Summary of constitutive_kalidinditwin subroutine

YUN JO RO

May 28, 2009

This document contains information for constitutive_kalidinditwin.f90 which is designed for HCP crystal. State variables in constitutive_kalidinditwin 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 24 slip and 24 twin systems, respectively, in this entire document. Slip system has four different families (i.e., basal, prism, pyr <a> and pyr <c+a>), and twin system has four diffrent families (i.e., 2 tensile twins and 2 compressive twins). Table 1 lists slip/twin systems implemented in the subroutine.

			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

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; hardening coefficient, 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 twin, 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.

$$\begin{bmatrix} \dot{s}^{\alpha} \\ \dot{s}^{\beta} \end{bmatrix}_{48\times1} = M_{48\times48} \begin{bmatrix} \dot{\gamma}^{\alpha} \\ \dot{f}^{\beta} \end{bmatrix}_{1\times48} \tag{3}$$

$M_{48\times48}$ consists of four interaction type matrices; i) slip-slip interaction type matrix ($M_{slip-slip}$), ii) slip-twin interaction type matrix ($M_{slip-twin}$), iii) twin-slip interaction type matrix ($M_{twin-slip}$), and iv) twin-twin interaction type matrix ($M_{twin-twin}$). Each interaction type matrix is 24×24 martix.

$$M_{48\times48} = \begin{bmatrix} M_{slip-slip} & M_{slip-twin} \\ M_{twin-slip} & M_{twin-twin} \end{bmatrix} \tag{4}$$

Detailed interaction type matrices in Equation 4 will be further discussed in the following Section.

2.2 Interaction type

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

- There are 11 types of slip-slip interaction as shown in Table 2. “1” in not included here, since ”1” is used for self-hardening for each slip system.
- In Table 2, types of latent hardening among slip systems are listed.
- Actual slip-slip interaction matrix, $M_{slip-slip}$, is listed in Equation 5.

	basal	prism	pyr <a>	pyr<c+a>
basal	2	6	7	8
prism		3	9	10
pyr <a>			4	11
pyra <c+a>				5

Table 2: Slip-slip interaction type

$$
M_{slip-slip} = \left[\begin{array}{ccc|ccc|cccccc|cccccccccccc}
1 & 2 & 2 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & 1 & 2 & \cdot & 6 & \cdot & \cdot & \cdot & 7 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 8 & \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 \\
\hline
 & & & 1 & 3 & 3 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & & 1 & 3 & \cdot & \cdot & 9 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 10 & \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 \\
\hline
 & & & & & & 1 & 4 & 4 & 4 & 4 & 4 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & & & & & 1 & 4 & 4 & 4 & 4 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & & & & & & 1 & 4 & 4 & 4 & \cdot & \cdot & \cdot & \cdot & \cdot & 11 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & & & & & & & 1 & 4 & 4 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & & & & & & & & 1 & 4 & \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 \\
\hline
 & & & & & & & & & & & & 1 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 \\
 & & & & & & & & & & & & & 1 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 \\
 & & & & & & & & & & & & & & 1 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 \\
 & & & & & & & & & & & & & & & 1 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 \\
 & & & & & & & & & & & & & & & & 1 & 5 & 5 & 5 & 5 & 5 & 5 & 5 \\
 & & & & & & & & & & & & & & & & & 1 & 5 & 5 & 5 & 5 & 5 & 5 \\
 & & & & & & & & & & & & & & & & & & 1 & 5 & 5 & 5 & 5 & 5 \\
 & & & & & & & & & & & & & & & & & & & 1 & 5 & 5 & 5 & 5 \\
 & & & & & & & & & & & & & & & & & & & & 1 & 5 & 5 & 5 \\
 & & & & & & & & & & & & & & & & & & & & & 1 & 5 & 5 \\
 & & & & & & & & & & & & & & & & & & & & & & 1 & 5 \\
 & & & & & & & & & & & & & & & & & & & & & & & 1
\end{array}\right] \tag{5}
$$

2.2.2 Slip-Twin interaction type

- 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 matrix, $M_{slip-twin}$, is listed in Equation 6.

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

Table 3: Slip-twin interaction type

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

2.2.3 Twin-Slip interaction type

- 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 matrix, $M_{twin-slip}$, is listed in Equation 7.

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

Table 4: Twin-slip interaction type

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

2.2.4 Twin-twin interaction type

- There are 11 types of twin-twin interaction as shown in Table 5. “1” in not included here, since ”1” is used for self-hardening for each twin system.
- In Table 5, types of latent hardening among twin systems are listed.
- Actual twin-twin interaction marix, $M_{twin-twin}$, is listed in Equation 8.

	T1	C1	T2	C2
T1	2	6	7	8
C1		3	9	10
T2			4	11
C2				5

Table 5: Twin-twin interaction type

$$M_{twin-twin} = \left[\begin{array}{cccccc|cccccc|cccccc|cccccc}
1 & 2 & 2 & 2 & 2 & 2 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & 1 & 2 & 2 & 2 & 2 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & 1 & 2 & 2 & 2 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & 1 & 2 & 2 & \cdot & \cdot & \cdot & 6 & \cdot & \cdot & \cdot & \cdot & \cdot & 7 & \cdot & \cdot & \cdot & \cdot & \cdot & 8 & \cdot & \cdot \\
 & & & & 1 & 2 & \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 \\
\hline
 & & & & & & 1 & 3 & 3 & 3 & 3 & 3 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & & & & & 1 & 3 & 3 & 3 & 3 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & & & & & & 1 & 3 & 3 & 3 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & & & & & & & 1 & 3 & 3 & \cdot & \cdot & \cdot & 9 & \cdot & \cdot & \cdot & \cdot & \cdot & 10 & \cdot & \cdot \\
 & & & & & & & & & & 1 & 3 & \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 \\
\hline
 & & & & & & & & & & & & 1 & 4 & 4 & 4 & 4 & 4 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & & & & & & & & & & & 1 & 4 & 4 & 4 & 4 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & & & & & & & & & & & & 1 & 4 & 4 & 4 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & & & & & & & & & & & & & 1 & 4 & 4 & \cdot & \cdot & \cdot & 11 & \cdot & \cdot \\
 & & & & & & & & & & & & & & & & 1 & 4 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 & & & & & & & & & & & & & & & & & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\hline
 & & & & & & & & & & & & & & & & & & 1 & 5 & 5 & 5 & 5 & 5 \\
 & & & & & & & & & & & & & & & & & & & 1 & 5 & 5 & 5 & 5 \\
 & & & & & & & & & & & & & & & & & & & & 1 & 5 & 5 & 5 \\
 & & & & & & & & & & & & & & & & & & & & & 1 & 5 & 5 \\
 & & & & & & & & & & & & & & & & & & & & & & 1 & 5 \\
 & & & & & & & & & & & & & & & & & & & & & & & 1
\end{array}\right] \qquad (8)$$

2.3 Prefactor (nonlinear factor)

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

$M_{slip-slip}$ and $M_{slip-twin}$ use for slip resistance evolution ($\dot{s}^{\alpha}$). Equation 9 is for a slip resistance rate evolution. This currently shows the prefactor for slip-slip interaction matrix, $M_{slip-slip}$.

$$[\dot{s}^{\alpha}]_{24\times1} = h_s^{\alpha}\left(1-\frac{s^{\alpha}}{s_s^{\alpha}}\right)M_{slip-slip}\,[\dot{\gamma}^{\alpha}]_{1\times24} \quad or \quad \dot{s}^{\alpha} = h_s^{\alpha}\left(1-\frac{s^{\alpha}}{s_s^{\alpha}}\right)\sum_{l}^{N^S}\dot{\gamma}^{l} \tag{9}$$

, where $h_s^{\alpha}$and S_s^{α} represent hardening rate and saturation slip resistance for slip system, respectively. $N^S$is the total number of slip system, 24. $h_s^{\alpha}$and S_s^{α} depend on total twin volume fraction as describing in Equations 10 and 11, respectively. Thus, deformation twin and slip interaction is indirectly implemented in Equation 9.

$$h_s^{\alpha} = \begin{cases} h_{so}^{bas}\left(1+C\left(\sum_{\beta} f^{\beta}\right)^{b}\right) & if\ \alpha \in basal \\ h_{so}^{pri}\left(1+C\left(\sum_{\beta} f^{\beta}\right)^{b}\right) & if\ \alpha \in prism \\ h_{so}^{pyr<a>}\left(1+C\left(\sum_{\beta} f^{\beta}\right)^{b}\right) & if\ \alpha \in pyr<a> \\ h_{so}^{pyr<c+a>}\left(1+C\left(\sum_{\beta} f^{\beta}\right)^{b}\right) & if\ \alpha \in pyr<c+a> \end{cases} \tag{10}$$

, where h_{so}^{α} presents the hardeing rate without twin volume fraction (i.e.,$\left(\sum_{\beta} f^{\beta}=0\right)$, and b is exponent to control the effect of twin volume fraction on the hardening rate. C is coefficient for twin effect.

$$s_s^{\alpha} = \begin{cases} s_{so}^{bas} + s_{pr}\left(\sum_{\beta} f^{\beta}\right)^{0.5} & if\ \alpha \in basal \\ s_{so}^{pri} + s_{pr}\left(\sum_{\beta} f^{\beta}\right)^{0.5} & if\ \alpha \in prism \\ s_{so}^{pyr<a>} + s_{pr}\left(\sum_{\beta} f^{\beta}\right)^{0.5} & if\ \alpha \in pyr<a> \\ s_{so}^{pyr<c+a>} + s_{pr}\left(\sum_{\beta} f^{\beta}\right)^{0.5} & if\ \alpha \in pyr<c+a> \end{cases} \tag{11}$$

, where s_{so}^{α} presents the saturation slip resistance without twin volume fraction (i.e.,$\left(\sum_{\beta} f^{\beta}=0\right)$, and s_{pr} is coefficient.

Slip-twin interaction matrix, $M_{slip-twin}$, has not been implemented with any prefactor yet. We need to decide whether Equations 10 and 11 remove from the current subroutine or not. Current way to implement the nonlinear factor for the effet of twin on $\dot{s}^{\alpha}$ is intertwined with Equation 9, so that it is hard to sperate from it. Either we do not use $M_{slip-twin}$ or we need to provide additional prefactor for $M_{slip-twin}$ without using Equations 10 and 11.

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

$M_{twin-slip}$ and $M_{twin-twin}$ use for twin resistance evolution $\left(\dot{s}^{\beta}\right)$. The first part in Equation 12 ($\dot{s}^{\beta}_{twin-twin}$) is twin-twin interaction contribution to twin resistance evolution, and the second part in Equation 12($\dot{s}^{\beta}_{twin-slip}$) is twin-slip interaction contribution to twin resistance evolution. Equations for each contribution is listed in Equations 13 and 14.

$$\dot{s}^{\beta} = \dot{s}^{\beta}_{twin-twin} + \dot{s}^{\beta}_{twin-slip} \tag{12}$$

$$\left[\dot{s}^{\beta}_{twin-twin}\right]_{24\times1} = h_{tw}\left(\sum_{m} f^{m}\right)^{d} M_{twin-twin}\left[\gamma^{\beta} f^{\beta}\right]_{1\times24} \quad or \quad \dot{s}^{\beta}_{twin-twin} = h_{tw}\left(\sum_{m} f^{m}\right)^{d} \sum_{k} \gamma^{k} \dot{f}^{k} \tag{13}$$

,where h_{tw} and d are coefficients for twin-twin contribution. γ^{β} is shear strain for each twin system.

$$\left[\dot{s}^{\beta}_{twin-slip}\right]_{24\times1} = h_{tw-sl}\left(\sum_{\alpha} \gamma^{\alpha}\right)^{e} M_{twin-slip}\left[\dot{\gamma}^{\alpha}\right]_{1\times24} \quad or \quad \dot{s}^{\beta}_{twin-slip} = h_{tw-sl}\left(\sum_{\alpha} \gamma^{\alpha}\right)^{e} \sum_{k} \dot{\gamma}^{k} \tag{14}$$

,where h_{tw-sl} and e are coefficients for twin-slip contribution.

3 Material Parameters (Material Configuration file)

Parameters for phenomenological modeling (kalidinditwin)

Parameter	Description	Value	Equation
s0_bas s0_pri s0_pyr s0_pyr_ca	initial slip resistance (s^{α})	65e6 22e6 50e6 50e6	Eqs. (1) & (9)
s0_t1 s0_c1 s0_t2 s0_c2	initial twin resistance (s^{β})	70e6 70e6 250e8 250e8	Eq (2)
s_sat_bas s_sat_pri s_sat_pyr s_sat_pyr_ca	initial saturation slip resistance (s_x^{α})	180e6 80e6 180e6 180e6	Eq. (11)
gdot0_slip gdot0_twin	reference shear strain ($\gamma^{\alpha}, \gamma^{\beta}$)	0.001 0.001	Eqs. (1) & (2)
n_slip n_twin	Exponent for Kinetic eqs.	50.0 50.0	
h0_bas h0_pri h0_pyr h0_pyr_ca	hardening coeff. for s^{α}	60e6 60e6 600e6 600e6	Eq. (10)
h0_tw h0_tw_sl	hardening coeff. for s^{β}	0.0 0.0	Eqs. (13) & (14)
twinC twinB s_pr	hardening coeff. for s^{α}	25 2 100e6	Eqs. (10) & (11)
twinD twinE	hardening coeff. for s^{β}	0.0 0.0	Eqs. (13) & (14)

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
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

Figure 1: Example of phenomenological modelling parameters.

- The sequence for latent hardening coefficients in Figure 1 (I need to implement this part if we agree to do this way.)
  - SlipSlip_hardening_coefficients (11 types); interacting between pairs listed below
    - self-hardening, basal-basal, prism-prism, pyr<a>-pyr<a>, pyr<c+a>-pyr<c+a>, basal-prism, basal-pyr<a>, basal-pyr<c+a>, prism-pyr<a>, prism-pyr<c+a>
  - SlipTwin_hardening_coefficients (16 types) and TwinSlip_hardening_coefficients (16 types); the sequence is the same as numbering in Tables 3 and 4. Numbers are 1 to 16.

- TwinTwin_hardening_coefficients (11 types); interacting between pairs listed below
  * self-hardening, T1-T1, C1-C1, T2-T2, C2-C2, T1-C1, T1-T2, T1-C2, C1-T2, C1-C2, T2-C1

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.