

# Simulation of texture formation of body-centered-cubic metals by three kinds of intersections of two $\{110\}$ slip planes

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**Abstract.** Based on the rotational symmetry of the principal axes of X[100], Y[010] and Z[001], 72 possible combinations of the five slips on  $\{110\}$  planes based on Taylor's formidable restriction rule of the five slips are calculated among three kinds of intersections of two  $\{110\}$  planes on  $\langle 111 \rangle$  direction in bcc metal. Crystal rotation is carried out by only one solution among the 72 by the minimum total slip at every strain and simulates properly length of accumulated researcher's experimental results such as the three stable orientations of bcc metal in rolling  $\{112\}\langle 110 \rangle$ ,  $\{111\}8\langle 4411 \rangle$  and  $\{100\}\langle 011 \rangle$ .

## 1. Introduction

The pencil glide theory combining  $\{110\}$ ,  $\{112\}$  and  $\{123\}$  planes with common direction  $\langle 111 \rangle$  gave a very clear account of prediction about crystal rotation of body-centered-cubic (bcc) metal.<sup>1-4)</sup> Barrett et al found that high silicon steel slips by only  $\{110\}\langle 111 \rangle$  and is less ductile than mild steel.<sup>5)</sup> But they also reported in other experiment that the high silicon steel forms finally almost same cold rolling textures as those of low carbon mild steel, although the latter are supposed to have been formed by the pencil glide.<sup>6)</sup> This led directly to a motivation in this study to investigate whether crystal rotation could take place by only slip on  $\{110\}$  plane on direction  $\langle 111 \rangle$  in bcc metal.

## 2. Model

The principal axes of X[100], Y[010] and Z[001] are perpendicular to each other as the three orbits of  $\{\pm X\}$ ,  $\{\pm Y\}$  and  $\{\pm Z\}$  by a rotational symmetry of mathematical group theory in such way that component X is not related to Y or Z one another whichever.<sup>7)</sup> There is a conservation quantity in the symmetry.<sup>8)</sup> For example, a small ball at the top of Mexican hat may drop down on the bottom everywhere equally and symmetrically within  $360^\circ$  around the top due to existence of potential energy of the ball as a conservation quantity. Once the hat inclined, the ball would lose both the quantity and symmetry. As Taylor proved, crystal rotates so that slips occurs associating themselves with the minimum total slip amount<sup>9)</sup>. The minimum total slip amount in crystal by Taylor corresponds to the conservation quantity in the rotational symmetry of cubic crystal.

There are three kinds of  $\{110\}$  planes having a common glide axis  $\langle 111 \rangle$  in bcc crystal such as those illustrated on Fig.1 in case around Z[001] axis.

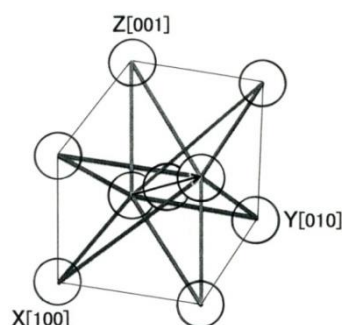


Fig.1 Three kinds of  $\{110\}$  planes composed of  $\{110\}$ ,  $\{101\}$  and  $\{011\}$  ones around the principal Z[001] axis with a common slip direction  $\langle 111 \rangle$  in bcc crystal.

Calculation method is exemplified as follows.

Firstly, an intersection of two kinds of  $\{110\}$  planes from the three ones composed of  $\{110\}$ ,  $\{101\}$  and  $\{011\}$  as illustrated on Fig.1 is chosen. As example, an intersection between  $\{101\}$  and  $\{011\}$  in Fig.1 is chosen and shears on  $\{101\}$  group planes on four  $\langle 111 \rangle$  directions in case around Z[001] axis are named by turns  $dX_1$ ,  $dX_2$ ,  $dX_3$  and  $dX_4$  and



those on  $\{011\}$  group planes are done  $dY_1$ ,  $dY_2$ ,  $dY_3$  and  $dY_4$  correspondently as shown in Fig.2. These are geometrically correlated to strain components  $d\varepsilon_{11}$ ,  $d\varepsilon_{22}$ ,  $d\varepsilon_{33}$ ,  $d\varepsilon_{12}$ ,  $d\varepsilon_{13}$  and  $d\varepsilon_{23}$  and crystal rotation  $d\phi_1$ ,  $d\phi_2$  and  $d\phi_3$  around the principal axes X, Y and Z respectively and accordingly a crystal rotation and texture formation can be calculated for the bcc crystal during any of compression, elongation, rolling and others.

Second the eight slips, however, must be reduced to five shears according to Taylor's formidable combination rule of the five slips as follows.<sup>9)</sup> The geometrical condition rule for a given strain cannot be satisfied if the five shears are chosen so that two are taken from one group, *i.e.* one slip plane, and the remaining three are chosen one from each of the three remaining groups, in other words, all of which must be chosen so that two shears occur on each of two planes, one on the third and none on the fourth. This rule was properly applied to the present model as exemplified in Fig.2. By the Taylor's combination rule of the five, Fig.2 in case of  $dX_1 = dY_1 = 0$  shows two possible combinations (○) of the five slips and two impossible ones (×). This phenomenon of two possible combinations on Fig.2 appears in each case of  $dX_i = dY_i = 0$  for four  $\langle 111 \rangle$  directions ( $i=1\sim 4$ ), and furthermore every for each group around X, Y and Z axes.

This shows  $24(=2 \times 4 \times 3)$  possible combinations in the intersection of two groups of  $\{110\}$  planes (in this example case  $\{101\}$  and  $\{011\}$ ) from the three ones. There are three kinds of intersections of two  $\{110\}$  planes as illustrated on Fig.1 and the model accordingly provides with  $72(=24 \times 3)$  possible combinations of the five slips as a whole.

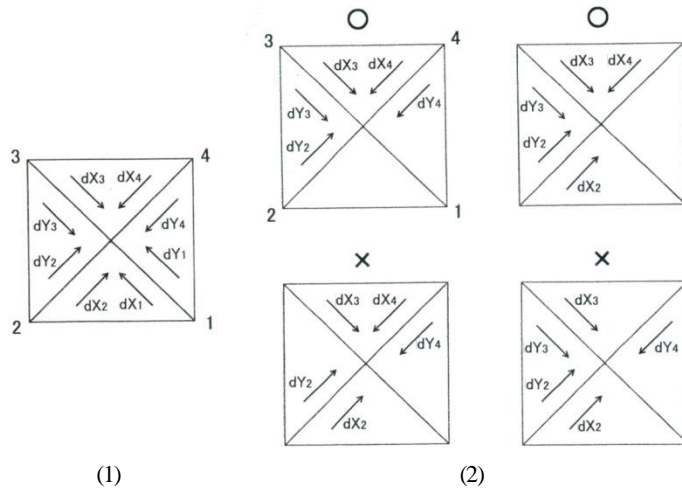


Fig.2 Example of an intersection between  $\{101\}$  and  $\{011\}$  in Fig.1.

(1) Eight slips in bcc cubic metal wherefrom five slips are needed for deformation and crystal rotation.

(2) Two possible combinations of the five slips (○) and two impossible ones (×) in the model by the rule of the Taylor's formidable restriction of the five slips, "all of which must be chosen so that two shears occur on each of two planes, one on the third and none on the fourth", are exemplified in case of  $dX_1 = dY_1 = 0$  ( $dX_2 = 0$  or  $dY_4 = 0$  is possible).

In this case of the intersection example between  $\{101\}$  and  $\{011\}$  from the three kinds of intersections around Z[001] axis in Fig.1, there are geometrical relations as demonstrated in equation (1) among the shears  $dX_1, dX_2, dX_3$  and  $dX_4$  on  $\{101\}$  group planes on four  $\langle 111 \rangle$  directions as well as  $dY_1, dY_2, dY_3$  and  $dY_4$  on  $\{011\}$  group planes, and strain components, crystal rotations. Similar equations exist also in each case around X[100] and Y[010] cases. Further, applied to equation (1), a calculation is carried out as example for crystal rotation in the possible case (○) of  $dX_1 = dY_1 = 0$ ,  $dX_2 = 0$  on Fig.2 according to the Taylor's combination rule of the five slips and its solution is introduced as in equation (2). The above example is only one of total 72 possible combinations of the five slips by the three kinds of intersections of two  $\{110\}$  planes on  $\langle 111 \rangle$  directions in bcc metal and each of the 72 has respectively similar equations as equation (2). Third an actual crystal rotation by equation (2) proceeds only for the case of which the total slip amount  $\Gamma$  (gamma) defined by equation (3) is minimum among the 72 cases. Calculation of equation (3) is performed by inserting both equation (1) and equation (2) to equation (3). Suppose one of the 72 cases is selected in the model.

$$\begin{aligned}
 dX_1 &= (\sqrt{6}/4)(d\varepsilon_{11} + d\varepsilon_{12} + d\varepsilon_{13} - 2d\varepsilon_{23} + d\phi_2 - d\phi_3) \\
 dX_2 &= (\sqrt{6}/4)(-d\varepsilon_{11} + d\varepsilon_{12} - d\varepsilon_{13} - 2d\varepsilon_{23} - d\phi_2 - d\phi_3) \\
 &\dots\dots\dots \\
 dY_4 &= (\sqrt{6}/4)(-d\varepsilon_{22} + d\varepsilon_{12} - 2d\varepsilon_{13} - d\varepsilon_{23} + d\phi_1 + d\phi_3)
 \end{aligned}
 \tag{1}$$

$$d\phi_1 = d\varepsilon_{22} + 2d\varepsilon_{12} - 2d\varepsilon_{13} - d\varepsilon_{23}, \quad d\phi_2 = -d\varepsilon_{11} - d\varepsilon_{13}, \quad d\phi_3 = d\varepsilon_{12} - 2d\varepsilon_{23} \quad (2)$$

$$\Gamma = \sqrt{dX_1 + dY_1} + \sqrt{dX_2 + dY_2} + \sqrt{dX_3 + dY_3} + \sqrt{dX_4 + dY_4} \quad (3)$$

### 3. Experimental results

According to the model Table 1 demonstrates how final stable rolling orientation in bcc (112)[ $\bar{1}10$ ] is derived from initial orientation (111)[ $\bar{1}10$ ] with increase of strain. At each strain the model selects one solution among the 72 cases composed of 24 ones each belonging to any one of X, Y and Z group. In this Table, it may be noted i) how the model gains the orientation with strain by way of selecting one of the partitions  $\{\pm X\}$ ,  $\{\pm Y\}$  and  $\{\pm Z\}$  independently in the rotational symmetrical system and ii) how it holds a continuous value of  $\Gamma$  (gamma), the minimum total slip by way of equation (3) throughout X,Y and Z group at each strain so smoothly as not to give a fatal discontinuity in the value of  $\Gamma$  (gamma). This is in reasonable accord with an expectation that amount of the external work by applied force to material shall be continuously changed with strain.

Table 1. Simulation results by the model how a final stable rolling orientation (112)[ $\bar{1}10$ ] of bcc metal is derived from initial orientation (111)[ $\bar{1}10$ ] with increase of strain.

initial			phi2	Phi	phil	ND			RD		
			45.00	54.74	180.00	0.58	0.58	0.58	-0.71	0.71	0.00
strain	mode	gamma	phi2	Phi	phil	ND	ND	ND	RD	RD	RD
0.069	Y	3.31	45.00	52.87	181.15	0.56	0.56	0.60	-0.70	0.72	-0.02
0.139	X	3.28	45.12	51.21	180.19	0.55	0.55	0.63	-0.70	0.71	0.00
0.208	X	3.28	45.18	49.74	179.40	0.54	0.54	0.65	-0.71	0.70	0.01
0.277	Y	3.26	45.03	48.43	180.12	0.53	0.53	0.66	-0.71	0.71	0.00
0.347	X	3.25	45.11	47.25	179.55	0.52	0.52	0.68	-0.71	0.70	0.01
0.416	Y	3.24	44.98	46.20	180.06	0.51	0.51	0.69	-0.71	0.71	0.00
0.485	X	3.23	45.07	45.26	179.63	0.50	0.50	0.70	-0.71	0.70	0.00
0.555	Y	3.22	44.96	44.41	180.00	0.49	0.50	0.71	-0.71	0.71	0.00
0.624	Y	3.21	44.90	43.65	180.29	0.49	0.49	0.72	-0.71	0.71	0.00
0.693	X	3.20	45.00	42.96	180.02	0.48	0.48	0.73	-0.71	0.71	0.00
0.762	X	3.19	45.06	42.33	179.80	0.48	0.48	0.74	-0.71	0.71	0.00
0.832	Y	3.18	44.99	41.76	179.99	0.47	0.47	0.75	-0.71	0.71	0.00
0.901	Y	3.17	44.94	41.24	180.15	0.47	0.47	0.75	-0.71	0.71	0.00
0.970	Z	3.16	45.00	40.77	180.00	0.46	0.46	0.76	-0.71	0.71	0.00
1.040	X	3.16	45.04	40.34	179.89	0.46	0.46	0.76	-0.71	0.71	0.00
1.109	Y	3.15	44.99	39.94	179.99	0.45	0.45	0.77	-0.71	0.71	0.00
1.178	Y	3.14	44.97	39.58	180.08	0.45	0.45	0.77	-0.71	0.71	0.00
1.248	X	3.13	45.00	39.25	180.00	0.45	0.45	0.78	-0.71	0.71	0.00
1.317	Y	3.13	44.98	38.95	180.06	0.44	0.44	0.78	-0.71	0.71	0.00
1.386	X	3.12	45.00	38.67	180.01	0.44	0.44	0.78	-0.71	0.71	0.00
1.456	X	3.11	45.02	38.42	179.96	0.44	0.44	0.78	-0.71	0.71	0.00
1.525	Y	3.11	45.00	38.18	180.00	0.44	0.44	0.79	-0.71	0.71	0.00
1.594	X	3.10	45.01	37.97	179.97	0.44	0.43	0.79	-0.71	0.71	0.00
1.664	Y	3.10	45.00	37.77	180.00	0.43	0.43	0.79	-0.71	0.71	0.00
1.733	X	3.09	45.01	37.58	179.97	0.43	0.43	0.79	-0.71	0.71	0.00
1.802	Y	3.09	45.00	37.41	180.00	0.43	0.43	0.79	-0.71	0.71	0.00
1.872	Y	3.08	44.99	37.26	180.02	0.43	0.43	0.80	-0.71	0.71	0.00
1.941	Z	3.08	45.00	37.11	180.00	0.43	0.43	0.80	-0.71	0.71	0.00
2.010	Y	3.08	44.99	36.98	180.01	0.43	0.43	0.80	-0.71	0.71	0.00
2.079	X	3.07	45.00	36.85	180.00	0.42	0.42	0.80	-0.71	0.71	0.00
2.149	Y	3.07	45.00	36.74	180.01	0.42	0.42	0.80	-0.71	0.71	0.00
2.218	X	3.07	45.00	36.63	180.00	0.42	0.42	0.80	-0.71	0.71	0.00
2.287	X	3.06	45.00	36.54	179.99	0.42	0.42	0.80	-0.71	0.71	0.00
2.357	Y	3.06	45.00	36.44	180.00	0.42	0.42	0.80	-0.71	0.71	0.00
2.426	Y	3.06	45.00	36.36	180.01	0.42	0.42	0.81	-0.71	0.71	0.00
2.495	X	3.06	45.00	36.28	180.00	0.42	0.42	0.81	-0.71	0.71	0.00
2.565	X	3.05	45.00	36.21	180.00	0.42	0.42	0.81	-0.71	0.71	0.00
2.634	Y	3.05	45.00	36.14	180.00	0.42	0.42	0.81	-0.71	0.71	0.00
2.703	Y	3.05	45.00	36.08	180.00	0.42	0.42	0.81	-0.71	0.71	0.00
2.773	Z	3.05	45.00	36.02	180.00	0.42	0.42	0.81	-0.71	0.71	0.00
2.842	X	3.05	45.00	35.97	180.00	0.42	0.42	0.81	-0.71	0.71	0.00
2.911	Y	3.05	45.00	35.92	180.00	0.41	0.41	0.81	-0.71	0.71	0.00
2.981	Y	3.05	45.00	35.87	180.00	0.41	0.41	0.81	-0.71	0.71	0.00
3.050	X	3.04	45.00	35.83	180.00	0.41	0.41	0.81	-0.71	0.71	0.00

Fig.3 illustrates by the model dynamically how orientations in ODFs map at rolling ratio of (a)6%,(b)38%,(c)62% and (d)95% are rigorously accumulated from initial random ones with strain in rolling by the present model and consequently

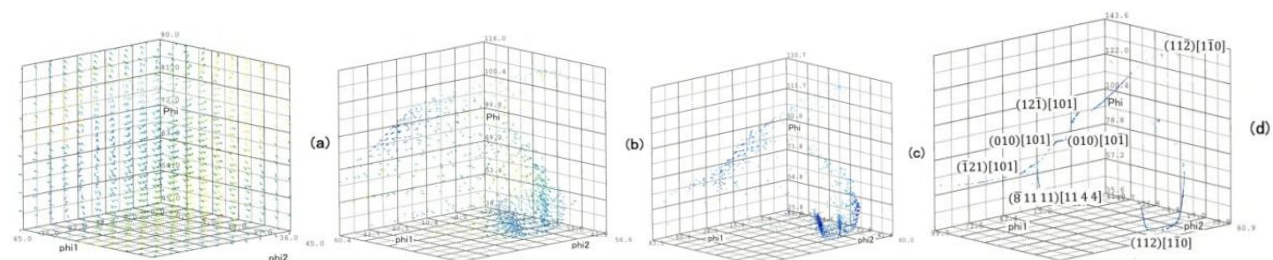


Fig.3 A visible demonstration by the model how and when the rolling orientation in bcc metal changes and appears in the ODFs map which shows the orientations at rolling ratio of (a)6%,(b)38%,(c)62% and (d)95%.

the three stable orientations of bcc metal in rolling<sup>3,10,11)</sup> such as  $\{112\}\langle 110 \rangle$ ,  $\{11\ 11\ 8\}\langle 4\ 4\ 11 \rangle$  and  $\{100\}\langle 011 \rangle$  are attained as drawn on Fig.3(d).

#### 4. Discussion

According to the model Table 1 illustrates how final stable rolling orientation in bcc  $(112)[\bar{1}10]$  is derived from initial orientation  $(111)[\bar{1}10]$  with increase of strain sequentially selecting one among the 72 cases composed of 24 ones each belonging to any one of X, Y and Z group. As in Table 1,  $\Gamma$  (gamma), the minimum total slip by way of equation (3) in the three X, Y and Z group, is not constant and changes but so gradually as not to give a fatal discontinuity in the value of  $\Gamma$  (gamma) so that the model may hold the symmetry in the system. As generally known, even in the stable system composed of extreme symmetry, it can lose the symmetry immediately and transiently when exposed to external forces or other physical energy. Even in this case, however, as it is still the orthodoxy accepted by the majority, if a break of symmetry is so small where the symmetry recovers immediately and sustains still continuously the original symmetric state that the symmetry may still give birth to forceful analytical means to the phenomenon.<sup>12)</sup> Besides example of Table 1, it is supposed that such phenomena by the model may happen throughout the whole orientation as shown in Fig.3.

Similar model on face-centered-cubic(fcc) metal already reported by the author requires 24 cases in total for one solution where two combinations of five slips are accepted by the Taylor's formidable combination rule of the five slips as similarly as in Fig.2 on  $\{111\}$  planes on every four directions of  $\langle 110 \rangle$  for each group of X, Y and Z principal axes of fcc metal.<sup>13-15)</sup> A ratio of the  $24(=2 \times 4 \times 3)$  of fcc metal to the 72 of bcc metal which has three intersections of  $\{110\}$  planes, implies a ratio of one  $\{111\}$  slip plane on direction  $\langle 110 \rangle$  of fcc metal to at least three slip planes  $\{110\}$ ,  $\{112\}$  and  $\{123\}$  on direction of  $\langle 111 \rangle$  in the pencil glide theory of bcc metal. The idea which utilized the rotational symmetry among X, Y and Z principal axes was also applied for texture formation of NaCl structure.<sup>16)</sup>

#### 5. Conclusion

There are 72 combinations of the five slips on  $\{110\}$  planes based on Taylor's formidable restriction rule of the five slips among three kinds of intersections of two  $\{110\}$  planes on  $\langle 111 \rangle$  direction in bcc metal based on the rotational symmetry of the principal axes of X[100], Y[010] and Z[001]. One solution of crystal rotation among the 72 is selected by the minimum total slip at every strain and simulates properly lengthly of accumulated researcher's experimental results such as the three stable orientations of bcc metal in rolling  $\{112\}\langle 110 \rangle$ ,  $\{11\ 11\ 8\}\langle 4\ 4\ 11 \rangle$  and  $\{100\}\langle 011 \rangle$ .

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