

PRISMS-Plasticity

Crystal Plasticity

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 $\alpha = 1, \dots, N$ slip systems defined by ortho-normal vector pairs $(\mathbf{m}_0^\alpha, \mathbf{n}_0^\alpha)$ 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 \mathbf{F} which can be decomposed into elastic and plastic parts as $\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$ (with $\det(\mathbf{F}^p) = 1$), 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 $\mathbf{E}^e = \frac{1}{2} (\mathbf{F}^{eT} \mathbf{F}^e - \mathbf{I})$ defined on the relaxed configuration (plastically deformed, unstressed configuration) is utilized. The conjugate stress measure is then defined as $\bar{\mathbf{T}} = \det(\mathbf{F}^e) (\mathbf{F}^e)^{-1} \boldsymbol{\sigma} (\mathbf{F}^e)^{-T}$. Kinematics of single crystal slip is illustrated in Fig. 1.

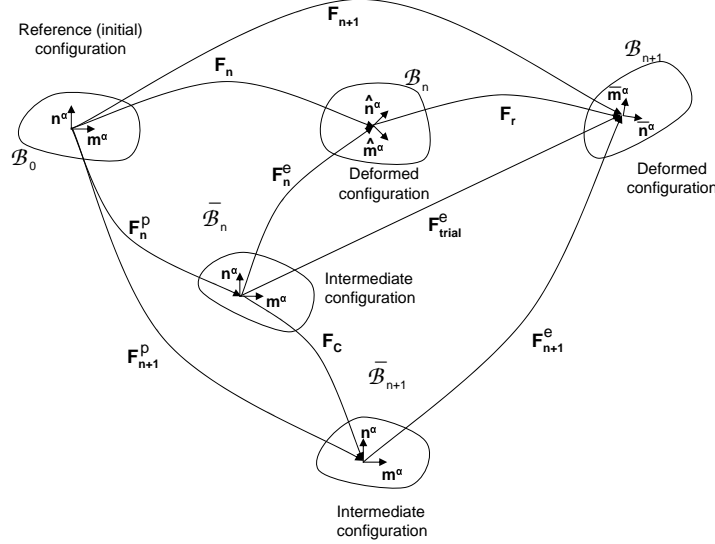


Figure 1: *Schematic of the various material configurations, for a single crystal, used in the integration of the constitutive model. The slip systems $(\mathbf{m}^\alpha, \mathbf{n}^\alpha)$ are known on the reference (initial) configuration. Also, $\hat{\mathbf{m}}^\alpha, \hat{\mathbf{n}}^\alpha$ are the slip directions (different from \mathbf{m}^α 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 $\bar{\mathbf{T}} = \mathcal{C}^e [\mathbf{E}^e]$ where \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:

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

where $\mathbf{S}_0^\alpha = \mathbf{m}_0^\alpha \otimes \mathbf{n}_0^\alpha$ is the Schmid tensor and $\dot{\gamma}^\alpha$ is the plastic shearing rate on the α -th slip system.

The resolved stress on the α^{th} slip system is given by $\tau^\alpha = (\mathbf{C}^e \bar{\mathbf{T}}) \cdot \mathbf{S}_0^\alpha$. This follows from Anand [2] that the plastic power per unit volume in this configuration may be defined by $\dot{\omega} = (\mathbf{C}^e \bar{\mathbf{T}}) \cdot \mathbf{L}_p$ with $\mathbf{C}^e = \mathbf{F}^{eT} \mathbf{F}^e$. The resolved shear stress is defined through the relation $\dot{\omega} = \sum_\alpha \tau^\alpha \dot{\gamma}^\alpha$.

A rate independent algorithm is employed to solve the single crystal model [1]. 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 $\dot{\gamma}^\alpha > 0$, where $\dot{\gamma}^\alpha$ is assumed to be constant during the time step. There is no plastic shearing rate, i.e., $\dot{\gamma}^\alpha = 0$ 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:

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

where

$$h^{\alpha\beta} = \begin{cases} h_o^\beta \left(1 - \frac{s^\beta(t)}{s_s^\beta}\right)^a, & \text{if } \alpha = \beta \\ h_o^\beta q \left(1 - \frac{s^\beta(t)}{s_s^\beta}\right)^a, & \text{otherwise} \end{cases}$$

Subsequently, the plastic part of the deformation gradient is updated using Eq. (4), the elastic part computed from $\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$. The conjugate stress measure, $\bar{\mathbf{T}}$ is then computed from $\bar{\mathbf{T}} = \mathbf{C}^e [\mathbf{E}^e]$ and converted to Cauchy stress and the Piola-Kirchhoff-I stress, $\mathbf{P} = (\det \mathbf{F}) \boldsymbol{\sigma} \mathbf{F}^{-T}$ for further use. The slip resistances are also updated at the end of the time step using Eq. 2. Finally, the tangent modulus $\frac{\partial \mathbf{P}}{\partial \mathbf{F}}$ for use in the weak form is computed using a fully implicit algorithm described in the following section.

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,

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p \quad (3)$$

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

$$\mathbf{L}^p = \dot{\mathbf{F}}^p (\mathbf{F}^p)^{-1} = \sum_\alpha \dot{\gamma}^\alpha \mathbf{S}_0^\alpha (\tau^\alpha) \quad (4)$$

where $\mathbf{S}_0^\alpha = \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha$ is the Schmid tensor and $\dot{\gamma}^\alpha$ is the plastic shearing rate on the α^{th} slip system. The solution of \mathbf{F}^p is computed by assuming a constant shearing rate $\dot{\gamma}^\alpha$ for the time-step:

$$\mathbf{F}_{n+1}^p = \exp\left(\sum_\alpha \Delta \gamma^\alpha \mathbf{S}_0^\alpha (\tau^\alpha)\right) \mathbf{F}_n^p \quad (5)$$

$\dot{\gamma}$ from Eq. 4 changes to $\Delta\gamma$ here, because it is now the increment in infinitesimal time Δt . \mathbf{F}^e can be obtained from Eq. 3 as:

$$\mathbf{F}^e = \mathbf{F}_{tr}^e \exp\left(-\sum_{\alpha} \Delta\gamma^{\alpha} \mathbf{S}_0^{\alpha}(\tau^{\alpha})\right) \quad (6)$$

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

$$\mathbf{E}^e = \frac{1}{2}((\mathbf{F}^e)^T \mathbf{F}^e - \mathbf{I}) \quad (7)$$

Let t denote the current time, Δt and infinitesimal time increment, and $\tau = t + \Delta t$. Then, given $\mathbf{F}(t), \mathbf{F}(\tau), \mathbf{m}_0^{\alpha}, \mathbf{n}_0^{\alpha}, \boldsymbol{\sigma}(t), \mathbf{F}^p(t)$ and $s^{\alpha}(t), \mathbf{F}^p(\tau), s^{\alpha}(\tau), \boldsymbol{\sigma}(\tau)$ need to be found out. First deformation gradient and Lagrangian strain are shown as

$$\mathbf{F}_{tr}^e(\tau) = \mathbf{F}(\tau) \mathbf{F}^p(t)^{-1} \quad (8)$$

$$\mathbf{E}_{tr}^e(\tau) = \frac{1}{2}((\mathbf{F}_{tr}^e(\tau))^T \mathbf{F}_{tr}^e(\tau) - \mathbf{I}) \quad (9)$$

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

$$\mathbf{T} = \det \mathbf{F}^e (\mathbf{F}^e)^{-1} \boldsymbol{\sigma} (\mathbf{F}^e)^{-T} \quad (10)$$

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

$$\mathbf{T}(\tau) = \mathcal{L}^e [\mathbf{E}^e(\tau)] \quad (11)$$

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

$$\tau^{\alpha} = (\mathbf{C}^e(\tau) \mathbf{T}(\tau)) \cdot \mathbf{S}_0^{\alpha} \quad (12)$$

while trial resolved shear stress is defined in the same way as $\tau_{tr}^{\alpha}(\tau) = (\mathbf{C}_{tr}^e(\tau) \mathbf{T}_{tr}(\tau)) \cdot \mathbf{S}_0^{\alpha}$. In crystal plastic theory the hardening law for the slip resistance s^{α} at time τ is given as:

$$s^{\alpha}(\tau) = s^{\alpha}(t) + \sum_{\beta} h^{\alpha\beta}(t) \Delta\gamma^{\beta} \quad (13)$$

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 $\alpha, \beta \in \mathcal{A}$:

$$\sum_{\beta \in \mathcal{A}} A^{\alpha\beta} \Delta\gamma^{\beta} = b^{\alpha} \quad (14)$$

where,

$$\begin{aligned} A^{\alpha\beta} &= h^{\alpha\beta}(t) + (\tau_{tr}^{\alpha}(\tau))(\tau_{tr}^{\beta}(\tau))(\mathbf{C}_{tr}^e(\tau) \mathcal{L}^e [\mathbf{B}^{\beta}] + 2\mathbf{B}^{\beta} \mathbf{T}_{tr}(\tau)) \cdot \mathbf{S}_0^{\alpha} \\ b^{\alpha} &= |\tau_{tr}^{\alpha}(\tau)| - s^{\alpha}(t) \end{aligned} \quad (15)$$

where $\mathbf{B} = (\mathbf{S}_0^{\alpha})^T (\mathbf{F}_{tr}^e)^T \mathbf{F}_{tr}^e + (\mathbf{F}_{tr}^e)^T \mathbf{F}_{tr}^e \mathbf{S}_0^{\alpha}$

only values of $\Delta\gamma$ bigger than 0 will be kept. The equation is solved repeatedly with $b^\alpha = |\tau^\alpha(\tau)|_n - s^\alpha(t)$ and $A^{\alpha\beta} = h^{\alpha\beta}(t) + (\tau_{tr}^\alpha(\tau))(\tau_{tr}^\beta(\tau))(C_{tr}^e(\tau)\mathcal{L}^e[B^\beta] + 2B^\beta T_{tr}(\tau)) \cdot S_0^\alpha$ until $b^\alpha < tol$ is reached.

Then, $\mathbf{F}^p(\tau)$ can be updated by Eq.5, $\mathbf{F}^e(\tau)$ updates through Eq.3 or Eq.6. $\boldsymbol{\sigma}(\tau)$ needs $\mathbf{T}(\tau)$ first, which can be updated through Eq.11. Then $\boldsymbol{\sigma}(\tau)$ can be found by $\boldsymbol{\sigma}(\tau) = \mathbf{F}^e(\tau) [\det(\mathbf{F}^e(\tau))]^{-1} \mathbf{T}(\tau) \mathbf{F}^e(\tau)^T$ from Eq.10, $s^\alpha(\tau)$ can be specified by Eq.13.

Tangent Modulus

The kinematic problem can be expressed in Lagrangian framework as

$$\nabla_0 \cdot \mathbf{P} + \mathbf{f} = \mathbf{0} \quad (16)$$

where ∇_0 is the divergence in the initial reference configuration, \mathbf{P} is the polycrystal Piola-Kirchhoff-I stress, shown as and \mathbf{f} is the reference body force.

$$\mathbf{P} = \det \mathbf{F} \boldsymbol{\sigma} \mathbf{F}^{-T} \quad (17)$$

Principle of Virtual Work states that \mathcal{B}_0 is in equilibrium if and only if the Piola-Kirchhoff stress field, \mathbf{P} , satisfies the virtual work functional for any kinematically admissible test function $\tilde{\mathbf{u}}$,

$$\mathcal{G}(\mathbf{u}, \tilde{\mathbf{u}}) \equiv \int_{\mathcal{B}_0} \mathbf{P} \cdot \nabla_0 \tilde{\mathbf{u}} dV - \int_{\partial \mathcal{B}_0} \boldsymbol{\lambda} \cdot \tilde{\mathbf{u}} dA - \int_{\mathcal{B}_0} \mathbf{f} \cdot \tilde{\mathbf{u}} dV = 0 \quad \forall \tilde{\mathbf{u}} \in \mathcal{V} \quad (18)$$

where \mathcal{V} is the function space in finite dimensions of all admissible shape functions in the material domain, \mathbf{f} and $\boldsymbol{\lambda}$ denote, respectively, the reference body force and surface traction fields.

The dependence of \mathcal{G} on the unknown function \mathbf{u} follows from the constitutive dependence of the stress tensor on the strain tensor which, in turn depends on the field \mathbf{u} . In the above, \mathbf{P} is a functional of the displacement field due to its constitutive dependence on the deformation gradient $\mathbf{F} = \mathbf{I} + \nabla_0 \mathbf{u}$.

Newton-Raphson iterative scheme with a line search procedure is employed. The directional derivative of \mathcal{G} at \mathbf{u}_n in the direction of $\Delta \mathbf{u}$ is given by

$$\frac{\partial \mathcal{G}(\mathbf{u}_n, \tilde{\mathbf{u}})}{\partial \mathbf{u}_n} \Delta \mathbf{u} = \int_{\mathcal{B}_0} \mathbf{A} \frac{\partial \mathbf{F}}{\partial \mathbf{u}_n} \cdot \nabla_0 \tilde{\mathbf{u}} dV \Delta \mathbf{u} = \int_{\mathcal{B}_0} \mathbf{A} \nabla_0 \Delta \mathbf{u} \cdot \nabla_0 \tilde{\mathbf{u}} dV \Delta \mathbf{u} \quad (19)$$

where

$$\mathbf{A} \equiv \left. \frac{\partial \mathbf{P}}{\partial \mathbf{F}} \right|_{\mathbf{F}_n} \quad (20)$$

is generally termed the material tangent modulus.

The Piola-Kirchhoff-I stress, shown as \mathbf{P} can be expanded as

$$\begin{aligned} \mathbf{P} &= \det \mathbf{F} \boldsymbol{\sigma} \mathbf{F}^{-T} \\ &= \det \mathbf{F} ((\det \mathbf{F}^e)^{-1} \mathbf{F}^e \mathbf{T} (\mathbf{F}^e)^T) \mathbf{F}^{-T} \\ &= \mathbf{F}^e \mathbf{T} (\mathbf{F}^e)^T \mathbf{F}^{-T} \end{aligned} \quad (21)$$

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

$$\begin{aligned}\delta \mathbf{P} &= \delta(\mathbf{F}^e \mathbf{T} (\mathbf{F}^e)^T \mathbf{F}^{-T}) \\ &= \delta(\mathbf{F}^e) \mathbf{T} (\mathbf{F}^e)^T \mathbf{F}^{-T} + \mathbf{F}^e \delta(\mathbf{T}) (\mathbf{F}^e)^T \mathbf{F}^{-T} + \mathbf{F}^e \mathbf{T} \delta((\mathbf{F}^e)^T) \mathbf{F}^{-T} \\ &\quad + \mathbf{F}^e \mathbf{T} (\mathbf{F}^e)^T \delta(\mathbf{F}^{-T})\end{aligned}\tag{22}$$

$$\begin{aligned}&= \delta(\mathbf{F}^e) \mathbf{T} (\mathbf{F}^e)^T \mathbf{F}^{-T} + \mathbf{F}^e \delta(\mathbf{T}) (\mathbf{F}^e)^T \mathbf{F}^{-T} + \mathbf{F}^e \mathbf{T} (\delta \mathbf{F}^e)^T \mathbf{F}^{-T} \\ &\quad + \mathbf{F}^e \mathbf{T} (\mathbf{F}^e)^T \delta(\mathbf{F}^{-1})^T\end{aligned}\tag{23}$$

$$\begin{aligned}&= \delta(\mathbf{F}^e) \mathbf{T} (\mathbf{F}^e)^T \mathbf{F}^{-T} + \mathbf{F}^e \delta(\mathbf{T}) (\mathbf{F}^e)^T \mathbf{F}^{-T} + \mathbf{F}^e \mathbf{T} (\delta \mathbf{F}^e)^T \mathbf{F}^{-T} \\ &\quad - \mathbf{F}^e \mathbf{T} (\mathbf{F}^e)^T (\mathbf{F}^{-1})^T \delta(\mathbf{F})^T (\mathbf{F}^{-1})^T\end{aligned}\tag{24}$$

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

$$\begin{aligned}\delta(\mathbf{F}^e) &= \delta \mathbf{F} (\mathbf{F}^p)^{-1} + \mathbf{F} \delta((\mathbf{F}^p)^{-1}) \\ &= \delta \mathbf{F} (\mathbf{F}^p)^{-1} - \mathbf{F} (\mathbf{F}^p)^{-1} \delta(\mathbf{F}^p) (\mathbf{F}^p)^{-1}\end{aligned}\tag{25}$$

Then the computation of $\delta \mathbf{T}$ can be obtained as from Eq. 11,

$$\delta \mathbf{T} = \mathcal{L}^e [\delta \mathbf{E}^e]\tag{26}$$

while

$$\begin{aligned}\delta \mathbf{E}^e &= \frac{1}{2} (\delta((\mathbf{F}^e)^T) \mathbf{F}^e + (\mathbf{F}^e)^T \delta(\mathbf{F}^e)) \\ &= \frac{1}{2} ((\delta \mathbf{F}^e)^T \mathbf{F}^e + (\mathbf{F}^e)^T \delta(\mathbf{F}^e))\end{aligned}\tag{27}$$

The variation of plastic deformation gradient, $\delta(\mathbf{F}^p)$ is computed in a iterative manner as follows

$\delta \mathbf{F}_{trial}^e$ is obtained as:

$$\begin{aligned}\delta(\mathbf{F}_{trial}^e) &= \delta \mathbf{F} (\mathbf{F}_{i-1}^p)^{-1} + \mathbf{F} \delta((\mathbf{F}_{i-1}^p)^{-1}) \\ &= \delta \mathbf{F} (\mathbf{F}_{i-1}^p)^{-1} - \mathbf{F} (\mathbf{F}_{i-1}^p)^{-1} \delta(\mathbf{F}_{i-1}^p) (\mathbf{F}_{i-1}^p)^{-1}\end{aligned}\tag{28}$$

where \mathbf{F}_i^p is the plastic deformation gradient in the i th iteration, $\mathbf{F}_0^p = \mathbf{F}_n^p$

$$\delta \mathbf{E}_{trial}^e = \frac{1}{2} ((\delta \mathbf{F}_{trial}^e)^T \mathbf{F}^e + (\mathbf{F}^e)^T \delta(\mathbf{F}_{trial}^e))\tag{29}$$

$$\delta \mathbf{T}_{trial} = \mathcal{L}^e [\delta \mathbf{E}_{trial}^e]\tag{30}$$

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

$$\delta b_i^\alpha = (\tau_{trial}^\alpha) \delta(\mathbf{C}_{trial}^e \mathbf{T}_{trial}) \cdot \mathbf{S}_0^\alpha - \delta(s_{i-1}^\alpha)\tag{31}$$

$$= (\tau_{trial}^\alpha) (\delta(\mathbf{C}_{trial}^e) \mathbf{T}_{trial} + \mathbf{C}_{trial}^e \delta(\mathbf{T}_{trial})) \cdot \mathbf{S}_0^\alpha - \delta(s_{i-1}^\alpha)\tag{32}$$

$$= (\tau_{trial}^\alpha) (2\delta(\mathbf{E}_{trial}^e) \mathbf{T}_{trial} + \mathbf{C}_{trial}^e \delta(\mathbf{T}_{trial})) \cdot \mathbf{S}_0^\alpha - \delta(s_{i-1}^\alpha)\tag{33}$$

The variation of slip system resistance s^α is computed as follows

$$\begin{aligned}
\delta(s_i^\alpha) &= \delta(s_{i-1}^\alpha) + \sum_\beta \delta h^{\alpha\beta} \Delta\gamma^\beta + \sum_\beta h^{\alpha\beta} \delta(\Delta\gamma^\beta) \\
&= \delta(s_{i-1}^\alpha) + \sum_\beta h_o^\beta (q + (1-q)\delta^{\alpha\beta}) (1 - \frac{s_i^\beta}{s_s^\beta})^{(a-1)} (\frac{-1}{s_s^\beta}) \delta(s_{i-1}^\beta) \Delta\gamma^\beta + \sum_\beta h^{\alpha\beta} \delta\Delta\gamma^\beta
\end{aligned} \tag{34}$$

$$\delta(\Delta\gamma^\beta) = (A^{\alpha\beta})^{-1} (\delta b^\alpha - \delta A^{\alpha\beta} \Delta\gamma^\beta) \tag{35}$$

$$\delta b^\alpha = (\tau_{tr}^\alpha) \mathcal{L}^e [\delta \mathbf{E}_{tr}^e] \cdot \mathbf{S}_0^\alpha \tag{36}$$

$$\delta A^{\alpha\beta} = (\tau_{tr}^\alpha) (\tau_{tr}^\beta) \mathbf{S}_0^\alpha \cdot \mathcal{L}^e \left[\mathbf{S}_0^{\beta T} \delta \mathbf{E}_{tr}^e + \delta \mathbf{E}_{tr}^e \mathbf{S}_0^\beta \right] \tag{37}$$

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

References

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