Crystal Plasticity Formulation

Crystal plasticity constitutive model

Classical single-crystal plasticity theory is used to model the deformation within each grain. The theory is based on the notion that plastic flow takes place through slip on prescribed slip systems. For a material with $\alpha = 1, \ldots, N$ slip systems defined by ortho-normal vector pairs $(\boldsymbol{m}_0^\alpha, \boldsymbol{n}_0^\alpha)$ denoting the slip direction and slip plane normal respectively at time $t = 0$, the constitutive equations relate the following basic fields (all quantities expressed in crystal lattice coordinate frame): the deformation gradient defined with respect to the initial undeformed crystal $\boldsymbol{F}$ which can be decomposed into elastic and plastic parts as $\boldsymbol{F} = \boldsymbol{F}^e \, \boldsymbol{F}^p$ (with $\det(\boldsymbol{F}^p) = 1$), the Cauchy stress $\boldsymbol{\sigma}$ and the slip resistances $s^\alpha > 0$. In the constitutive equations to be defined below, the Green elastic strain measure $\boldsymbol{E}^e = \frac{1}{2} \left(\boldsymbol{F}^{eT} \boldsymbol{F}^e - \boldsymbol{I} \right)$ defined on the relaxed configuration (plastically deformed, unstressed configuration) is utilized. The conjugate stress measure is then defined as $\bar{\boldsymbol{T}} = \det \boldsymbol{F}^e (\boldsymbol{F}^e)^{-1} \boldsymbol{\sigma} (\boldsymbol{F}^e)^{-T}$. Kinematics of single crystal slip is illustrated in Fig. 1.
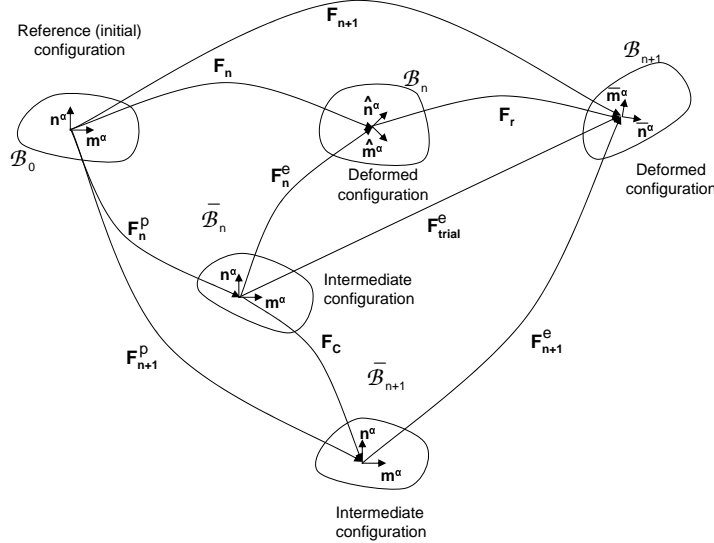

Figure 1: *Schematic of the various material configurations, for a single crystal, used in the integration of the constitutive model. The slip systems $(\boldsymbol{m}^\alpha, \boldsymbol{n}^\alpha$ are known on the reference (initial) configuration. Also, $\hat{\boldsymbol{m}}^\alpha$, $\bar{\boldsymbol{m}}^\alpha$ are the slip directions (different from $\boldsymbol{m}^\alpha$ because of crystal re-orientation) in the deformed configurations $\mathcal{B}_n$ and $\mathcal{B}_{n+1}$, respectively.*

The constitutive relation, for stress, is given by $\bar{\boldsymbol{T}} = \boldsymbol{\mathcal{C}}^e [\boldsymbol{E}^e]$ where $\boldsymbol{\mathcal{C}}^e$ is the fourth-order anisotropic elasticity tensor. It is assumed that deformation takes place through dislocation glide and the evolution of the plastic velocity gradient is given by:

$$\boldsymbol{L}^p = \dot{\boldsymbol{F}}^p (\boldsymbol{F}^p)^{-1} = \sum_\alpha \dot{\gamma}^\alpha \boldsymbol{S}_0^\alpha sign(\tau^\alpha) \tag{1}$$

where $\boldsymbol{S}_0^\alpha = \boldsymbol{m}_0^\alpha \otimes \boldsymbol{n}_0^\alpha$ is the Schmid tensor and $\dot{\gamma}^\alpha$ is the plastic shearing rate on the αth slip system. The resolved stress on the αth slip system is given by $\tau^\alpha = \bar{\boldsymbol{T}} \cdot \boldsymbol{S}_0^\alpha$.

A rate independent algorithm is employed to solve the single crystal model. The resolved shear stress τ^α is taken to attain a critical value s^α (the slip system resistance) on the systems where slip occurs. These active systems have a plastic shearing rate $\dot\gamma^\alpha > 0$. There is no plastic shearing rate ($\dot\gamma^\alpha = 0$) on inactive slip systems where the resolved shear stress does not exceed s^α. The evolution of slip system resistance given by the following expression:

$$\dot{s}^\alpha(t) = \sum_\beta h^{\alpha\beta}\dot\gamma^\beta(t), \text{ with } s^\alpha(0) = \tau_0^\alpha \tag{2}$$

$$\text{where, } h^{\alpha\beta} = h_o^\beta(q + (1-q)\delta^{\alpha\beta})(1 - \frac{s^\beta(t)}{s_s^\beta})^a \text{ (no sum on } \beta) \tag{3}$$

The algorithm for computing the plastic shear increment $\Delta\gamma^\beta$ from this model be found in the appendix **??**. Subsequently, the plastic part of the deformation gradient is updated using Eq. (5), the elastic part computed from $\boldsymbol{F} = \boldsymbol{F}^e\ \boldsymbol{F}^p$. The conjugate stress measure, $\bar{\boldsymbol{T}}$ is then computed from $\bar{\boldsymbol{T}} = \boldsymbol{\mathcal{C}}^e[\boldsymbol{E}^e]$ and converted to Cauchy stress and the Piola-Kirchhoff-I stress, $\boldsymbol{P} = (\det\boldsymbol{F})\boldsymbol{\sigma}\boldsymbol{F}^{-T}$ for further use. The slip resistances are also updated at the end of the time step using Eq. **??**. Finally, the tangent modulus $\frac{\partial\boldsymbol{\sigma}}{\partial\boldsymbol{F}}$ for use in the weak form is computed using a fully implicit algorithm described in appendix **??**.
The rate independent model is used to find the PKI stress and tangent modulus for getting the finite element nodes displacement. The deformation gradient can be decomposed as elastic and plastic parts as followed,

$$\boldsymbol{F} = \boldsymbol{F}^e\ \boldsymbol{F}^p \tag{4}$$

$\boldsymbol{F}^e$ is the elastic deformation gradient, while $\boldsymbol{F}^p$ is plastic deformation gradient with $\det(\boldsymbol{F}^p) = 1$. The velocity gradient $\boldsymbol{L}$ can be decomposed as $\boldsymbol{L}^e + \boldsymbol{L}^p$, while plastic velocity gradient is the sum of strain rate over all slip systems,

$$\boldsymbol{L}^p = \dot{\boldsymbol{F}}^p(\boldsymbol{F}^p)^{-1} = \sum_\alpha \dot\gamma^\alpha \boldsymbol{S}_0^\alpha sign(\tau^\alpha) \tag{5}$$

where $\boldsymbol{S}_0^\alpha = \boldsymbol{m}^\alpha \otimes \boldsymbol{n}^\alpha$ is the Schmid tensor and $\dot\gamma^\alpha$ is the plastic shearing rate on the αth slip system. The solution of $\boldsymbol{F}^p$ from Euler-backward scheme is:

$$\boldsymbol{F}_{n+1}^p \approx (\boldsymbol{I} + \sum_\alpha \Delta\gamma^\alpha \boldsymbol{S}_0^\alpha sign(\tau^\alpha))\boldsymbol{F}_n^p \tag{6}$$

$\dot\gamma$ from Eq. 5 changes to $\Delta\gamma$ here, because it is now the increment in infinitesimal time Δt. $\boldsymbol{F}^e$ can be obtained from Eq. 4 as:

$$\boldsymbol{F}^e = \boldsymbol{F}_{tr}^e(\boldsymbol{I} - \sum_\alpha \Delta\gamma^\alpha \boldsymbol{S}_0^\alpha sign(\tau^\alpha)) \tag{7}$$

where $\boldsymbol{F}_{tr}^e$ is $\boldsymbol{F}_{n+1}(\boldsymbol{F}_n^p)^{-1}$. Lagrange strain can be written as:

$$\begin{aligned} \boldsymbol{E}^e &= \frac{1}{2}(\boldsymbol{F}^{eT}\boldsymbol{F}^e - \boldsymbol{I}) \\ &= \boldsymbol{E}_{tr}^e - \frac{1}{2}\sum_\alpha sign(\tau^\alpha)\Delta\gamma^\alpha \boldsymbol{B}^\alpha \end{aligned} \tag{8}$$

where $\boldsymbol{E}^e_{tr} = \frac{1}{2}((\boldsymbol{F}^e_{tr})^T \boldsymbol{F}^e_{tr} - \boldsymbol{I})$ and $\boldsymbol{B} = (\boldsymbol{S}^\alpha_0)^T(\boldsymbol{F}^e_{tr})^T \boldsymbol{F}^e_{tr} + (\boldsymbol{F}^e_{tr})^T \boldsymbol{F}^e_{tr} \boldsymbol{S}^\alpha_0$

Let t denote the current time, Δt and infinitesimal time increment, and $\tau = t + \Delta t$. Then, given $\boldsymbol{F}(t), \boldsymbol{F}(\tau), \boldsymbol{m}^\alpha_0, \boldsymbol{n}^\alpha_0, \boldsymbol{\sigma}(t), \boldsymbol{F}^p(t)$ and $s^\alpha(t)$, $\boldsymbol{F}^p(\tau), s^\alpha(\tau), \sigma(\tau)$ need to be found out. First deformation gradient and Lagrangian strain are shown as

$$\boldsymbol{F}^e_{tr}(\tau) = \boldsymbol{F}(\tau)\ \boldsymbol{F}^p(t)^{-1} \tag{9}$$

$$\boldsymbol{E}^e_{tr}(\tau) = \frac{1}{2}(\boldsymbol{F}^e_{tr}(\tau))^T \boldsymbol{F}^e_{tr}(\tau) \tag{10}$$

In order to find the resolved shear stress, the conjugate stress measure is then defined by

$$\boldsymbol{T} = \det\boldsymbol{F}^e(\boldsymbol{F}^e)^{-1}\boldsymbol{\sigma}(\boldsymbol{F}^e)^{-T} \tag{11}$$

while $\boldsymbol{T}(\tau)$ is expressed as

$$\boldsymbol{T}(\tau) = \boldsymbol{\mathcal{L}}^e \left[\boldsymbol{E}^e(\tau)\right] \tag{12}$$

$\boldsymbol{T}_{tr}(\tau)$ is calculated in the same manner as $\boldsymbol{\mathcal{L}}^e \left[\boldsymbol{E}^e_{tr}(\tau)\right]$, where $\boldsymbol{\mathcal{L}}^e$ is the fourth-order anisotropic elasticity tensor. The resolved shear stress is approximated by

$$\tau^\alpha = \boldsymbol{T}(\tau) \cdot \boldsymbol{S}^\alpha_0 \tag{13}$$

while trial resolved shear stress is defined in the same way as $\tau^\alpha_{tr}(\tau) = \boldsymbol{T}_{tr}(\tau) \cdot \boldsymbol{S}^\alpha_0$. By substitute Eq.8 to Eq.12, we obtain,

$$\boldsymbol{T}(\tau) = \boldsymbol{T}_{tr}(\tau) - \frac{1}{2}\sum_\beta sign(\tau^\beta_{tr}(\tau))\Delta\gamma^\beta \boldsymbol{\mathcal{L}}^e\left[\boldsymbol{B}^\beta\right] \tag{14}$$

then apply new $\boldsymbol{T}(\tau)$ to Eq.13, we will get

$$\tau^\alpha(\tau) = |\tau^\alpha_{tr}| - \frac{1}{2}\sum_\beta sign(\tau^\alpha_{tr}(\tau))sign(\tau^\beta_{tr}(\tau))\Delta\gamma^\beta \boldsymbol{\mathcal{L}}^e\left[\boldsymbol{B}^\beta\right] \cdot \boldsymbol{S}^\alpha_0 \tag{15}$$

In crystal plastic theory the hardening law for the slip resistance s^α at time τ is given as:

$$s^\alpha(\tau) = s^\alpha(t) + \sum_\beta h^{\alpha\beta}(t)\Delta\gamma^\beta \tag{16}$$

where $h^{\alpha\beta}$ describes the rate of increase of the deformation resistance on slip system α due to shearing on slip system β. Now we can determine $\Delta\gamma$ now, with $\alpha, \beta \in \mathcal{A}$:

$$\sum_{\beta\in\mathcal{A}} A^{\alpha\beta}\Delta\gamma^\beta = b^\alpha \tag{17}$$

where,

$$\begin{aligned}A^{\alpha\beta} &= h^{\alpha\beta}(t) + sign(\tau^\alpha_{tr}(\tau))sign(\tau^\beta_{tr}(\tau))\boldsymbol{\mathcal{L}}^e\left[\boldsymbol{B}^\beta\right] \cdot \boldsymbol{S}^\alpha_0 \\ b^\alpha &= |\tau^\alpha_{tr}(\tau)| - s^\alpha(t)\end{aligned} \tag{18}$$

only values of $\Delta\gamma$ bigger than 0 will be kept. Then, $\boldsymbol{F}^p(\tau)$ can be updated by Eq.6, $\boldsymbol{F}^e(\tau)$ updates through Eq.4 or Eq.7. $\boldsymbol{\sigma}(\tau)$ needs $\boldsymbol{T}(\tau)$ first, which can be updated through Eq.12. Then $\boldsymbol{\sigma}(\tau)$ can be found by $\boldsymbol{\sigma}(\tau) = \boldsymbol{F}^e(\tau)\left[\det(\boldsymbol{F}^e(\tau))\right]^{-1}\boldsymbol{T}(\tau)\boldsymbol{F}^e(\tau)^T$ from Eq.11, $s^\alpha(\tau)$ can be specified by Eq.16.

Tangent modulus

Kinematic problem can be expressed in Lagrangian framework by

$$\nabla_0 \cdot \langle \boldsymbol{P} \rangle + \boldsymbol{f} = \boldsymbol{0} \tag{19}$$

where ∇_0 is the divergence int the initial reference configuration. The polycrystal Piola-Kirchhoff-I stress, $\langle \boldsymbol{P} \rangle$ shown as

$$\langle \boldsymbol{P} \rangle = \det \boldsymbol{F} \langle \boldsymbol{\sigma} \rangle \boldsymbol{F}^{-T} \tag{20}$$

For any kinematically admissible test function $\tilde{\boldsymbol{u}}$, the weak form of the virtual work equation is like:

$$\mathcal{G}(\boldsymbol{u}_{n+1}, \tilde{\boldsymbol{u}}) \equiv \int_{\mathcal{B}_0} \langle \boldsymbol{P} \rangle \cdot \nabla_0 \tilde{\boldsymbol{u}} dV - \int_{\partial \mathcal{B}_0} \boldsymbol{\lambda} \cdot \tilde{\boldsymbol{u}} dA - \int_{\mathcal{B}_0} \boldsymbol{f} \cdot \tilde{\boldsymbol{u}} dV = 0 \tag{21}$$

The Newton-Raphson iterative scheme with a line search procedure is employed,

$$\frac{\partial \mathcal{G}(\boldsymbol{u}_n, \tilde{\boldsymbol{u}})}{\partial \boldsymbol{u}_n} \Delta \boldsymbol{u} = \int_{\mathcal{B}_0} \frac{\partial \langle \boldsymbol{P} \rangle}{\partial \boldsymbol{F}} \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{u}_n} \cdot \nabla_0 \tilde{\boldsymbol{u}} dV \Delta \boldsymbol{u} = \mathcal{G}(\boldsymbol{u}_n, \tilde{\boldsymbol{u}}) \tag{22}$$

The variation of PKI stress at time τ is given by:

$$\delta \langle \boldsymbol{P} \rangle = \det \boldsymbol{F} \left(\text{tr}(\delta \boldsymbol{F} \boldsymbol{F}^{-1}) \langle \boldsymbol{\sigma} \rangle - \langle \boldsymbol{\sigma} \rangle (\delta \boldsymbol{F} \boldsymbol{F}^{-1})^T + \langle \delta \boldsymbol{\sigma} \rangle \right) \boldsymbol{F}^{-T} \tag{23}$$

From Eq. 11, $\delta \boldsymbol{\sigma}$ can be deduced as:

$$
\begin{aligned}
\delta \boldsymbol{\sigma} &= \delta \left(-\frac{1}{\det \boldsymbol{F}^e} \boldsymbol{F}^e \boldsymbol{T} (\boldsymbol{F}^e)^T \right) \\
&= -tr(\boldsymbol{F}^{-1} \delta \boldsymbol{F}) \boldsymbol{\sigma} + \delta \boldsymbol{F}^e (\boldsymbol{F}^e)^{-T} \boldsymbol{\sigma} + \boldsymbol{\sigma} (\boldsymbol{F}^e)^{-1} \delta (\boldsymbol{F}^e)^T + \frac{1}{\det \boldsymbol{F}^e} \boldsymbol{F}^e \delta \boldsymbol{T} (\boldsymbol{F}^e)^T
\end{aligned} \tag{24}
$$

where $\delta \boldsymbol{F}^e$ is obtained as:

$$\delta(\boldsymbol{F}^e) = \delta \boldsymbol{F} (\boldsymbol{F}^p)^{-1} - \boldsymbol{F}^e_{tr} \sum_\beta sign(\tau^\beta_{tr}) \delta(\Delta \gamma^\beta) \boldsymbol{S}^\beta_0 \tag{25}$$

Then the computation of $\delta \boldsymbol{T}$ can be obtained as from Eq. 14,

$$
\begin{aligned}
\delta \boldsymbol{T} = \; & \mathcal{L}^e \left[\delta \boldsymbol{E}^e_{tr} \right] - \frac{1}{2} \sum_\beta sign(\tau^\beta_{tr}) \delta(\Delta \gamma^\beta) \mathcal{L}^e \left[\boldsymbol{B}^\beta \right] \\
& - \sum_\beta sign(\tau^\beta_{tr}) \Delta \gamma^\beta \mathcal{L}^e \left[\boldsymbol{S}^{\beta T}_0 \delta \boldsymbol{E}^e_{tr} + \delta \boldsymbol{E}^e_{tr} \boldsymbol{S}^\beta_0 \right]
\end{aligned} \tag{26}
$$

$\delta(\Delta \gamma^\beta)$ in this equation is evaluated as following:

$$\delta(\Delta \gamma^\beta) = (A^{\alpha\beta})^{-1} (\delta b^\alpha - \delta A^{\alpha\beta} \Delta \gamma^\beta) \tag{27}$$

$$\delta b^\alpha = sign(\tau^\alpha_{tr}) \mathcal{L}^e \left[\delta \boldsymbol{E}^e_{tr} \right] \cdot \boldsymbol{S}^\alpha_0 \tag{28}$$

$$\delta A^{\alpha\beta} = sign(\tau^\alpha_{tr}) sign(\tau^\beta_{tr}) \boldsymbol{S}^\alpha_0 \cdot \mathcal{L}^e \left[\boldsymbol{S}^{\beta T}_0 \delta \boldsymbol{E}^e_{tr} + \delta \boldsymbol{E}^e_{tr} \boldsymbol{S}^\beta_0 \right] \tag{29}$$

while $\delta \boldsymbol{E}^e_{tr} = \text{sym}(\boldsymbol{F}^{eT}_{tr} \delta \boldsymbol{F} \delta \boldsymbol{F}^{p-1})$.