Summary of constitutive_phenoPowerlaw

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This document contains information for constitutive_phenoPowerlaw.f90. This constitutive subroutine is modified from the current contitutive_phenomenological.f90. We introduce slip and twin family as additional index (or input) for each crystal structure in lattice.f90 subroutine (e.g., for HCP crystal: slip and twin system has four faimilies, respectively). The current State variables in constitutive_phenoPowerlaw are "slip resistance (s^{α})", "twin resistance $\left(s^{\beta}\right)$", "cumulative shear strain (γ^{α})", and "twin volume fraction $\left(f^{\beta}\right)$". Superscript α and β denote to slip and twin systems, respectively, in this entire document. Table 1 lists slip/twin systems for the "hex (hcp)" case.

			No. of slip system
slip system	basal	$\{0001\}\langle 1\bar{2}10\rangle$	3
	prism	$\{10\bar{1}0\}\langle 1\bar{2}10\rangle$	3
	pyr <a>	$\{10\bar{1}1\}\langle 1\bar{2}10\rangle$	6
	pyr <c+a>	$\{10\bar{1}1\}\langle 2\bar{1}\bar{1}3\rangle$	12
twin system	tensile (T1)	$\{10\bar{1}2\}\langle \bar{1}011\rangle$	6
	compressive (C1)	$\{11\bar{2}2\}\langle 11\bar{2}\bar{3}\rangle$	6
	tensile (T2)	$\{11\bar{2}1\}\langle \bar{1}\bar{1}26\rangle$	6
	compressive (C1)	$\{10\bar{1}1\}\langle 10\bar{1}\bar{2}\rangle$	6

Table 1: Implemented deformation mechanims in α-Ti

Slip/twin system figure for HCP is coming soon.

1 Kinetics

Shear strain rate due to slip is described by following eqation [1, 2]:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_o \left| \frac{\tau^{\alpha}}{s^{\alpha}} \right|^n sign\left(\tau^{\alpha}\right) \tag{1}$$

, where $\dot{\gamma}^{\alpha}$; shear strain rate, $\dot{\gamma}_o$; reference shear strain rate, τ^{α}; resolved shear stress on the slip system, n; stress exponent, and s^{α}; slip resistance.

Twin volume fraction rate is described by following eqation [1, 2]:

$$\dot{f}^{\beta} = \frac{\dot{\gamma}_o}{\gamma^{\beta}} \left| \frac{\tau^{\beta}}{s^{\beta}} \right|^n \mathcal{H}\left(\tau^{\beta}\right) \tag{2}$$

, where $\dot{f}^{\beta}$; twin volume fraction rate, $\dot{\gamma}_o$; reference shear strain rate, γ^{β};shear strain due to mechanical twinning, τ^{β}; resolved shear stress on the twin system, and s^{β}; twin resistance. $\mathcal{H}$ is Heaviside function.

2 Structure Evolution

In this present section, we attempt to show how we establish the relationship between the evolutoin of slip/twin resistance and the evolution of shear strain/twin volume fraction.

2.1 Interaction matrix.

Conceptual relationship between the evolution of state and kinetic variables is shown in Equation 3.

$$\begin{bmatrix} \dot{s}^{\alpha} \\ \dot{s}^{\beta} \end{bmatrix} = \begin{bmatrix} M_{\text{slip}-\text{slip}} & M_{\text{slip}-\text{twin}} \\ M_{\text{twin}-\text{slip}} & M_{\text{twin}-\text{twin}} \end{bmatrix} \begin{bmatrix} \dot{\gamma}^{\alpha} \\ \dot{f}^{\beta} \end{bmatrix} \tag{3}$$

Four interaction martices are followings; i) slip-slip interaction matrix ($M_{\text{slip}-\text{slip}}$), ii) slip-twin interaction matrix ($M_{\text{slip}-\text{twin}}$), iii) twin-slip interaction matrix ($M_{\text{twin}-\text{slip}}$), and iv) twin-twin interaction matrix ($M_{\text{twin}-\text{twin}}$).

Detailed interaction type matrices in Equation 3 will be further discussed in the following Section.

2.2 Interaction type matrix

Following sections are sparated into four based on each interaction type matrix alluded. Numbers in Tables 2, 3, 4, and 5 denote the type of interaction between deformation systems (The first column vs. The first row).

2.2.1 Slip-Slip interaction type matrix

- There are 20 types of slip-slip interaction as shown in Table 2.
- In Table 2, types of latent hardening among slip systems are listed.
- Actual slip-slip interaction type matrix, $M'_{\text{slip}-\text{slip}}$, is listed in Equation 4.

	basal	prism	pyr <a>	pyr<c+a>
basal	1, 5	9	12	14
prism	15	2, 6	10	13
pyr <a>	18	16	3, 7	11
pyr <c+a>	20	19	17	4, 8

Table 2: Slip-slip interaction type

$$M'_{\text{slip-slip}} = \left[\begin{array}{ccc|ccc|cccccc|cccccccccccc}
1 & 5 & 5 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & 1 & 5 & \cdot & 9 & \cdot & \cdot & \cdot & 12 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 14 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
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\cdot & \cdot & \cdot & 2 & 6 & 6 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & 15 & \cdot & & 2 & 6 & \cdot & \cdot & 10 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 13 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
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\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 3 & 7 & 7 & 7 & 7 & 7 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
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\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & 3 & 7 & 7 & 7 & \cdot & \cdot & \cdot & \cdot & \cdot & 11 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & 18 & \cdot & \cdot & 16 & \cdot & & & & 3 & 7 & 7 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
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\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & & & & 3 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\hline
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 4 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & 4 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & 4 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & & 4 & 8 & 8 & 8 & 8 & 8 & 8 & 8 & 8 \\
\cdot & 20 & \cdot & \cdot & 19 & \cdot & \cdot & \cdot & 17 & \cdot & \cdot & \cdot & & & & & 4 & 8 & 8 & 8 & 8 & 8 & 8 & 8 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & & & & 4 & 8 & 8 & 8 & 8 & 8 & 8 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & & & & & 4 & 8 & 8 & 8 & 8 & 8 \\
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\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & & & & & & & & 4 & 8 & 8 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & & & & & & & & & 4 & 8 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & & & & & & & & & & 4
\end{array}\right] \tag{4}$$

2.2.2 Slip-Twin interaction type matrix

- There are 16 types of slip-twin interaction in Table 3.
- Meaning of T1, C1, T2, C2 is listed in Table 1.
- Actual slip-twin interaction type matrix, $M'_{\text{slip}-\text{twin}}$, is listed in Equation 5.

	T1	C1	T2	C1
basal	1	2	3	4
prism	5	6	7	8
pyr <a>	9	10	11	12
pyr <c+a>	13	14	15	16

Table 3: Slip-twin interaction type

$$M'_{\text{slip}-\text{twin}} = \left[\begin{array}{c|c|c|c} 1 & 2 & 3 & 4 \\ \hline 5 & 6 & 7 & 8 \\ \hline 9 & 10 & 11 & 12 \\ \hline 13 & 14 & 15 & 16 \end{array}\right] \tag{5}$$

2.2.3 Twin-Slip interaction type matrix

- There 16 types of twin-slip interaction in Table 4.
- Meaning of T1, C1, T2, C2 is listed in Table 1.
- Actual twin-slip interaction type matrix, $M'_{\text{twin}-\text{slip}}$, is listed in Equation 6.

	basal	prism	pyr <a>	pyr <c+a>
T1	1	5	9	13
C1	2	6	10	14
T2	3	7	11	15
C2	4	8	12	16

Table 4: Twin-slip interaction type

$$M'_{\text{twin}-\text{slip}} = \left[\begin{array}{c|c|c|c} 1 & 5 & 9 & 13 \\ \hline 2 & 6 & 10 & 14 \\ \hline 3 & 7 & 11 & 15 \\ \hline 4 & 8 & 12 & 16 \end{array}\right] \tag{6}$$

2.2.4 Twin-twin interaction type matrix

- There are 20 types of twin-twin interaction as shown in Table 5.
- In Table 5, types of latent hardening among twin systems are listed.
- Actual twin-twin interaction type marix, $M'_{\text{twin}-\text{twin}}$, is listed in Equation 7.

	T1	C1	T2	C2
T1	1, 5	9	12	14
C1	15	2, 6	10	13
T2	18	16	3, 7	11
C2	20	19	17	4, 8

Table 5: Twin-twin interaction type

$$M'_{\text{twin}-\text{twin}} = \left[\begin{array}{cccccc|cccccc|cccccc|cccccc}
1 & 5 & 5 & 5 & 5 & 5 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & 1 & 5 & 5 & 5 & 5 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & 1 & 5 & 5 & 5 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & 1 & 5 & 5 & \cdot & \cdot & \cdot & 9 & \cdot & \cdot & \cdot & \cdot & \cdot & 12 & \cdot & \cdot & \cdot & \cdot & \cdot & 14 & \cdot & \cdot \\
 & & & & 1 & 5 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & & & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
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\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 2 & 6 & 6 & 6 & 6 & 6 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & 2 & 6 & 6 & 6 & 6 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
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\cdot & \cdot & \cdot & 15 & \cdot & \cdot & & & & 2 & 6 & 6 & \cdot & \cdot & \cdot & 10 & \cdot & \cdot & \cdot & \cdot & \cdot & 13 & \cdot & \cdot \\
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\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & 3 & 7 & 7 & 7 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & 18 & \cdot & \cdot & \cdot & \cdot & \cdot & 16 & \cdot & \cdot & & & & 3 & 7 & 7 & \cdot & \cdot & \cdot & 11 & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & & & 3 & 7 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & & & & 3 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
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\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 4 & 8 & 8 & 8 & 8 & 8 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & 4 & 8 & 8 & 8 & 8 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & 4 & 8 & 8 & 8 \\
\cdot & \cdot & \cdot & 20 & \cdot & \cdot & \cdot & \cdot & \cdot & 19 & \cdot & \cdot & \cdot & \cdot & \cdot & 17 & \cdot & \cdot & & & & 4 & 8 & 8 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & & & 4 & 8 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & & & & 4
\end{array}\right] \tag{7}$$

2.3 Prefactor (nonlinear factor)

2.3.1 Prefactors for slip resistance (s^α); $M_{\text{slip-slip}}$ and $M_{\text{slip-twin}}$ [2]

$M_{\text{slip-slip}}$ and $M_{\text{slip-twin}}$ use for slip resistance evolution $(\dot{s}^\alpha)$. Equation 8 is for a slip resistance rate evolution. This currently shows the prefactor for "slip-slip interaction matrix, $M_{\text{slip-slip}}$".

$$M_{\text{slip-slip}} = h_{\text{slip}} \left(1 + C \cdot F^b\right) \left(1 - \frac{s^\alpha}{s_{so}^\alpha + s_{\text{pr}} \cdot \sqrt{F}}\right) \cdot M'_{\text{slip-slip}} \tag{8}$$

, where h_{slip}represent a hardening rate, and S_{so}^α saturation slip resistance for slip system without mechanical twinning $\left(\sum_\beta f^\beta = 0\right)$, respectively. And, F is $\sum_\beta f^\beta$, and $N^S$is the total number of slip system.C, s_{pr}, and b are coefficients to introduce the effect of interaction between slip and mechanical twin in Equation 8.

- Slip-twin interaction matrix, $M_{\text{slip-twin}}$, has not been implemented with any prefactor in the present version.

2.3.2 Prefactors for twin resistance $\left(s^\beta\right)$; $M_{\text{twin-slip}}$ and $M_{\text{twin-twin}}$ [1]

$M_{\text{twin-sli}p}$ and $M_{\text{twin-twin}}$ use for twin resistance evolution $\left(\dot{s}^\beta\right)$. Twin-twin and twin-slip interaction matrices are described in Equations 9 and 10.

$$M_{\text{twin-twin}} = h_{\text{tw}} \cdot F^d \cdot M'_{\text{twin-twin}} \tag{9}$$

,where h_{tw} and d are coefficients for twin-twin contribution. F is $\sum_\beta f^\beta$.

$$M_{\text{twin-slip}} = h_{\text{tw-sl}} \cdot \Gamma^e \cdot M'_{\text{twin-slip}} \tag{10}$$

,where $h_{\text{tw-sl}}$ and e are coefficients for twin-slip contribution, and $\Gamma = \sum_\alpha \gamma^\alpha$.

3 Material Parameters (Material Configuration file)

Parameters for phenomenological modeling (kalidinditwin)

s0_slip	22e6	50e6	50e6	65e6	initial slip resistance (s^{α})
s0_twin	70e6	70e6	250e8	250e8	initial twin resistance (s^{β})
s_sat_slip	180e6	80e6	180e6	180e6	initial saturation slip resistance (s_x^{α})
gdot0_slip	0.001				reference shear strain (γ^{α}, γ^{β})
gdot0_twin	0.001				Exponent for Kinetic eqs.
n_slip	50.0				
n_twin	50.0				
h0_slip	60e6				hardening coeff. for s^{α}
h0_tw	0.0				hardening coeff. for s^{β}
h0_tw_sl	0.0				
twinC	25				hardening coeff. for s^{α}
twinB	2				
s_pr	100e6				
twinD	0.0				hardening coeff. for s^{β}
twinE	0.0				

```
# self and latent hardening coefficients

SlipSlip_hardening_coefficients   1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
SlipTwin_hardening_coefficients   1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
TwinSlip_hardening_coefficients   1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
TwinTwin_hardening_coefficients   1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
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Figure 1: Expected of phenomenological modelling parameters.

- The sequence for hardening coefficients in Figure 1 is the sequence of numbering in Tables 2, 3, 4, and 5 above.

References

[1] A.A. Salem, S.R. Kalidindi, and S.L. Semiatin. Strain hardening due to deformation twinning in [alpha]-titanium: Constitutive relations and crystal-plasticity modeling. *Acta Materialia*, 53(12):3495 – 3502, 2005.

[2] Xianping Wu, Surya R. Kalidindi, Carl Necker, and Ayman A. Salem. Prediction of crystallographic texture evolution and anisotropic stress-strain curves during large plastic strains in high purity [alpha]-titanium using a taylor-type crystal plasticity model. *Acta Materialia*, 55(2):423 – 432, 2007.