A Multiscale Model to Incorporate Texture Evolution into Phenomenological Plasticity Models

CP Kohar¹, JL Bassani², RK Mishra⁴, K Inal¹

¹Department of Mechanical and Mechatronics Engineering, University of Waterloo, Waterloo, Ontario, Canada, N2L 3G1
² Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA, USA, 19104
³ General Motors Research and Development Center, 20500 Mound Road, Warren, MI, USA, 48090-9055

Email: kinal@uwaterloo.ca

Abstract. Crystal plasticity is a micromechanics-based model that is regularly used to simulate plastic spin during large deformation. Although crystal plasticity can provide an accurate description of local deformation behaviour, it is often computationally expensive and usually replaced by flow rule-based phenomenological models that do not capture this phenomenon. This work presents a phenomenological-based texture evolution (PBTE) model that allows for the enhancement of flow rule-based models to capture microstructural spin in a phenomenological manner. A numerical framework is presented for generating and calibrating the microstructural evolution for the PBTE model using crystal plasticity. The PBTE Model is calibrated and employed to predict the macroscopic mechanical response and the generated microstructural spin for single crystal FCC cube during non-proportional strain paths.

1. Introduction

Crystal plasticity is a physics-based model that computes the crystallographic slip due to dislocation glide [1]. This model typically uses an electron backscatter diffraction (EBSD) map and a single uniaxial stress-strain curve to characterize a material. When implemented into numerical frameworks, such as the finite element method, crystal plasticity can be used to simulate localized deformation phenomenon [2, 3, 4] for lightweighting applications with large and complex strain paths. Yet, these crystal plasticity models are often sacrificed for phenomenological models that require substantially fewer resources for lab scale simulations of sheet metal formability [5, 6] and crashworthiness [7, 8]. Phenomenological constitutive models are derived from fitting a yield function to the macroscopic anisotropy that is observed experimentally. However, these phenomenological plasticity models typically do not capture the microstructural evolution that develops during large plastic strain.

Attempts have been made to scale up deformation mechanisms from crystal plasticity to phenomenological models [9, 10]; Yet, these frameworks do not allow for microstructural evolution during off-axis loading or non-proportional strain paths. Recently, Bassani and Pan [11] proposed a phenomenological-based texture evolution (PBTE) model that was implemented into a multiscaling framework by Kohar et al. [12] to relate the rotation of the orthotropic axes of anisotropy to the plastic shear components in a phenomenological manner. The results of their work show promise in the ability of phenomenological models to capture detailed microstructural information in an efficient manner.

This work presents the multiscaling framework by Kohar et al. [12] that utilizes the PBTE model proposed Bassani and Pan [11] for incorporating microstructural evolution into phenomenological plasticity that is obtained from crystal plasticity. This framework employs the crystal plasticity formulations presented in Inal et al. [2, 10] with the non-quadratic multi-transformation yield function proposed by Cazacu, Plunkett and Barlat [13, 14]. Measurements of the orthotropic axis evolution are
generated by crystal plasticity following the test program proposed by Kim and Yin [15] and Bunge and Nielsen [16]. The objective of this framework is to calibrate the phenomenological-based texture evolution constitutive model by using the predictions obtained from the crystal plasticity theory. This framework is demonstrated for single face-centered cubic (FCC) cube crystals to highlight the ability of the constitutive model to capture microstructure evolution.

2. Constitutive Model

A complete description of the constitutive model can be found in Kohar et al. [12] and is summarized as follows. This framework assumes that three mutually orthogonal symmetry planes represent the axes of anisotropy, which can evolve with deformation. Figure 1 presents a 2D schematic of these orthonormal axes.

\[
\hat{e}_i = \omega e_i = (W - \hat{W}^P)e_i \tag{1}
\]

where \(\hat{W}^P\) is the plastic spin on the intermediate configuration. On the lab frame, \(e_1 - e_2\), the velocity gradient, \(L\), is derived as

\[
L = \dot{F}F^{-1} \tag{2}
\]

where \(F\) is the deformation gradient. The stretching rates, \(D\), and spin tensors, \(W\), can be defined accordingly as

\[
L = D + W, \quad D = \frac{1}{2}(L + L^T), \quad W = \frac{1}{2}(L - L^T) \tag{3}
\]

The elastic and plastic component of the stretching and spin tensors can be decomposed into

\[
D = D^* + D^p, \quad W = W^* + W^p \tag{4}
\]

An intermediate Cauchy stress tensor, \(\Sigma\), can be defined on the orthotropic axes

\[
\Sigma = R(\beta): \sigma \tag{5}
\]

where the Cauchy stress tensor, \(\sigma\), is related through the direction cosine matrix, \(R(\beta)\) that evolve with \(\omega\). The plastic stretch rate on the intermediate frame rate, \(\dot{D}^p\)

\[
\dot{D}^p = \dot{\varepsilon}^p \frac{\partial \phi}{\partial \Sigma} \tag{6}
\]

where \(\dot{\varepsilon}^p\) is the effective plastic strain rate and \(\frac{\partial \phi}{\partial \Sigma}\) is the normality of a yield function on the intermediate configuration. The plastic stretch rate, \(D^p\), in the reference configuration can be defined as

\[
D^p = \dot{\varepsilon}^p \frac{\partial \phi}{\partial \sigma} \frac{\partial \phi}{\partial \Sigma} \frac{\partial \Sigma}{\partial \sigma} \tag{7}
\]

Bassani and Pan [11] proposed that the plastic shear components of the plastic stretch rate tensor can be related to the plastic spin rate tensor in a phenomenological manner

\[
\hat{W}^p_{12} = \eta_3 \hat{D}^p_{12}, \quad \hat{W}^p_{13} = \eta_2 \hat{D}^p_{13}, \quad \hat{W}^p_{23} = \eta_1 \hat{D}^p_{23} \tag{8}
\]
where \( \eta_i \) is a phenomenological parameter that can be related to a function of stress invariants. Nesterova et al. [17] reported that the orthotropic axes off-axis loading during uniaxial tension (i.e. uniaxial tension along the \( \beta_0 \) direction) tend to rotate towards a stable orientation that is typically aligned with the pulling direction. Assuming small strains \( (W^p_{12} \approx \hat{W}^p_{12}) \) and an even function formulation of \( \eta_i \) leads to

\[
\eta_3 = \eta_{o3} + \xi_3 \frac{\partial \Phi}{\partial \sum_{33}} \frac{\partial \Phi}{\partial \sum_{22}} \frac{\partial \Phi}{\partial \sum_{11}}
\]

(9)

3. Model Calibration using Crystal Plasticity

The crystal plasticity framework presented in Inal et al. [10] is used to generate the yield loci that is needed for calibration of the phenomenological-based texture evolution model. An idealized single crystal FCC cube is utilized that follows the crystal plasticity framework presented in Inal et al. [2] with power law hardening (Peirce et al. [18, 19]) obtained from Brahme et al. [20]. Table 1 presents the single crystal hardening parameters used for the single cube texture. For details about the crystal plasticity formulation, please refer to Inal et al. [10] and Brahme et al. [20].

| \( C_{11} \) [GPa] | \( C_{12} \) [GPa] | \( C_{44} \) [GPa] | \( \tau_0 \) [MPa] | \( h_0 \) [MPa] | \( n_x \) | \( m_x \) | \( \gamma_0 \) (s\(^{-1}\)) | q |
|----------------|----------------|----------------|----------------|----------------|-----|-----|----------------|-----|
| 230            | 132            | 60            | 12.5           | 3125           | 0.370 | 0.002 | 1.0 \times 10^{-3} | 1.00 |

3.1 Measuring Orthotropic Axis Evolution

This framework is adopted from Kim and Yin [15] and Bunge and Nielsen [16] where the orthotropic axis of a material is defined as the symmetry axis of a pole figure. A pole figure is a 2-dimensional representation in polar space \( (R, \theta) \) of the 3-dimensional Bunge Euler angles \( (\theta_1, \Phi, \theta_2) \) for an orientation distribution function (ODF), which is commonly used to describe the texture of a material. The intensity of a pole figure, \( W(R, \theta) \), is evaluated as the number of crystallographic orientations that occur within bins of \( 0 \leq R \leq 1 \) and \( 0 \leq \theta \leq 2\pi \). As off-axis deformation is applied to the material, the symmetry axis of the pole figure rotates towards the loading direction accordingly.

In a general framework, the angle of the orthotropic axis from the sample reference direction, \( \beta \), is determined by minimizing an error function that measures the degree of symmetry of the pole figure. For a given symmetry axis, \( \beta_k \), the local error in the degree of symmetry of the pole figure is defined as

\[
\psi_{ijk} = \left| W(R_i, \theta_j + \beta_k) - W(R_i, 2\pi - (\theta_j + \beta_k)) \right|
\]

and the total error in symmetry, \( \psi_k \), is calculated as

\[
\psi_k = \sum_{i=1}^{N} \sum_{j=1}^{M} \frac{\left| W(R_i, \theta_j + \beta_k) - W(R_i, 2\pi - (\theta_j + \beta_k)) \right|}{(R_i^2 - R_{i-1}^2)(\theta_j - \theta_{j-1})}
\]

where \( N \) and \( M \) are the number of bins used to discretize the polar domain of the pole figure [12]. Figure 2 presents a schematic of the error function for a single crystal FCC cube that was initially rotated 30° from the loading axis and deformed 20% strain in uniaxial tension. The error function reaches a minimum at \( \beta = 26.5° \) and 116.5°, which indicates a rotation of \( \Delta \beta = -3.5° \) in the orthotropic axes during uniaxial tension.

3.2 Calibration for Ideal Cube Texture using Crystal Plasticity

Phenomenological parameters for ideal single crystal FCC cube were obtained from Kohar et al. [12] and were used in this study. These parameters were obtained by fitting the phenomenological model to the measurements and responses obtained from crystal plasticity. Table 2 presents the phenomenological hardening parameters for single crystal FCC cube. The phenomenological power-law hardening relationship was used to describe the flow stress response, \( \bar{\sigma} \), where

\[
\bar{\sigma} = K(e_0 + \varepsilon)_{ph}^n
\]

(12)
A five transformation form of the Cazacu, Plunket and Barlat [13, 14] (CPB06) anisotropic yield function without yield surface asymmetry was selected to capture the yield surface curvature. The coefficients used for the CPB06 yield function are presented in Table 3. The single crystal FCC cube was rotated about the normal direction axis at various initial angles and deformed to various levels of uniaxial tension using crystal plasticity to generate off-axis loading. A non-linear regression scheme was used to calibrate the phenomenological parameters for microstructural spin (\(n_0 = -2.026 \times 10^{-4}\) and \(\xi = 1.0658\)) to capture the orthotropic axis rotation observed in crystal plasticity.

### Table 2. Phenomenological Plasticity Hardening Parameters for Single Crystal FCC Cube [12]

| E [GPa] | \(\nu\) | K [MPa] | \(\varepsilon_0\) (\(10^{-3}\)) | \(n_{ph}\) | \(\dot{\varepsilon}_0\) (\(10^{-3}\)) |
|---------|---------|---------|-----------------|--------|-----------------|
| 145.1   | 0.4191  | 496.66  | 0.4103          | 0.368  | 1.00            |

### Table 3. CPB06 Coefficients for Single Crystal FCC Cube (\(\alpha = 100\)) [12]

| \(C_{11}\) | \(C_{12}\) | \(C_{13}\) | \(C_{22}\) | \(C_{23}\) | \(C_{33}\) | \(C_{44}\) |
|------------|------------|------------|------------|------------|------------|------------|
| 1.8793     | 0.3528     | 1.8776     | -0.0070    | 0.8738     | 0.3254     | 0.9974     |
| 1.2711     | 1.1983     | -0.0428    | 0.9222     | 1.5097     | 1.4986     | 0.9860     |
| 2.6622     | 1.8815     | 0.7680     | 1.9895     | 0.4580     | 0.9174     | -1.0021    |
| 2.0239     | 2.0499     | 3.0241     | 0.1227     | 1.1079     | 2.0806     | 0.6891     |
| -2.5478    | -1.2956    | -0.8376    | -0.3070    | 0.6708     | 0.6985     | 0.9764     |

### 4. Simulations of Non-proportional Strain Paths

Simulations of in-plane non-proportional shear-tension paths are performed to highlight the effect of microstructure evolution using crystal plasticity and the calibrated phenomenological model for single crystal FCC cube. Figure 3 presents the strain paths used in this study. In each strain path, the single crystal FCC cube undergoes a total shear and normal strain of \(\gamma_{12}=0.75\) and \(\varepsilon_{11}=0.25\) respectively with \(D_{23} = D_{13} = \sigma_{33} = 0\). Equation (13) presents the boundary conditions for Strain Path #1.

For \(\int_0^{t_1} 2D_{12} dt < 0.75: D_{12} = 1 \times 10^{-6} s^{-1}, D_{11} = D_{22} = 0\) (13)

The single crystal FCC cube is initially deformed in simple shear until \(\gamma_{12}=0.75\). After, the single crystal FCC cube is then deformed in uniaxial tension until \(\varepsilon_{11}=0.25\). Equation (14) presents the boundary conditions for Strain Path #2, which is a reversal in the order of the deformation from Strain Path #1.

For \(\int_0^{t_1} D_{11} dt < 0.25: D_{11} = 1 \times 10^{-6} s^{-1}, D_{12} = \sigma_{22} = 0\) (14)
Figure 4 presents the resulting stress-strain responses for the given strain paths using crystal plasticity (dots) and the calibrated phenomenological model with microstructural evolution (solid line). Simulations were also performing using the calibrated phenomenological model without evolution (dashed line) for comparison. The stress-strain response for Strain Path #1 and #2 are presented in red and blue respectively. In general, the phenomenological model with evolution is able to capture the stress-strain response of crystal plasticity for both strain paths. The model without evolution estimates the normal stress-strain response well for Strain Path #2; yet, it begins to deviate in the shear stress response. More noticeably, the phenomenological model without evolution shows significant over-predictions for Strain Path #1. During the first phase of loading Strain Path #1, there is a significant error introduced in the simple shear when no microstructural evolution is accounted for (Figure 4b). This error is approximately the same error introduced at the end of Strain Path #2 during shear. However, during the subsequent loading cycle in uniaxial tension, the normal stress response severely over-estimates the crystal plasticity response (Figure 4a). Thus, it is important to capture the evolution of the orthotropic axes during large deformation where off-axis modes of deformation can occur.

\[ \sigma_{11} - \varepsilon_{11} \]

\[ \sigma_{12} - \gamma_{12} \]

**Figure 3.** Non-proportional Strain Path of Combined Uniaxial Tension + Simple Shear

**Figure 4.** a) \( \sigma_{11} - \varepsilon_{11} \), b) \( \sigma_{12} - \gamma_{12} \) Stress-Strain Response for Strain Path #1 (Red) and Strain Path #2 (Blue).

5. Conclusions

This work presented a multiscaling framework for incorporating microstructure evolution from crystal plasticity into phenomenological plasticity. Crystal plasticity theory was used to calibrate the phenomenological-based texture evolution (PBTE) model to capture microstructural evolution. This was accomplished through a numerical framework for measuring microstructural evolution during off-axis uniaxial tension. This framework was demonstrated for single crystal FCC cube texture with high fidelity. Two phenomenological coefficients were used to capture the microstructural evolution of the orthotropic axes of symmetry. Non-proportional strain simulations of shear-tension showed that the phenomenological model with evolution could capture the microstructural evolution observed in the stress-strain response of crystal plasticity.
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