

Summary of constitutive_phenoPowerlaw

YunJo Ro Philip Eisenlohr

June 21, 2011

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_phenoPowerlaw.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.

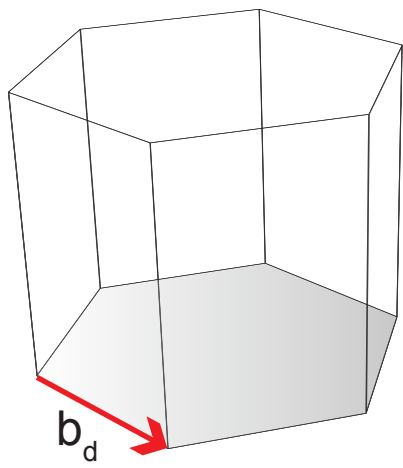
2 Considered Deformation Mechanisms

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

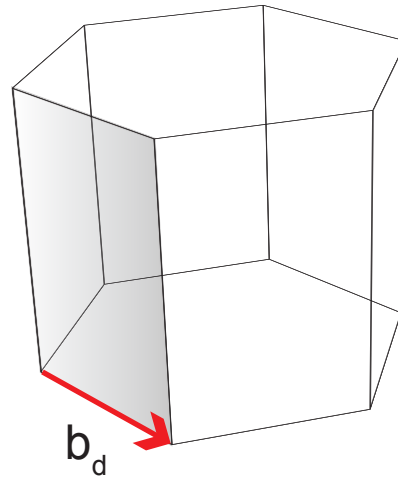
type	system	plane / direction	multiplicity
slip	basal	$\{0001\} \langle 1\bar{2}10 \rangle$	3
	prism	$\{10\bar{1}0\} \langle 1\bar{2}10 \rangle$	3
	pyr $\langle a \rangle$	$\{10\bar{1}1\} \langle 1210 \rangle$	6
	pyr $\langle c + a \rangle$	$\{10\bar{1}1\} \langle 2\bar{1}\bar{1}3 \rangle$	12
twin	T1	$\{10\bar{1}2\} \langle \bar{1}011 \rangle$	6
	C1	$\{11\bar{2}2\} \langle 11\bar{2}\bar{3} \rangle$	6
	T2	$\{11\bar{2}1\} \langle \bar{1}\bar{1}26 \rangle$	6
	C2	$\{10\bar{1}1\} \langle 10\bar{1}\bar{2} \rangle$	6

Table 1: Implemented deformation mechanisms in α -Ti

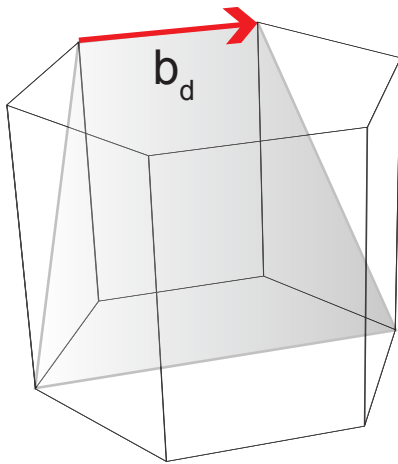
Slip/twin system for HCP are illustrated in Figures 1 and 2.



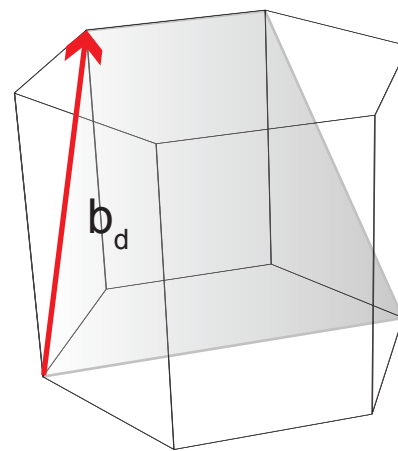
(a) Basal $\langle a \rangle$ slip



(b) Prismatic $\langle a \rangle$ slip

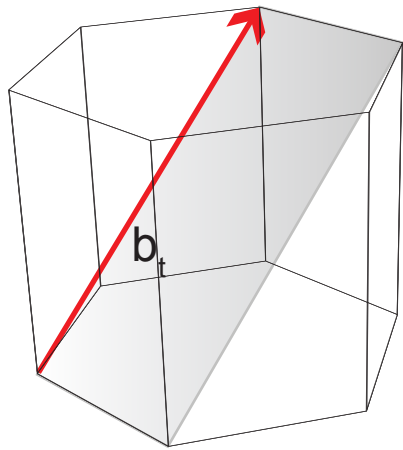


(c) Pyramidal $\langle a \rangle$ slip

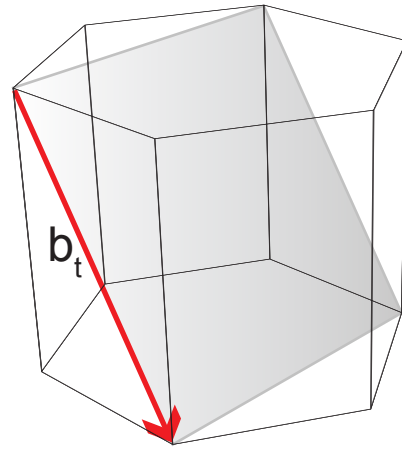


(d) Pyramidal $\langle c + a \rangle$ slip

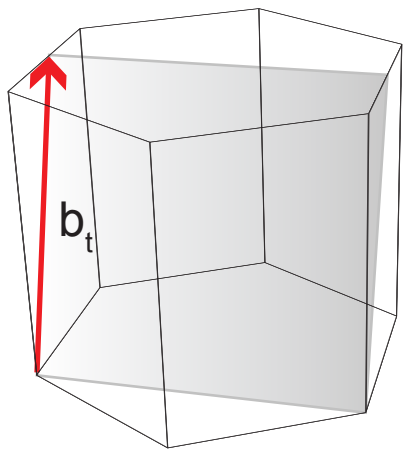
Figure 1: Dislocation slip systems considered for hexagonal lattice structure.



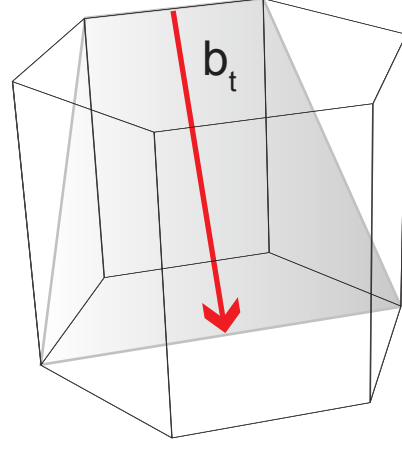
(a) Extension (T1)



(b) Contraction (C1)



(c) Extension (T2)



(d) Contraction (C2)

Figure 2: Mechanical twinning systems considered for hexagonal lattice structure. Burgers vectors are not drawn to scale.

3 Kinetics

Shear strain rate due to slip is described by following equation Salem et al. [2005], Wu et al. [2007]:

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

, 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 Salem et al. [2005], Wu et al. [2007]:

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

, 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).

4.2.2 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.

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

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.

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

4.2.4 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 matrix, $M'_{\text{twin-twin}}$, is listed in Equation 7.

- 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 $M_{\text{twin-twin}}$ **Salem et al. [2005]**

$M_{\text{twin-slip}}$ 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 $\Gamma = \sum_{\alpha} \gamma^\alpha$.

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

Table 2: Slip-slip interaction type

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

Table 3: Slip-twin interaction type

	basal	prism	pyr $\langle a \rangle$	pyr $\langle c + a \rangle$
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

	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

5 Material Parameters (Material Configuration file)

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## Parameters for phenomenological modeling (kalidinditwin)

s0_slip      22e6    50e6    50e6    65e6    initial slip resistance (sα)
-----

s0_twin      70e6    70e6    250e8    250e8    initial twin resistance (sβ)
-----

s_sat_slip   180e6    80e6    180e6    180e6    initial saturation slip resistance (sxα)
-----

gdot0_slip   0.001                                reference shear strain (γα, γβ)
gdot0_twin   0.001                                Exponent for Kinetic eqs.
n_slip       50.0
n_twin       50.0
-----

h0_slip      60e6                                hardening coeff. for sα
-----

h0_tw        0.0                                hardening coeff. for sβ
h0_tw_sl     0.0
-----

twinC        25                                hardening coeff. for sα
twinB        2
s_pr         100e6
-----

twinD        0.0                                hardening coeff. for sβ
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
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
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
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

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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

- 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. ISSN 1359-6454. doi: DOI:10.1016/j.actamat.2005.04.014. URL <http://www.sciencedirect.com/science/article/B6TW8-4G94J1C-2/2/9745b826d50791e36598ba02e5b0d4e1>. 4, 8
- 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. ISSN 1359-6454. doi: DOI:10.1016/j.actamat.2006.08.034. URL <http://www.sciencedirect.com/science/article/B6TW8-4M63RXJ-6/2/b13d16ac5a205e5218141b1a25b85a27>. 4, 7