Crystal Plasticity Formulation

Elasto-plastic constitutive model

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,

$$\boldsymbol{F} = \boldsymbol{F}^e \ \boldsymbol{F}^p \tag{1}$$

$\boldsymbol{F}^e$ 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,

$$\boldsymbol{L}^p = \dot{\boldsymbol{F}}^p(\boldsymbol{F}^p)^{-1} \ = \ \sum_\alpha \dot{\gamma}^\alpha \boldsymbol{S}_0^\alpha sign(\tau^\alpha) \tag{2}$$

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 α^{th} slip system. The solution of $\boldsymbol{F}^p$ from Euler-backward scheme is:

$$\boldsymbol{F}^p_{n+1} \approx (\boldsymbol{I} + \sum_\alpha \Delta\gamma^\alpha \boldsymbol{S}_0^\alpha sign(\tau^\alpha))\boldsymbol{F}^p_n \tag{3}$$

$\dot{\gamma}$ from Eq. 2 changes to $\Delta\gamma$ here, because it is now the increment in infinitesimal time Δt. $\boldsymbol{F}^e$ can be obtained from Eq. 1 as:

$$\boldsymbol{F}^e = \boldsymbol{F}^e_{tr}(\boldsymbol{I} - \sum_\alpha \Delta\gamma^\alpha \boldsymbol{S}_0^\alpha sign(\tau^\alpha)) \tag{4}$$

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

$$\begin{aligned} \boldsymbol{E}^e &= \frac{1}{2}(\boldsymbol{F}^{eT}\boldsymbol{F}^e - \boldsymbol{I}) \\ &= \boldsymbol{E}^e_{tr} - \frac{1}{2}\sum_\alpha sign(\tau^\alpha)\Delta\gamma^\alpha \boldsymbol{B}^\alpha \end{aligned} \tag{5}$$

where $\boldsymbol{E}^e_{tr} = \frac{1}{2}((\boldsymbol{F}^e_{tr})^T\boldsymbol{F}^e_{tr} - \boldsymbol{I})$ and $\boldsymbol{B} = (\boldsymbol{S}_0^\alpha)^T(\boldsymbol{F}^e_{tr})^T\boldsymbol{F}^e_{tr} + (\boldsymbol{F}^e_{tr})^T\boldsymbol{F}^e_{tr}\boldsymbol{S}_0^\alpha$

Let t denote the current time, Δt and infinitesimal time increment, and $\tau = t + \Delta t$. Then, given $\boldsymbol{F}(t), \boldsymbol{F}(\tau)$, $\boldsymbol{m}_0^\alpha, \boldsymbol{n}_0^\alpha, \boldsymbol{\sigma}(t), \boldsymbol{F}^p(t)$ 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

$$\boldsymbol{F}^e_{tr}(\tau) = \boldsymbol{F}(\tau) \ \boldsymbol{F}^p(t)^{-1} \tag{6}$$

$$\boldsymbol{E}^e_{tr}(\tau) = \frac{1}{2}(\boldsymbol{F}^e_{tr}(\tau))^T\boldsymbol{F}^e_{tr}(\tau) \tag{7}$$

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

$$\boldsymbol{T} \ = \ \det\boldsymbol{F}^e(\boldsymbol{F}^e)^{-1}\boldsymbol{\sigma}(\boldsymbol{F}^e)^{-T} \tag{8}$$

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

$$\boldsymbol{T}(\tau) \;=\; \boldsymbol{\mathcal{L}}^e \left[\boldsymbol{E}^e(\tau)\right] \tag{9}$$

$\boldsymbol{T}_{tr}(\tau)$ 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

$$\tau^\alpha = \boldsymbol{T}(\tau) \cdot \boldsymbol{S}^\alpha_0 \tag{10}$$

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.5 to Eq.9, we obtain,

$$\boldsymbol{T}(\tau) = \boldsymbol{T}_{tr}(\tau) - \frac{1}{2}\sum_\beta sign(\tau^\beta_{tr}(\tau))\Delta\gamma^\beta \boldsymbol{\mathcal{L}}^e \left[\boldsymbol{B}^\beta\right] \tag{11}$$

then apply new $\boldsymbol{T}(\tau)$ to Eq.10, we will get

$$\tau^\alpha(\tau) = |\tau^\alpha_{tr}| - \frac{1}{2}\sum_\beta sign(\tau^\alpha_{tr}(\tau))sign(\tau^\beta_{tr}(\tau))\Delta\gamma^\beta \boldsymbol{\mathcal{L}}^e \left[\boldsymbol{B}^\beta\right] \cdot \boldsymbol{S}^\alpha_0 \tag{12}$$

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

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

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

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

where,

$$\begin{aligned} A^{\alpha\beta} &= h^{\alpha\beta}(t) + sign(\tau^\alpha_{tr}(\tau))sign(\tau^\beta_{tr}(\tau))\boldsymbol{\mathcal{L}}^e \left[\boldsymbol{B}^\beta\right] \cdot \boldsymbol{S}^\alpha_0 \\ b^\alpha &= |\tau^\alpha_{tr}(\tau)| - s^\alpha(t) \end{aligned} \tag{15}$$

only values of $\Delta\gamma$ bigger than 0 will be kept. Then, $\boldsymbol{F}^p(\tau)$ can be updated by Eq.3, $\boldsymbol{F}^e(\tau)$ updates through Eq.1 or Eq.4. $\boldsymbol{\sigma}(\tau)$ needs $\boldsymbol{T}(\tau)$ first, which can be updated through Eq.9. 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.8, $s^\alpha(\tau)$ can be specified by Eq.13.

Tangent modulus

Kinematic problem can be expressed in Lagrangian framework by

$$\nabla_0 \cdot \langle\boldsymbol{P}\rangle + \boldsymbol{f} = \boldsymbol{0} \tag{16}$$

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

$$\langle\boldsymbol{P}\rangle = \det\boldsymbol{F}\langle\boldsymbol{\sigma}\rangle\boldsymbol{F}^{-T} \tag{17}$$

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

$$\mathcal{G}(\boldsymbol{u}_{n+1}, \tilde{\boldsymbol{u}}) \equiv \int_{\mathcal{B}_0} \langle \boldsymbol{P} \rangle \cdot \nabla_0 \tilde{\boldsymbol{u}} dV - \int_{\partial \mathcal{B}_0} \boldsymbol{\lambda} \cdot \tilde{\boldsymbol{u}} dA - \int_{\mathcal{B}_0} \boldsymbol{f} \cdot \tilde{\boldsymbol{u}} dV = 0 \tag{18}$$

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

$$\frac{\partial \mathcal{G}(\boldsymbol{u}_n, \tilde{\boldsymbol{u}})}{\partial \boldsymbol{u}_n} \Delta \boldsymbol{u} = \int_{\mathcal{B}_0} \frac{\partial \langle \boldsymbol{P} \rangle}{\partial \boldsymbol{F}} \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{u}_n} \cdot \nabla_0 \tilde{\boldsymbol{u}} dV \Delta \boldsymbol{u} = \mathcal{G}(\boldsymbol{u}_n, \tilde{\boldsymbol{u}}) \tag{19}$$

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

$$\delta \langle \boldsymbol{P} \rangle = \det \boldsymbol{F} \left(\mathrm{tr}(\delta \boldsymbol{F} \boldsymbol{F}^{-1}) \langle \boldsymbol{\sigma} \rangle - \langle \boldsymbol{\sigma} \rangle (\delta \boldsymbol{F} \boldsymbol{F}^{-1})^T + \langle \delta \boldsymbol{\sigma} \rangle \right) \boldsymbol{F}^{-T} \tag{20}$$

From Eq. 8, $\delta \boldsymbol{\sigma}$ can be deduced as:

$$\begin{aligned} \delta \boldsymbol{\sigma} &= \delta \left(-\frac{1}{\det \boldsymbol{F}^e} \boldsymbol{F}^e \boldsymbol{T} (\boldsymbol{F}^e)^T \right) \\ &= -tr(\boldsymbol{F}^{-1} \delta \boldsymbol{F}) \boldsymbol{\sigma} + \delta \boldsymbol{F}^e (\boldsymbol{F}^e)^{-T} \boldsymbol{\sigma} + \boldsymbol{\sigma} (\boldsymbol{F}^e)^{-1} \delta (\boldsymbol{F}^e)^T + \frac{1}{\det \boldsymbol{F}^e} \boldsymbol{F}^e \delta \boldsymbol{T} (\boldsymbol{F}^e)^T \end{aligned} \tag{21}$$

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

$$\delta(\boldsymbol{F}^e) = \delta \boldsymbol{F} (\boldsymbol{F}^p)^{-1} - \boldsymbol{F}^e_{tr} \sum_\beta sign(\tau^\beta_{tr}) \delta(\Delta \gamma^\beta) \boldsymbol{S}^\beta_0 \tag{22}$$

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

$$\begin{aligned} \delta \boldsymbol{T} &= \boldsymbol{\mathcal{L}}^e \left[\delta \boldsymbol{E}^e_{tr} \right] - \frac{1}{2} \sum_\beta sign(\tau^\beta_{tr}) \delta(\Delta \gamma^\beta) \boldsymbol{\mathcal{L}}^e \left[\boldsymbol{B}^\beta \right] \\ &- \sum_\beta sign(\tau^\beta_{tr}) \Delta \gamma^\beta \boldsymbol{\mathcal{L}}^e \left[\boldsymbol{S}^{\beta T}_0 \delta \boldsymbol{E}^e_{tr} + \delta \boldsymbol{E}^e_{tr} \boldsymbol{S}^\beta_0 \right] \end{aligned} \tag{23}$$

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

$$\delta(\Delta \gamma^\beta) = (A^{\alpha\beta})^{-1} (\delta b^\alpha - \delta A^{\alpha\beta} \Delta \gamma^\beta) \tag{24}$$

$$\delta b^\alpha = sign(\tau^\alpha_{tr}) \boldsymbol{\mathcal{L}}^e \left[\delta \boldsymbol{E}^e_{tr} \right] \cdot \boldsymbol{S}^\alpha_0 \tag{25}$$

$$\delta A^{\alpha\beta} = sign(\tau^\alpha_{tr}) sign(\tau^\beta_{tr}) \boldsymbol{S}^\alpha_0 \cdot \boldsymbol{\mathcal{L}}^e \left[\boldsymbol{S}^{\beta T}_0 \delta \boldsymbol{E}^e_{tr} + \delta \boldsymbol{E}^e_{tr} \boldsymbol{S}^\beta_0 \right] \tag{26}$$

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