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Co-yield surfaces for $\{111\}\langle 110\rangle$ slip and $\{111\}\langle 112\rangle$ twinning in fcc metals

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The co-yield surfaces in fcc single crystals for slip on $\{111\}\langle 110\rangle$ and twinning on $\{111\}\langle 112\rangle$ systems have been analyzed and derived systematically for the first time. The results demonstrated that only if the ratio ξ of the critical resolved shear stress (CRSS) for twinning to that for slip is within the range of $1/\sqrt{3} \leq \xi \leq 2/\sqrt{3}$, slip and twinning can occur together. There are only two types of co-yield surfaces when ξ is within this range. The corresponding analytical expressions of all possible types of yield vertices are also derived and tabulated. One type consists of 259 co-yield stress states when $\sqrt{3}/2 < \xi < 2/\sqrt{3}$, which can be classified into 21 groups in stress space according to the crystal symmetry. The other type contains 259 co-yield stress states also when $1/\sqrt{3} < \xi < \sqrt{3}/2$, which can be subdivided into 19 groups. Of the two types of the co-yield stress states, 139 ones are common and 120 ones are different.

1. Introduction

The single crystal yield surfaces (SCYS) are extremely important to the study of the yield and deformation behavior of polycrystalline materials, texture development and plastic anisotropy. The crystal plastic theory points out that activation of five independent slip systems is required in order to fulfill an arbitrary shape change of a deforming crystal, if slip is the only deformation mechanism. For the stress states that can activate five independent slip systems simultaneously, they are the yield vertices that lie on the yield surfaces. For an arbitrary strain state, the principle of maximum work of Bishop-Hill [1, 2] can be used to determine the appropriate stress state (s), hence the corresponding active slip systems can be decided also. On the other hand, one can decide the combination of active slip systems by applying the minimum shear principle of Taylor [3]. Both methods have been proved to be equivalent [4, 5]. When less than five strain components are imposed, the yield stress states can be derived on the basis of the knowledge of the yield vertices [6]. Therefore, only the yield stress states of single crystal that can satisfy an arbitrary shape change have been investigated in this paper.

Since the investigation of Bishop and Hill [1, 2], the SCYS of fcc crystals for slip on $\{111\}\langle 110\rangle$ systems is well known. But there is little investigation for the case that slip and twinning can take place simultaneously. In fact, both slip and twinning can occur for fcc metals in many cases [7, 8] (such as for fcc metals with medium, low stacking fault energy, particularly, when deformed at low temperatures and high strain rates). Since the SCYS are the fundamental to the study of polycrystalline plastic deformation, the mixed yield surfaces of fcc single crystals and its characteristics for slip on the $\{111\}\langle 110\rangle$ and twinning on the $\{111\}\langle 112\rangle$ systems have been investigated systematically for the first time on the basis of Taylor/Bishop-Hill theory in this article.

2. Single crystal yield surfaces

2.1. The Schmid law and stress strain-increment vectors

Each slip system of single crystal can be characterized by the normal to the slip plane **n** and the slip direction unit vector **b**, respectively, and each twinning system by the normal to the twinning plane and twinning direction as well. Here **n** and **b** are assumed to be normalized. For the rate-insensitive materials, if the stress state is specified by the tensor σ_{ij}, the yield surfaces can be decided by the Schmid law [9]

$$m_{ij}{}^{s}\sigma_{ij} \leq \tau_{c}{}^{s} \qquad (i, j = 1, 2, 3) \qquad (1)$$

where $m_{ij}{}^{s}$ are the generalized Schmid factors for different shear systems, $m_{ij}{}^{s} = (b_i{}^{s}n_j{}^{s} + b_j{}^{s}n_i{}^{s})/2$. The equality sign in Equation 1 holds for every active shear system and the inequality for inactive systems. The strain-increment associated with the microscopic shear that takes place in the system is decided by

$$d\varepsilon_{ij} = m_{ij}{}^{s}d\gamma^{s} \qquad (2)$$

TABLE I {111}⟨110⟩ slip systems and generalized Schmid vectors $m_{ks}{}^{s}$

Number of slip systems		Slip systems						$m^{s}_{ks} = 1/\sqrt{6}\times$								Notations of slip systems	
								5D space:			$m53$	$m54$	$m55$	$m51$	$m52$		
Pos	Neg	$n = 1/\sqrt{3}\times$			$b = 1/\sqrt{2}\times$			$m61$	$m62$	$m63$	$m64$	$m65$	$m66$	6D space		Pos	Neg
1	13	1	1	1	0	1	−1	0	1	−1	0	−1	1	−1	−1	s1	s13
2	14	1	1	1	−1	0	1	−1	0	1	1	0	−1	−1	1	s2	s14
3	15	1	1	1	1	−1	0	1	−1	0	−1	1	0	2	0	s3	s15
4	16	−1	−1	1	0	−1	−1	0	1	−1	0	1	1	−1	−1	s4	s16
5	17	−1	−1	1	1	0	1	−1	0	1	−1	0	−1	−1	1	s5	s17
6	18	−1	−1	1	−1	1	0	1	−1	0	1	−1	0	2	0	s6	s18
7	19	−1	1	1	0	1	−1	0	1	−1	0	1	−1	−1	−1	s7	s19
8	20	−1	1	1	1	0	1	−1	0	1	1	0	1	−1	1	s8	s20
9	21	−1	1	1	−1	−1	0	1	−1	0	−1	−1	0	2	0	s9	s21
10	22	1	−1	1	0	−1	−1	0	1	−1	0	−1	−1	−1	−1	s10	s22
11	23	1	−1	1	−1	0	1	−1	0	1	−1	0	1	−1	1	s11	s23
12	24	1	−1	1	1	1	0	1	−1	0	1	1	0	2	0	s12	s24

TABLE II {111}⟨112⟩ twinning systems and generalized Schmid vectors $m_{kt}{}^{s}$

Number of twinning systems	Twinning systems						$m^{s}_{ks} = 1/\sqrt{18}\times$								Notations of twinning systems
							5D space			$m53$	$m54$	$m55$	$m51$	$m52$	
	$n = 1/\sqrt{3}\times$			$b = 1/\sqrt{6}\times$			$m61$	$m62$	$m63$	$m64$	$m65$	$m66$	6D space		
25	1	1	1	−2	1	1	−2	1	1	2	−1	−1	−3	1	t1
26	1	1	1	1	−2	1	1	−2	1	−1	2	−1	3	1	t2
27	1	1	1	1	1	−2	1	1	−2	−1	−1	2	0	−2	t3
28	−1	−1	1	2	−1	1	−2	1	1	−2	1	−1	−3	1	t4
29	−1	−1	1	−1	2	1	1	−2	1	1	−2	−1	3	1	t5
30	−1	−1	1	−1	−1	−2	1	1	−2	1	1	2	0	−2	t6
31	−1	1	1	2	1	1	−2	1	1	2	1	1	−3	1	t7
32	−1	1	1	−1	−2	1	1	−2	1	−1	−2	1	3	1	t8
33	−1	1	1	−1	1	−2	1	1	−2	−1	1	−2	0	−2	t9
34	1	−1	1	−2	−1	1	−2	1	1	−2	−1	1	−3	1	t10
35	1	−1	1	1	2	1	1	−2	1	1	2	1	3	1	t11
36	1	−1	1	1	−1	−2	1	1	−2	1	−1	−2	0	−2	t12

For convenience, it is often to represent them by vector. The vector representations introduced by Kocks [6] in five- or six-dimensional stress space are used in this paper.

Using the concept of stress vector, the Schmid law can be expressed by

$$m_k{}^{s}\sigma_k \leq \tau_c{}^{s} \qquad (k = 1\text{–}5 \text{ or } 6) \tag{3}$$

The corresponding strain-increment is given by

$$d\varepsilon_k = m_k{}^{s}\, d\gamma^{s} \tag{4}$$

For the five- or six-dimensional stress vectors, the $m_k{}^{s}$ are the different linear combinations of the $m_{ij}{}^{s}$.

2.2. The shear systems and Schmid factor vectors

Tables I and II list all the {111}⟨110⟩ slip systems and {111}⟨112⟩ twinning systems and the generalized Schmid vector components $m_{ks}{}^{s}$ and $m_{kt}{}^{s}$ in the cubic crystallographic axes. They are given in two different vector representations. The second column labeled Neg in Table I represents the opposite slip direction, for which all the components of **m** must be replaced by their negatives. Assuming that twinning can not happen in the anti-twinning directions, so there is not the Neg column in Table II.

2.3. {111}⟨110⟩ slip yield surfaces P_s and {111}⟨112⟩ twinning yield surfaces P_t

The polyhedra P_s will be used to denote the {111}⟨110⟩ slip yield surfaces, P_t for the {111}⟨112⟩ twinning yield surfaces, and P_m for the mixed yield surfaces that both slip and twinning are possible. Bishop and Hill derived the yield surfaces P_s including 56 stress states using an analytical method in 1954 [1]. By duality, they are identical to those of bcc crystals for slip on {110}⟨111⟩ systems. The yield vertices can be classified into 5 groups according to the crystal symmetry. Kocks *et al.* tabulated the characteristics of yield surfaces P_s for fcc metals in detail [6]. The yield surfaces for twinning on the {111}⟨112⟩ systems have been calculated using the stress and strain notations in this paper, there are 25 yield vertices altogether, which can be subdivided into 4 groups. Tables III and IV give the yield vertices, the number of equivalent vertices and the number of the sets of 5 independent slip and twinning systems associated with each particular group.

3. Results and discussion

3.1. The range of CRSS ratios for mixed slip and twinning

Assuming that the critical shear stresses are τ_{cs} for all the {111}⟨110⟩ slip systems and τ_{ct} for all the {111}

TABLE III Yield vertices, the number of sets of 5 independent slip systems and active systems for {111}⟨110⟩ slip systems

5 groups of yield vertices	Number of equivalent vertices	$\vec{M}$ (units of τ_{cs}) $= \sqrt{6}\times$								Number of sets of 5 independent slip systems	Active slip systems
		M_{61}	M_{62}	M_{63}	M_{64}	M_{65}	M_{66}				
					M_{53}	M_{54}	M_{55}	M_{51}	M_{52}		
1	6	1/3	1/3	−2/3	0	0	0	0	−1	32	s1 s4 s7 s10 s14 s17 s20 s23
2	6	0	0	0	0	−1	0	0	0	32	s1 s6 s9 s10 s15 s16 s19 s24
3	12	0	1/2	−1/2	−1/2	0	0	−1/4	−3/4	36	s1 s4 s7 s10 s14 s18 s20 s24
4	24	−1/6	1/3	−1/6	1/2	0	1/2	−1/4	−1/4	4	s1 s4 s8 s15 s17 s21
5	8	0	0	0	−1/2	−1/2	1/2	0	0	6	s1 s6 s8 s15 s17 s19

The first subscript stands for the dimensions and the second subscript for stress vector components.

TABLE IV Yield vertices, the number of sets of 5 independent twinning systems, and active systems for {111}⟨112⟩ twinning systems

4 groups of yield vertices	Number of equivalent vertices	$\vec{M}$ (units of τ_{ct}) $= \sqrt{18}\times$								Number of sets of 5 independent twinning systems	Active twinning systems
		M_{61}	M_{62}	M_{63}	M_{64}	M_{65}	M_{66}				
					M_{53}	M_{54}	M_{55}	M_{51}	M_{52}		
1	3	−1/3	−1/3	2/3	0	0	0	0	1	56	t1 t2 t4 t5 t7 t8 t10 t11
2	6	−1/12	−1/12	1/6	0	0	−3/4	0	1/4	6	t1 t2 t4 t5 t9 t12
3	4	0	0	0	1/2	1/2	−1/2	0	0	6	t1 t2 t7 t9 t11 t12
4	12	−1/6	1/12	1/12	1/4	1/2	−1/2	−1/8	−1/8	1	t1 t2 t4 t7 t9

The first subscript stands for the dimensions and the second subscript for stress vector components.

⟨110⟩ twinning systems. For convenience, the stress vector $\boldsymbol{\sigma}$ is normalized as **M** with respect to the CRSS of the {111}⟨110⟩ slip system τ_{cs}. At the same time, the CRSS ratio for twinning on the {111}⟨112⟩ is denoted ζ and slip on {111}⟨110⟩ and for active systems.

$$\left.\begin{aligned} m^{s}_{ks}M_k &= 1 \quad \text{for slip systems} \\ m^{s}_{kt}M_k &= \xi \quad \text{for twinning systems} \end{aligned}\right\} \tag{5}$$

The above equations define a series of hyperplanes in five- or six-dimensional stress space, the $m_{ks}{}^{s}$ and $m_{kt}{}^{s}$ are the inverse intercepts on the k axis of the s plane, the distances from the origin to the planes are dependent on **b** and **n** of different slip and twinning systems. The stress states that can fulfill an arbitrary shape change (i.e. the FC Taylor model) are called yield vertices. All the M_k, $m_{ks}{}^{s}$ and $m_{kt}{}^{s}$ components are calculated with respect to the cubic crystallographic axes.

Only the CRSS ratio ξ is within a certain range, slip and twinning can occur simultaneously. The twinning becomes more and more difficult as ξ increases within the range, eventually, at some upper critical value, only slip deformation is possible. From geometry point of view, increasing ξ means the expansion of the polyhedra P_t, which makes the distance from origin to the P_t planes become further and further, finally, only slip is possible. At this time, P_t lies completely outside P_s. Conversely, reducing ξ to some lower critical value, P_t lies entirely inside P_s, then only twinning is possible.

Based on the above analysis, if only slip occurs, all the vertices of polyhedra P_s must lie within P_t, then

$$m^{s}_{kt}M_{kp_s} < \xi \tag{6}$$

The M_{kp_s} is the component of the yield vertices for {111}⟨110⟩ slip. As a result, for any one vertex in each group, the ξ value at which the P_s vertex belongs to the P_t facet can be calculated, then their crossing area can be determined as well. The upper limit value $2/\sqrt{3}$ can be obtained, excluding $2/\sqrt{3}$. The same method can be used to determine the lower bound for ξ, if only twinning happens, in that case

$$m^{s}_{ks}M_{kp_t} < 1 \tag{7}$$

The M_{kp_t} is the component of the yield vertices for {111}⟨112⟩ twinning. The obtained lower limited value is $1/\sqrt{3}$, also excluding $1/\sqrt{3}$.

So, only if the ratio ξ of the critical resolved shear stress (CRSS) for twinning to that for slip is within the range of $1/\sqrt{3} \le \xi \le 2/\sqrt{3}$, slip and twinning can occur together. The above calculated results are consistent with those obtained by Chin [10] using an analytical method.

3.2. Characterization of the mixed yield surfaces

It has proved with the crystal plastic theory that slip and twinning can co-occur only if ξ is within the range: $1/\sqrt{3} \le \xi \le 2/\sqrt{3}$. The remainder to do is to calculate the mixed yield surfaces and analyze their characteristics in the allowed whole range. Firstly, we calculate the yield surfaces when their CRSS are equal, that is, $\xi = 1$, then test the vadility of the obtained polyhedra over the full range of ξ.

All the resolved shear stresses on slip and twinning systems can be obtained in five- or six-dimensional stress space according to the corresponding Schmid factors. Since slip is reversible and twinning is unidirectional, there are 36 slip and twinning systems, that is, there are 36 equations altogether.

According to the Schmid law, if the resolved shear stress on slip system s $\tau^{s} = \tau_{cs}$, crystal yields and slip occurs; if the resolved shear stress on twining system t $\tau^{t} = \tau_{ct}$, crystal yields and twinning occurs. In order to accommodate an arbitrary shape change, solving the simultaneous equations, Equation 5 should be fulfilled on five or more than five shear systems (five independent active systems are needed, including slip and twinning). At the same time, the following conditions should be satisfied

$$\left.\begin{array}{ll} m^{s}_{ks} M_{kp_{m}} < 1 & \text{for slip systems} \\ m^{s}_{kt} M_{kp_{m}} < \xi & \text{for twinning systems} \end{array}\right\} \qquad (8)$$

on all the remainder inactive systems.

The $M_{kp_{m}}$ is the component of the mixed yield vertices for $\{111\}\langle 110\rangle$ slip and $\{111\}\langle 112\rangle$ twinning. For slip on $\{111\}\langle 110\rangle$ and twinning on $\{111\}\langle 112\rangle$ systems. Solving the simultaneous equations discussed above, the coordinate values of yield vertices together with the associated active systems can be derived. It is found out that there are 259 stress states that can be subdivided into 21 groups (21 basic stress states) according to the crystal symmetry. Then, substituting ξ into the yield condition equations associated with $\{111\}\langle 112\rangle$ twinning systems, the analytical expressions can be obtained as a function of ξ. They are listed in Table V:

(i) 3 groups of them activate 8 systems, there are 21 vertices, and each of them activates 8, 6 or 4 $\{111\}\langle 110\rangle$ slip systems and 0, 2, 4 $\{111\}\langle 112\rangle$ twinning system (s), the group of them activating 8 slip systems is the particular case of Bishop-Hill yield vertices (the 1st group).

(ii) 9 groups activate 6 systems, there are 70 vertices, and 8 groups of them activate 4 $\{111\}\langle 110\rangle$slip systems and 2 $\{111\}\langle 112\rangle$ twinning systems (66 vertices), the other group which activates 6 slip systems is the particular case of Bishop-Hill yield vertices (the 9th group).

(iii) the remainder 9 groups activate 5 systems simultaneously, there are 168 vertices. 3 groups of them activate 4 $\{111\}\langle 110\rangle$ slip systems and 1 $\{111\}\langle 112\rangle$ twinning systems (60 vertices), 3 groups of them activate 3 $\{111\}\langle 110\rangle$slip systems and 2 $\{111\}\langle 112\rangle$ twinning systems (72 vertices), the other 3 groups activate 2 $\{111\}\langle 110\rangle$slip systems and 3 $\{111\}\langle 112\rangle$ twinning systems (36 vertices).

Table V gives the 21 group of basic yield vertices, the number of sets of 5 independent shear systems and the number of equivalent yield vertices according to the crystal symmetry associated with each particular group. All the other yield stresses can be found out according to Table V and the appendix in reference [11, 12]. From the known yield vertices, the resolved shear stress on every system can be worked out in terms of the $m_{ks}{}^{s}$ and $m_{kt}{}^{s}$ in Tables I and II.

The results showed that most of the resolved shear stresses on the inactive system are not zero, this is quite different from $\{111\}\langle 110\rangle$ slip systems. For slip

TABLE V Co-yield vertices, the number of sets of 5 independent $\{110\}\langle 111\rangle$slip and $\{111\}\langle 112\rangle$ twinning systems, and active systems

Basic yield vertices	Number of equivalent vertices	$\vec{M}$ (units of τ_{cs}) $= \sqrt{6}\times$ (M_{51}, M_{52}, M_{53}, M_{54}, M_{55})	Number of sets of 5 independent slip or/and twinning systems	Active systems
1	3	$(-1/2, -1/2, 0, 0, 0)$	32	s1 s4 s7 s10 s15 s18 s21 s24
2	12	$(-3/4+\sqrt{3}\xi/4, -1/4-\sqrt{3}\xi/4, -1/2+\sqrt{3}\xi/2, 0, 0)$	40	s1 s4 s7 s10 s15 s21 t6 t12
3	6	$(\sqrt{3}\xi/2-1, -\sqrt{3}\xi/2, 0, 0, 0)$	44	s1 s4 s7 s10 t3 t6 t9 t12
4[a]	6	$(\sqrt{3}\xi/2-1, 0, 0, 0\ \sqrt{3}\xi/2)$	6	s1 s4 s8 s11 t3 t6
5[a]	6	$(-\sqrt{3}\xi/2+1, 0, 0, 0, -\sqrt{3}\xi/2)$	6	s13 s16 s20 s23 t9 t12
6[a]	6	$(1/2-\sqrt{3}\xi/2, 0, 0, 0, 3/2-\sqrt{3}\xi/2)$	6	s1 s4 s8 s11 t7 t10
7[a]	6	$(-1/2+\sqrt{3}\xi/2, 0, 0, 0, -3/2+\sqrt{3}\xi/2)$	6	s13 s16 s20 s23 t2 t5
8	12	$(\sqrt{3}\xi/4-3/4, \sqrt{3}\xi/4-3/4, \sqrt{3}\xi/2-1/2, 0, \sqrt{3}\xi/2-1/2)$	4	s1 s4s15 s21 t6 t7
9	4	$(0, 0, 1/2, -1/2, 1/2)$	6	s1 s6 s8 s15 s17 s19
10	12	$(0, 0, 1-\sqrt{3}\xi/2, -\sqrt{3}\xi/2, 1-\sqrt{3}\xi/2)$	6	s1 s6 s15 s19 t5 t8
11	12	$(\sqrt{3}\xi/4-1/4, 1/4-\sqrt{3}\xi/4, 1-\sqrt{3}\xi/2, -1/2, 1/2)$	6	s1 s6 s17 s19 t3 t8
12	6	$(\sqrt{3}\xi/8-1/4, \sqrt{3}\xi/8-1/4, 0, -\sqrt{3}\xi/4-1/2, 0)$	6	s1 s10 s15 s24 t5 t8
13[a]	24	$(0, 1/2-\sqrt{3}\xi/2, \sqrt{3}\xi/2-1/2, \sqrt{3}\xi/2-3/2, 0)$	1	s1 s6 s10 s15 t12
14[a]	24	$(0, \sqrt{3}\xi/2-1, 1-\sqrt{3}\xi/2, -\sqrt{3}\xi/2, 0)$	1	s1 s6 s10 s15 t5
15	12	$(0, -\sqrt{3}\xi/4, 1/2, -1/2, 1/2-\sqrt{3}\xi/4)$	1	s1 s6 s15 s17 t12
16[a]	24	$(-1/4, 3/4-\sqrt{3}\xi/2, \sqrt{3}\xi-3/2, 0, 3/2-\sqrt{3}\xi/2)$	1	s1 s4 s8 t6 t7
17	24	$(\sqrt{3}\xi/4-1/4, 1/4-\sqrt{3}\xi/2, 1-\sqrt{3}\xi/2, -1/2, 1/2-\sqrt{3}\xi/4)$	1	s1 s6 s17 t3 t12
18[a]	24	$(0, \sqrt{3}\xi/2-1, 1/2-\sqrt{3}\xi/2, \sqrt{3}\xi/2-3/2, \sqrt{3}\xi-3/2)$	1	s1 s9 s24 t3 t8
19	12	$(0, 1/2-3\sqrt{3}\xi/4, 1-\sqrt{3}\xi/2, \sqrt{3}\xi/2-1, 1/2-\sqrt{3}\xi/4)$	1	s1 s17 t3 t6 t12
20	12	$(\sqrt{3}\xi/8-1/4, 1/4-\sqrt{3}\xi/8, 1-3\sqrt{3}\xi/4-1/2, 1/2)$	1	s1 s19 t3 t8 t10
21	12	$(\sqrt{3}\xi/8-1/4, \sqrt{3}\xi/8-1/4, 1/2-\sqrt{3}\xi/2,$ $\sqrt{3}\xi/4-1, \sqrt{3}\xi/2-1/2)$	1	s1 s24 t3 t8 t10
22[b]	12	$(\sqrt{3}\xi/2-1, \sqrt{3}\xi-3/2, 0, 0, 3\sqrt{3}\xi/2-3/2)$	6	s1 s4 t3 t6 t7 t10
23[b]	12	$(\sqrt{3}\xi/2-5/8, 3/8-\sqrt{3}\xi/2, 0, -3/4, 0)$	6	s1 s10 t3 t5 t8 t12
24[b]	24	$(\sqrt{3}\xi/4-3/8, 1/8-\sqrt{3}\xi/4, \sqrt{3}\xi/2-1/2, -3/4, 0)$	1	s1 s10 s15 t5 t12
25[b]	24	$(0, -1/4, 1-\sqrt{3}\xi/2, -\sqrt{3}\xi/2, 3/4-\sqrt{3}\xi/2)$	1	s1 s6 s15 t5 t12
26[b]	24	$(\sqrt{3}\xi/4-1/4, 3/4-3\sqrt{3}\xi/4, 3/2-\sqrt{3}\xi, -\sqrt{3}\xi/2, 3/2-\sqrt{3}\xi)$	1	s1 s6 t3 t5 t8
27[b]	24	$(\sqrt{3}\xi/4-1/4, -\sqrt{3}\xi/4, 3/2-\sqrt{3}\xi, \sqrt{3}\xi/2, 3/4-\sqrt{3}\xi/2)$	1	s1 s6 t3 t5 t12

[a] The yield stress states that can satisfy the yield condition only when $\sqrt{3}/2 < \xi < 2/\sqrt{3}$.
[b] The yield stress states that can satisfy the yield condition only when $1/\sqrt{3} < \xi < \sqrt{3}/2$.

on {111}⟨110⟩ systems, all the resolved shear stresses of the yield vertices on inactive systems are zero. In particular, for twinning systems, the resolved shear stress of yield vertices on anti-twinning directions can be more than τ_{ct}. These stress states can be validity when the direction of twinning is considered. It also should be pointed out that the number of yield vertices for which there is active system ambiguity (i.e. more than 5 active systems) are 91. The 1st group and the 9th group in Table V are the vertices of Bishop-Hill yield surfaces, but the numbers of the equivalent yield vertices are only the half of the latter. Furthermore, in Table V, the yield vertices of the 4th and 5th, 6th and 7th groups are equal but the sign is opposite. However, they can not be classified into the same group, it is because that the twinning yield surfaces are unidirectional (that is not reversible), while the slip yield surfaces are symmetry about the original (this amounts to that the crystal symmetry includes inversion center for slip, but not for twinning). In addition, not every symmetry operation can obtain a new vertex when a different symmetry operation is applied to the basic yield vertex, some of them may be redundant, so the number of the equivalent yield vertices for different groups may be different.

In order to test the vadility of the obtained analytical expressions according to $\xi = 1$ within the allowed whole range, it should be calculated whether the resolved shear stress on every system fulfills the yield condition, that is

$$\left.\begin{array}{ll} m_{ks}^{s} M_{kp_m} \leq 1 & \text{for slip systems} \\ m_{kt}^{s} M_{kp_m} \leq \xi & \text{for twinning systems} \end{array}\right\} \quad (9)$$

Undoubtedly, these stress states should fulfill the condition that the resolved shear stress are 1 or ξ on 5 or more than 5 slip and twinning systems also. In reality, it is more visualized to represent the above relations graphically. Obviously, the resolved shear stress on every slip or twinning system is a function of ξ, that is

$$m_{ks(t)}^{s} M_{kp_m} = f(\xi) \quad (10)$$

The above expressions are straight line equations that should fulfill the condition (9).

From the analysis and calculation discussed above, it is found out that the critical value is $\sqrt{3}/2$. The number 4, 5, 6, 7, 13, 14, 16, 18 groups (there are 120 equivalent stress states labeled notation[a]) in Table V can not always satisfy the yield conditions within the allowed whole range, only satisfy them when $\sqrt{3}/2 < \xi < 2/\sqrt{3}$. For the mixed yield surfaces of $1/\sqrt{3} < \xi < \sqrt{3}/2$, also 259 stress states have been found out using the above method. They can be subdivided into 19 basic yield states according to the crystal symmetry. In the meantime, the analytical expressions are derived also. 13 groups of them (The number 1, 2, 3, 8, 9, 10, 11, 12, 15, 17, 19, 20, 21 groups, there are 139 equivalent stress states) are the same as those results when $\sqrt{3}/2 < \xi < 2/\sqrt{3}$. The 6 groups of yield vertices (The number 22, 23, 24, 25, 26, 27 groups, 120 vertices) labeled notation[b] in Table V are the yield vertices which only satisfied the yield condition when $1/\sqrt{3} < \xi < \sqrt{3}/2$.

Table V lists the analytical expressions of the two types of basic yield vertices when $1/\sqrt{3} < \xi < 2/\sqrt{3}$. All the remainder yield stress states can be found out in terms of Table V and those equivalent stress states obtained by use of the symmetric operations. Since the yield stress states have been known, the resolved shear stress on every shear system can be calculated in terms of the components of generalized Schmid factors $m_{ks}{}^{s}$ and $m_{kt}{}^{s}$. It also should be pointed out that, for {111}⟨110⟩ slip and {111}⟨112⟩ twinning, the fraction of ambiguous vertices for which there is slip system ambiguity (i.e. more than 5 slip systems) is reduced greatly compared to the {111}⟨110⟩ pure slip. So, if {111}⟨110⟩ slip and {111}⟨112⟩ twinning are the main deformation mechanism, correspondingly, the ambiguity of deformation textures also should be reduced very much. Besides, by duality, the obtained yield vertices in this paper are identified to those of bcc metals for slip on {110}⟨111⟩ and twinning on {112} ⟨111⟩.

As far as the yield stress states in the special cases that ξ is equal to $1/\sqrt{3}$, $\sqrt{3}/2$, $2/\sqrt{3}$, these critical values can be substituted into the analytical expressions in Table V, then the resolved shear stresses on all systems and the coordinates values of yield vertices can be obtained.

Using the calculated stress states in this paper, for an arbitrary deformation mode of an arbitrarily orientated crystal, one can calculate its Taylor factor and predict the behavior of plastic deformation by invoking of the principle of maximum work. In addition, the corresponding active systems are also decided, hence the change of the crystal orientation.

In a word, the calculated yield vertices of single crystal establish a foundation for further investigation of plastic deformation of polycrystalline materials, the formation and development of deformation textures and the prediction of macroscopic mechanical properties.

4. Conclusion

The mixed yield surfaces of fcc single crystals for slip on {111}⟨110⟩ and twinning on {111}⟨112⟩ systems have been determined for the first time on the basis of Taylor-Bishop-Hill Theory. It is showed that only slip is possible when $\xi > 2/\sqrt{3}$, and only twinning is possible if $\xi < 1/\sqrt{3}$. Both slip and twinning are possible when $1/\sqrt{3} \leq \xi \leq 2/\sqrt{3}$. The analyzed and calculated results show that only two types of mixed yield surfaces exist in fcc metals for slip on {111}⟨110⟩ and twinning on {111}⟨112⟩ systems. There are 259 stress states when $\sqrt{3}/2 < \xi < 2/\sqrt{3}$, which can be subdivided into 21 groups according to the crystal symmetry; there are also 259 stress states if $1/\sqrt{3} < \xi < \sqrt{3}/2$, which can be classified into 19 groups. Within the two types of co-yield stress states, 139 are the common and 120 are different.

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