ME 531 - Crystal Plasticity (WARP3D)

Objective Stress Rates & WARP 3D

Jaumman Rate

$$\overset{\circ}{\sigma} = \dot{\sigma} - \Omega\sigma + \sigma\Omega$$

is used in constitutive equations because this rate is objective (invariant to rotations)

It is used in finite strain plasticity and also in crystal plasticity (see Pierce Asaro - Needleman).

The meaning of Ω is given in our lecture notes for crystal plasticity.

$$\Omega = \Omega^e + \Omega^p$$

$$= \Omega^e + \sum_{\alpha=1}^{N} \Omega^\alpha \dot{\gamma}^\alpha$$

$$= \dot{R}^e R^{eT} + \sum_{\alpha=1}^{N} \Omega^\alpha \dot{\gamma}^\alpha$$

Indeed, R^e needs to be determined as part of solution.

Havner refers to the second term as plastic spin it comes from lattice response while R^e comes from overall kinematics. The ABAQUS and many FEM codes use this formulation.

Now we consider the formulation in WARP3D. They use the Green-Naghdi rate.

In finite strain plasticity, the Green-Naghdi rate is written as,

$$\overset{\diamond}{\sigma}_{ik} = \dot{\sigma}_{ik} + \sigma\left(\dot{R}R^T\right) - \left(\dot{R}R^T\right)\sigma$$

In general the spin tensor is (applicable to plasticity in general)

$$\Omega = \dot{R}R^T + \frac{1}{2}R\left(\dot{U}U^{-1} - U^{-1}\dot{U}\right)R^T$$

$$W = \dot{R}R^T \quad \text{(name calling)}$$

or if elastic strains are small, we have

rigid body rotation — Deformation Induced Rotation

$$\Omega = \dot{R}R^T + \frac{1}{2}R\left(\dot{U}^P U^{P-1} - U^{P-1}\dot{U}^P\right)R^T$$

but in Green Naghdi only $\dot{R}R^T$ is used.

Now back to the definitions of F.

$$F = R\,U$$

Any tensor can be described via polar decomposition. We recall that

$$F F^T = (RU)^T RU = U^T R^T R U = U^T U$$

$$U^2 = F^T F$$

$$U = (F^T F)^{1/2}$$

Then $R = F U^{-1}$

So given F U & R can be determined uniquely as shown above.

This is a general statement (not necessarily crystal plasticity).

In crystal plasticity $(\dot{U}^P U^{P-1} - U^{P-1}\dot{U}^P)$ is non-zero in general. For a proportional loading case such as

$$U = \begin{bmatrix} \lambda_x & & \\ & \lambda_y & \\ & & \lambda_z \end{bmatrix}$$

$$\dot{U} = \begin{bmatrix} \dot{\lambda}_x & & \\ & \dot{\lambda}_y & \\ & & \dot{\lambda}_z \end{bmatrix}$$

$$U^{-1} = \begin{bmatrix} 1/\lambda_x & & \\ & 1/\lambda_y & \\ & & 1/\lambda_3 \end{bmatrix}$$

$$\dot{U}U^{-1} = \begin{bmatrix} \dot{\lambda}_x/\lambda_x & & \\ & \dot{\lambda}_y/\lambda_y & \\ & & \dot{\lambda}_3/\lambda_3 \end{bmatrix}$$

$$= U^{-1}\dot{U}$$ so two terms cancel.

Then in this case $\Omega = \dot{R}R^T$

Now, we are ready to pursue WARP 3D's formulation, first polar decomposition

$$F = R U$$

note in general $R = R^e R^p$

we note that U has elastic & plastic parts as well.

Then $F = V^e R^e R^p U^p$

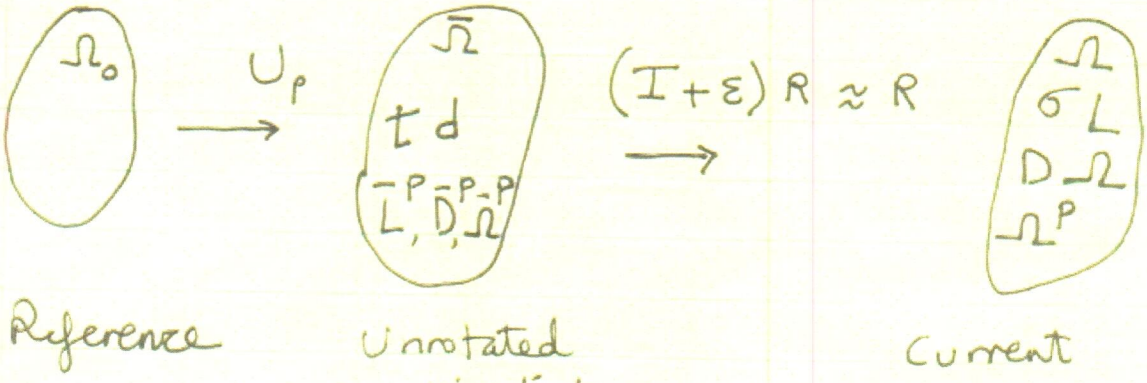
or if elasticity is infinitesimal

$$V^e = I + \varepsilon$$

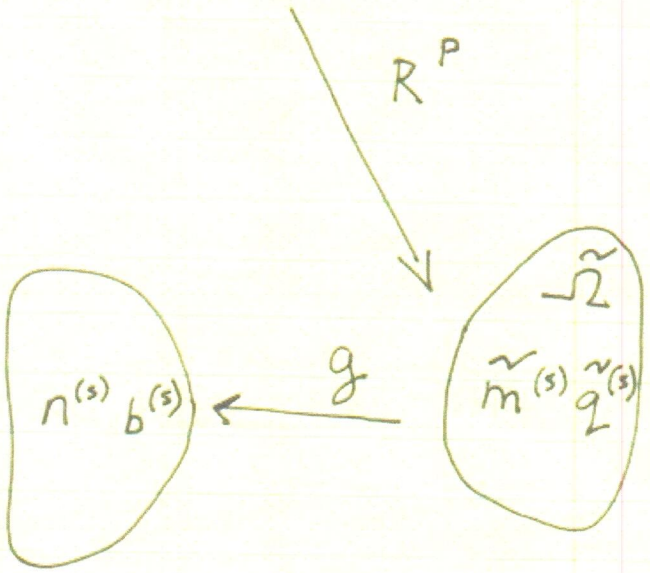
$$F = (I + \varepsilon) R U^p$$

where ε represents the elastic strain.

Now we look at a figure to illustrate these deformations that are implemented in WARP3D



Reference — Unrotated intermediate — Current



Crystallographic — lattice

(crystallographic directions are known in the lattice frame).

Now, substituting F into L expression

$$L = \dot{F}F^{-1} = \dot{R}R^T + \dot{\varepsilon}$$
$$+ \dot{R}R^T\varepsilon - \varepsilon\dot{R}R^T$$
$$+ R\bar{L}^P R^T + \varepsilon R\bar{L}^P R^T$$
$$- R\bar{L}^P R^T\varepsilon$$

Of course for elastic case $L = \dot{\varepsilon}$ (if there is no rotation). This eqn shows the coupling of elastic & plastic strains, in general. Note,

$\bar{L}^P = \dot{F}^P F^{P-1}$ in above equation.

Symmetric & skew parts of L are (current coordinates)

$$D = \frac{1}{2}(L + L^T)$$
$$= \dot{\varepsilon} + \varepsilon\Omega - \Omega\varepsilon + R\bar{D}^P R^T$$
$$+ \varepsilon R\bar{\Omega}^P R^T - R\bar{\Omega}^P R^T\varepsilon$$

$$\Omega = \frac{1}{2}(L - L^T)$$

$$= \dot{R}R^T + R\bar{\Omega}^P R^T + \varepsilon R \bar{D}^P R^T - R\bar{D}^P R^T \varepsilon$$

$\bar{D}^P$ is symmetric part of $\bar{L}^P$ and $\bar{\Omega}^P$ is the skew symmetric part (also known as plastic vorticity) ~~or plastic spin~~). $\dot{R}R^T$ denotes the total spin (call it W)

Ω = overall antisymmetric portion of velocity gradient.

plastic vorticity $\bar{\Omega}^P$ is not equal to plastic spin $\dot{R}^P R^{PT}$.

R^P = plastic spin (WARP 3D rotation)

We make the D expression to stress rate, we assume small elastic strains and Apply elasticity tensor,

$$\dot{\sigma} = C\,\dot{\varepsilon}$$

then,

$$C : D = \dot{\sigma} + \sigma W - W\sigma + C : (R\,\bar{D}^{p} R^{T}) + \sigma R\,\bar{\Omega}^{p} R^{T} - R\,\bar{\Omega}^{p} R^{T}\sigma \qquad (*)$$

$$\overset{\diamond}{\sigma} = C : (D - R\,\bar{D}^{p} R^{T})$$

$$- \sigma R\,\bar{\Omega}^{p} R^{T} + R\,\bar{\Omega}^{p} R^{T}\sigma$$

$$= \dot{\sigma} + \sigma W - W\sigma$$

What is remarkable is that with this formulation the $\overset{\nabla}{\sigma}$ recovered is actually the Green-Naghdi Rate.

note $W-\Omega$ relation was given earlier,

$$\Omega = W + R\bar{\Omega}^p R^T + \varepsilon R\bar{D}^p R^T - R\bar{D}^p R^T \varepsilon$$

extract W and substitute into (*) we get (where $W = \dot{R}R^T$)

$$\overset{\nabla}{\sigma} = C : \left[D - (R\bar{D}^p R^T) + \varepsilon^2 R\bar{D}^p R^T - 2\varepsilon R\bar{D}^p R^T \varepsilon + R\bar{D}^p R^T \varepsilon^2 \right]$$

Recall, $\overset{\nabla}{\sigma} = \dot{\sigma} + \sigma\Omega - \Omega\sigma$

can be shown to conform to the Jaumann stress rate.

If quadratic terms are dropped in terms of ε, the Jaumann rate becomes

$$\overset{\nabla}{\sigma} = C : (D - R\bar{D}^P R^T)$$

If $\bar{\Omega}^P = 0$ both objective rates become identical.

Now, we take another look at the Green Naghdi rate which is written in corotational frame as

$$\dot{t} = C_0 : (D - \bar{D}^P) + R\bar{\Omega}^P R^T t - t R\bar{\Omega}^P R^T$$

The material model in WARP3D integrates this rate of unrotated Cauchy stress, $t = R^T \sigma R$.

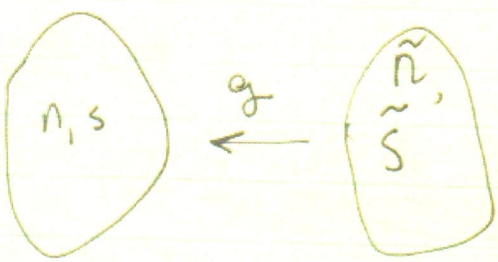
as a function of D_o, the unrotated rate of deformation. Note that macroscale rotational response is uncoupled from the macroscale rotations, only global rotation R appears. The elasticity tensor C_o has the appropriate form of the crystal frame rotated from the initial lattice frame to the reference frame.

We would like to obtain expression for $\bar{D}^p$. The velocity gradient is defined as

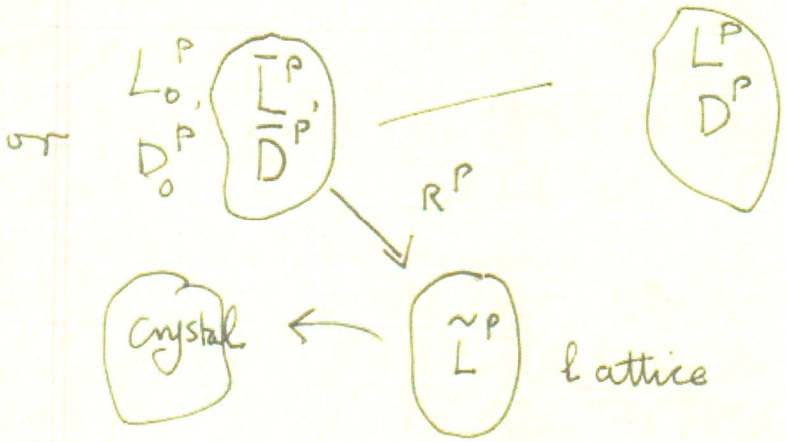
$$\tilde{L}^p = \sum_{s=1}^{n\text{slip}} \dot{\gamma}^{(s)} \, \tilde{s}^{(s)} \otimes \tilde{n}^{(s)}$$

$s^{(s)}$ slip system direction
$n^{(s)}$ slip system normal

A rigid rotation q calculated from original grain orientations relate the crystal frame to the lattice axis frame $(\tilde{s}^{(s)}, \tilde{n}^{(s)})$



Then, as our figure below indicates we must transform this velocity gradient tensor into the unrotated frame the rotation defining this is R^p. The kinematics of macroscale deformation does not define this plastic rotation, the constitutive response does.



or

$$\bar{D}^p = \sum_{s=1}^{n\,slip} \dot{\gamma}^{(s)}\, R^{pT}\, \tilde{P}^{(s)}\, R^p$$

or $D_o^p = \bar{D}^p$ (same expression)

Then,

$$\bar{D}^p = \sum_{s=1}^{n_{slip}} \dot{\gamma}^{(s)} \tilde{P}^{(s)} R^p$$

$$\bar{\Omega}^p = \sum_{s=1}^{n_{slip}} \dot{\gamma}^{(s)} \left(R^{pT} \tilde{\Omega}^{(s)} R^p \right)$$

This is consistent with our early notation. As noted before $\bar{D}^p$ is same D_0^p, and $\bar{\Omega}^p$ is same as Ω_0.

The slip rate is given ~~in~~ in WARP 3D as

$$\dot{\gamma}^{(s)} = \frac{\dot{\gamma}_0}{\tilde{\tau}} \left| \frac{\tau^{(s)}}{\tilde{\tau}} \right|^{n-1} \tau^{(s)}$$

where $\dot{\gamma}_0$ a reference slip rate, $\tilde{\tau}$ is the slip system strength and $\tau^{(s)}$ is the resolved shear on slip system s.

The rate of plastic rotation is given as

$$\dot{R}^p = \bar{\Omega}^p R^p$$

This relation is used to approximate

texture evolution. See WARP3D theory manual ad also Messner, Dodds, Beaudoin, Engineering Computations, V. 32, No. 6 pp 1526-1548, 2015

elements. The homogenized behavior of the polycrystalline material is achieved through a Taylor [23] approximation which enforces identical strain increments (rates) in each material at the integration point. The resulting (not necessarily equilibrium) stresses are averaged. This approach creates a simple reduced, multi-scale model. A single finite element on the scale of centimeters can represent a polycrystal with a length-scale on the order of microns.

To facilitate the various types of simulations anticipated to use the CP material model, the input of properties is separated into three parts: (1) the crystal elastic and flow properties *i.e.*, a crystal *type* is defined and identified by an integer value, (2) the initial lattice orientations relative to the model (global system), and (3) other values including the thermal expansion coefficient, mass density, local (iterative) solver/parameters in the CP routines, etc. The end result in each case is a named *material* in the WARP3D scheme for assignment of material information to finite elements. Many such named materials may be defined as required to meet the complexity of representing the construction of a component. Materials other than the CP model available in WARP3D may be defined and associated with other finite elements in the mesh. The options to define a *material* for association with finite elements are summarized briefly here to illustrate the modeling capabilities with details provided later in this section.

- One or more *crystals* numbered 1, 2, 3, ... are defined. Provided information includes the lattice structure (fcc, bcc, hcp18, single ...), type of elasticity, selection of the hardening model to couple shear stress to slip strain rates and values of associated parameters.
- One or more named *materials*, *e.g.*, AlLi2099, Gr91, Ti, ... is defined each making reference to a single crystal (by number) and having a single orientation. This approach works well when material specification for a simulation model requires only a few crystals and/or orientations. Input for the named material includes the crystal number, one set of (3) orientation angles, thermal properties, mass density, algorithms/tolerances for internal CP computations. Each named material may be then associated with any number of finite elements via the usual input commands employed for all other material models in WARP3D (see Section 2.3), *e.g.*, `elements 2000-10000 type l3disop nonlinear material Gr91 bbar center_output` ...
- The next approach proves more suitable for models where only a few crystals but many different orientations are needed. Each finite element is assigned a single crystal and a single lattice orientation. The named material now provides the crystal number but the 3 orientation angles are replaced by the name of a flat (text) file; this file lists finite element numbers and the three Euler angles (one line per element).
- In the most general scheme, polycrystal homogenization via the Taylor approximation is achieved through a flat text file with each line containing: an element number, a crystal number and 3 Euler angles. Each line thus associates a crystal number and orientation angles with an element. Multiple lines may be defined for an element listing different (or same) crystal numbers and angles as needed to represent material properties. The number of lines (crystals) per element and the file name are specified in properties of the named material. This approach provides considerable flexibility to define complex and spatially varying material properties throughout the model.

This section continues with a brief summary of key features of the CP formulation within the WARP3D framework for implicit solutions including large rotations and finite strains. The CP model formulation draws heavily on the concepts described in [1, 14] and in the new work by T. Truster (publications in progress).

3.12.1 Kinematics

This section summarizes key features of the kinematics for the Green-Naghdi objective stress rate adopted as the overall framework for large-rotations and finite-strains in WARP3D. The

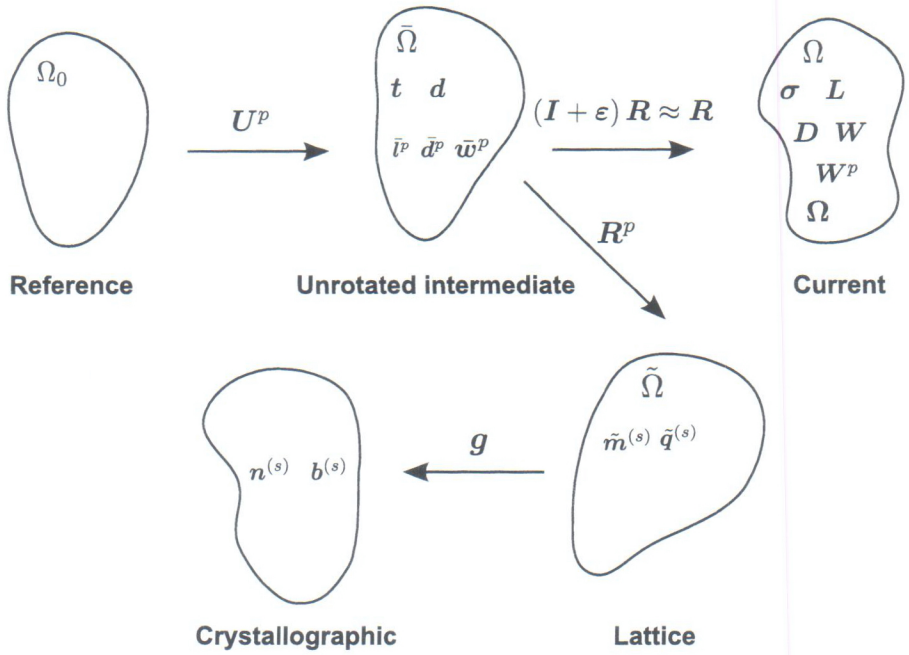


Figure 3.12.1: Coordinate systems for the crystal plasticity kinematic framework. Integration of the objective stress rate occurs in the unrotated (intermediate) configuration. The kinematics of crystal plasticity are defined in the lattice coordinates.

material stress rate differs in various objective rate theories that include plastic vorticity, *i.e.*, a material model designed for a Jaumann rate becomes kinematically incorrect in a solution framework that uses the Green-Naghdi rate and vice-versa. An interesting observation emerges from a rigorous derivation: stress integration for crystal plasticity requires either the macroscale, total vorticity or the microscale plastic vorticity, but does not require both [17, 18].

Figure 3.12.1 shows the kinematic framework. Stress integration with the Green-Naghdi rate takes place in the unrotated intermediate or corotational frame – the remainder of the configurations are standard for crystal plasticity kinematics. The corotational frame follows from a polar decomposition of the total deformation gradient $\mathbf{F}$ into a rotation and a stretch:

$$\mathbf{F} = \mathbf{R}\mathbf{U} \ . \tag{3.12.1}$$

A multiplicative decomposition of the deformation gradient yields $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p = \mathbf{V}^e\mathbf{R}^e\mathbf{R}^p\mathbf{U}^p$, which decomposes both the elastic and plastic deformations into an associated stretch and rotation. For the moment, neglect the elastic stretch $\mathbf{V}^e$, then

$$\mathbf{F} = \mathbf{R}^e\mathbf{R}^p\mathbf{U}^p.$$

The small-strain nature of metal elasticity justifies this assumption. On comparing this expression to the polar decomposition of the total deformation gradient in Eq. 3.12.1, we have:

$$\mathbf{R} = \mathbf{R}^e\mathbf{R}^p.$$

After substituting and rearranging $\mathbf{F} = \mathbf{R}\mathbf{U}^p$. The elastic stretch is now re-introduced as a small deviation from the identity tensor such that $\mathbf{V}^e = \mathbf{I} + \boldsymbol{\varepsilon}$. The final decomposition of the

deformation gradient becomes:

$$\mathbf{F} = (\mathbf{I} + \boldsymbol{\varepsilon})\,\mathbf{R}\mathbf{U}^p$$

The top part of Fig. 3.12.1 shows the three coordinate systems defined by this decomposition of the deformation gradient.

After eliminating quadratic terms in $\boldsymbol{\varepsilon}$ and $\dot{\boldsymbol{\varepsilon}}$, the spatial velocity gradient becomes:

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1} = \dot{\mathbf{R}}\mathbf{R}^T + \dot{\boldsymbol{\varepsilon}} + \dot{\mathbf{R}}\mathbf{R}^T\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}\dot{\mathbf{R}}\mathbf{R}^T + \mathbf{R}\bar{\mathbf{l}}^p\mathbf{R}^T + \boldsymbol{\varepsilon}\mathbf{R}\bar{\mathbf{l}}^p\mathbf{R}^T - \mathbf{R}\bar{\mathbf{l}}^p\mathbf{R}^T\boldsymbol{\varepsilon}.$$

In this equation $\bar{\mathbf{l}}^p = \dot{\mathbf{F}}^p\mathbf{F}^{p-1}$ defines a constitutive tensor; kinematically, this is the plastic velocity gradient pulled back to the corotational, intermediate frame. The symmetric and skew parts of this expression are:

$$\mathbf{D} = \frac{1}{2}\left(\mathbf{L} + \mathbf{L}^T\right) = \dot{\boldsymbol{\varepsilon}} + \boldsymbol{\varepsilon}\boldsymbol{\Omega} - \boldsymbol{\Omega}\boldsymbol{\varepsilon} + \mathbf{R}\bar{\mathbf{d}}^p\mathbf{R}^T + \boldsymbol{\varepsilon}\mathbf{R}\bar{\mathbf{w}}^p\mathbf{R}^T - \mathbf{R}\bar{\mathbf{w}}^p\mathbf{R}^T\boldsymbol{\varepsilon} \tag{3.12.2}$$

$$\mathbf{W} = \frac{1}{2}\left(\mathbf{L} - \mathbf{L}^T\right) = \boldsymbol{\Omega} + \mathbf{R}\bar{\mathbf{w}}^p\mathbf{R}^T + \boldsymbol{\varepsilon}\mathbf{R}\bar{\mathbf{d}}^p\mathbf{R}^T - \mathbf{R}\bar{\mathbf{d}}^p\mathbf{R}^T\boldsymbol{\varepsilon}. \tag{3.12.3}$$

Here, $\bar{\mathbf{d}}^p$ is the symmetric part of $\bar{\mathbf{l}}^p$, $\bar{\mathbf{w}}^p$ is the skew part, and $\boldsymbol{\Omega} = \dot{\mathbf{R}}\mathbf{R}^T$ denotes the total spin. The skew part of $\bar{\mathbf{l}}^p$ (the plastic vorticity $\bar{\mathbf{w}}^p$) is not equal, in general, to the plastic spin $\dot{\mathbf{R}}^p\mathbf{R}^{pT}$. There is no kinematic reason to neglect either the spin or the vorticity. To make Eq. 3.12.2 into a stress rate, we adopt the usual assumption of small elastic strains and apply the elasticity tensor $\mathbf{C}$ such that $\mathbf{C} : \dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\sigma}}$:

$$\mathbf{C} : \mathbf{D} = \dot{\boldsymbol{\sigma}} + \boldsymbol{\sigma}\boldsymbol{\Omega} - \boldsymbol{\Omega}\boldsymbol{\sigma} + \mathbf{C} : \left(\mathbf{R}\bar{\mathbf{d}}^p\mathbf{R}^T\right) + \boldsymbol{\sigma}\mathbf{R}\bar{\mathbf{w}}^p\mathbf{R}^T - \mathbf{R}\bar{\mathbf{w}}^p\mathbf{R}^T\boldsymbol{\sigma} \tag{3.12.4}$$

$$\check{\boldsymbol{\sigma}} = \mathbf{C} : \left(\mathbf{D} - \mathbf{R}\bar{\mathbf{d}}^p\mathbf{R}^T\right) - \boldsymbol{\sigma}\mathbf{R}\bar{\mathbf{w}}^p\mathbf{R}^T + \mathbf{R}\bar{\mathbf{w}}^p\mathbf{R}^T\boldsymbol{\sigma} = \dot{\boldsymbol{\sigma}} + \boldsymbol{\sigma}\boldsymbol{\Omega} - \boldsymbol{\Omega}\boldsymbol{\sigma}. \tag{3.12.5}$$

This $\check{\boldsymbol{\sigma}}$ is the Green-Naghdi objective stress rate. The material stress rate for a computational framework using the Green-Naghdi rate becomes:

$$\check{\boldsymbol{\sigma}} = \mathbf{C} : \left(\mathbf{D} - \mathbf{R}\bar{\mathbf{d}}^p\mathbf{R}^T - \boldsymbol{\varepsilon}\mathbf{R}\bar{\mathbf{w}}^p\mathbf{R}^T + \mathbf{R}\bar{\mathbf{w}}^p\mathbf{R}^T\boldsymbol{\varepsilon}\right).$$

In the absence of plastic spin ($\bar{\mathbf{w}}^p$), the stress rate becomes the usual rate form for conventional plasticity models (discussed in Chapter 1). As observed above, the Green-Naghdi rate has a correction term to include effects of plastic spin:

$$\check{\boldsymbol{\sigma}}^{corr} = \mathbf{C} : \left(-\boldsymbol{\varepsilon}\mathbf{R}\bar{\mathbf{w}}^p\mathbf{R}^T + \mathbf{R}\bar{\mathbf{w}}^p\mathbf{R}^T\boldsymbol{\varepsilon}\right).$$

The Green-Naghdi rate does not require the macroscopic vorticity $\mathbf{W}$ but does require the microscopic plastic vorticity $\bar{\mathbf{w}}^p$. This result holds after effects of lattice evolution are included in the plastic constitutive tensor $\bar{\mathbf{l}}^p$ (see below).

With this choice of stress rate, the stress integration simplifies considerably once stated in the corotational frame. A pull-back of Eq. 3.12.5 to the corotational frame yields:

$$\dot{\mathbf{t}} = \mathbf{C}_0 : \left(\mathbf{d} - \bar{\mathbf{d}}^p\right) + \mathbf{R}\bar{\mathbf{w}}^p\mathbf{R}^T\mathbf{t} - \mathbf{t}\mathbf{R}\bar{\mathbf{w}}^p\mathbf{R}^T\ . \tag{3.12.6}$$

Material models in WARP3D integrate this rate of unrotated Cauchy stress $\mathbf{t} = \mathbf{R}^T\boldsymbol{\sigma}\mathbf{R}$ as a function of $\mathbf{d}$, the unrotated rate of deformation. At this point, the macroscale rotational response uncouples completely from the microscale lattice rotations – only the global rotation $\mathbf{R}$ appears. In one advantage of this framework, the elasticity tensor $\mathbf{C}_0$, may have the appropriate form of an anisotropic tensor for the crystal system, rotated from the initial lattice frame to the reference frame. WARP3D handles all the rotations required for the elasticity tensor automatically. The user provides the appropriate anisotropic elasticity tensor in the *crystallographic frame*. The code will provide the constant rotation into the lattice frame as well as the rotation into the intermediate configuration, which changes with time. By enabling this definition of a constant elasticity tensor in the corotational frame, the total material rotation then updates the anisotropic elastic constants of a crystal. For small elastic stretches, this approach is equivalent to elasticity models derived from a hyperelastic potential.

With Eq. 3.12.6 taken to update stresses at a material (integration) point in a finite element, the constitutive model must then compute the plastic deformation $\overline{\mathbf{l}}^p$. For crystal plasticity, the common kinematic assumption is an additive decomposition of plastic shear deformations in a lattice frame [4]:

$$\tilde{\mathbf{l}}^p = \sum_{s=1}^{n_{slip}} \dot{\gamma}^{(s)} \left(\tilde{\mathbf{b}}^{(s)} \otimes \tilde{\mathbf{n}}^{(s)} \right) \tag{3.12.7}$$

where $\tilde{\mathbf{b}}^{(s)}$ and $\tilde{\mathbf{n}}^{(s)}$ denote collections of slip-system directions and normals in the lattice frame and $\dot{\gamma}^{(s)}$ is the slip rate along each slip system. The geometry of the crystal system, for example face centered cubic (FCC), defines these slip systems in the crystallographic frame and a rigid rotation $\mathbf{g}$, calculated from the initial grain orientations, defines the rotation between the lattice frame and the crystallographic frame. Finally, as Fig. 3.12.1 indicates, the model must transform this deformation tensor in the lattice frame into the unrotated frame to specify the plastic deformation in the corotational coordinates. The rotation defining this transformation is $\mathbf{R}^p$. The kinematics of macroscale deformation do not define this plastic rotation. Here, we define $\mathbf{R}^p$ as part of the constitutive response of the material. That is, the plastic rotation is part of the micro-constitutive response, not the global kinematics. This plastic rotation does not affect the elasticity tensor, only the plastic rate $\tilde{\mathbf{l}}^p$. This approximation appears acceptable for moderate plastic strains [8], where the elastic response of the material does not depend strongly on the plastic deformation.

From these definitions, the symmetric and skew parts of plastic deformation are:

$$\overline{\mathbf{d}}^p = \sum_{s=1}^{n_{slip}} \dot{\gamma}^{(s)} \left(\mathbf{R}^{pT} \tilde{\mathbf{m}}^{(s)} \mathbf{R}^p \right)$$

$$\overline{\mathbf{w}}^p = \sum_{s=1}^{n_{slip}} \dot{\gamma}^{(s)} \left(\mathbf{R}^{pT} \tilde{\mathbf{q}}^{(s)} \mathbf{R}^p \right)$$

with $\tilde{\mathbf{m}}^{(s)} = \text{sym}\left[\tilde{\mathbf{b}}^{(s)} \otimes \tilde{\mathbf{n}}^{(s)}\right]$ and $\tilde{\mathbf{q}}^{(s)} = \text{skew}\left[\tilde{\mathbf{b}}^{(s)} \otimes \tilde{\mathbf{n}}^{(s)}\right]$.

The CP model adopts a general constitutive framework for the slip rates $\dot{\gamma}^{(s)}$ on each system as a function of the current applied stress $\boldsymbol{\sigma}$ and other factors such as temperature and

microstructural state. Similarly, the hardening variables follow particular evolution equations depending on the user-selected constitutive model available as CP options (see subsequent sections). The generic form of the evolution equations is given by:

$$\dot{\gamma}^{(s)} = \dot{\gamma}^{(s)}\left(\tau^{(s)}, \boldsymbol{\xi}, \mathbf{d}; \boldsymbol{\nu}\right) \tag{3.12.8}$$

$$\dot{\boldsymbol{\xi}} = \dot{\boldsymbol{\xi}}\left(\mathbf{t}, \boldsymbol{\xi}, \mathbf{d}; \boldsymbol{\nu}\right) \tag{3.12.9}$$

where

$$\tau^{(s)} = \mathbf{t} : \left(\mathbf{R}^{pT}\tilde{\mathbf{m}}^{(s)}\mathbf{R}^{p}\right) \tag{3.12.10}$$

is the resolved shear stress on the slip system, $\boldsymbol{\xi}$ is a set of hardening variables, and $\mathbf{d}$ is the unrotated rate of deformation defined previously. These three fields are treated in an implicit fashion within the stress update algorithm – a coupled system of nonlinear equations is solved at an integration point for the current (global) estimate of the solution at $n+1$. Additionally, the model accommodates other parameters and field dependencies but treated in an explicit manner; these variables are denoted by $\boldsymbol{\nu}$. An example of such a field is the Nye tensor $\boldsymbol{\alpha}$ that drives features to approximate size effects in the Mechanical Threshold Stress (MTS) constitutive model.

The selection of a *hardening type* controls both the slip rate and hardening relationships. Options exist for both isotropic hardening and anisotropic hardening of the slip system resistances, and flow rules may have power-law or exponential form. Later sections describe the specific forms now available; the user can also implement their own models within the general framework.

Finally, define the rate of plastic rotation:

$$\dot{\mathbf{R}}^{p} = \overline{\mathbf{w}}^{p}\mathbf{R}^{p}. \tag{3.12.11}$$

Kinematically, this form is not rigorously correct, but it does approximate closely the experimentally observed texture evolution in a variety of situations (see Section 5.1 in [11], [12, 14, 19]). Substitution of the macroscopic vorticity via Eq. 3.12.3 eliminates the plastic vorticity from the above equation, thus making the lattice evolution dependent only on the macroscopic vorticity and the symmetric part of the microscopic plastic deformation. In the presence of lattice rotations, the formulation then continues to require only one of (1) the macroscale, total vorticity or (2) the microscale, plastic vorticity.

3.12.2 Generalized Implicit Material Update Algorithm

A backward Euler integration of Eq. 3.12.6 defines the stress update procedure. To reduce computational effort an explicit, exponential integration of Eq. 3.12.11 provides the plastic rotation update. The resulting implicit equations are:

$$\begin{aligned}\mathbf{0} = \mathbf{R}_1 &= \mathbf{t}_{n+1} - \overline{\mathbf{t}}\left(\mathbf{t}_{n+1}, \boldsymbol{\xi}_{n+1}, \Delta\mathbf{d}_{n+1}; \boldsymbol{\nu}_n\right) \\ &= \mathbf{t}_{n+1} - \left[\mathbf{t}_n + \dot{\mathbf{t}}\left(\mathbf{t}_{n+1}, \boldsymbol{\xi}_{n+1}, \Delta\mathbf{d}_{n+1}; \boldsymbol{\nu}_n\right)\Delta t\right]\end{aligned} \tag{3.12.12}$$