F}_{\mathrm{e}}^{\mathrm{T}} \cdot \boldsymbol{F}_{\mathrm{e}} + \boldsymbol{F}_{\mathrm{e}}^{\mathrm{T}} \cdot \delta \boldsymbol{F}_{\mathrm{e}} \\ &= (2{}^4\mathbb{I}^{\mathrm{S}} \cdot \boldsymbol{F}_{\mathrm{e}}^{\mathrm{T}}) : \delta \boldsymbol{F}_{\mathrm{e}}, \end{aligned} \tag{45} $$

where the relations $\boldsymbol{A} \cdot \boldsymbol{B} + \boldsymbol{B}^{\mathrm{T}} \cdot \boldsymbol{A}^{\mathrm{T}} = 2{}^4\mathbb{I}^{\mathrm{S}} : (\boldsymbol{A} \cdot \boldsymbol{B})$ and ${}^4\mathbb{A} : (\boldsymbol{B} \cdot \boldsymbol{C}) = ({}^4\mathbb{A} \cdot \boldsymbol{B}) : \boldsymbol{C}$ have been employed. This implies

$$ \boxed{\frac{\partial \boldsymbol{C}_{\mathrm{e}}}{\partial \boldsymbol{F}_{\mathrm{e}}^{\mathrm{T}}} = 2{}^4\mathbb{I}^{\mathrm{S}} \cdot \boldsymbol{F}_{\mathrm{e}}^{\mathrm{T}}.} \tag{46} $$

4.2.5 Elastic stress w.r.t. elastic strain

The variational form of eq. (4) and eq. (6) can be expressed as

$$ \delta \boldsymbol{S}_{\mathrm{e}} = \frac{1}{2}{}^4\mathbb{C} : \delta \boldsymbol{C}_{\mathrm{e}}, \tag{47} $$

which directly implies

$$ \boxed{\frac{\partial \boldsymbol{S}_{\mathrm{e}}}{\partial \boldsymbol{C}_{\mathrm{e}}^{\mathrm{T}}} = \frac{1}{2}{}^4\mathbb{C}} \tag{48} $$

4.2.6 Resolved shear stress w.r.t. elastic stress

The variational form of eq. (8) can be expressed as

$$ \begin{aligned} \delta \tau^{\alpha} &= (\delta \boldsymbol{S}_{\mathrm{e}} \cdot \boldsymbol{C}_{\mathrm{e}} + \boldsymbol{S}_{\mathrm{e}} \cdot \delta \boldsymbol{C}_{\mathrm{e}}) : \boldsymbol{P}_0^{\alpha} \\ &= \boldsymbol{P}_0^{\alpha} : (\delta \boldsymbol{S}_{\mathrm{e}} \cdot \boldsymbol{C}_{\mathrm{e}} + \boldsymbol{S}_{\mathrm{e}} \cdot \delta \boldsymbol{C}_{\mathrm{e}}) \\ &= \boldsymbol{P}_0^{\alpha} : \left({}^4\mathbb{I}^{\mathrm{RT}} : (\boldsymbol{C}_{\mathrm{e}}^{\mathrm{T}} \cdot \delta \boldsymbol{S}_{\mathrm{e}}^{\mathrm{T}}) + 2\boldsymbol{S}_{\mathrm{e}} \cdot {}^4\mathbb{S} : \delta \boldsymbol{S}_{\mathrm{e}}\right) \\ &= \boldsymbol{P}_0^{\alpha} : \left({}^4\mathbb{I}^{\mathrm{RT}} \cdot \boldsymbol{C}_{\mathrm{e}} + 2\boldsymbol{S}_{\mathrm{e}} \cdot {}^4\mathbb{S}\right) : \delta \boldsymbol{S}_{\mathrm{e}}, \end{aligned} \tag{49} $$

with the 4th-order compliance tensor defined as

$$
{}^4\mathbb{S} = \frac{\partial \boldsymbol{E}_\mathrm{e}}{\partial \boldsymbol{S}_\mathrm{e}^\mathrm{T}} = \frac{1}{2}\frac{\partial \boldsymbol{C}_\mathrm{e}}{\partial \boldsymbol{S}_\mathrm{e}^\mathrm{T}}. \tag{50}
$$

Here the relations ${}^4\mathbb{I}^\mathrm{RT} : \boldsymbol{A} = \boldsymbol{A}^\mathrm{T}$ and ${}^4\mathbb{A} : (\boldsymbol{B}\cdot\boldsymbol{C}) = ({}^4\mathbb{A}\cdot\boldsymbol{B}) : \boldsymbol{C}$ (also see Appendix) have been employed. Since $\delta\boldsymbol{S}_\mathrm{e}$ is symmetric, the derivative with respect to $\boldsymbol{S}_\mathrm{e}$ is imposed to be symmetric by post-multiplying with ${}^4\mathbb{I}^\mathrm{S}$. Thus, equation (49) implies

$$
\boxed{\left(\frac{\partial \underset{\sim}{\tau}}{\partial \boldsymbol{S}_\mathrm{e}^\mathrm{T}}\right)^\alpha = \frac{\partial \tau^\alpha}{\partial \boldsymbol{S}_\mathrm{e}^\mathrm{T}} = \frac{\partial \tau^\alpha}{\partial \boldsymbol{S}_\mathrm{e}} = \boldsymbol{P}_0^\alpha : \left({}^4\mathbb{I}^\mathrm{RT}\cdot\boldsymbol{C}_\mathrm{e} + 2\boldsymbol{S}_\mathrm{e}\cdot{}^4\mathbb{S}\right) : {}^4\mathbb{I}^\mathrm{S}.} \tag{51}
$$

Applying eqs. (31), (39), (44), (46), (48) and (51) to specify eq. (29). Then, substituting eqs. (28) and (29) to (23) finally results in an explicit form of $\underline{K}$ such that eq. (19) becomes solvable by following the Newton-Raphson iterative procedure.

5 Material tangent stiffness

After the converged solution of eq. (19) is obtained, one can readily extract the material tangent stiffness tensor required in Marc/Mentat (the geometrical tangent stiffness tensor is automatically taken into account), which in `hypela2.f` is defined by

$$
{}^4\mathbb{K} = \frac{\partial \boldsymbol{S}}{\partial \boldsymbol{E}}. \tag{52}
$$

The explicit form of $\frac{\partial \boldsymbol{S}}{\partial \boldsymbol{E}}$ is obtained by splitting eq. (52), reading

$$
\boxed{{}^4\mathbb{K} = \underbrace{\frac{\partial \boldsymbol{S}}{\partial \boldsymbol{F}^\mathrm{T}}}_{5.2} : \underbrace{\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{E}}}_{5.1}.} \tag{53}
$$

Two intermediate terms $\frac{\partial \boldsymbol{S}}{\partial \boldsymbol{F}^\mathrm{T}}$ and $\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{E}}$ can be separately derived in the following.

5.1 Deformation gradient w.r.t strain

$\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{E}}$ is rewritten as

$$
\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{E}} = \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{U}} : \frac{\partial \boldsymbol{U}}{\partial \boldsymbol{C}} : \frac{\partial \boldsymbol{C}}{\partial \boldsymbol{E}}, \tag{54}
$$

with $\boldsymbol{U} = \boldsymbol{R}^{-1}\cdot\boldsymbol{F}$, $\boldsymbol{C} = \boldsymbol{F}^\mathrm{T}\cdot\boldsymbol{F}$ and $\boldsymbol{E} = \frac{1}{2}(\boldsymbol{C}-\boldsymbol{I})$. Here $\boldsymbol{U}$ denotes the (symmetric) right stretch tensor, $\boldsymbol{C}$ the (symmetric) Cauchy-Green deformation tensor, $\boldsymbol{E}$ the (symmetric) Green-Lagrange strain tensor and $\boldsymbol{R}$ the rotation tensor, which can be regarded as constant during each time step (more details can be found in [3]).

The variational forms of $\boldsymbol{E} = \frac{1}{2}(\boldsymbol{C}-\boldsymbol{I})$ and $\boldsymbol{F} = \boldsymbol{R}\cdot\boldsymbol{U}$ can be individually expressed as

$$
\delta\boldsymbol{E} = \frac{1}{2}\delta\boldsymbol{C}, \tag{55a}
$$

$$
\delta\boldsymbol{F} = \boldsymbol{R}\cdot\delta\boldsymbol{U}, \tag{55b}
$$

which immediately implies

$$\frac{\partial \boldsymbol{C}}{\partial \boldsymbol{E}} = 2^4\mathbb{I}^{\mathrm{S}}, \tag{56a}$$

$$\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{U}} = \boldsymbol{R} \cdot {}^4\mathbb{I}^{\mathrm{S}}. \tag{56b}$$

Here the relation ${}^4\mathbb{I}^{\mathrm{S}} : \boldsymbol{A} = \boldsymbol{A} : {}^4\mathbb{I}^{\mathrm{S}} = \boldsymbol{A}^{\mathrm{S}}$ has been employed.

$\frac{\partial \boldsymbol{U}}{\partial \boldsymbol{C}}$ is relatively complicated to identify (detailed procedure can be found in [5]) and here given by

$$\frac{\partial \boldsymbol{U}}{\partial \boldsymbol{C}} = \sum_{m=1}^{3}\sum_{n=1}^{3} \frac{1}{\lambda_m + \lambda_n} \vec{n}_m \vec{n}_n \vec{n}_n \vec{n}_m, \tag{57}$$

with $\boldsymbol{U}$ in its spectral form $\boldsymbol{U} = \sum_{m=1}^{3} \lambda_m \vec{n}_m \vec{n}_m$, where λ_m denotes the principal strain component and $\vec{n}_m$ the principal basis vector.

Now collecting eqs. (54), (56) and (57) gives

$$\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{E}} = \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{U}} : \frac{\partial \boldsymbol{U}}{\partial \boldsymbol{C}} : \frac{\partial \boldsymbol{C}}{\partial \boldsymbol{E}}, \tag{58}$$

with

$$\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{U}} = \boldsymbol{R} \cdot {}^4\mathbb{I}^{\mathrm{S}}, \tag{59a}$$

$$\frac{\partial \boldsymbol{U}}{\partial \boldsymbol{C}} = \sum_{m=1}^{3}\sum_{n=1}^{3} \frac{1}{\lambda_m + \lambda_n} \vec{n}_m \vec{n}_n \vec{n}_n \vec{n}_m, \tag{59b}$$

$$\frac{\partial \boldsymbol{C}}{\partial \boldsymbol{E}} = 2^4\mathbb{I}^{\mathrm{S}}. \tag{59c}$$

5.2 Stress w.r.t deformation gradient

From (5), it can be derived that the relation for the 2nd Piola-Kichhoff stress tensor is expressed as

$$\boldsymbol{S} = \boldsymbol{F}_{\mathrm{p}}^{-1} \cdot \boldsymbol{S}_{\mathrm{e}} \cdot \boldsymbol{F}_{\mathrm{p}}^{-\mathrm{T}}. \tag{60}$$

As can be seen, $\boldsymbol{S}$ is dependent on both $\boldsymbol{S}_{\mathrm{e}}$ and $\boldsymbol{F}_{\mathrm{p}}$. Therefore, the derivative $\frac{\partial \boldsymbol{S}}{\partial \boldsymbol{F}^{\mathrm{T}}}$ is split as follows

$$\frac{\partial \boldsymbol{S}}{\partial \boldsymbol{F}^{\mathrm{T}}} = \underbrace{\frac{\partial \boldsymbol{S}}{\partial \boldsymbol{S}_{\mathrm{e}}^{\mathrm{T}}}}_{5.2.1} : \underbrace{\frac{\partial \boldsymbol{S}_{\mathrm{e}}}{\partial \boldsymbol{F}^{\mathrm{T}}}}_{5.2.3} + \underbrace{\frac{\partial \boldsymbol{S}}{\partial \boldsymbol{F}_{\mathrm{p}}^{\mathrm{T}}}}_{5.2.1} : \underbrace{\frac{\partial \boldsymbol{F}_{\mathrm{p}}}{\partial \boldsymbol{F}^{\mathrm{T}}}}_{5.2.2}. \tag{61}$$

The terms will be derived in the following sections.

5.2.1 Variational form of stress

In order to obtain $\frac{\partial \boldsymbol{S}}{\partial \boldsymbol{S}_{\mathrm{e}}^{\mathrm{T}}}$ and $\frac{\partial \boldsymbol{S}}{\partial \boldsymbol{F}_{\mathrm{p}}^{\mathrm{T}}}$, the variational form of $\boldsymbol{S}$ is expressed as

$$\begin{aligned} \delta\boldsymbol{S} &= \delta(\boldsymbol{F}_{\mathrm{p}}^{-1} \cdot \boldsymbol{S}_{\mathrm{e}} \cdot \boldsymbol{F}_{\mathrm{p}}^{-\mathrm{T}}) \\ &= \delta\boldsymbol{F}_{\mathrm{p}}^{-1} \cdot \boldsymbol{S}_{\mathrm{e}} \cdot \boldsymbol{F}_{\mathrm{p}}^{-\mathrm{T}} + \boldsymbol{F}_{\mathrm{p}}^{-1} \cdot \delta\boldsymbol{S}_{\mathrm{e}} \cdot \boldsymbol{F}_{\mathrm{p}}^{-\mathrm{T}} + \boldsymbol{F}_{\mathrm{p}}^{-1} \cdot \boldsymbol{S}_{\mathrm{e}} \cdot \delta\boldsymbol{F}_{\mathrm{p}}^{-\mathrm{T}}. \end{aligned} \tag{62}$$

The derivative $\frac{\partial \boldsymbol{S}}{\partial \boldsymbol{S}_\mathrm{e}^\mathrm{T}}$ can be obtained from the second term as follows

$$\boldsymbol{F}_\mathrm{p}^{-1} \cdot \delta \boldsymbol{S}_\mathrm{e} \cdot \boldsymbol{F}_\mathrm{p}^{-\mathrm{T}} = (\boldsymbol{F}_\mathrm{p}^{-1} \cdot {}^4\mathbb{I}^\mathrm{RT} \cdot \boldsymbol{F}_\mathrm{p}^{-1}) : \delta \boldsymbol{S}_\mathrm{e}, \tag{63}$$

where the relations ${}^4\mathbb{I}^\mathrm{RT} : \boldsymbol{A} = \boldsymbol{A}^\mathrm{T}$ and ${}^4\mathbb{A} : (\boldsymbol{B} \cdot \boldsymbol{C}) = ({}^4\mathbb{A} \cdot \boldsymbol{B}) : \boldsymbol{C}$ (also see Appendix) have been employed. Therefore, it holds that

$$\boxed{\frac{\partial \boldsymbol{S}}{\partial \boldsymbol{S}_\mathrm{e}^\mathrm{T}} = \boldsymbol{F}_\mathrm{p}^{-1} \cdot {}^4\mathbb{I}^\mathrm{RT} \cdot \boldsymbol{F}_\mathrm{p}^{-1}.} \tag{64}$$

The remaining two terms of eq. (62) are rewritten as follows

$$\begin{aligned} \delta \boldsymbol{F}_\mathrm{p}^{-1} \cdot \boldsymbol{S}_\mathrm{e} \cdot \boldsymbol{F}_\mathrm{p}^{-\mathrm{T}} &+ \boldsymbol{F}_\mathrm{p}^{-1} \cdot \boldsymbol{S}_\mathrm{e} \cdot \delta \boldsymbol{F}_\mathrm{p}^{-\mathrm{T}} \\ &= ({}^4\mathbb{I}^\mathrm{RT} \cdot \boldsymbol{F}_\mathrm{p}^{-1} \cdot \boldsymbol{S}_\mathrm{e}) : \delta \boldsymbol{F}_\mathrm{p}^{-\mathrm{T}} + (\boldsymbol{F}_\mathrm{p}^{-1} \cdot \boldsymbol{S}_\mathrm{e} \cdot {}^4\mathbb{I}) : \delta \boldsymbol{F}_\mathrm{p}^{-\mathrm{T}} \\ &= \left({}^4\mathbb{I}^\mathrm{RT} \cdot \boldsymbol{F}_\mathrm{p}^{-1} \cdot \boldsymbol{S}_\mathrm{e} + \boldsymbol{F}_\mathrm{p}^{-1} \cdot \boldsymbol{S}_\mathrm{e} \cdot {}^4\mathbb{I}\right) : \delta \boldsymbol{F}_\mathrm{p}^{-\mathrm{T}}, \end{aligned} \tag{65}$$

with

$$\begin{aligned} \delta \boldsymbol{F}_\mathrm{p}^{-\mathrm{T}} &= -\boldsymbol{F}_\mathrm{p}^{-\mathrm{T}} \cdot \delta \boldsymbol{F}_\mathrm{p}^\mathrm{T} \cdot \boldsymbol{F}_\mathrm{p}^{-\mathrm{T}} \\ &= -\boldsymbol{F}_\mathrm{p}^{-\mathrm{T}} \cdot \left({}^4\mathbb{I}^\mathrm{RT} \cdot \boldsymbol{F}_\mathrm{p}^{-1}\right) : \delta \boldsymbol{F}_\mathrm{p}, \end{aligned} \tag{66}$$

where the relations ${}^4\mathbb{I}^\mathrm{RT} : \boldsymbol{A} = \boldsymbol{A}^\mathrm{T}$, ${}^4\mathbb{A} : (\boldsymbol{B} \cdot \boldsymbol{C}) = ({}^4\mathbb{A} \cdot \boldsymbol{B}) : \boldsymbol{C}$, $\delta \boldsymbol{I} = \boldsymbol{A} \cdot \delta \boldsymbol{A}^{-1} + \delta \boldsymbol{A} \cdot \boldsymbol{A}^{-1} = \boldsymbol{0}$ and ${}^4\mathbb{I} : \boldsymbol{A} = \boldsymbol{A} : {}^4\mathbb{I} = \boldsymbol{A}$ (also see Appendix) have been employed. Substitution of eq. (66) into eq. (65) gives

$$\boxed{\frac{\partial \boldsymbol{S}}{\partial \boldsymbol{F}_\mathrm{p}^\mathrm{T}} = -\left({}^4\mathbb{I}^\mathrm{RT} \cdot \boldsymbol{F}_\mathrm{p}^{-1} \cdot \boldsymbol{S}_\mathrm{e} + \boldsymbol{F}_\mathrm{p}^{-1} \cdot \boldsymbol{S}_\mathrm{e} \cdot {}^4\mathbb{I}\right) : \left(\boldsymbol{F}_\mathrm{p}^{-\mathrm{T}} \cdot {}^4\mathbb{I}^\mathrm{RT} \cdot \boldsymbol{F}_\mathrm{p}^{-1}\right).} \tag{67}$$

5.2.2 Plastic deformation gradient w.r.t deformation gradient

Based on the chain rule, $\frac{\partial \boldsymbol{F}_\mathrm{p}}{\partial \boldsymbol{F}^\mathrm{T}}$ can be computed as

$$\boxed{\frac{\partial \boldsymbol{F}_\mathrm{p}}{\partial \boldsymbol{F}^\mathrm{T}} = \underbrace{\frac{\partial \boldsymbol{F}_\mathrm{p}}{\partial \boldsymbol{S}_\mathrm{e}^\mathrm{T}}}_{5.2.4} : \underbrace{\frac{\partial \boldsymbol{S}_\mathrm{e}}{\partial \boldsymbol{F}^\mathrm{T}}}_{5.2.3}.} \tag{68}$$

The individual terms will be derived in the upcoming sections.

5.2.3 Elastic stress w.r.t deformation gradient

In order to relate $\boldsymbol{S}_\mathrm{e}$ to $\boldsymbol{F}$, first eq. (42) is substituted in $\delta \boldsymbol{S}_\mathrm{e} = \frac{\partial \boldsymbol{S}_\mathrm{e}}{\partial \boldsymbol{F}_\mathrm{e}^\mathrm{T}} : \delta \boldsymbol{F}_\mathrm{e}$. This results in the following expression

$$\begin{aligned} \delta \boldsymbol{S}_\mathrm{e} &= \frac{\partial \boldsymbol{S}_\mathrm{e}}{\partial \boldsymbol{F}_\mathrm{e}^\mathrm{T}} : \left({}^4\mathbb{G} : \delta \boldsymbol{F} - \boldsymbol{F}_\mathrm{e} \cdot {}^4\mathbb{G} : \delta \boldsymbol{F}_\mathrm{p}\right) \\ &= \frac{\partial \boldsymbol{S}_\mathrm{e}}{\partial \boldsymbol{F}_\mathrm{e}^\mathrm{T}} : \left({}^4\mathbb{G} : \delta \boldsymbol{F} - \boldsymbol{F}_\mathrm{e} \cdot {}^4\mathbb{G} : \frac{\partial \boldsymbol{F}_\mathrm{p}}{\partial \boldsymbol{S}_\mathrm{e}} : \delta \boldsymbol{S}_\mathrm{e}\right). \end{aligned} \tag{69}$$

Recall that ${}^4\mathbb{G} = ({}^4\mathbb{I}^{\mathrm{RT}} \cdot \boldsymbol{F}_{\mathrm{p}}^{-\mathrm{T}}) : {}^4\mathbb{I}^{\mathrm{RT}}$ was adopted in order to obtain a more compact notation. Next, rearranging eq. (69) gives

$$\left({}^4\mathbb{I}^{\mathrm{S}} + \frac{\partial \boldsymbol{S}_{\mathrm{e}}}{\partial \boldsymbol{F}_{\mathrm{e}}^{\mathrm{T}}} : \left(\boldsymbol{F}_{\mathrm{e}} \cdot {}^4\mathbb{G} \right) : \frac{\partial \boldsymbol{F}_{\mathrm{p}}}{\partial \boldsymbol{S}_{\mathrm{e}}} \right) : \delta \boldsymbol{S}_{\mathrm{e}} = \frac{\partial \boldsymbol{S}_{\mathrm{e}}}{\partial \boldsymbol{F}_{\mathrm{e}}^{\mathrm{T}}} : {}^4\mathbb{G} : \delta \boldsymbol{F}, \tag{70}$$

where the relation ${}^4\mathbb{I}^{\mathrm{S}} : \boldsymbol{A} = \boldsymbol{A} : {}^4\mathbb{I}^{\mathrm{S}} = \boldsymbol{A}^{\mathrm{S}}$ has been employed. One can directly identify $\frac{\partial \boldsymbol{S}_{\mathrm{e}}}{\partial \boldsymbol{F}^{\mathrm{T}}}$ from eq. (70) as

$$\frac{\partial \boldsymbol{S}_{\mathrm{e}}}{\partial \boldsymbol{F}^{\mathrm{T}}} = {}^4\mathbb{N}_1^{-1} : {}^4\mathbb{N}_2, \tag{71}$$

with

$${}^4\mathbb{N}_1 = {}^4\mathbb{I}^{\mathrm{S}} + \frac{\partial \boldsymbol{S}_{\mathrm{e}}}{\partial \boldsymbol{F}_{\mathrm{e}}^{\mathrm{T}}} : \left(\boldsymbol{F}_{\mathrm{e}} \cdot {}^4\mathbb{G} \right) : \frac{\partial \boldsymbol{F}_{\mathrm{p}}}{\partial \boldsymbol{S}_{\mathrm{e}}}, \tag{72a}$$

$${}^4\mathbb{N}_2 = \frac{\partial \boldsymbol{S}_{\mathrm{e}}}{\partial \boldsymbol{F}_{\mathrm{e}}^{\mathrm{T}}} : {}^4\mathbb{G}. \tag{72b}$$

The inversion operation of the (left- and right) symmetric 4th-order tensor tensor ${}^4\mathbb{N}_1$ is detailed in the appendix. Furthermore,

$$\frac{\partial \boldsymbol{S}_{\mathrm{e}}}{\partial \boldsymbol{F}_{\mathrm{e}}^{\mathrm{T}}} = \frac{\partial \boldsymbol{S}_{\mathrm{e}}}{\partial \boldsymbol{C}_{\mathrm{e}}^{\mathrm{T}}} : \frac{\partial \boldsymbol{C}_{\mathrm{e}}}{\partial \boldsymbol{F}_{\mathrm{e}}^{\mathrm{T}}} \tag{73}$$

is already known from eq. (46) and eq. (48).

5.2.4 Plastic deformation gradient w.r.t. elastic stress

The derivative $\frac{\partial \boldsymbol{F}_{\mathrm{p}}}{\partial \boldsymbol{S}_{\mathrm{e}}^{\mathrm{T}}}$ is split using the chain rule as follows

$$\frac{\partial \boldsymbol{F}_{\mathrm{p}}}{\partial \boldsymbol{S}_{\mathrm{e}}^{\mathrm{T}}} = \underbrace{\frac{\partial \boldsymbol{F}_{\mathrm{p}}}{\partial \boldsymbol{M}^{\mathrm{T}}}}_{\text{eq. (39)}} : \underbrace{\frac{\partial \boldsymbol{M}}{\partial \Delta \underset{\sim}{\gamma}}}_{\text{eq. (31)}} \frac{\partial \Delta \underset{\sim}{\gamma}}{\partial \underset{\sim}{\tau}} \underbrace{\frac{\partial \underset{\sim}{\tau}}{\partial \boldsymbol{S}_{\mathrm{e}}^{\mathrm{T}}}}_{\text{eq. (51)}} . \tag{74}$$

Derivative $\frac{\partial \Delta \underset{\sim}{\gamma}}{\partial \underset{\sim}{\tau}}$ will be derived in the remainder of this section.

Notice that $r^\alpha(\Delta \underset{\sim}{\gamma}) = 0$ at the converged state and thereby the variational form of eq. (16) can be expressed as

$$\delta \Delta \gamma^\alpha = b^\alpha (s^\alpha \delta \tau^\alpha - \tau^\alpha \delta s^\alpha), \tag{75}$$

where the relation $\operatorname{sign}(\tau^\alpha)|\tau^\alpha| = \tau^\alpha$ has been employed. Recall that b^α is given by

$$b^\alpha = \frac{\Delta t}{2} \frac{1}{(s^\alpha)^2} \frac{\dot{\gamma}_0}{m} \left(\frac{|\tau^\alpha|}{s^\alpha} \right)^{1/m-1} . \tag{76}$$

In order to relate $\Delta \underset{\sim}{\gamma}$ to $\underset{\sim}{\tau}$, the chain rule is applied to split δs^α in eq. (75) such that

$$\delta \Delta \gamma^\alpha + b^\alpha \tau^\alpha \sum_{\beta=1}^{N_{\mathrm{s}}} \frac{\partial s^\alpha}{\partial \gamma^\beta} \delta \Delta \gamma^\beta = b^\alpha s^\alpha \delta \tau^\alpha, \tag{77}$$

where $\frac{\partial s^\alpha}{\partial \gamma^\beta}$ is already known from eq. (28). If the derivative is taken with respect to τ^β, the following expression is obtained

$$\frac{\partial \Delta \gamma^\alpha}{\partial \tau^\beta} + b^\alpha \tau^\alpha \sum_{\chi=1}^{N_{\mathrm{s}}} \frac{\partial s^\alpha}{\partial \Delta \gamma^\chi} \frac{\partial \Delta \gamma^\chi}{\partial \tau^\beta} = \delta^{\alpha\beta} b^\alpha s^\alpha . \tag{78}$$

Note that $\frac{\partial \tau^\alpha}{\partial \tau^\beta} = \delta^{\alpha\beta}$. The matrix notation of eq. (78) is written as

$$
\begin{aligned}
\frac{\partial \Delta \underset{\sim}{\gamma}}{\partial \underset{\sim}{\tau}} + \underline{T}\, \frac{\partial \underset{\sim}{s}}{\partial \Delta \underset{\sim}{\gamma}}\, \frac{\partial \Delta \underset{\sim}{\gamma}}{\partial \underset{\sim}{\tau}} &= \underline{H}_2 \\
\left(\underline{I} + \underline{T}\, \frac{\partial \underset{\sim}{s}}{\partial \Delta \underset{\sim}{\gamma}} \right) \frac{\partial \Delta \underset{\sim}{\gamma}}{\partial \underset{\sim}{\tau}} &= \underline{H}_2,
\end{aligned}
\tag{79}
$$

with

$$(\underline{I})^{\alpha\beta} = \delta^{\alpha\beta} \tag{80a}$$

$$(\underline{T})^{\alpha\beta} = b^\alpha \tau^\alpha \delta^{\alpha\beta} \tag{80b}$$

$$(\underline{H}_2)^{\alpha\beta} = \delta^{\alpha\beta} b^\alpha s^\alpha. \tag{80c}$$

This implies that

$$\frac{\partial \Delta \underset{\sim}{\gamma}}{\partial \underset{\sim}{\tau}} = \underline{H}_1^{-1} \underline{H}_2, \tag{81}$$

with

$$(\underline{H}_1)^{\alpha\beta} = \delta^{\alpha\beta} + b^\alpha \tau^\alpha \frac{\partial s^\alpha}{\partial \Delta \gamma^\beta}. \tag{82}$$

Eqs. (71) and (68) are substituted in (61). Then, eqs. (58) and (61) are substituted in eq. (53) finally yield the explicit form of $^4\mathbb{K}$, which is the overall material tangent stiffness matrix.

A Notations

The employed scalars, vectors, (2nd-order) tensors and 4th-order tensors are distinguished as follows:

- *Scalar* is denoted by the italic symbol, e.g. a.
- *Vector* is denoted by the symbol with an arrow above, e.g. $\vec{a}$. When the Einstein summation convention is adopted, the vector $\vec{a}$ can also be written in index notation as $a_i \vec{e}_i$, where $\vec{e}_i$ is the Cartesian vector basis.
- *Tensor* is denoted by the italic-bold symbol, e.g. $\boldsymbol{A}$. The tensor $\boldsymbol{A}$ can be written in index notation as $\boldsymbol{A} = A_{ij} \vec{e}_i \vec{e}_j$.
- *4th-order tensor* is denoted by the blackboard-bold symbol with a left superscript "4", e.g. $^4\mathbb{A}$. The 4th-order ensor $^4\mathbb{A}$ can be written in index notation as $^4\mathbb{A} = A_{ijkl} \vec{e}_i \vec{e}_j \vec{e}_k \vec{e}_l$.

B Operations

A series of employed operations are defined in the following:

- *Column* assembly of quantities is denoted by a tilde below as $(\underset{\sim}{\bullet})$.
- *Matrix* assembly of quantities is denoted by a line below as $(\underline{\bullet})$.
- *Determinant* of a tensor is directly denoted as $\det(\bullet)$.
- *Inverse* of a tensor is denoted using a right superscript "-1" as $(\bullet)^{-1}$.
- *Transpose* of a column, matrix, tensor or 4th-order tensor is denoted using a right superscript "T" as $(\bullet)^{\mathrm{T}}$.
- *Left transpose* of a 4th-order tensor is denoted using a right superscript "LT" as $(\bullet)^{\mathrm{LT}}$.

- *Right transpose* of a 4th-order tensor is denoted using a right superscript "RT" as $(\bullet)^{\mathrm{RT}}$.
- *Symmetrization* of a tensor is denoted using a right superscript "S" as $(\bullet)^{\mathrm{S}} = \frac{1}{2}[(\bullet)+(\bullet)^{\mathrm{T}}]$. In particular, the symmetric part of a 4th-order tensor exists and is defined as ${}^4\mathbb{I}^{\mathrm{S}} = \frac{1}{2}({}^4\mathbb{I}+{}^4\mathbb{I}^{\mathrm{RT}})$.
- *Dyadic product* is directly denoted as $(\bullet)(\circ)$.
- *Dot product* is denoted by a dot, as $(\bullet)\cdot(\circ)$.
- *Double dot product* is denoted by a double dot, as $(\bullet):(\circ)$.
- *Derivative* of a tensor w.r.t a tensor is specially defined as $\frac{\partial(\bullet)}{\partial(\circ)^{\mathrm{T}}}$ (NOT $\frac{\partial(\bullet)}{\partial(\circ)}$), which can be written in index notation as $\frac{\partial(\bullet)_{ij}}{\partial(\circ)_{lk}}\vec{e}_i\vec{e}_j\vec{e}_k\vec{e}_l$ for convenience to apply the chain rule. For instance, if $\boldsymbol{B} = \boldsymbol{B}(\boldsymbol{C})$, we can have

$$\delta\boldsymbol{A} = \frac{\partial\boldsymbol{A}}{\partial\boldsymbol{A}^{\mathrm{T}}} : \frac{\partial\boldsymbol{B}}{\partial\boldsymbol{C}^{\mathrm{T}}} : \delta\boldsymbol{C}. \tag{83}$$

The details about the common operations above can be found in [3, 5].

B.1 Inversion of a 4th-order tensor

The inversion operation for a 4th-order order tensor is relatively complicated and most easily done as follows:

- Convert this tensor to a 9x9 matrix.
- In case of a left (${}^4\mathbb{A}^{\mathrm{LT}} = {}^4\mathbb{A}$) or right-symmetric (${}^4\mathbb{A}^{\mathrm{RT}} = {}^4\mathbb{A}$) 4th-order tensor, reduce corresponding 9x9 matrix to a 6x6 matrix.
- Take the inverse of this matrix.
- Convert the resulted matrix back to fourth order tensor notation.

B.2 Expansion and reduction of stiffness matrix

Since the shear component in a strain tensor is half of the engineering shear strain, e.g. $\epsilon_{12} = \frac{1}{2}\gamma_{12}$, associated expansion and reduction operations of stiffness matrix may be necessary, depending on the adopted formulation to implement the constitutive relations. For instance of the expansion operation:

- A stiffness matrix is specified by

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{31} \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} A \\ C \end{bmatrix} & \begin{bmatrix} B \\ D \end{bmatrix} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{12} \\ 2\varepsilon_{23} \\ 2\varepsilon_{31} \end{bmatrix}, \tag{84}$$

and can then be expanded as

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{21} \\ \sigma_{32} \\ \sigma_{13} \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} A \\ C \\ C \end{bmatrix} & \begin{bmatrix} B \\ D \\ D \end{bmatrix} & \begin{bmatrix} B \\ D \\ D \end{bmatrix} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \varepsilon_{12} \\ \varepsilon_{23} \\ \varepsilon_{31} \\ \varepsilon_{21} \\ \varepsilon_{32} \\ \varepsilon_{13} \end{bmatrix} \tag{85}$$

.

- A compliance matrix is specified by

$$\begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{12} \\ 2\varepsilon_{23} \\ 2\varepsilon_{31} \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} P \end{bmatrix} & \begin{bmatrix} Q \end{bmatrix} \\ \begin{bmatrix} R \end{bmatrix} & \begin{bmatrix} S \end{bmatrix} \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{31} \end{bmatrix}, \tag{86}$$

  and can then be expanded as

$$\begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \varepsilon_{12} \\ \varepsilon_{23} \\ \varepsilon_{31} \\ \varepsilon_{21} \\ \varepsilon_{32} \\ \varepsilon_{13} \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} P \end{bmatrix} & \begin{bmatrix} Q/2 \end{bmatrix} & \begin{bmatrix} Q/2 \end{bmatrix} \\ \begin{bmatrix} R/2 \end{bmatrix} & \begin{bmatrix} S/4 \end{bmatrix} & \begin{bmatrix} S/4 \end{bmatrix} \\ \begin{bmatrix} R/2 \end{bmatrix} & \begin{bmatrix} S/4 \end{bmatrix} & \begin{bmatrix} S/4 \end{bmatrix} \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{21} \\ \sigma_{32} \\ \sigma_{13} \end{bmatrix} \tag{87}$$

The reduction operation is similar.

C Unit tensors and useful relations

The unit tensor and 4th-order unit tensor together with their useful properties are highlighted as follows:

- *Unit tensor* $\boldsymbol{I}$ is defined such that $\boldsymbol{I} \cdot \vec{a} = \vec{a} \cdot \boldsymbol{I}$, which maps a vector $\vec{a}$ to itself and can be written in index notation as $\boldsymbol{I} = I_{ij} = \delta_{ij}$. A few useful relations involving $\boldsymbol{I}$ are given as

$$\boldsymbol{A} \cdot \boldsymbol{A}^{-1} = \boldsymbol{A}^{-1} \cdot \boldsymbol{A} = \boldsymbol{I}, \tag{88a}$$
$$\boldsymbol{I} \cdot \boldsymbol{A} = \boldsymbol{A} \cdot \boldsymbol{I} = \boldsymbol{A}, \tag{88b}$$
$$\boldsymbol{I} : \boldsymbol{A} = \boldsymbol{A} : \boldsymbol{I} = \mathrm{tr}(\boldsymbol{A}), \tag{88c}$$
$$\det(\boldsymbol{I} + \delta \boldsymbol{A}) \approx 1 + \mathrm{tr}(\delta \boldsymbol{A}), \tag{88d}$$
$$\delta \boldsymbol{I} = \boldsymbol{A} \cdot \delta \boldsymbol{A}^{-1} + \delta \boldsymbol{A} \cdot \boldsymbol{A}^{-1} = \boldsymbol{0}, \tag{88e}$$

  where $\mathrm{tr}(\bullet)$ and $\det(\bullet)$ are the trace (or 1st-invariant) and determinant (or 3rd-invariant) of a tensor, respectively and $\delta(\bullet)$ the variation.

- *4th-order unit tensor* ${}^4\mathbb{I}$ is defined such that ${}^4\mathbb{I} : \boldsymbol{A} = \boldsymbol{A} : {}^4\mathbb{I} = \boldsymbol{A}$, which maps a tensor to itself and can be written in index notation as ${}^4\mathbb{I} = I_{ijkl}\vec{e}_i\vec{e}_j\vec{e}_k\vec{e}_l = \delta_{il}\delta_{jk}\vec{e}_i\vec{e}_j\vec{e}_k\vec{e}_l$. A few useful relations involving ${}^4\mathbb{I}$ are given as

$${}^4\mathbb{I}^{\mathrm{RT}} : \boldsymbol{A} = \boldsymbol{A} : {}^4\mathbb{I}^{\mathrm{RT}} = \boldsymbol{A}^{\mathrm{T}}, \tag{89a}$$
$${}^4\mathbb{I}^{\mathrm{S}} : \boldsymbol{A} = \boldsymbol{A} : {}^4\mathbb{I}^{\mathrm{S}} = \boldsymbol{A}^{\mathrm{S}}. \tag{89b}$$

  Other useful relations include

$$(\boldsymbol{A} \cdot \boldsymbol{B})^{\mathrm{T}} = \boldsymbol{B}^{\mathrm{T}} \cdot \boldsymbol{A}^{\mathrm{T}}, \tag{90a}$$
$$(\boldsymbol{A} \cdot \boldsymbol{B})^{-1} = \boldsymbol{B}^{-1} \cdot \boldsymbol{A}^{-1}, \tag{90b}$$
$$\boldsymbol{A} : \boldsymbol{B} = \boldsymbol{A}^{\mathrm{T}} : \boldsymbol{B}^{\mathrm{T}} = \boldsymbol{B} : \boldsymbol{A} = \mathrm{tr}(\boldsymbol{A} \cdot \boldsymbol{B}); \tag{90c}$$
$$\boldsymbol{A} : (\boldsymbol{B} \cdot \boldsymbol{C}) = (\boldsymbol{A} \cdot \boldsymbol{B}) : \boldsymbol{C}, \tag{90d}$$
$${}^4\mathbb{A} : (\boldsymbol{B} \cdot \boldsymbol{C}) = ({}^4\mathbb{A} \cdot \boldsymbol{B}) : \boldsymbol{C}, \tag{90e}$$
$$\boldsymbol{A} \cdot \boldsymbol{B} + \boldsymbol{B}^{\mathrm{T}} \cdot \boldsymbol{A}^{\mathrm{T}} = 2\,{}^4\mathbb{I}^{\mathrm{S}} : (\boldsymbol{A} \cdot \boldsymbol{B}), \tag{90f}$$
$$\mathrm{tr}(\boldsymbol{A} + \boldsymbol{B}) = \mathrm{tr}(\boldsymbol{A}) + \mathrm{tr}(\boldsymbol{B}), \tag{90g}$$
$$\det(\boldsymbol{A} \cdot \boldsymbol{B}) = \det(\boldsymbol{A})\det(\boldsymbol{B}). \tag{90h}$$

D Definition of the rotation matrix

The rotation tensor rotates is defined as follows

$$\vec{e}_i^{\,\mathrm{c}} = \boldsymbol{R}^* \cdot \vec{e}_i \tag{91}$$

With

- $\vec{e}_i$ the **global** coordinate system base vectors,
- $\vec{e}_i^{\,\mathrm{c}}$ the **crystal** coordinate system base vectors.

The components of the rotation matrix $\underline{R}^*$ are determined with respect to the **global** coordinate system:

$$\boldsymbol{R}^* = R^*_{ij}\vec{e}_i\vec{e}_j \tag{92}$$

A vector $\vec{n}$ in terms of the **crystal** coordinate system can be expressed as

$$\vec{n} = n_1^{\mathrm{c}}\vec{e}_1^{\,\mathrm{c}} + n_2^{\mathrm{c}}\vec{e}_2^{\,\mathrm{c}} + n_3^{\mathrm{c}}\vec{e}_3^{\,\mathrm{c}} \quad \text{and} \quad \underset{\sim}{n}^{\mathrm{c}} = \begin{bmatrix} n_1^{\mathrm{c}} \\ n_2^{\mathrm{c}} \\ n_3^{\mathrm{c}} \end{bmatrix} \tag{93}$$

The **same** vector can also be expressed in terms of the **global** coordinate system:

$$\vec{n} = n_1\vec{e}_1 + n_2\vec{e}_2 + n_3\vec{e}_3 \quad \text{and} \quad \underset{\sim}{n} = \begin{bmatrix} n_1 \\ n_2 \\ n_3 \end{bmatrix} \tag{94}$$

Conversion between the components can be written as

$$\underset{\sim}{n} = \underline{R}^*\underset{\sim}{n}^{\mathrm{c}}. \tag{95}$$

Details of the derivation of this relation can be found in [4]. Eq. (95) holds for an arbitrary vector $\vec{n}$. A similar relation holds for the components of an arbitrary tensor $\boldsymbol{A}$:

$$\underline{A} = \underline{R}^*\underline{A}^{\mathrm{c}}\underline{R}^{*\mathrm{T}} \tag{96}$$

The texture-file which dictates the orientation of each grain should have the following structure. The first line contains the number of orientations in the file. Each consecutive line starts with an identification number, followed by the 9 components of the rotation matrix $\underline{R}^*$ in the following order: $[\underline{R}^*_{11}, \underline{R}^*_{22}, \underline{R}^*_{33}, \underline{R}^*_{12}, \underline{R}^*_{23}, \underline{R}^*_{31}, \underline{R}^*_{21}, \underline{R}^*_{32}, \underline{R}^*_{13}]$.

Note that $\underline{R}^*$ is a rotation matrix and should therefore satisfy the following conditions

$$\det\left(\underline{R}^*\right) = 1 \tag{97}$$

$$\left(\underline{R}^*\right)^{-1} = \left(\underline{R}^*\right)^{\mathrm{T}} \tag{98}$$

The rotation matrix is applied in the code for rotating the (non-)Schmid tensor according to equation (96).

$$\underline{P}_0 = \underline{R}^*\underline{P}_0^{\mathrm{c}}\underline{R}^{*\mathrm{T}} \tag{99}$$

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