

Mathematical Notes on the Crystal Plasticity UMAT

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1 Introduction

Huang's UMAT [1] was released in June 1991 to integrate crystal plasticity into Abaqus FEA. In November 1997, Jeffrey W. Kysar added modifications to correct an error in the implementation of the Bassani and Wu hardening law. At the time of release, computing power was substantially lower than today. To put it in context, the Cray C90 series, which was a vector processor supercomputer, was launched by Cray Research in 1991 and delivered, at peak performance, 16 GFLOPS [2, 3], while the recently released Intel® Core™ Ultra 9 processor (285K GMac/s, up to 5.70 GHz) for desktop computing delivers a peak performance of 1420.8 GFLOPS [4]. Therefore, a current desktop computer can process approximately 88.8 times faster than a supercomputer in 1991. As a result, the simulation of crystals was difficult and the code had to be extremely efficient with the use of memory. However, the advances in computational power of the previous decades since Huang's UMAT release opened new frontiers of research in the multi-scale space which make the UMAT relevant for process–microstructure–service modelling.

As an example, in a recent review published by Enrico Salvati [5], the Scopus database was mined to extract papers from 1980 to 2023 dealing with fatigue. The review showed that the increase per year of papers with fatigue-related sub-topics in crystal plasticity is of 13.4%, with AI being 33.6% and fatigue in metals, creep, corrosion, and residual stress being 3.8%, 2.3%, 3.6%, and 6.0%, respectively. The growing trend of papers using the crystal plasticity finite element method (CPFEM) is no coincidence, but a result of the evolution of computer hardware which now allows to model polycrystals.

Considering the current scenario, it is worthwhile to revisit older Fortran UMAT implementations and add enhanced modelling equations based on the progress of physics,

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and also modify them according to modern software engineering practices, such as testing and modularity. In particular, Huang's UMAT was written in a very efficient and compact way. However, without proper documentation, this makes the code difficult to follow and expand. The goal of this document is not to re-explain the entirety of crystal plasticity theory, but rather to present the key equations and derivations that underpin the implementation. This should help researchers and engineers understand the numerical methods behind the UMAT, and allow them to adapt and extend the code with confidence.

2 Schmid Law for a General Stress State

Schmid's law [6] establishes the relationship between the shear stress in a slip plane and the stress applied to the material. In Figure 1, a single crystal subjected to a load in the direction of the vector \mathbf{t} is shown. The resolved shear stress $\tau^{(\alpha)}$ in the slip system α can be calculated according to Schmid's law as follows:

$$\tau^{(\alpha)} = \sigma \cos \lambda \cos \phi \quad (1)$$

where σ is the uniaxial stress, and λ and ϕ are the angles between the load direction and the slip direction and normal, respectively. Equation (1) is applicable in the context of a tensile stress applied to the single crystal as shown in Figure 1. For a general stress state, the equation can be expressed as:

$$\tau^{(\alpha)} = \boldsymbol{\sigma} : (\mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)}) = \mathbf{s}^{(\alpha)} : \boldsymbol{\sigma} : \mathbf{m}^{(\alpha)} = \mathbf{m}^{(\alpha)} : \boldsymbol{\sigma} : \mathbf{s}^{(\alpha)} \quad (2)$$

where $\mathbf{s}^{(\alpha)}$ and $\mathbf{m}^{(\alpha)}$ are directional cosines that represent the slip direction and the normal to the slip plane, respectively.

For any two second-order tensors \mathbf{A} and \mathbf{B} , if \mathbf{A} is symmetric (i.e. $\mathbf{A} = \mathbf{A}^T$), it can be proved that $\mathbf{A} : \mathbf{B} = \mathbf{A} : \text{sym}(\mathbf{B})$. Thus, Equation (2) can be written in the following way:

$$\begin{aligned} \tau^{(\alpha)} &= \boldsymbol{\sigma} : (\mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)}) = \boldsymbol{\sigma} : \text{sym}(\mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)}) \\ \tau^{(\alpha)} &= \boldsymbol{\sigma} : \frac{1}{2} \left[\mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)} + (\mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)})^T \right] \\ \tau^{(\alpha)} &= \boldsymbol{\sigma} : \frac{1}{2} (\mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)} + \mathbf{m}^{(\alpha)} \otimes \mathbf{s}^{(\alpha)}) \\ \tau^{(\alpha)} &= \boldsymbol{\sigma} : \boldsymbol{\mu}^{(\alpha)} \end{aligned} \quad (3)$$

where $\boldsymbol{\mu}^{(\alpha)}$ is the symmetric projection tensor or *Schmid factor*. In the UMAT, $\boldsymbol{\mu}^{(\alpha)}$ is the variable `SLPDEF`. Since the matrix is symmetric, it is possible to store it as a vector following Voigt notation, resulting in the components $\mu_{11}^{(\alpha)}$, $\mu_{22}^{(\alpha)}$, $\mu_{33}^{(\alpha)}$, $2\mu_{12}^{(\alpha)}$, $2\mu_{13}^{(\alpha)}$, and $2\mu_{23}^{(\alpha)}$.

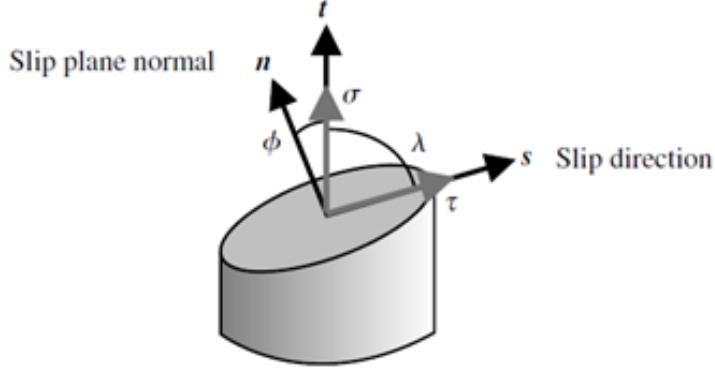


Figure 1: A single crystal with a slip direction defined by vector s , slip normal \mathbf{m} , and load direction by \mathbf{t} [7].

It is important to also note that $\boldsymbol{\omega}^{(\alpha)}$ is the skew-symmetric tensor so that:

$$\boldsymbol{\mu}^{(\alpha)} + \boldsymbol{\omega}^{(\alpha)} = \mathbf{s}^{(\alpha)} \otimes \mathbf{m}^{(\alpha)} \quad (4)$$

3 Derivation of the Rate of Change of Schmid Stress in a Crystal Lattice

This section derives Equation (2.2.4) in Huang's technical report.

First, it is worth noting that in Huang's formulation the deformation gradient \mathbf{F} is decomposed into \mathbf{F}^* and \mathbf{F}^p , the elastic and plastic components, respectively, using the multiplicative decomposition. The inelastic component arises solely from crystallographic slip. Elastic properties are not affected by slip, and stress is generated only by \mathbf{F}^* . Consequently, plastic flow does not directly contribute to the stress rate; instead, plastic flow evolves the slip systems and relaxes stress.

Schmid's law expressed in terms of the Kirchhoff stress, corresponding to Equation (2.2.3) in Huang's technical report, can be written as follows:

$$\tau^\alpha = \mathbf{m}^{*(\alpha)} : \left(\frac{\rho_0}{\rho} \boldsymbol{\sigma} \right) : \mathbf{s}^{*(\alpha)} \quad (5)$$

Here, the Cauchy stress tensor is replaced by the Kirchhoff stress $\boldsymbol{\tau}$:

$$\boldsymbol{\tau} = J \boldsymbol{\sigma} \quad (6)$$

with $J = \det(\mathbf{F}) = \rho_0/\rho$. Huang states that τ^α represents a *mixed* stress measure, since the Kirchhoff stress is defined in the spatial (Eulerian) frame while it is projected onto purely material (lattice-frame) directions. The stress and the geometric basis therefore reside in different frames.

At finite strains, the Kirchhoff stress is used instead of the Cauchy stress because it

is work-conjugate to the rate of deformation tensor. This choice, originally motivated by Hill and Rice [8], ensures that the macroscopic stress power equals the sum of the slip-system contributions, which in turn guarantees compliance with the Clausius–Duhem inequality:

$$\boldsymbol{\tau} : \mathbf{D} = \sum_{\alpha=1}^{N_\alpha} \tau^{(\alpha)} \dot{\gamma}^{(\alpha)} \quad (7)$$

where \mathbf{D} is the rate of deformation tensor, $\dot{\gamma}^{(\alpha)}$ is the slip rate of slip system α (i.e. the time derivative of the shear strain $\gamma^{(\alpha)}$), and N_α is the total number of slip systems. In practice, this formulation amounts to projecting the Kirchhoff stress onto the lattice slip systems, thereby producing the so-called *mixed* resolved shear stress. The energetically conjugate resolved shear stress $\tau^{(\alpha)}$ is therefore no longer identical to the classical Schmid resolved shear stress. Under common metal material assumptions, namely nearly incompressible behaviour ($J \approx 1$) and an elastic part of the lattice motion that is approximately a rigid rotation (so that starred directions coincide with spatial unit directions), the result of Equation (5) is approximately equivalent to that of Equation (2).

The time derivative of Equation (5) is given by

$$\begin{aligned} \dot{\tau}^{(\alpha)} &= \dot{\mathbf{m}}^{*(\alpha)} : \left(\frac{\rho_0}{\rho} \boldsymbol{\sigma} \right) : \mathbf{s}^{*(\alpha)} + \mathbf{m}^{*(\alpha)} : \frac{d}{dt} \left(\frac{\rho_0}{\rho} \boldsymbol{\sigma} \right) : \mathbf{s}^{*(\alpha)} \\ &\quad + \mathbf{m}^{*(\alpha)} : \left(\frac{\rho_0}{\rho} \boldsymbol{\sigma} \right) : \dot{\mathbf{s}}^{*(\alpha)} \\ \dot{\tau}^{(\alpha)} &= -\mathbf{m}^{*(\alpha)} \mathbf{L}^* : \left(\frac{\rho_0}{\rho} \boldsymbol{\sigma} \right) : \mathbf{s}^{*(\alpha)} + \mathbf{m}^{*(\alpha)} : \frac{d}{dt} \left(\frac{\rho_0}{\rho} \boldsymbol{\sigma} \right) : \mathbf{s}^{*(\alpha)} \\ &\quad + \mathbf{m}^{*(\alpha)} : \left(\frac{\rho_0}{\rho} \boldsymbol{\sigma} \right) : \mathbf{L}^* \mathbf{s}^{*(\alpha)} \\ \dot{\tau}^{(\alpha)} &= \mathbf{m}^{*(\alpha)} : \left[\frac{d}{dt} \left(\frac{\rho_0}{\rho} \boldsymbol{\sigma} \right) + \left(\frac{\rho_0}{\rho} \right) \boldsymbol{\sigma} \mathbf{L}^* - \left(\frac{\rho_0}{\rho} \right) \mathbf{L}^* \boldsymbol{\sigma} \right] : \mathbf{s}^{*(\alpha)} \end{aligned} \quad (8)$$

where \mathbf{L} is the velocity gradient. In Equation (8), the time derivative must be expressed in an alternative form in order to obtain Equation (2.2.4). For this purpose, the principle of mass conservation is used:

$$\frac{d}{dt} \int_{\Omega_t} \rho(\mathbf{x}, t) dV = 0 \quad (9)$$

Here, ρ is the density of a volume Ω_t . The Reynolds transport theorem states that the rate of change of the integral of a quantity in a moving volume equals the local time derivative plus the flux across the moving boundary. Implementing it in Equation (9) gives:

$$\frac{d}{dt} \int_{\Omega_t} \rho(\mathbf{x}, t) dV = \int_{\Omega_t} \frac{\partial \rho}{\partial t} dV + \int_{\partial \Omega_t} \rho (\mathbf{v} \cdot \mathbf{n}) dA \quad (10)$$

where \mathbf{v} is the velocity field. Applying the divergence theorem yields:

$$\int_{\partial\Omega_t} \rho (\mathbf{v} \cdot \mathbf{n}) dA = \int_{\Omega_t} \nabla \cdot (\rho \mathbf{v}) dV$$

Equation (10) can therefore be expressed as:

$$\begin{aligned} \frac{d}{dt} \int_{\Omega_t} \rho(\mathbf{x}, t) dV &= \int_{\Omega_t} \frac{\partial \rho}{\partial t} dV + \int_{\Omega_t} \nabla \cdot (\rho \mathbf{v}) dV \\ &= \int_{\Omega_t} \left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) \right] dV \end{aligned} \quad (11)$$

The partial time derivative $\partial \rho / \partial t$ is Eulerian, as it represents the change of ρ at a fixed point in space. The Lagrangian (material) derivative can be expressed as:

$$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} \Big|_{\mathbf{x}} + \mathbf{v} \cdot \nabla \rho$$

Expanding the divergence in Equation (11) yields:

$$\begin{aligned} \int_{\Omega_t} \left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) \right] dV &= \int_{\Omega_t} \left[\frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{v} \right] dV \\ &= \int_{\Omega_t} (\dot{\rho} + \rho \nabla \cdot \mathbf{v}) dV \end{aligned} \quad (12)$$

Considering that $\text{tr}(\nabla \mathbf{v}) = \nabla \cdot \mathbf{v}$, Equation (12) can be written as:

$$\int_{\Omega_t} (\dot{\rho} + \rho \nabla \cdot \mathbf{v}) dV = \int_{\Omega_t} (\dot{\rho} + \rho \text{tr}(\mathbf{L})) dV \quad (13)$$

Since the integral in Equation (11) must vanish for any arbitrary material subvolume, the integrand itself must vanish:

$$\dot{\rho} + \rho \text{tr}(\mathbf{L}) = 0 \quad (14)$$

The velocity gradient \mathbf{L} can be expressed as the sum of the rate of deformation tensor \mathbf{D} and the continuum spin tensor $\boldsymbol{\Omega}$:

$$\mathbf{L} = \mathbf{D} + \boldsymbol{\Omega} = \frac{1}{2} (\mathbf{L} + \mathbf{L}^T) + \frac{1}{2} (\mathbf{L} - \mathbf{L}^T)$$

The symmetric part, represented by \mathbf{D} , measures the local strain rate, while the skew-symmetric tensor $\boldsymbol{\Omega}$ measures the local rigid-body rotation. The trace of $\boldsymbol{\Omega}$ is zero since its diagonal components vanish. Consequently,

$$\frac{\dot{\rho}}{\rho} = -\text{tr}(\mathbf{L}) = -\mathbf{I} : \mathbf{D} \quad (15)$$

Using Equation (15), the following expression can be derived:

$$\frac{d}{dt} \left(\frac{\rho_0}{\rho} \right) = \rho_0 \frac{d}{dt} \left(\frac{1}{\rho} \right) = -\rho_0 \frac{\dot{\rho}}{\rho^2} = \frac{\rho_0}{\rho} (\mathbf{I} : \mathbf{D}) \quad (16)$$

And differentiating the Kirchhoff stress considering the multiplicative decomposition:

$$\begin{aligned} \frac{d}{dt} \left(\frac{\rho_0}{\rho} \boldsymbol{\sigma} \right) &= \frac{d}{dt} \left(\frac{\rho_0}{\rho} \right) \boldsymbol{\sigma} + \frac{\rho_0}{\rho} \dot{\boldsymbol{\sigma}} \\ \frac{d}{dt} \left(\frac{\rho_0}{\rho} \boldsymbol{\sigma} \right) &= \frac{\rho_0}{\rho} [\dot{\boldsymbol{\sigma}} + (\mathbf{I} : \mathbf{D}^*) \boldsymbol{\sigma}] \end{aligned} \quad (17)$$

Introducing Equation (17) into Equation (8):

$$\begin{aligned} \dot{\tau}^{(\alpha)} &= \mathbf{m}^{*(\alpha)} : \left[\frac{d}{dt} \left(\frac{\rho_0}{\rho} \boldsymbol{\sigma} \right) + \left(\frac{\rho_0}{\rho} \right) \boldsymbol{\sigma} \mathbf{L}^* - \left(\frac{\rho_0}{\rho} \right) \mathbf{L}^* \boldsymbol{\sigma} \right] : \mathbf{s}^{*(\alpha)} \\ \dot{\tau}^{(\alpha)} &= \mathbf{m}^{*(\alpha)} : [J(\dot{\boldsymbol{\sigma}} + (\mathbf{I} : \mathbf{D}^*) \boldsymbol{\sigma}) + J\boldsymbol{\sigma} \mathbf{L}^* - J\mathbf{L}^* \boldsymbol{\sigma}] : \mathbf{s}^{*(\alpha)} \\ \dot{\tau}^{(\alpha)} &= J\mathbf{m}^{*(\alpha)} : [\dot{\boldsymbol{\sigma}} + (\mathbf{I} : \mathbf{D}^*) \boldsymbol{\sigma} + \boldsymbol{\sigma}(\mathbf{D}^* + \boldsymbol{\Omega}^*) - (\mathbf{D}^* + \boldsymbol{\Omega}^*) \boldsymbol{\sigma}] : \mathbf{s}^{*(\alpha)} \\ \dot{\tau}^{(\alpha)} &= J\mathbf{m}^{*(\alpha)} : [\dot{\boldsymbol{\sigma}} + \boldsymbol{\sigma}\boldsymbol{\Omega}^* - \boldsymbol{\Omega}^* \boldsymbol{\sigma} + (\mathbf{I} : \mathbf{D}^*) \boldsymbol{\sigma} + \boldsymbol{\sigma}\mathbf{D}^* - \mathbf{D}^* \boldsymbol{\sigma}] : \mathbf{s}^{*(\alpha)} \\ \dot{\tau}^{(\alpha)} &= J\mathbf{m}^{*(\alpha)} : \left[\nabla \boldsymbol{\sigma} + (\mathbf{I} : \mathbf{D}^*) \boldsymbol{\sigma} + \boldsymbol{\sigma} \mathbf{D}^* - \mathbf{D}^* \boldsymbol{\sigma} \right] : \mathbf{s}^{*(\alpha)} \\ \dot{\tau}^{(\alpha)} &= \mathbf{m}^{*(\alpha)} : \left[\nabla \boldsymbol{\sigma} + (\mathbf{I} : \mathbf{D}^*) \boldsymbol{\sigma} + \boldsymbol{\sigma} \mathbf{D}^* - \mathbf{D}^* \boldsymbol{\sigma} \right] : \mathbf{s}^{*(\alpha)} \end{aligned} \quad (18)$$

Equation (18) results from absorbing the Jacobian into the Kirchhoff stress and it is the form in which Huang presented the equation in the technical note.

4 Derivation of the Increment of Resolved Shear Stress

Using Equation (2.2.1) in Huang's technical note and Equation (18):

$$\dot{\tau}^{(\alpha)} = \mathbf{m}^{*(\alpha)} : [\mathbb{L} : \mathbf{D}^* + \boldsymbol{\sigma} \mathbf{D}^* - \mathbf{D}^* \boldsymbol{\sigma}] : \mathbf{s}^{*(\alpha)} \quad (19)$$

where \mathbb{L} is the elasticity tensor. The fourth-order tensor \mathbb{L} is symmetric in its first index pair. As a result,

$$L_{ijkl} \omega_{ij}^\alpha = 0.$$

Distributing the double-dot product:

$$\dot{\tau}^{(\alpha)} = \underbrace{\mathbf{m}^{*(\alpha)} : (\mathbb{L} : \mathbf{D}^*) : \mathbf{s}^{*(\alpha)}}_{\text{Term 1}} + \underbrace{\mathbf{m}^{*(\alpha)} : (\boldsymbol{\sigma} \mathbf{D}^* - \mathbf{D}^* \boldsymbol{\sigma}) : \mathbf{s}^{*(\alpha)}}_{\text{Term 2}}$$

Term 1

$$\mathbf{m}^{*(\alpha)} : (\mathbb{L} : \mathbf{D}^*) : \mathbf{s}^{*(\alpha)} = m_i^{*(\alpha)} L_{ijkl} D_{kl}^* s_j^{*(\alpha)}$$

Since every index is dummy, the result of the product is a scalar. Scalars are invariant to re-ordering, so the factors can be permuted:

$$L_{ijkl} \left(m_i^{*(\alpha)} s_j^{*(\alpha)} \right) D_{kl}^*$$

The term in parentheses is the dyadic (outer) product of two vectors. Consequently:

$$L_{ijkl} \left(\mu_{ij}^{(\alpha)} + \omega_{ij}^{(\alpha)} \right) D_{kl}^* = L_{ijkl} \mu_{ij}^{(\alpha)} D_{kl}^* + L_{ijkl} \omega_{ij}^{(\alpha)} D_{kl}^*$$

Using the minor symmetry of the elasticity tensor $L_{ijkl} = L_{jikl}$ and the skew-symmetry of the spin tensor $\omega_{ij} = -\omega_{ji}$:

$$L_{ijkl} \omega_{ij}^{(\alpha)} = \frac{1}{2} \left(L_{ijkl} \omega_{ij}^{(\alpha)} + L_{jikl} \omega_{ij}^{(\alpha)} \right) = \frac{1}{2} \left(L_{ijkl} \omega_{ij}^{(\alpha)} + L_{jikl} \omega_{ji}^{(\alpha)} \right)$$

$$L_{ijkl} \omega_{ij}^{(\alpha)} = \frac{1}{2} \left(L_{ijkl} \omega_{ij}^{(\alpha)} - L_{ijkl} \omega_{ij}^{(\alpha)} \right) = \frac{1}{2} L_{ijkl} \left(\omega_{ij}^{(\alpha)} - \omega_{ij}^{(\alpha)} \right) = 0$$

$$L_{ijkl} \omega_{ij}^{(\alpha)} = 0$$

Consequently:

$$L_{ijkl} \left(\mu_{ij}^{(\alpha)} + \omega_{ij}^{(\alpha)} \right) D_{kl}^* = L_{ijkl} \mu_{ij}^{(\alpha)} D_{kl}^* + L_{ijkl} \omega_{ij}^{(\alpha)} D_{kl}^* = L_{ijkl} \mu_{ij}^{(\alpha)} D_{kl}^*$$

Using the major symmetry $L_{ijkl} = L_{klij}$ of the elasticity tensor and renaming dummy indices ($i \rightarrow k, j \rightarrow l, k \rightarrow i, l \rightarrow j$):

$$\text{Term 1} = L_{ijkl} \mu_{ij}^{(\alpha)} D_{kl}^* = L_{klij} \mu_{ij}^{(\alpha)} D_{kl}^* = L_{ijkl} \mu_{kl}^{(\alpha)} D_{ij}^*$$

Term 2

$$\mathbf{m}^{*(\alpha)} : (\boldsymbol{\sigma} \mathbf{D}^* - \mathbf{D}^* \boldsymbol{\sigma}) : \mathbf{s}^{*(\alpha)} = m_i^{*(\alpha)} \left(\sigma_{ik} D_{kj}^* - D_{ik}^* \sigma_{kj} \right) s_j^{*(\alpha)}$$

As before, the terms can be rearranged since the result is a scalar:

$$m_i^{*(\alpha)} \left(\sigma_{ik} D_{kj}^* - D_{ik}^* \sigma_{kj} \right) s_j^{*(\alpha)} = \left(m_i^{*(\alpha)} s_j^{*(\alpha)} \right) \left(\sigma_{ik} D_{kj}^* - D_{ik}^* \sigma_{kj} \right)$$

$$\left(m_i^{*(\alpha)} s_j^{*(\alpha)}\right) \left(\sigma_{ik} D_{kj}^* - D_{ik}^* \sigma_{kj}\right) = \mu_{ij}^{(\alpha)} \left(\sigma_{ik} D_{kj}^* - D_{ik}^* \sigma_{kj}\right) + \omega_{ij}^{(\alpha)} \left(\sigma_{ik} D_{kj}^* - D_{ik}^* \sigma_{kj}\right)$$

The Schmid tensor $\mu_{ij}^{(\alpha)}$ is symmetric and since the commutator of two symmetric tensors is antisymmetric, $\mu_{ij}^{(\alpha)} \left(\sigma_{ik} D_{kj}^* - D_{ik}^* \sigma_{kj}\right) = 0$.

$$\mu_{ij}^{(\alpha)} \left(\sigma_{ik} D_{kj}^* - D_{ik}^* \sigma_{kj}\right) + \omega_{ij}^{(\alpha)} \left(\sigma_{ik} D_{kj}^* - D_{ik}^* \sigma_{kj}\right) = \omega_{ij}^{(\alpha)} \left(\sigma_{ik} D_{kj}^* - D_{ik}^* \sigma_{kj}\right)$$

$$\begin{aligned} \omega_{ij}^{(\alpha)} \left(\sigma_{ik} D_{kj}^* - D_{ik}^* \sigma_{kj}\right) &= \omega_{ij}^{(\alpha)} \sigma_{ik} D_{kj}^* - \omega_{ij}^{(\alpha)} D_{ik}^* \sigma_{kj} = \left(\omega_{ik}^{(\alpha)} \sigma_{jk} + \omega_{jk}^{(\alpha)} \sigma_{ik}\right) D_{ij}^* \\ \text{Term 2} &= \left(\omega_{ik}^{(\alpha)} \sigma_{jk} + \omega_{jk}^{(\alpha)} \sigma_{ik}\right) D_{ij}^* \end{aligned}$$

Using Term 1 and Term 2 and replacing in Equation (19):

$$\dot{\tau}^{(\alpha)} = L_{ijkl} \mu_{kl}^{(\alpha)} D_{ij}^* + \left(\omega_{ik}^{(\alpha)} \sigma_{jk} + \omega_{jk}^{(\alpha)} \sigma_{ik}\right) D_{ij}^* \quad (20)$$

The constitutive formulation is expressed in the lattice corotational frame and the objective stress rate is the Jaumann corotational rate. In Abaqus FEA, the strain increment passed to the UMAT as **DSTRAN** is already rotation-free; it does not include the contribution from rigid-body spin. Instead, it represents the corotational strain increment, i.e. the time integral of the symmetric part of the velocity gradient in the corotating axes. Therefore, in the Jaumann corotational frame adopted by Abaqus FEA, the strain increment is obtained as:

$$\Delta \boldsymbol{\varepsilon}^J = \int_t^{t+\Delta t} \mathbf{D}^J dt \quad (21)$$

where $\mathbf{D}^J = \mathbf{Q}^T \mathbf{D} \mathbf{Q}$ is the rate of deformation expressed in the corotating axes. Abaqus FEA passes the increment $\Delta \boldsymbol{\varepsilon}^J$ as **DSTRAN**, and the incremental corotational rotation as **DROT** (i.e. \mathbf{Q}). The rate of deformation \mathbf{D} can then be expressed as:

$$\mathbf{D}^* = \mathbf{D} - \mathbf{D}^P = \dot{\boldsymbol{\varepsilon}} - \sum_{\beta} \dot{\gamma}^{(\beta)} \boldsymbol{\mu}^{(\beta)} \quad (22)$$

Factoring D_{ij}^* out from Equation (20) and replacing it with the integrated form of Equation (22), Equation (3.2.3) in Huang's technical note is obtained:

$$\Delta \tau^{(\alpha)} = \left[L_{ijkl} \mu_{kl}^{(\alpha)} + \omega_{ik}^{(\alpha)} \sigma_{jk} + \omega_{jk}^{(\alpha)} \sigma_{ik} \right] \left[\Delta \varepsilon_{ij} - \sum_{\beta} \mu_{ij}^{(\beta)} \Delta \gamma^{(\beta)} \right] \quad (23)$$

5 Derivation of the Increment of Corotational Stress

Equation (2.2.2) of Huang's technical note relates the corotational stress rate on axes that rotate with the lattice axes with the corotational stress rate on axes rotating with

the material:

$$\overset{\nabla}{\sigma}^* = \overset{\nabla}{\sigma} + (\Omega - \Omega^*) \sigma - \sigma (\Omega - \Omega^*) \quad (24)$$

where $\overset{\nabla}{\sigma}$ is the Jaumann stress rate:

$$\overset{\nabla}{\sigma} = \dot{\sigma} - \Omega \sigma + \sigma \Omega \quad (25)$$

Additionally, Equation (2.2.1) in Huang's work establishes a relationship between the corotational stress in the lattice frame with the rate of deformation of the lattice:

$$\overset{\nabla}{\sigma}^* + \sigma (\mathbf{I} : \mathbf{D}^*) = \mathbb{L} : \mathbf{D}^* \quad (26)$$

Solving for $\overset{\nabla}{\sigma}$ in Equation (24) and substituting $\overset{\nabla}{\sigma}^*$ with Equation (26):

$$\overset{\nabla}{\sigma} = \overset{\nabla}{\sigma}^* - (\Omega - \Omega^*) \sigma + \sigma (\Omega - \Omega^*)$$

$$\overset{\nabla}{\sigma} = \mathbb{L} : \mathbf{D}^* - \sigma (\mathbf{I} : \mathbf{D}^*) - (\Omega - \Omega^*) \sigma + \sigma (\Omega - \Omega^*)$$

In indicial notation:

$$\overset{\nabla}{\sigma}_{ij} = L_{ijkl} D_{kl}^* - \sigma_{ij} D_{mm}^* - (\Omega_{ik} - \Omega_{ik}^*) \sigma_{kj} + \sigma_{ik} (\Omega_{kj} - \Omega_{kj}^*) \quad (27)$$

From Equation (2.1.4) in Huang's technical note:

$$\mathbf{D} = \mathbf{D}^* + \mathbf{D}^P \quad \Omega = \Omega^* + \Omega^P \quad (28)$$

Replacing Equation (28) in Equation (27):

$$\overset{\nabla}{\sigma}_{ij} = L_{ijkl} (D_{kl} - D_{kl}^P) - \sigma_{ij} (D_{mm} - D_{mm}^P) - (\Omega_{ik} - \Omega_{ik}^*) \sigma_{kj} + \sigma_{ik} (\Omega_{kj} - \Omega_{kj}^*) \quad (29)$$

From Equation (2.1.5) in Huang's technical note:

$$\mathbf{D}^P + \Omega^P = \sum_{\alpha} \dot{\gamma}^{(\alpha)} \mathbf{s}^{*(\alpha)} \otimes \mathbf{m}^{*(\alpha)} = \sum_{\alpha} \dot{\gamma}^{(\alpha)} [\boldsymbol{\mu}^{(\alpha)} + \boldsymbol{\omega}^{(\alpha)}] \quad (30)$$

$$\mathbf{D}^P = \sum_{\alpha} \dot{\gamma}^{(\alpha)} \boldsymbol{\mu}^{(\alpha)}$$

$$\Omega^P = \sum_{\alpha} \dot{\gamma}^{(\alpha)} \boldsymbol{\omega}^{(\alpha)}$$

Expanding the products of Equation (29), using the definition of plastic spin and inserting Equation (30):

$$\overset{\nabla}{\sigma}_{ij} = L_{ijkl} D_{kl} - L_{ijkl} D_{kl}^P - \sigma_{ij} (D_{mm} - D_{mm}^P) - \Omega_{ik}^P \sigma_{kj} + \sigma_{ik} \Omega_{ik}^P$$

$$\overset{\nabla}{\sigma}_{ij} = L_{ijkl}D_{kl} - \sigma_{ij}(D_{mm} - D_{mm}^P) - \sum_{\alpha} \left[L_{ijkl}\mu_{kl}^{(\alpha)} + \omega_{ik}^{(\alpha)}\sigma_{jk} + \omega_{jk}^{(\alpha)}\sigma_{ik} \right] \dot{\gamma}^{(\alpha)}$$

Expressing the equation in incremental form, the equation presented in Huang's technical note is obtained:

$$\Delta\sigma_{ij} = L_{ijkl}\Delta\varepsilon_{kl} - \sigma_{ij}\Delta\varepsilon_{kk} - \sum_{\alpha} \left[L_{ijkl}\mu_{kl}^{(\alpha)} + \omega_{ik}^{(\alpha)}\sigma_{jk} + \omega_{jk}^{(\alpha)}\sigma_{ik} \right] \Delta\gamma^{(\alpha)} \quad (31)$$

6 Linearisation of the Slip Increment Equation

Hutchingson [9] used a power law for crystalline creep to describe the relationship between slipping rate, which is the derivative of the shear strain for a specific slip system α , and resolved shear stress $\tau^{(\alpha)}$ and slip resistance $g^{(\alpha)}$:

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0^{(\alpha)} \left| \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right|^{n-1} \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \quad (32)$$

where the constant coefficient $\dot{\gamma}_0^{(\alpha)}$ is the reference strain rate on slip system α . It is worth noting that Equation (32) is equivalent to:

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0^{(\alpha)} \left| \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right|^n \text{sign} \left(\frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right) = \dot{\gamma}_0^{(\alpha)} \left| \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right|^n \text{sign} (\tau^{(\alpha)}) \quad (33)$$

where $\text{sign}(\tau^{(\alpha)}/g^{(\alpha)}) = \text{sign}(\tau^{(\alpha)})$ because the slip resistance $g^{(\alpha)}$ is always positive. Following Huang's work, the tangent modulus method for rate dependent solids developed by Peirce, Shih and Needleman [10] can be expressed as:

$$\Delta\gamma^{(\alpha)} = \gamma^{(\alpha)}(t + \Delta t) - \gamma^{(\alpha)}(t) \quad (34)$$

Employing a linear interpolation:

$$\Delta\gamma^{(\alpha)} = \Delta t \left[(1 - \theta)\dot{\gamma}_t^{(\alpha)} + \theta\dot{\gamma}_{t+\Delta t}^{(\alpha)} \right] \quad (35)$$

The slipping rate at $t + \Delta t$ can be written utilising a Taylor expansion to approximate it:

$$\dot{\gamma}_{t+\Delta t}^{(\alpha)} = \dot{\gamma}_t^{(\alpha)} + \frac{\partial\dot{\gamma}^{(\alpha)}}{\partial\tau^{(\alpha)}}\Delta\tau^{(\alpha)} + \frac{\partial\dot{\gamma}^{(\alpha)}}{\partial g^{(\alpha)}}\Delta g^{(\alpha)} \quad (36)$$

Replacing $\dot{\gamma}_{t+\Delta t}^{(\alpha)}$ in Equation (35) with Equation (36):

$$\Delta\gamma^{(\alpha)} = \Delta t(1 - \theta)\dot{\gamma}_t^{(\alpha)} + \Delta t\theta\dot{\gamma}_{t+\Delta t}^{(\alpha)}$$

$$\Delta\gamma^{(\alpha)} = \Delta t(1 - \theta)\dot{\gamma}_t^{(\alpha)} + \Delta t\theta \left(\dot{\gamma}_t^{(\alpha)} + \frac{\partial\dot{\gamma}^{(\alpha)}}{\partial\tau^{(\alpha)}}\Delta\tau^{(\alpha)} + \frac{\partial\dot{\gamma}^{(\alpha)}}{\partial g^{(\alpha)}}\Delta g^{(\alpha)} \right)$$

$$\begin{aligned}
\Delta\gamma^{(\alpha)} &= \Delta t \dot{\gamma}_t^{(\alpha)} - \Delta t \theta \dot{\gamma}_t^{(\alpha)} + \Delta t \theta \dot{\gamma}_t^{(\alpha)} + \Delta t \theta \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \tau^{(\alpha)}} \Delta \tau^{(\alpha)} + \Delta t \theta \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial g^{(\alpha)}} \Delta g^{(\alpha)} \\
\Delta\gamma^{(\alpha)} &= \Delta t \dot{\gamma}_t^{(\alpha)} + \Delta t \theta \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \tau^{(\alpha)}} \Delta \tau^{(\alpha)} + \Delta t \theta \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial g^{(\alpha)}} \Delta g^{(\alpha)} \\
\Delta\gamma^{(\alpha)} &= \Delta t \left(\dot{\gamma}_t^{(\alpha)} + \theta \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \tau^{(\alpha)}} \Delta \tau^{(\alpha)} + \theta \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial g^{(\alpha)}} \Delta g^{(\alpha)} \right)
\end{aligned} \tag{37}$$

To solve for the $\Delta\gamma^{(\alpha)}$ using the Taylor expansion, the increments in resolved shear stress and the slip resistance must be substituted by their expressions since they depend on $\Delta\gamma^{(\alpha)}$. The form of $\Delta\tau^{(\alpha)}$ was obtained in a previous section and it was labelled as Equation (22). The strain hardening equation (2.3.2) in Huang's report is as follows:

$$\dot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^{(\beta)} \tag{38}$$

Expressed in incremental form:

$$\Delta g^{(\alpha)} = \sum_{\beta} h_{\alpha\beta} \Delta \gamma^{(\beta)} \operatorname{sign}(\dot{\gamma}_t^{(\beta)}) \tag{39}$$

where the sign function was included to consider the sign of the slip direction. This avoids cases in which $\Delta\gamma^{(\alpha)}$ is negative which could artificially reduce the slip resistance. A negative $\Delta\gamma^{(\beta)}$ would imply a reversal of slip direction in the slip system. The sign function ensures that no matter whether the slip increment is positive or negative, the slip resistance never decreases.

The addition of the sign function seems counterintuitive when considering the Bauschinger effect. However, $g^{(\alpha)}$ has the role of modelling the average dislocation density and how does it change with the effect of external forces. The slip resistance acts as a scalar that cannot distinguish loading direction. Huang's original implementation does not take into consideration the Bauschinger effect. This will be addressed in a later section of this document, as the UMAT presented in this work implements the Bauschinger effect through a set of backstresses that shift the driving force.

Inserting Equation (23) and Equation (39) into Equation (37):

$$\begin{aligned}
\Delta\gamma^{(\alpha)} &= \Delta t \left(\dot{\gamma}_t^{(\alpha)} + \theta \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \tau^{(\alpha)}} \left(L_{ijkl} \mu_{kl}^{(\alpha)} + \omega_{ik}^{(\alpha)} \sigma_{jk} + \omega_{jk}^{(\alpha)} \sigma_{ik} \right) \left[\Delta \varepsilon_{ij} - \sum_{\beta} \mu_{ij}^{(\beta)} \Delta \gamma^{(\beta)} \right] \right. \\
&\quad \left. + \theta \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial g^{(\alpha)}} \sum_{\beta} h_{\alpha\beta} \Delta \gamma^{(\beta)} \operatorname{sign}(\dot{\gamma}_t^{(\beta)}) \right)
\end{aligned}$$

$$\begin{aligned}\Delta\gamma^{(\alpha)} &= \Delta t \dot{\gamma}_t^{(\alpha)} + \Delta t \theta \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \tau^{(\alpha)}} \left(L_{ijkl} \mu_{kl}^{(\alpha)} + \omega_{ik}^{(\alpha)} \sigma_{jk} + \omega_{jk}^{(\alpha)} \sigma_{ik} \right) \left[\Delta \varepsilon_{ij} - \sum_{\beta} \mu_{ij}^{(\beta)} \Delta \gamma^{(\beta)} \right] \\ &\quad + \Delta t \theta \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial g^{(\alpha)}} \sum_{\beta} h_{\alpha\beta} \Delta \gamma^{(\beta)} \operatorname{sign}(\dot{\gamma}_t^{(\beta)})\end{aligned}$$

Using the Kronecker delta, the increment of shear strain in slip system α can be written as:

$$\Delta\gamma^{(\beta)} = \sum_{\beta} \delta_{\alpha\beta} \Delta\gamma^{(\beta)}$$

Consequently:

$$\begin{aligned}& \sum_{\beta} \delta_{\alpha\beta} \Delta\gamma^{(\beta)} + \Delta t \theta \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \tau^{(\alpha)}} \left[L_{ijkl} \mu_{kl}^{(\alpha)} + \omega_{ik}^{(\alpha)} \sigma_{jk} + \omega_{jk}^{(\alpha)} \sigma_{ik} \right] \sum_{\beta} \mu_{ij}^{(\beta)} \Delta\gamma^{(\beta)} \\ &\quad - \Delta t \theta \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial g^{(\alpha)}} \sum_{\beta} h_{\alpha\beta} \Delta\gamma^{(\beta)} \operatorname{sign}(\dot{\gamma}_t^{(\beta)}) \\ &= \Delta t \dot{\gamma}_t^{(\alpha)} + \Delta t \theta \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \tau^{(\alpha)}} \left[L_{ijkl} \mu_{kl}^{(\alpha)} + \omega_{ik}^{(\alpha)} \sigma_{jk} + \omega_{jk}^{(\alpha)} \sigma_{ik} \right] \Delta \varepsilon_{ij} \\ & \sum_{\beta} \left\{ \delta_{\alpha\beta} + \theta \Delta t \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \tau^{(\alpha)}} \left[L_{ijkl} \mu_{kl}^{(\alpha)} + \omega_{ik}^{(\alpha)} \sigma_{jk} + \omega_{jk}^{(\alpha)} \sigma_{ik} \right] \mu_{ij}^{(\beta)} \right. \\ &\quad \left. - \theta \Delta t \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial g^{(\alpha)}} h_{\alpha\beta} \operatorname{sign}(\dot{\gamma}_t^{(\beta)}) \right\} \Delta\gamma^{(\beta)} \quad (40) \\ &= \dot{\gamma}_t^{(\alpha)} \Delta t + \theta \Delta t \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \tau^{(\alpha)}} \left[L_{ijkl} \mu_{kl}^{(\alpha)} + \omega_{ik}^{(\alpha)} \sigma_{jk} + \omega_{jk}^{(\alpha)} \sigma_{ik} \right] \Delta \varepsilon_{ij}\end{aligned}$$

Equation (40) corresponds to Equation (3.2.5) in Huang's technical report and allows the increment of shear strain in each slip system to be calculated using Taylor's expansion. Equation (40) is solved using LU decomposition.

7 Lattice Rotation Derivations

Equations (2.1.2a) and (2.1.2b) in Huang's technical report define the slip direction and slip plane normal vectors and the mapping between the reference crystal basis (before deformation) and the current lattice basis (after deformation):

$$\mathbf{s}^{*(\alpha)} = \mathbf{F}^* \mathbf{s}^{(\alpha)} \quad (41)$$

$$\mathbf{m}^{*(\alpha)} = \mathbf{m}^{(\alpha)} \mathbf{F}^{*-1} \quad (42)$$

Differentiating Equation (41) with respect to time results in Equation (3.3.1a):

$$\begin{aligned}\dot{\mathbf{s}}^{*(\alpha)} &= \dot{\mathbf{F}}^* \mathbf{s}^{(\alpha)} = \dot{\mathbf{F}}^* \mathbf{F}^{*-1} \mathbf{s}^{*(\alpha)} = \mathbf{L}^* \mathbf{s}^{*(\alpha)} = (\mathbf{D}^* + \boldsymbol{\Omega}^*) \mathbf{s}^{*(\alpha)} \\ \dot{\mathbf{s}}^{*(\alpha)} &= (\mathbf{D}^* + \boldsymbol{\Omega}^*) \mathbf{s}^{*(\alpha)}\end{aligned}\quad (43)$$

Using the lattice and plastic decomposition of the velocity gradient and Equation (30):

$$\mathbf{D}^* + \boldsymbol{\Omega}^* = (\mathbf{D} + \boldsymbol{\Omega}) - (\mathbf{D}^P + \boldsymbol{\Omega}^P)$$

$$\mathbf{D}^* + \boldsymbol{\Omega}^* = (\mathbf{D} + \boldsymbol{\Omega}) - \sum_{\alpha} \dot{\gamma}^{(\alpha)} [\boldsymbol{\mu}^{(\alpha)} + \boldsymbol{\omega}^{(\alpha)}] \quad (44)$$

Inserting Equation (44) into Equation (43), using Equation (21) and using indicial and incremental form, Equation (3.3.2a) is obtained:

$$\Delta s_i^{*(\alpha)} = \left(\Delta \varepsilon_{ij} + \Omega_{ij} \Delta t - \sum_{\beta} [\mu_{ij}^{(\beta)} + \omega_{ij}^{(\beta)}] \Delta \gamma^{(\beta)} \right) s_i^{*(\alpha)} \quad (45)$$

For the slip plane mapping defined in Equation (42), applying the temporal derivative operator yields Equation (3.3.1b):

$$\dot{\mathbf{m}}^{*(\alpha)} = \mathbf{m}^{(\alpha)} \dot{\mathbf{F}}^{*-1}$$

The derivative of the inverse of the deformation gradient can be expressed as follows:

$$\begin{aligned}\frac{\partial (\mathbf{F}^* \mathbf{F}^{*-1})}{\partial t} &= \mathbf{I} \\ \dot{\mathbf{F}}^* \mathbf{F}^{*-1} + \mathbf{F}^* \frac{\partial (\mathbf{F}^{*-1})}{\partial t} &= \mathbf{0} \\ \frac{\partial \mathbf{F}^{*-1}}{\partial t} &= -\mathbf{F}^{*-1} \dot{\mathbf{F}}^* \mathbf{F}^{*-1}\end{aligned}$$

Therefore:

$$\begin{aligned}\dot{\mathbf{m}}^{*(\alpha)} &= \mathbf{m}^{(\alpha)} \dot{\mathbf{F}}^{*-1} = -\mathbf{m}^{(\alpha)} \mathbf{F}^{*-1} \dot{\mathbf{F}}^* \mathbf{F}^{*-1} = -\mathbf{m}^{*(\alpha)} \mathbf{L}^* \\ &= -\mathbf{m}^{*(\alpha)} (\mathbf{D}^* + \boldsymbol{\Omega}^*) \\ \dot{\mathbf{m}}^{*(\alpha)} &= -\mathbf{m}^{*(\alpha)} (\mathbf{D}^* + \boldsymbol{\Omega}^*)\end{aligned}\quad (46)$$

Replacing $\mathbf{D}^* + \boldsymbol{\Omega}^*$ with Equation (44) and using Equation (21) results in Equation (3.3.2b) of Huang's technical report:

$$\Delta m_i^{*(\alpha)} = -m_j^{*(\alpha)} \left(\Delta \varepsilon_{ij} + \Omega_{ij} \Delta t - \sum_{\beta} [\mu_{ij}^{(\beta)} + \omega_{ij}^{(\beta)}] \Delta \gamma^{(\beta)} \right) \quad (47)$$

8 Newton–Raphson Solution of Nonlinear Incremental Slip Equations

Instead of relying solely on Equation (40), i.e. the previously derived linear approximation, Huang used the Newton–Raphson method to enforce a null residual which leads to a more accurate and consistent solution for the increment of shear strain $\Delta\gamma^{(\alpha)}$. For $t + \Delta t$:

$$\dot{\gamma}_{t+\Delta t}^{(\alpha)} = \dot{\gamma}_0^{(\alpha)} \left| \frac{\tau^{(\alpha)} + \Delta\tau^{(\alpha)}}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^n \text{sign} (\tau^{(\alpha)} + \Delta\tau^{(\alpha)}) \quad (48)$$

Rearranging Equation (35):

$$\Delta\gamma^{(\alpha)} - \Delta t(1 - \theta)\dot{\gamma}_t^{(\alpha)} - \Delta t\theta\dot{\gamma}_{t+\Delta t}^{(\alpha)} = 0 \quad (49)$$

Inserting Equation (48) into Equation (49) and defining $R^{(\alpha)}(\Delta\gamma^{(\alpha)})$ as the residual from an approximated slip increment $\Delta\gamma_k^{(\alpha)}$ at iteration k :

$$\begin{aligned} R^{(\alpha)} \left(\Delta\gamma_k^{(\alpha)} \right) &= \Delta\gamma_k^{(\alpha)} - \Delta t(1 - \theta)\dot{\gamma}_t^{(\alpha)} \\ &\quad - \Delta t\theta\dot{\gamma}_0^{(\alpha)} \left| \frac{\tau_t^{(\alpha)} + \Delta\tau^{(\alpha)}}{g_t^{(\alpha)} + \Delta g^{(\alpha)}} \right|^n \text{sign} (\tau_t^{(\alpha)} + \Delta\tau^{(\alpha)}) \end{aligned} \quad (50)$$

Where $\dot{\gamma}_t^{(\alpha)}$, $\tau_t^{(\alpha)}$ and $g_t^{(\alpha)}$ are the slip rate, the shear stress and slip resistance from the previous converged step. The increment $\Delta\gamma_k^{(\alpha)}$ is a trial value that can be obtained with Equation (40). Equation (50) expresses a nonlinear function and it can be linearised via a first-order Taylor expansion as follows:

$$R^{(\alpha)} \left(\Delta\gamma_k^{(\alpha)} + \Delta\gamma_{\text{corr}}^{(\alpha)} \right) \approx R^{(\alpha)} \left(\Delta\gamma_k^{(\alpha)} \right) + \sum_{\beta} \frac{\partial R^{(\alpha)}}{\partial \Delta\gamma^{(\beta)}} \Big|_{\Delta\gamma_k^{(\alpha)}} \Delta\gamma_{\text{corr}}^{(\beta)} \quad (51)$$

where $\Delta\gamma_{\text{corr}}^{(\alpha)}$ is a correction increment such as:

$$\Delta\gamma_{k+1}^{(\alpha)} = \Delta\gamma_k^{(\alpha)} + \Delta\gamma_{\text{corr}}^{(\alpha)} \quad (52)$$

Setting the linearised residual in Equation (51) to zero results in the Newton step:

$$\sum_{\beta} \frac{\partial R^{(\alpha)}}{\partial \Delta\gamma^{(\beta)}} \Big|_{\Delta\gamma_k^{(\alpha)}} \Delta\gamma_{\text{corr}}^{(\beta)} = -R^{(\alpha)} \left(\Delta\gamma_k^{(\alpha)} \right) \quad (53)$$

At each Newton iteration, the current guess $\Delta\gamma_k^{(\alpha)}$ is updated by adding a correction $\Delta\gamma_{\text{corr}}^{(\alpha)}$, obtained by solving the linearised residual. The correction $\Delta\gamma_{\text{corr}}^{(\alpha)}$ is a numerical adjustment to the trial slip increment $\Delta\gamma_k^{(\alpha)}$, chosen so that the nonlinear residual is driven towards zero.

Equation (53) defines the Jacobian $K_{\alpha\beta}$ for constitutive updates (also called the tangent operator):

$$K_{\alpha\beta} \left(\Delta\gamma_k^{(\alpha)} \right) = \frac{\partial R^{(\alpha)}}{\partial \Delta\gamma^{(\beta)}} \Big|_{\Delta\gamma_k^{(\alpha)}} \quad (54)$$

The Jacobian results from the derivative of Equation (50) with respect to the shear strain increments. For clarity, each term is derived separately:

$$\begin{aligned} R^{(\alpha)} \left(\Delta\gamma_k^{(\alpha)} \right) &= \underbrace{\Delta\gamma_k^{(\alpha)}}_{\text{Term 1}} - \underbrace{\Delta t(1-\theta)\dot{\gamma}_t^{(\alpha)}}_{\text{Term 2}} \\ &\quad - \underbrace{\Delta t\theta\dot{\gamma}_0^{(\alpha)} \left| \frac{\tau^{(\alpha)} + \Delta\tau^{(\alpha)}}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^{n-1} \frac{\tau^{(\alpha)} + \Delta\tau^{(\alpha)}}{g^{(\alpha)} + \Delta g^{(\alpha)}}}_{\text{Term 3}} \end{aligned}$$

Term 1:

$$\frac{\partial \Delta\gamma_k^{(\alpha)}}{\partial \Delta\gamma^{(\beta)}} = \delta_{\alpha\beta}$$

Term 2:

$$\frac{\partial \left[\Delta t(1-\theta)\dot{\gamma}_k^{(\alpha)} \right]}{\partial \Delta\gamma^{(\beta)}} = 0$$

The derivative of Term 2 is zero since Δt , θ , and $\dot{\gamma}_k^{(\alpha)}$ are fixed at the current time step and at the previous iteration (time step k), respectively.

Term 3:

$$\Delta t \theta \dot{\gamma}_0^{(\alpha)} \left| \frac{\tau^{(\alpha)} + \Delta\tau^{(\alpha)}}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^{n-1} \text{sign}(\tau^{(\alpha)} + \Delta\tau^{(\alpha)}) = f \left(\frac{\tau^{(\alpha)} + \Delta\tau^{(\alpha)}}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right)$$

$$\frac{\partial (\text{Term 3})}{\partial \Delta\gamma^{(\beta)}} = \Delta t \theta \frac{\partial \left[\dot{\gamma}_0^{(\alpha)} f(\tau^{(\alpha)} + \Delta\tau^{(\alpha)}, g^{(\alpha)} + \Delta g^{(\alpha)}) \right]}{\partial \Delta\gamma^{(\beta)}}$$

$$\frac{\partial (\text{Term 3})}{\partial \Delta\gamma^{(\beta)}} = \Delta t \theta \left[\frac{\partial \dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial \Delta\tau^{(\alpha)}} \frac{\partial \Delta\tau^{(\alpha)}}{\partial \Delta\gamma^{(\beta)}} + \frac{\partial \dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial g^{(\alpha)}} \frac{\partial \Delta g^{(\alpha)}}{\partial \Delta\gamma^{(\beta)}} \right] = \Delta t \theta [T1 T2 + T3 T4] \quad (55)$$

T1

Considering $X = \tau^{(\alpha)} + \Delta\tau^{(\alpha)}/g^{(\alpha)} + \Delta g^{(\alpha)}$:

$$\dot{\gamma}_{t+\Delta t}^{(\alpha)} = \dot{\gamma}_0^{(\alpha)} |X|^n \text{sign}(X) = \dot{\gamma}_0^{(\alpha)} X |X|^{n-1} = \dot{\gamma}_0^{(\alpha)} h$$

Applying the chain rule:

$$T1 = \frac{\partial \dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial \Delta \tau^{(\alpha)}} = \frac{\partial h}{\partial X} \frac{\partial X}{\partial \Delta \tau^{(\alpha)}}$$

$$\frac{\partial h}{\partial X} = |X|^{n-1} + X(n-1)|X|^{n-2} \operatorname{sign}(X) = |X|^{n-2} [|X| + X(n-1) \operatorname{sign}(X)]$$

$$\frac{\partial h}{\partial X} = |X|^{n-2} [|X| + |X|(n-1)] = |X|^{n-2} [|X|(1 + (n-1))] = |X|^{n-2}|X|n = n|X|^{n-1}$$

$$\frac{\partial X}{\partial \Delta \tau^{(\alpha)}} = \frac{1}{g^{(\alpha)} + \Delta g^{(\alpha)}}$$

Therefore:

$$T1 = \frac{\partial \dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial \Delta \tau^{(\alpha)}} = \dot{\gamma}_0^{(\alpha)} n \left| \frac{\tau^{(\alpha)} + \Delta \tau^{(\alpha)}}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^{n-1} \frac{1}{g^{(\alpha)} + \Delta g^{(\alpha)}}$$

T2

Let $S_{ij}^{(\alpha)} = L_{ijkl}\mu_{kl}^{(\alpha)} + \omega_{ik}^{(\alpha)}\sigma_{jk} + \omega_{jk}^{(\alpha)}\sigma_{ik}$:

$$\Delta \tau^{(\alpha)} = S_{ij}^{(\alpha)} \left[\Delta \varepsilon_{ij} - \sum_{\beta} \mu_{ij}^{(\beta)} \Delta \gamma^{(\beta)} \right]$$

$$\frac{\partial \Delta \tau^{(\alpha)}}{\partial \Delta \gamma^{(\beta)}} = S_{ij}^{(\alpha)} \left[0 - \mu_{ij}^{(\beta)} \right] = -S_{ij}^{(\alpha)} \mu_{ij}^{(\beta)}$$

$$T2 = -S_{ij}^{(\alpha)} \mu_{ij}^{(\beta)}$$

T3

Upon setting $X = \tau^{(\alpha)} + \Delta \tau^{(\alpha)}/g^{(\alpha)} + \Delta g^{(\alpha)}$ and applying the chain rule analogously to that used for T1:

$$T3 = \frac{\partial \dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial \Delta g^{(\alpha)}} = \frac{\partial h}{\partial X} \frac{\partial X}{\partial \Delta g^{(\alpha)}}$$

$$\frac{\partial h}{\partial X} = n|X|^{n-1}$$

$$\frac{\partial X}{\partial \Delta g^{(\alpha)}} = -\frac{\tau^{(\alpha)} + \Delta \tau^{(\alpha)}}{(g^{(\alpha)} + \Delta g^{(\alpha)})^2}$$

Consequently:

$$T3 = \dot{\gamma}_0^{(\alpha)} n \left| \frac{\tau^{(\alpha)} + \Delta\tau^{(\alpha)}}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^{n-1} \left(-\frac{\tau^{(\alpha)} + \Delta\tau^{(\alpha)}}{(g^{(\alpha)} + \Delta g^{(\alpha)})^2} \right)$$

T4

Defining the cumulative shear slip on slip system β as:

$$\Gamma_\beta = \int_0^t |\dot{\gamma}^{(\beta)}| dt \quad (56)$$

Equation (39) can be expressed as:

$$\Delta g^{(\alpha)} = \sum_{\beta} h_{\alpha\beta}(\Gamma) \Delta\gamma^{(\beta)} \operatorname{sign}(\dot{\gamma}_t^{(\beta)}) \quad (57)$$

where Γ represents a state variable that depends on the accumulated slip. The hardening modulus $h_{\alpha\beta}$ depends on all cumulative slips $\Gamma = \{\Gamma_1, \Gamma_2, \dots\}$. Hence:

$$\begin{aligned} \frac{\partial \Delta g^{(\alpha)}}{\partial \Delta\gamma^{(\beta)}} &= \sum_{\mu} h_{\alpha\mu}(\Gamma) \frac{\partial \Delta\gamma^{(\mu)}}{\partial \Delta\gamma^{(\beta)}} \operatorname{sign}(\dot{\gamma}_t^{(\mu)}) + \sum_{\mu} \frac{\partial h_{\alpha\mu}(\Gamma)}{\partial \Delta\gamma^{(\beta)}} \Delta\gamma^{(\mu)} \operatorname{sign}(\dot{\gamma}_t^{(\mu)}) \\ \frac{\partial \Delta g^{(\alpha)}}{\partial \Delta\gamma^{(\beta)}} &= \sum_{\mu} h_{\alpha\mu}(\Gamma) \delta_{\mu\beta} \operatorname{sign}(\dot{\gamma}_t^{(\mu)}) + \sum_{\mu} \frac{\partial h_{\alpha\mu}(\Gamma)}{\partial \Delta\gamma^{(\beta)}} \Delta\gamma^{(\mu)} \operatorname{sign}(\dot{\gamma}_t^{(\mu)}) \end{aligned}$$

The Kronecker delta nullifies the summation for all cases where $\mu \neq \beta$. Thus:

$$\frac{\partial \Delta g^{(\alpha)}}{\partial \Delta\gamma^{(\beta)}} = h_{\alpha\beta}(\Gamma) \operatorname{sign}(\dot{\gamma}_t^{(\beta)}) + \sum_{\mu} \frac{\partial h_{\alpha\mu}(\Gamma)}{\partial \Delta\gamma^{(\beta)}} \Delta\gamma^{(\mu)} \operatorname{sign}(\dot{\gamma}_t^{(\mu)})$$

The derivative $\partial h_{\alpha\mu}(\Gamma)/\partial \Delta\gamma^{(\beta)}$ is explicitly expanded as follows:

$$\frac{\partial h_{\alpha\mu}(\Gamma)}{\partial \Delta\gamma^{(\beta)}} = \frac{\partial h_{\alpha\mu}}{\partial \Delta\Gamma} \frac{\partial \Delta\Gamma}{\partial \Delta\gamma^{(\beta)}} = \frac{\partial h_{\alpha\mu}}{\partial \Gamma} \frac{\partial |\Delta\gamma^{(\beta)}|}{\partial \Delta\gamma^{(\beta)}} = \frac{\partial h_{\alpha\mu}}{\partial \Gamma} \operatorname{sign}(\Delta\gamma^{(\beta)})$$

As a result:

$$\frac{\partial \Delta g^{(\alpha)}}{\partial \Delta\gamma^{(\beta)}} = h_{\alpha\beta}(\Gamma) \operatorname{sign}(\dot{\gamma}_t^{(\beta)}) + \sum_{\mu} \frac{\partial h_{\alpha\mu}}{\partial \Gamma} \operatorname{sign}(\Delta\gamma^{(\beta)}) \Delta\gamma^{(\mu)} \operatorname{sign}(\dot{\gamma}_t^{(\mu)})$$

The sign-consistency approximation is adopted, assuming that the sign functions remain unchanged over a sufficiently small increment. Therefore:

$$T4 = \frac{\partial \Delta g^{(\alpha)}}{\partial \Delta\gamma^{(\beta)}} = h_{\alpha\beta}(\Gamma) \operatorname{sign}(\dot{\gamma}_t^{(\beta)}) + \sum_{\mu} \frac{\partial h_{\alpha\mu}}{\partial \Gamma_{\beta}} |\Delta\gamma^{(\mu)}|$$

By consolidating the four previously derived terms, the full relation for the derivative

of *Term 3* is obtained:

$$\begin{aligned} \frac{\partial(\text{Term 3})}{\partial\Delta\gamma^{(\beta)}} &= \Delta t \theta \left[\dot{\gamma}_0^{(\alpha)} n \left| \frac{\tau^{(\alpha)} + \Delta\tau^{(\alpha)}}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^{n-1} \frac{1}{g^{(\alpha)} + \Delta g^{(\alpha)}} \left(-S_{ij}^{(\alpha)} : \mu_{ij}^{(\beta)} \right) \right. \\ &\quad + \dot{\gamma}_0^{(\alpha)} n \left| \frac{\tau^{(\alpha)} + \Delta\tau^{(\alpha)}}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^{n-1} \frac{-(\tau^{(\alpha)} + \Delta\tau^{(\alpha)})}{(g^{(\alpha)} + \Delta g^{(\alpha)})^2} \left(h_{\alpha\beta}(\Gamma) \operatorname{sign}(\dot{\gamma}_t^{(\beta)}) \right. \\ &\quad \left. \left. + \sum_{\mu} \frac{\partial h_{\alpha\mu}}{\partial\Gamma_{\beta}} |\Delta\gamma^{(\mu)}| \right) \right] \end{aligned}$$

It is worth noting that the resolved shear stress and slip resistance are expressed as:

$$\begin{aligned} \tau &= \tau_t + \Delta\tau \\ g &= g_t + \Delta g \end{aligned}$$

Therefore, they are affine functions of the corresponding increments, with unit slope. Consequently, the partial derivatives with respect to totals and with respect to increments are identical, that is:

$$\begin{aligned} \frac{\partial\dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial\Delta\tau^{(\alpha)}} &= \frac{\partial\dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial\tau^{(\alpha)}} \\ \frac{\partial\dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial\Delta g^{(\alpha)}} &= \frac{\partial\dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial g^{(\alpha)}} \end{aligned}$$

Having derived the individual contributions, the left-hand side (LHS) expression of Equation (53) can now be written as follows:

$$\begin{aligned} \sum_{\beta} \left\{ \delta_{\alpha\beta} - \Delta t \theta \left[\dot{\gamma}_0^{(\alpha)} n \left| \frac{\tau^{(\alpha)} + \Delta\tau^{(\alpha)}}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^{n-1} \frac{1}{g^{(\alpha)} + \Delta g^{(\alpha)}} \left(-S_{ij}^{(\alpha)} : \mu_{ij}^{(\beta)} \right) \right. \right. \\ \left. \left. + \dot{\gamma}_0^{(\alpha)} n \left| \frac{\tau^{(\alpha)} + \Delta\tau^{(\alpha)}}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^{n-1} \frac{-(\tau^{(\alpha)} + \Delta\tau^{(\alpha)})}{(g^{(\alpha)} + \Delta g^{(\alpha)})^2} \left(h_{\alpha\beta}(\Gamma) \operatorname{sign}(\dot{\gamma}_t^{(\beta)}) \right. \right. \right. \\ \left. \left. \left. + \sum_{\mu} \frac{\partial h_{\alpha\mu}}{\partial\Gamma_{\beta}} |\Delta\gamma^{(\mu)}| \right) \right) \right\} \Delta\gamma_{\text{corr}}^{(\alpha)} = -R^{(\alpha)} \left(\Delta\gamma_k^{(\alpha)} \right) \end{aligned} \quad (58)$$

Inserting Equation (50) into Equation (58):

$$\begin{aligned}
& \sum_{\beta} \left\{ \delta_{\alpha\beta} - \Delta t \theta \left[\dot{\gamma}_0^{(\alpha)} n \left| \frac{\tau^{(\alpha)} + \Delta\tau^{(\alpha)}}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^{n-1} \frac{1}{g^{(\alpha)} + \Delta g^{(\alpha)}} (-S_{ij}^{(\alpha)} : \mu_{ij}^{(\beta)}) \right. \right. \\
& \quad \left. \left. + \dot{\gamma}_0^{(\alpha)} n \left| \frac{\tau^{(\alpha)} + \Delta\tau^{(\alpha)}}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^{n-1} \frac{-(\tau^{(\alpha)} + \Delta\tau^{(\alpha)})}{(g^{(\alpha)} + \Delta g^{(\alpha)})^2} (h_{\alpha\beta}(\Gamma) \operatorname{sign}(\dot{\gamma}_t^{(\beta)}) \right. \right. \\
& \quad \left. \left. + \sum_{\mu} \frac{\partial h_{\alpha\mu}}{\partial \Gamma_{\beta}} |\Delta\gamma^{(\mu)}|) \right] \right\} \Delta\gamma_{\text{corr}}^{(\alpha)} \\
& = -\Delta\gamma_k^{(\alpha)} + \Delta t (1 - \theta) \dot{\gamma}_t^{(\alpha)} + \Delta t \theta \dot{\gamma}_0^{(\alpha)} \left| \frac{\tau_t^{(\alpha)} + \Delta\tau^{(\alpha)}}{g_t^{(\alpha)} + \Delta g^{(\alpha)}} \right|^n \operatorname{sign}(\tau^{(\alpha)} + \Delta\tau^{(\alpha)}) \tag{59}
\end{aligned}$$

Equation (59) can be expressed in a compact form as:

$$\begin{aligned}
& \sum_{\beta} \left\{ \delta_{\alpha\beta} + \Delta t \theta \frac{\partial \dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial \tau^{(\alpha)}} (S_{ij}^{(\alpha)} : \mu_{ij}^{(\beta)}) \right. \\
& \quad \left. - \frac{\partial \dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial g^{(\alpha)}} \left[h_{\alpha\beta}(\Gamma) \operatorname{sign}(\dot{\gamma}_t^{(\beta)}) + \sum_{\mu} \frac{\partial h_{\alpha\mu}}{\partial \Gamma_{\beta}} |\Delta\gamma^{(\mu)}| \right] \right\} \Delta\gamma_{\text{corr}}^{(\alpha)} \tag{60} \\
& = -\Delta\gamma_k^{(\alpha)} + \Delta t (1 - \theta) \dot{\gamma}_t^{(\alpha)} \\
& \quad + \Delta t \theta \dot{\gamma}_0^{(\alpha)} \left| \frac{\tau_t^{(\alpha)} + \Delta\tau^{(\alpha)}}{g_t^{(\alpha)} + \Delta g^{(\alpha)}} \right|^n \operatorname{sign}(\tau^{(\alpha)} + \Delta\tau^{(\alpha)})
\end{aligned}$$

The form of Equation (60) is similar to that of Equation (40). The reason is that the Newton–Raphson method is essentially a first-order Taylor expansion of the residual function R about the current estimate. The only distinction is the additional term arising from the derivative of the hardening moduli $h_{\alpha\mu}$ with respect to the cumulative slip Γ_{β} , weighted by the magnitude of the slip increment. This distinction is explicitly exploited in Huang’s numerical implementation: the derivative of the hardening moduli with respect to the cumulative slip is accounted for only after the first iteration, through the inclusion of the DHDGDG term in the Jacobian update. When considering a base point $\Delta\gamma_0 = 0$, both expressions are equal:

$$-R_0^{(\alpha)} = \Delta t (1 - \theta) \dot{\gamma}_t^{(\alpha)} + \Delta t \theta \dot{\gamma}^{(\alpha)} \left(\frac{\tau_t^{(\alpha)} + \mathbf{S}^{(\alpha)} : \Delta\boldsymbol{\varepsilon}}{g_t^{(\alpha)}} \right)$$

Expanding the rate function about time t :

$$\dot{\gamma}^{(\alpha)} \left(\frac{\tau_t^{(\alpha)} + \mathbf{S}^{(\alpha)} : \Delta\boldsymbol{\varepsilon}}{g_t^{(\alpha)}} \right) \approx \dot{\gamma}_t^{(\alpha)} + \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \tau} \Big|_t (\mathbf{S}^{(\alpha)} : \Delta\boldsymbol{\varepsilon}) + \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial g} \Big|_{t=0} \underbrace{\Delta g}_{=0}$$

$$\begin{aligned}
-R_0^{(\alpha)} &= \Delta t(1 - \theta) \dot{\gamma}_t^{(\alpha)} + \Delta t \theta \left[\dot{\gamma}_t^{(\alpha)} + \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \tau} \Big|_t (\mathbf{S}^{(\alpha)} : \Delta \boldsymbol{\varepsilon}) \right] \\
-R_0^{(\alpha)} &= \Delta t \dot{\gamma}_t^{(\alpha)} + \Delta t \theta \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \tau} \Big|_t (\mathbf{S}^{(\alpha)} : \Delta \boldsymbol{\varepsilon})
\end{aligned} \tag{61}$$

Equation (61) coincides with the right-hand side (RHS) of Equation (40). The left-hand side (LHS) of Equation (60) is also the same as the LHS of Equation (40) when $\Delta \gamma_0 = 0$.

9 Inclusion of the Bauschinger Effect in the Linearisation of the Slip Increment Equation

In the previous sections, the linearised form of the Taylor expansion of the shear rates per slip system and the Newton–Raphson equation were derived. However, the Bauschinger effect was not considered, despite being fundamental for the modelling of cyclic loading. To account for the Bauschinger effect, a backstress formulation based on the Armstrong–Frederick [11] nonlinear kinematic hardening model is adopted:

$$\dot{\chi}^{(\alpha)} = C \dot{\gamma}^{(\alpha)} - D \chi^{(\alpha)} |\dot{\gamma}^{(\alpha)}| \tag{62}$$

where the constant C causes the backstress to proportionally grow relative to the slip rate and D generates dynamic recovery, i.e. a reduction of the backstress as cyclic loading continues. The Bauschinger effect is directional, and after slip occurs in one direction, dislocation structures oppose reverse slip more weakly. This loss of resistance does not apply to all directions, but specifically in the effective resolved shear stress for the reversed system. Therefore, mathematically, shifting the driving force represents best this effect:

$$\tau_{\text{eff}}^{(\alpha)} = \tau^{(\alpha)} - \chi^{(\alpha)} \tag{63}$$

Equation (63) is inserted in Equation (32) or (33) to include the Bauschinger effect. Dislocation structures possess fast and slow recovery components and a single backstress is hardly capable to fit the early Bauschinger effect and the long-term cyclic stabilisation. Consequently, the Chaboche model [12] superimposes multiple backstress to better fit the experimental cyclic curves:

$$\tau_{\text{eff}}^{(\alpha)} = \tau^{(\alpha)} - \sum_m \chi_m^{(\alpha)} \tag{64}$$

Where m denotes the number of backstresses considered in the formulation. Adding backstresses to Equation (33) results in:

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0^{(\alpha)} \left| \frac{\tau^{(\alpha)} - \sum_m \chi_m^{(\alpha)}}{g^{(\alpha)}} \right|^n \text{sign} \left(\tau^{(\alpha)} - \sum_m \chi_m^{(\alpha)} \right) \quad (65)$$

As it was shown in the previous section, the Newton–Raphson scheme is based on the first-order Taylor expansion of the residual function around the current iteration point. Therefore, the derivation in the previous section will be utilised to derive the final expression when adding backstresses to the formulation. The residual in Equation (50) is modified by the inclusion of the backstresses as follows:

$$\begin{aligned} R^{(\alpha)} (\Delta\gamma_k^{(\alpha)}) &= \Delta\gamma_k^{(\alpha)} - \Delta t(1-\theta)\dot{\gamma}_t^{(\alpha)} \\ &\quad - \Delta t\theta\dot{\gamma}_0^{(\alpha)} \left| \frac{(\tau_t^{(\alpha)} + \Delta\tau^{(\alpha)}) - (\sum_m \chi_m^{(\alpha)} + \Delta\chi_m^{(\alpha)})}{g_t^{(\alpha)} + \Delta g^{(\alpha)}} \right|^n \\ &\quad \text{sign} \left((\tau_t^{(\alpha)} + \Delta\tau^{(\alpha)}) - \left(\sum_m \chi_m^{(\alpha)} + \Delta\chi_m^{(\alpha)} \right) \right) \end{aligned} \quad (66)$$

As shown in Equation (66), only the last term changes when the Bauschinger effect is considered. Consequently, following the derivation of the previous section, the only expression that varies when constructing the Newton-Raphson scheme is Equation (55):

$$\begin{aligned} \frac{\partial(Term\ 3)}{\partial\Delta\gamma^{(\beta)}} &= \Delta t\theta \left[\frac{\partial\dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial\Delta\tau^{(\alpha)}} \frac{\partial\Delta\tau^{(\alpha)}}{\partial\Delta\gamma^{(\beta)}} + \frac{\partial\dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial\Delta g^{(\alpha)}} \frac{\partial\Delta g^{(\alpha)}}{\partial\Delta\gamma^{(\beta)}} + \sum_m \frac{\partial\dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial\Delta\chi_m^{(\alpha)}} \frac{\partial\Delta\chi_m^{(\alpha)}}{\partial\Delta\gamma^{(\beta)}} \right] \\ &= \Delta t\theta [T1\ T2 + T3\ T4 + T5\ T6] \end{aligned} \quad (67)$$

It is worth noting that to implement the Bauschinger effect in all the derivations made previously the variable X is taken as

$$X = \frac{(\tau_t^{(\alpha)} + \Delta\tau^{(\alpha)}) - (\sum_m \chi_m^{(\alpha)} + \Delta\chi_m^{(\alpha)})}{g^{(\alpha)} + \Delta g^{(\alpha)}}.$$

T5

Applying the chain rule:

$$T5 = \frac{\partial\dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial\Delta\chi_m^{(\alpha)}} = \frac{\partial h}{\partial X} \frac{\partial X}{\partial\Delta\chi_m^{(\alpha)}}$$

$$\frac{\partial h}{\partial X} = n|X|^{n-1}$$

$$\frac{\partial X}{\partial\Delta\chi_m^{(\alpha)}} = \frac{-1}{g^{(\alpha)} + \Delta g^{(\alpha)}}$$

Consequently:

$$T5 = -\dot{\gamma}_0^{(\alpha)} \left| \frac{(\tau_t^{(\alpha)} + \Delta\tau^{(\alpha)}) - (\sum_m \chi_m^{(\alpha)} + \Delta\chi_m^{(\alpha)})}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^{n-1} \frac{1}{g^{(\alpha)} + \Delta g^{(\alpha)}}$$

T6

By discretising Equation (62) over the time increment Δt , the following incremental form is obtained:

$$\Delta\chi^{(\alpha)} = C\Delta\gamma^{(\alpha)} - D\chi^{(\alpha)} |\Delta\gamma^{(\alpha)}| \quad (68)$$

Hence:

$$T6 = \frac{\partial \Delta\chi_m^{(\alpha)}}{\partial \Delta\gamma^{(\beta)}} = \delta_{\alpha\beta} [C_m^{(\alpha)} - D_m^{(\alpha)} \chi_m^{(\alpha)} \operatorname{sign}(\Delta\gamma^{(\alpha)})]$$

By collecting terms, the resulting expression is:

$$\begin{aligned} \frac{\partial(Term\ 3)}{\partial \Delta\gamma^{(\beta)}} &= \Delta t \theta \left[\dot{\gamma}_0^{(\alpha)} n \left| \frac{(\tau_t^{(\alpha)} + \Delta\tau^{(\alpha)}) - (\sum_m \chi_m^{(\alpha)} + \Delta\chi_m^{(\alpha)})}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^{n-1} \frac{1}{g^{(\alpha)} + \Delta g^{(\alpha)}} (-S_{ij}^{(\alpha)} \mu_{ij}^{(\beta)}) \right. \\ &\quad + \dot{\gamma}_0^{(\alpha)} n \left| \frac{(\tau_t^{(\alpha)} + \Delta\tau^{(\alpha)}) - (\sum_m \chi_m^{(\alpha)} + \Delta\chi_m^{(\alpha)})}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^{n-1} \left(-\frac{(\tau_t^{(\alpha)} + \Delta\tau^{(\alpha)}) - (\sum_m \chi_m^{(\alpha)} + \Delta\chi_m^{(\alpha)})}{(g^{(\alpha)} + \Delta g^{(\alpha)})^2} \right) \\ &\quad \left(h_{\alpha\beta}(\Gamma) \operatorname{sign}(\dot{\gamma}_t^{(\beta)}) + \sum_{\mu} \frac{\partial h_{\alpha\mu}}{\partial \Gamma_{\beta}} |\Delta\gamma^{(\mu)}| \right) \right. \\ &\quad \left. + \sum_m \left(-\dot{\gamma}_0^{(\alpha)} n \left| \frac{(\tau_t^{(\alpha)} + \Delta\tau^{(\alpha)}) - (\sum_m \chi_m^{(\alpha)} + \Delta\chi_m^{(\alpha)})}{g^{(\alpha)} + \Delta g^{(\alpha)}} \right|^{n-1} \frac{1}{g^{(\alpha)} + \Delta g^{(\alpha)}} \delta_{\alpha\beta} [C_m^{(\alpha)} - D_m^{(\alpha)} \chi_m^{(\alpha)} \operatorname{sign}(\Delta\gamma^{(\alpha)})] \right) \right] \end{aligned}$$

Finally, introducing the derived term that considers backstresses into Equation (60):

$$\begin{aligned}
& \sum_{\beta} \left\{ \delta_{\alpha\beta} + \Delta t \theta \frac{\partial \dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial \tau^{(\alpha)}} \left(S_{ij}^{(\alpha)} : \mu_{ij}^{(\beta)} \right) \right. \\
& \quad - \frac{\partial \dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial g^{(\alpha)}} \left[h_{\alpha\beta}(\Gamma) \operatorname{sign}(\dot{\gamma}_t^{(\beta)}) + \sum_{\mu} \frac{\partial h_{\alpha\mu}}{\partial \Gamma_{\beta}} |\Delta \gamma^{(\mu)}| \right] \\
& \quad \left. + \sum_m \frac{\partial \dot{\gamma}_{t+\Delta t}^{(\alpha)}}{\partial \chi_m^{(\alpha)}} \delta_{\alpha\beta} [C_m^{(\alpha)} - D_m^{(\alpha)} \chi_m^{(\alpha)} \operatorname{sign}(\Delta \gamma^{(\alpha)})] \right\} \Delta \gamma_{\text{corr}}^{(\alpha)} \\
& = -\Delta \gamma_k^{(\alpha)} + \Delta t (1 - \theta) \dot{\gamma}_t^{(\alpha)} \\
& \quad + \Delta t \theta \dot{\gamma}_0^{(\alpha)} \left| \frac{(\tau_t^{(\alpha)} + \Delta \tau^{(\alpha)}) - (\sum_m \chi_m^{(\alpha)} + \Delta \chi_m^{(\alpha)})}{g_t^{(\alpha)} + \Delta g^{(\alpha)}} \right|^n \\
& \quad \operatorname{sign} \left((\tau_t^{(\alpha)} + \Delta \tau^{(\alpha)}) - (\sum_m \chi_m^{(\alpha)} + \Delta \chi_m^{(\alpha)}) \right) \\
& \quad + \Delta \tau^{(\alpha)} - \left(\sum_m \chi_m^{(\alpha)} + \Delta \chi_m^{(\alpha)} \right).
\end{aligned} \tag{69}$$

10 Consistent Tangent Stiffness Derivation

The material Jacobian matrix or consistent tangent stiffness matrix $\partial \Delta \boldsymbol{\sigma} / \partial \Delta \boldsymbol{\varepsilon}$ is required in the FEM when running a nonlinear material model. The derivative can be obtained by deriving Equation (31):

$$\begin{aligned}
\frac{\partial \Delta \boldsymbol{\sigma}}{\partial \Delta \boldsymbol{\varepsilon}} &= \frac{\partial (\mathbb{L} \Delta \boldsymbol{\varepsilon} - \boldsymbol{\sigma}(\mathbf{I} : \Delta \boldsymbol{\varepsilon}) - \sum_{\alpha} \mathbf{S}^{(\alpha)} \Delta \gamma^{(\alpha)})}{\partial \Delta \boldsymbol{\varepsilon}} \\
\frac{\partial \Delta \boldsymbol{\sigma}}{\partial \Delta \boldsymbol{\varepsilon}} &= \mathbb{L} - \boldsymbol{\sigma} \boldsymbol{\delta} - \sum_{\alpha} \mathbf{S}^{(\alpha)} \frac{\partial \Delta \gamma^{(\alpha)}}{\partial \Delta \boldsymbol{\varepsilon}}
\end{aligned} \tag{70}$$

To compute Equation (70), the derivative of the increments of shear strain per slip system is required. The derivative can be obtained by using the LU decomposition in Equation (53):

$$K_{\alpha\beta} \frac{\partial \Delta \gamma^{(\alpha)}}{\partial \Delta \boldsymbol{\varepsilon}} = -\frac{\partial R^{(\alpha)}}{\partial \Delta \boldsymbol{\varepsilon}} \tag{71}$$

Consequently, the derivative of the residual is as follows:

$$\begin{aligned}
\frac{\partial R^{(\alpha)}}{\partial \Delta \boldsymbol{\varepsilon}} &= -\theta \Delta t \left[\frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \tau} \frac{\partial \Delta \tau}{\partial \Delta \boldsymbol{\varepsilon}} + \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial g} \frac{\partial \Delta g^{(\alpha)}}{\partial \Delta \boldsymbol{\varepsilon}} + \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \chi} \frac{\partial \Delta \chi^{(\alpha)}}{\partial \Delta \boldsymbol{\varepsilon}} \right] \\
\frac{\partial R^{(\alpha)}}{\partial \Delta \boldsymbol{\varepsilon}} &= -\theta \Delta t \frac{\partial \dot{\gamma}^{(\alpha)}}{\partial \tau} \mathbf{S}^{(\alpha)}
\end{aligned} \tag{72}$$

By substituting Equation (72) into Equation (71), solving for $\partial\Delta\gamma^{(\alpha)}/\partial\Delta\varepsilon$, and subsequently inserting this expression into Equation (70), the Jacobian is obtained.

11 Step-by-Step Description of the UMAT Computations

The following set of steps is a high level description of the UMAT computations considering that the theory of finite strain and rotations and the Newton-Raphson iterative solver are used.

1. Calculate the elasticity matrix DLOCAL in the local cubic crystal system.
2. Calculate the rotation matrix \mathbf{D} which transforms from local to global coordinates.
3. Define NSET, THETA, NLGEOM, ITRATN, ITRMAX and GAMERR.
4. Calculate the spin increment $\Delta\Omega$ using Rodriguez formula.
5. Calculate the increment of dilatation strain for future computations that involve $\Delta\varepsilon_{kk}$.
6. In the first step of the simulation, the initial state is defined (number of slip systems and their corresponding orientation vectors) and the stress and Jacobian computed are purely elastic. From the second increment of the simulation onwards, the current state is retrieved.
7. The $\mathbf{S}_{ij}^{(\alpha)} = L_{ijkl}\mu_{kl}^{(\alpha)} + \omega_{jk}^{(\alpha)}\sigma_{ik} + \omega_{ik}^{(\alpha)}\sigma_{jk}$ tensor is calculated.
8. The $\dot{\gamma}^{(\alpha)}$ and $\partial\dot{\gamma}^{(\alpha)}/\partial X$ are calculated for each slip system where
$$X = \frac{\left(\tau_t^{(\alpha)} + \Delta\tau^{(\alpha)}\right) - \left(\sum_m \chi_m^{(\alpha)} + \Delta\chi_m^{(\alpha)}\right)}{g^{(\alpha)} + \Delta g^{(\alpha)}}.$$
9. The $h_{\alpha\beta}$ matrix is computed.
10. The Jacobian of the Newton-Raphson scheme is calculated and the matrix is decomposed in its LU form.
11. The right-hand side of the equation to solve for the $\Delta\gamma^{(\alpha)}$ is computed. The form of the equation depends on whether the Taylor expansion is used or the NR scheme is already operational.
12. Using the lower upper backwards substitution the $\Delta\gamma_{\text{corr}}^{(\alpha)}$ are obtained and the $\Delta\gamma_{k+1}^{(\alpha)}$ is computed.
13. The shear strain $\gamma^{(\alpha)}$, the current strength $g^{(\alpha)}$ and the kinematic hardening variables $\chi^{(\alpha)}$ are updated using the recently computed $\Delta\gamma^{(\alpha)}$.

14. The increment of strain associated with lattice stretching $\Delta\boldsymbol{\varepsilon}^* = \Delta\boldsymbol{\varepsilon} - \sum_\alpha \boldsymbol{\mu}^{(\alpha)} \Delta\gamma^{(\alpha)}$ (DELATS) is computed. Since DSTRAN is provided as a corotational measure of strain, it already excludes spin, and therefore only the symmetric slip contribution is subtracted.
15. The lattice velocity gradient \mathbf{L}^* is computed (DVGRAD).
16. The resolved shear stress $\tau^{(\alpha)}$ is updated.
17. The increment of stress $\Delta\boldsymbol{\sigma}$ is calculated and the stress $\boldsymbol{\sigma}$ is updated.
18. Using the lattice velocity gradient \mathbf{L}^* , the slip plane and slip direction are updated.
19. The material Jacobian $\partial\Delta\boldsymbol{\sigma}/\partial\Delta\boldsymbol{\varepsilon}$ is computed.
20. If the iterative solver is on the first iteration, the solution arrays are saved in alternative arrays. The logic behind this step is to provide a solution even when the iterative solver does not converge within maximum number of iterations.
21. The increments of the current iteration are saved to be used for future updates.
22. The convergence of the iterative solution is evaluated. If no convergence is achieved and the number of iterations is lower than the configured number, the derivative of the hardening moduli $h_{\alpha\mu}$ with respect to the cumulative slip Γ_β , weighted by the magnitude of the slip increment, is calculated via subroutine call (ITERATION). Otherwise, if the iteration number exceeds the input parameter, the solution without iterations is used.
23. If the number of iterations is less than the specified limit and the tolerance has not been reached, a GO TO statement redirects program execution to step 6.
24. The total cumulative shear strain is computed both for all slip systems collectively and for each individual slip system at the integration point.
25. The effective plastic slip parameter is calculated.

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