

Summary of constitutive _phenoPowerlaw

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This document contains information for constitutive _phenoPowerlaw.f90. This constitutive subroutine is modified from the current constitutive _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 families, respectively).

1 State Variables in constitutive _phenoPowelaw.f90

The current State variables in constitutive _phenoPowerlaw are “slip resistance (s^α)”, “twin resistance (s^β)”, “cumulative shear strain (γ^α)”, and “twin volume fraction (f^β)”. Superscript α and β denote to slip and twin systems, respectively, in this entire document.

2 Considered Deformation Mechanisms

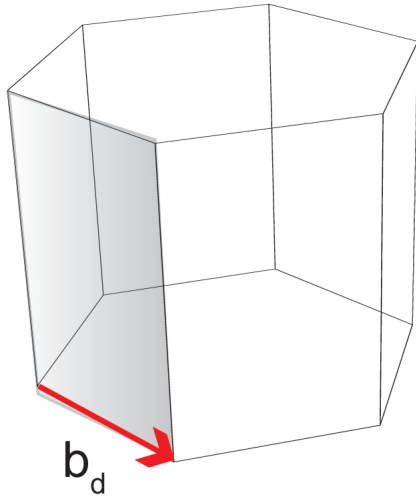
Table 1 lists slip/twin systems for the “hex (hcp)” case.

			No. of slip system
slip system	basal	$\{0001\} \langle 1\bar{2}10 \rangle$	3
	prism	$\{10\bar{1}0\} \langle 1210 \rangle$	3
	pyr $\langle a \rangle$	$\{10\bar{1}1\} \langle 1\bar{2}10 \rangle$	6
	pyr $\langle c+a \rangle$	$\{10\bar{1}1\} \langle 2\bar{1}\bar{1}3 \rangle$	12
twin system	tensile (T1)	$\{10\bar{1}2\} \langle \bar{1}011 \rangle$	6
	compressive (C1)	$\{1122\} \langle 1123 \rangle$	6
	tensile (T2)	$\{1121\} \langle \bar{1}\bar{1}26 \rangle$	6
	compressive (C1)	$\{10\bar{1}1\} \langle 10\bar{1}\bar{2} \rangle$	6

Table 1: Implemented deformation mechanisms in α -Ti

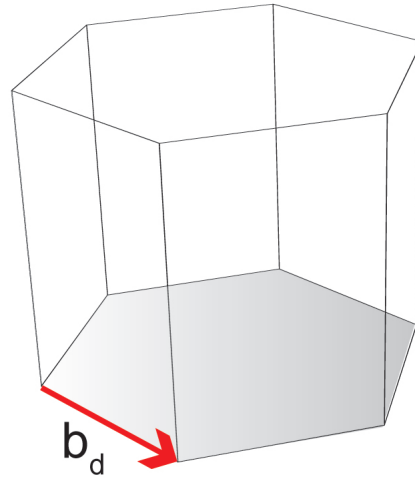
- Slip/twin system for HCP are illustrated in Figures 1 and 2.

Prism $\langle a \rangle$ slip



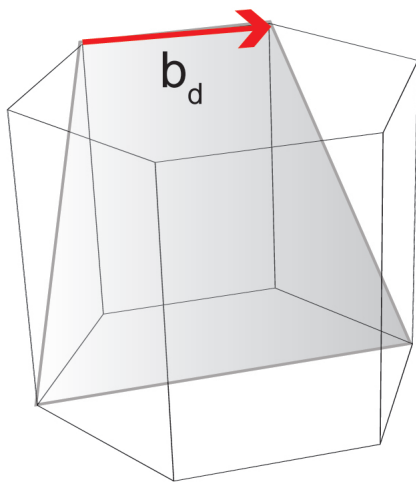
(a)

Basal $\langle a \rangle$ slip



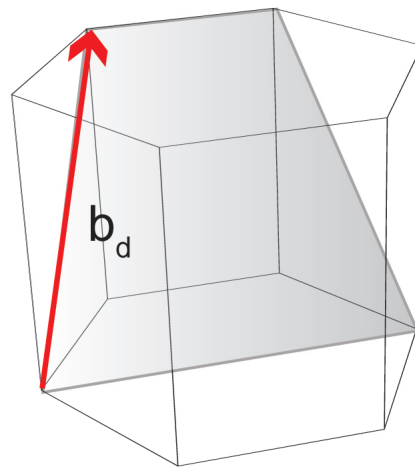
(c)

Pyramidal $\langle a \rangle$ slip



(b)

Pyramidal $\langle c+a \rangle$ slip



(d)

Figure 1: Drawing for slip system for HCP. Burgers vectors were scaled.

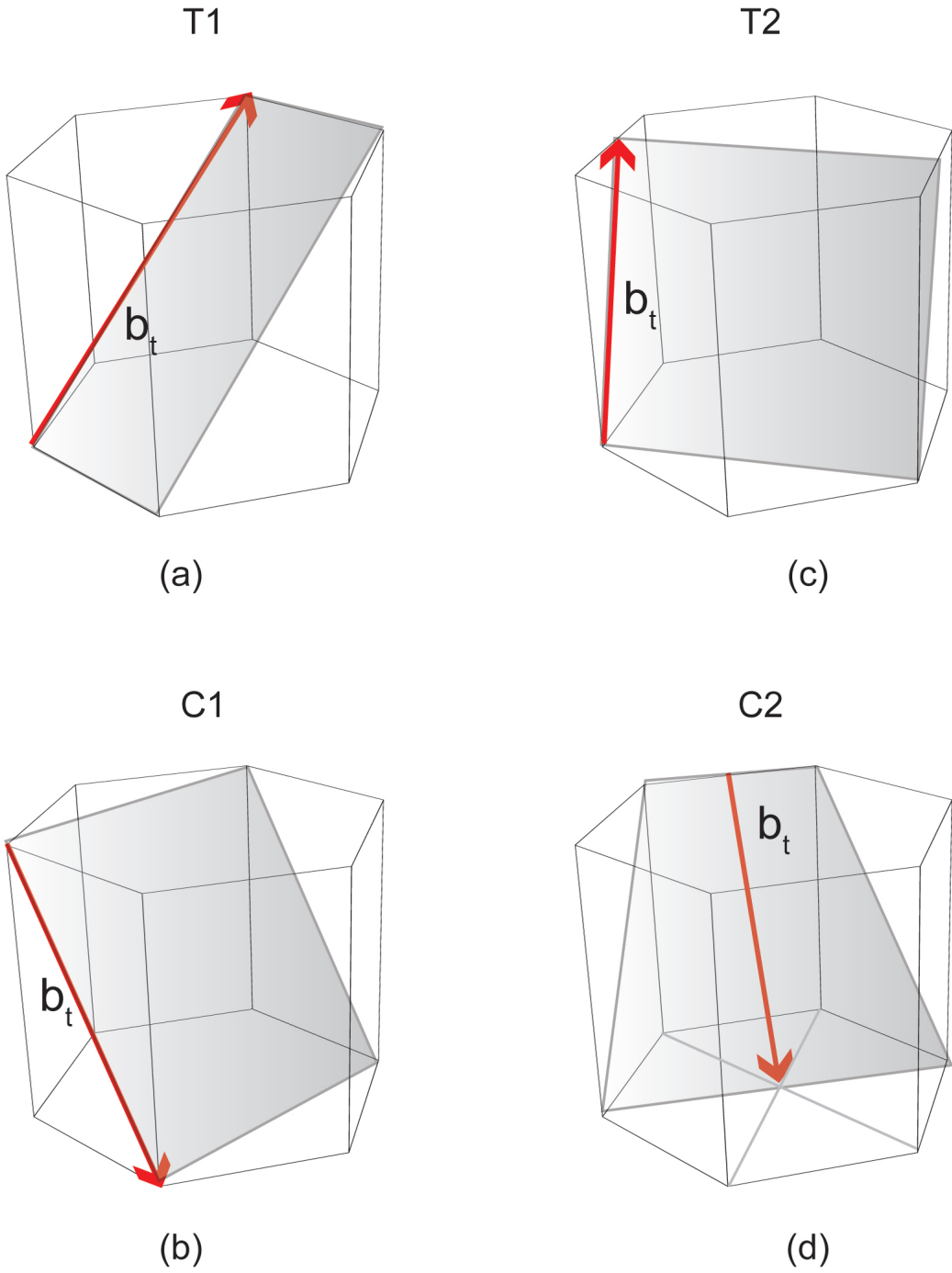


Figure 2: Drawing for twin system for HCP (α -Ti). Twin directions are not scaled yet.

3 Kinetics

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

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

, 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 equation [1, 2]:

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

, where \dot{f}^β ; 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.

4 Structure Evolution

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

4.1 Interaction matrix.

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

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

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

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

4.2 Interaction type matrix

Following sections are separated 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).

4.2.1 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, $M'_{\text{slip-slip}}$, is listed in Equation 4.

4.2.2 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, $M'_{\text{slip-twin}}$, 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

$$M'_{\text{slip-twin}} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \\ 13 & 14 & 15 & 16 \end{bmatrix} \quad (5)$$

4.2.3 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, $M'_{\text{twin-slip}}$, 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

$$M'_{\text{twin-slip}} = \begin{bmatrix} 1 & 5 & 9 & 13 \\ 2 & 6 & 10 & 14 \\ 3 & 7 & 11 & 15 \\ 4 & 8 & 12 & 16 \end{bmatrix} \quad (6)$$

4.3 Prefactor (nonlinear factor)

4.3.1 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}^α). Equation 8 is for a slip resistance rate evolution. This currently shows the prefactor for “slip-slip interaction matrix, $M_{\text{slip-slip}}$ ”.

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

, where h_{slip} represent a hardening rate, and S_{so}^α saturation slip resistance for slip system without mechanical twinning ($\sum_\beta f^\beta = 0$), 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.

4.3.2 Prefactors for twin resistance (s^β); $M_{\text{twin-slip}}$ and $M_{\text{twin-twin}}$ [1]

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

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

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

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

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

5 Material Parameters (Material Configuration file)

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## Parameters for phenomenological modeling (kalidinditwin)

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

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Figure 3: Expected of phenomenological modelling parameters.

- The sequence for hardening coefficients in Figure 3 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.