FCC Crystal Plasticity Framework with ABAQUS/Explicit (VUMAT) Implementation

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1 Kinematics

The total deformation gradient $\mathbf{F}$ is multiplicatively decomposed into elastic and plastic parts. Elastic deformation is caused by lattice distortion and rotation, while plastic deformation is dominated by slip.

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$$

where:

- $\mathbf{F}^e$: Elastic deformation gradient (includes lattice rotation and stretch).
- $\mathbf{F}^p$: Plastic deformation gradient (accumulates slip system shear).

2 Slip System Definition

FCC crystals have 12 slip systems defined by the Schmid tensor in the **reference configuration**:

$$\mathbf{S}_0^\alpha = \mathbf{s}_0^\alpha \otimes \mathbf{n}_0^\alpha$$

where:

- $\mathbf{s}_0^\alpha \in \langle 110 \rangle$: Slip direction.
- $\mathbf{n}_0^\alpha \in \{111\}$: Slip plane normal.

3 Current Configuration Schmid Tensor

When considering the effect of elastic deformation (including rotation and stretching) on the Schmid tensor, the Schmid tensor of the current configuration should be transformed by the full elastic deformation gradient $\mathbf{F}^e$.

- **Slip direction** is mapped to the current configuration through:

$$\mathbf{s}^\alpha = \mathbf{F}^e \mathbf{s}_0^\alpha$$

- **Slip plane normal** is mapped to the current configuration through:

$$\mathbf{n}^\alpha = \mathbf{F}^{e-T}\mathbf{n}_0^\alpha$$

Thus, the Schmid tensor in the current configuration is:

$$\mathbf{S}^\alpha = \mathbf{s}^\alpha \otimes \mathbf{n}^\alpha = \mathbf{F}^e\mathbf{s}_0^\alpha \otimes \mathbf{F}^{e-T}\mathbf{n}_0^\alpha = \mathbf{F}^e(\mathbf{s}_0^\alpha \otimes \mathbf{n}_0^\alpha)\mathbf{F}^{e-T} = \mathbf{F}^e\mathbf{S}_0^\alpha\mathbf{F}^{e-T}$$

4 Cauchy Stress

The Cauchy stress $\boldsymbol{\sigma}$ is computed as:

$$\boldsymbol{\sigma} = \frac{1}{\det \mathbf{F}^e}\mathbf{F}^e\mathbf{S}^e\mathbf{F}^{eT}$$

where $\mathbf{S}^e$ is the second Piola-Kirchhoff stress in the intermediate configuration:

$$\mathbf{S}^e = \mathbb{C} : \mathbf{E}^e$$

and $\mathbf{E}^e$ is the elastic Green strain:

$$\mathbf{E}^e = \frac{1}{2}\left(\mathbf{F}^{eT}\mathbf{F}^e - \mathbf{I}\right).$$

5 Resolved Shear Stress

Key Principle: Stress and Schmid tensor must be calculated in the same configuration to ensure consistency in physical projection.

- The resolved shear stress on slip system α is:

$$\tau^\alpha = \boldsymbol{\sigma} : \mathbf{S}^\alpha.$$

- If Second Piola-Kirchhoff stress $\mathbf{S}^e$ is used to calculate the resolved shear stress, the Schmid tensor needs to be pulled back to the intermediate configuration:

$$\tau^\alpha = \mathbf{S}^e : \left(\mathbf{F}^{e-T}\mathbf{S}^\alpha\mathbf{F}^{e-1}\right)$$

6 Slip System Evolution

6.1 Flow Rule

The shear strain rate is given by:

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left(\frac{|\tau^\alpha|}{g^\alpha}\right)^{1/m} \mathrm{sign}(\tau^\alpha),$$

where:

- $\dot{\gamma}_0$: Reference shear rate.
- m: Strain rate sensitivity exponent.
- g^α: Critical resolved shear stress.

6.2 Hardening Law

The evolution of the critical resolved shear stress is:

$$\dot{g}^{\alpha} = \sum_{\beta=1}^{12} h_{\alpha\beta} |\dot{\gamma}^{\beta}|,$$

where the hardening modulus $h_{\alpha\beta}$ is:

$$h_{\alpha\beta} = q_{\alpha\beta} h_0 \left(1 - \frac{g^{\beta}}{g_{\text{sat}}}\right)^{a_h}$$

and

$$q_{\alpha\beta} = q_1 + (1 - q_1)\delta_{ij}$$

7 Velocity Gradient

7.1 Elastic Velocity Gradient

- Elastic velocity gradient

$$\mathbf{L}^e = \dot{\mathbf{F}}^e \mathbf{F}^{e-1}$$

- Plastic velocity gradient

$$\mathbf{L}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p-1}$$

- Total velocity gradient

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1} = \left(\dot{\mathbf{F}}^e \mathbf{F}^p + \mathbf{F}^e \dot{\mathbf{F}}^p\right)\left(\mathbf{F}^{p-1}\mathbf{F}^{e-1}\right) = \underbrace{\dot{\mathbf{F}}^e \mathbf{F}^{e-1}}_{\mathbf{L}^e} + \mathbf{F}^e \underbrace{\left(\dot{\mathbf{F}}^p \mathbf{F}^{p-1}\right)}_{\mathbf{L}^p} \mathbf{F}^{e-1}$$

Therefore

$$\mathbf{L}^e = \mathbf{L} - \mathbf{F}^e \mathbf{L}^p \mathbf{F}^{e-1}$$

7.2 Plastic Velocity Gradient

Plastic deformation is dominated by the shear of the slip system, and its velocity gradient is defined as:

$$\mathbf{L}^p = \sum_{\alpha=1}^{12} \dot{\gamma}^{\alpha} \mathbf{S}_0^{\alpha} = \sum_{\alpha=1}^{12} \dot{\gamma}^{\alpha} \left(\mathbf{s}_0^{\alpha} \otimes \mathbf{n}_0^{\alpha}\right)$$

Where:

- $\mathbf{S}_0^{\alpha}$ is the Schmid tensor in the reference configuration.
- $\dot{\gamma}^{\alpha}$ is the shear strain rate of the slip system α.

Physical Meaning:

- Plastic deformation occurs in the intermediate configuration (the configuration after elastic unloading), and the slip system direction is defined by the initial reference configuration.

- $\mathbf{L}^p$ describes the local flow induced by slip in the intermediate configuration of the material, which is independent of the elastic deformation of the current configuration.

The Role of the Schmid Tensor in the Current Configuration

The Schmid tensor $\mathbf{S}^\alpha$ in the current configuration is used to calculate the resolved shear stress τ^α:

$$\tau^\alpha = \boldsymbol{\sigma} : \mathbf{S}^\alpha = \boldsymbol{\sigma} : \left(\mathbf{F}^e \mathbf{S}_0^\alpha \mathbf{F}^{e-T}\right)$$

- Here, the Schmid tensor $\mathbf{S}^\alpha$ of the current configuration must be used because the resolved shear stress reflects the projection of the current stress state onto the slip system.

- Elastic deformation (rotation and stretch) dynamically adjusts the spatial orientation of the slip system through $\mathbf{F}^e$, affecting the resolved shear stress, but does not change the definition of plastic flow.

8 Lattice Rotation Update

8.1 Elastic Velocity Gradient

Plastic Deformation Gradient Update (Explicit Integration):

$$\mathbf{F}_{n+1}^p = \exp\left(\mathbf{L}^p \Delta t\right) \mathbf{F}_n^p$$

Elastic Deformation Gradient Update

$$\mathbf{F}_{n+1}^e = \mathbf{F}_{n+1} \mathbf{F}_{n+1}^{p-1}$$

Total Velocity Gradient:

$$\mathbf{L} = \frac{\mathbf{F}_{n+1} - \mathbf{F}_n}{\Delta t} \mathbf{F}_{n+1}^{-1}$$

Elastic Velocity Gradient:

$$\mathbf{L}^e = \mathbf{L} - \mathbf{F}_{n+1}^e \mathbf{L}^p \mathbf{F}_{n+1}^{e-1}$$

8.2 Elastic Spin and Rotation Update

The elastic velocity gradient $\mathbf{L}^e$ can be decomposed into a symmetric part (stretch rate $\mathbf{D}^e$) and an antisymmetric part (spin rate $\mathbf{W}^e$):

$$\mathbf{L}^e = \mathbf{D}^e + \mathbf{W}^e,$$

where

$$\mathbf{D}^e = \frac{1}{2}\left(\mathbf{L}^e + (\mathbf{L}^e)^T\right), \quad \mathbf{W}^e = \frac{1}{2}\left(\mathbf{L}^e - (\mathbf{L}^e)^T\right).$$

From the polar decomposition $\mathbf{F}^e = \mathbf{R}^e\mathbf{U}^e$, differentiate with respect to time:

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

Combining with the definition of the elastic velocity gradient $\mathbf{L}^e = \dot{\mathbf{F}}^e(\mathbf{F}^e)^{-1}$, and substituting the polar decomposition, we get:

$$\mathbf{L}^e = \underbrace{\dot{\mathbf{R}}^e(\mathbf{R}^e)^{-1}}_{\text{anti-symmetric}} + \underbrace{\mathbf{R}^e\dot{\mathbf{U}}^e(\mathbf{U}^e)^{-1}(\mathbf{R}^e)^{-1}}_{\text{symmetric}}$$

Thus,

$$\dot{\mathbf{R}}^e = \mathbf{W}^e\mathbf{R}^e.$$

Within the time step Δt, solve the differential equation $\dot{\mathbf{R}}^e = \mathbf{W}^e\mathbf{R}^e$. Assuming $\mathbf{W}^e$ is constant over the step, the solution is given by the matrix exponential:

$$\mathbf{R}^e_{n+1} = \exp(\mathbf{W}^e\Delta t)\mathbf{R}^e_n.$$

- For the spin tensor $\mathbf{W}^e$, its matrix exponential can be expressed analytically using Rodrigues' formula. Let the rotation vector corresponding to $\mathbf{W}^e$ be $\boldsymbol{\omega} = [\omega_1, \omega_2, \omega_3]^T$, then:

$$\mathbf{W}^e = \begin{bmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{bmatrix}.$$

  Define the rotation angle $\theta = \|\boldsymbol{\omega}\|\Delta t$ and the unit vector $\mathbf{n} = \boldsymbol{\omega}/\|\boldsymbol{\omega}\|$, then:

$$\exp(\mathbf{W}^e\Delta t) = \mathbf{I} + \sin\theta\mathbf{K} + (1-\cos\theta)\mathbf{K}^2,$$

  where $\mathbf{K}$ is the skew-symmetric matrix:

$$\mathbf{K} = \begin{bmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{bmatrix}.$$

- Numerical integration may cause $\mathbf{R}^e_{n+1}$ to lose orthogonality, which needs to be corrected using the Gram-Schmidt orthogonalization:

  1. Take the three column vectors of $\mathbf{R}^e_{n+1}$, $\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3$.
  2. Orthogonalize:

$$\mathbf{u}_1 = \frac{\mathbf{r}_1}{\|\mathbf{r}_1\|}, \quad \mathbf{u}_2 = \frac{\mathbf{r}_2 - (\mathbf{r}_2\cdot\mathbf{u}_1)\mathbf{u}_1}{\|\mathbf{r}_2 - (\mathbf{r}_2\cdot\mathbf{u}_1)\mathbf{u}_1\|}, \quad \mathbf{u}_3 = \mathbf{u}_1 \times \mathbf{u}_2.$$

  3. Reconstruct the orthogonal matrix:

$$\mathbf{R}^e_{n+1} = [\mathbf{u}_1\,\mathbf{u}_2\,\mathbf{u}_3].$$

9 ABAQUS/Explicit (VUMAT) Implementation I

9.1 Input Variables

- $\mathbf{F}_n$: Deformation gradient at step n (from ABAQUS).
- $\mathbf{F}_{n+1}$: Deformation gradient at step $n+1$ (from ABAQUS).
- Δt: Time increment.
- State variables at step n: $\mathbf{F}_n^p$, $\mathbf{R}_n^e$, g_n^α.

9.2 Output Variables

- $\boldsymbol{\sigma}_{n+1}$: Cauchy stress at step $n+1$.
- State variables at step $n+1$: $\mathbf{F}_{n+1}^p$, $\mathbf{R}_{n+1}^e$, g_{n+1}^α.

9.3 Explicit Update Procedure

1. Compute elastic deformation gradient:
$$\mathbf{F}_{n+1}^e = \mathbf{F}_{n+1}\mathbf{F}_n^{p-1}.$$
2. Update Schmid tensor:
$$\mathbf{S}_{n+1}^\alpha = \mathbf{F}_{n+1}^e \mathbf{S}_0^\alpha \mathbf{F}_{n+1}^{e-T}.$$
3. Compute Cauchy stress:
$$\boldsymbol{\sigma}_{n+1} = \frac{1}{\det \mathbf{F}_{n+1}^e}\mathbf{F}_{n+1}^e \mathbf{S}_{n+1}^e \mathbf{F}_{n+1}^{eT}.$$
4. Calculate resolved shear stress:
$$\tau_{n+1}^\alpha = \boldsymbol{\sigma}_{n+1} : \mathbf{S}_{n+1}^\alpha.$$
5. Update shear strain rate:
$$\dot{\gamma}_{n+1}^\alpha = \dot{\gamma}_0 \left(\frac{|\tau_{n+1}^\alpha|}{g_n^\alpha}\right)^{1/m} \operatorname{sign}(\tau_{n+1}^\alpha).$$
6. Update critical resolved shear stress:
$$g_{n+1}^\alpha = g_n^\alpha + \Delta t \sum_{\beta=1}^{12} h_{\alpha\beta} |\dot{\gamma}_{n+1}^\beta|.$$
7. Update plastic deformation gradient:
$$\mathbf{F}_{n+1}^p = \left(\mathbf{I} + \mathbf{L}_{n+1}^p \Delta t\right) \mathbf{F}_n^p$$
8. Update lattice rotation:
$$\mathbf{R}_{n+1}^e = \exp\left(\mathbf{W}_{n+1}^e \Delta t\right) \mathbf{R}_n^e.$$

10 ABAQUS/Explicit (VUMAT) Implementation II

10.1 Input Variables

- Total deformation gradients: $\mathbf{F}_n$ (step n), $\mathbf{F}_{n+1}$ (step $n+1$)
- Time increment: Δt
- State variables from step n:
  - Plastic deformation gradient: $\mathbf{F}_n^p$
  - Elastic rotation tensor: $\mathbf{R}_n^e$
  - Critical resolved shear stress: g_n^α
  - Slip rates: $\dot{\gamma}_n^\alpha$

10.2 Output Variables

- $\boldsymbol{\sigma}_{n+1}$: Cauchy stress at step $n+1$.
- State variables at step $n+1$: $\mathbf{F}_{n+1}^p$, $\mathbf{R}_{n+1}^e$, g_{n+1}^α, $\dot{\gamma}_{n+1}^\alpha$.

10.3 Explicit Update Procedure

1. Compute $\mathbf{L}_{n+1}^p$ using previous slip rates:

$$\mathbf{L}_{n+1}^p = \sum_{\alpha=1}^{12} \dot{\gamma}_n^\alpha \mathbf{S}_0^\alpha$$

   where $\mathbf{S}_0^\alpha = \mathbf{s}_0^\alpha \otimes \mathbf{n}_0^\alpha$ is the reference Schmid tensor.

2. Update Plastic Deformation Gradient

$$\mathbf{F}_{n+1}^p = \left(\mathbf{I} + \mathbf{L}_{n+1}^p \Delta t\right) \mathbf{F}_n^p$$

3. Compute Elastic Deformation Gradient

$$\mathbf{F}_{n+1}^e = \mathbf{F}_{n+1} \cdot (\mathbf{F}_{n+1}^p)^{-1}$$

4. Elastic Green Strain

$$\mathbf{E}_{n+1}^e = \frac{1}{2}\left((\mathbf{F}_{n+1}^e)^T \mathbf{F}_{n+1}^e - \mathbf{I}\right)$$

5. Second Piola-Kirchhoff Stress

$$\mathbf{S}_{n+1}^e = \mathbb{C} : \mathbf{E}_{n+1}^e$$

   where $\mathbb{C}$ is the fourth-order elasticity tensor

6. Cauchy Stress

$$\boldsymbol{\sigma}_{n+1} = \frac{1}{\det \mathbf{F}^e_{n+1}} \mathbf{F}^e_{n+1} \mathbf{S}^e_{n+1} (\mathbf{F}^e_{n+1})^T$$

7. Resolved Shear Stress

$$\tau^\alpha_{n+1} = \boldsymbol{\sigma}_{n+1} : \mathbf{S}^\alpha_{n+1}$$

where

$$\mathbf{S}^\alpha_{n+1} = \mathbf{F}^e_{n+1} \mathbf{S}^\alpha_0 \mathbf{F}^{e-T}_{n+1}$$

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8. Slip Rate Update

$$\dot{\gamma}^\alpha_{n+1} = \dot{\gamma}_0 \left(\frac{|\tau^\alpha_{n+1}|}{g^\alpha_n} \right)^{1/m} \operatorname{sign}(\tau^\alpha_{n+1})$$

9. Hardening Law

$$g^\alpha_{n+1} = g^\alpha_n + \Delta t \sum_{\beta=1}^{12} h_{\alpha\beta} |\dot{\gamma}^\beta_{n+1}|$$

10. Total Velocity Gradient

$$\mathbf{L}_{n+1} = \frac{\mathbf{F}_{n+1} - \mathbf{F}_n}{\Delta t} \mathbf{F}^{-1}_{n+1}$$

11. Elastic Velocity Gradient

$$\mathbf{L}^e_{n+1} = \mathbf{L}_{n+1} - \mathbf{F}^e_{n+1} \mathbf{L}^p_{n+1} (\mathbf{F}^e_{n+1})^{-1}$$

12. Elastic Spin Tensor

$$\mathbf{W}^e_{n+1} = \frac{1}{2} \left(\mathbf{L}^e_{n+1} - (\mathbf{L}^e_{n+1})^\top \right)$$

13. Update Elastic Rotation

$$\mathbf{R}^e_{n+1} = \exp\left(\mathbf{W}^e_{n+1} \Delta t \right) \mathbf{R}^e_n$$

where $\exp(\cdot)$ is calculated via Rodrigues' formula.

10.4 State Variable Transfer

Variable	**Step** n	**Step** $n+1$
Plastic deformation gradient	$\mathbf{F}^p_n$	$\mathbf{F}^p_{n+1}$
Elastic rotation tensor	$\mathbf{R}^e_n$	$\mathbf{R}^e_{n+1}$
Critical resolved shear stress	g^α_n	g^α_{n+1}
Slip rates	$\dot{\gamma}^\alpha_n$	$\dot{\gamma}^\alpha_{n+1}$