Effects of Elastic Anisotropy on the Properties of $a+c$ Dislocations in H.C.P. Metals

H. Numakura*, M. Koiwa*, T. Ando*[†]
and M. H. Yoo**

*Department of Metal Science and Technology, Kyoto University, Kyoto 606-01, Japan

**Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6115, USA

The elastic energy, displacement field, and Peierls stress of $a+c$ dislocations have been calculated on the basis of anisotropic elasticity theory for several h.c.p. metals. The preferences of glide planes predicted from the self-energy of an edge dislocation and the profile of nonuniform displacement distribution around a screw dislocation agree with the experimental observations for the strongly anisotropic metals, Zn and Cd, but not for the others. The Peierls stress of an $a+c$ edge dislocation exhibits little correlation with experiments; the plane of the lowest Peierls stress is not always the observed glide plane. The calculated Peierls stress is primarily governed by the geometry of the slip system, i.e. the magnitude of the Burgers vector and the interplanar spacing, rather than the elastic anisotropy.

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I. Introduction

In metals with the h.c.p. structure, plastic deformation occurs primarily by slip in the a direction. The slip in the $a+c$ direction is a secondary but an important deformation mode giving rise to the strain in the c direction. Table 1 lists the slip systems observed in several h.c.p. metals. The slip plane of the a slip is either the basal plane, (0002), or the prismatic plane, $\{10\bar{1}0\}$, while that of $a+c$ slip is $\{11\bar{2}2\}$ or $\{10\bar{1}1\}$. The choice of the glide plane of a dislocations has been discussed in terms of the self energy and the Peierls stress on the basis of anisotropic elasticity theory⁽¹⁾⁻⁽³⁾. However, such arguments could not satisfactorily explain the whole experimental observations. Tyson⁽¹⁾ pointed out that dislocation core effect, i.e. spreading of the core, would be the most important.

In the last decade, computer simulation has been applied to h.c.p. metals, with the intention of clarifying the variety of deformation behaviour from an atomistic point of view (see, e.g. Ref. (4)): the choice of the slip planes of a dislocations has been explained in terms of the stability of stacking faults with the aid of atomistic calculations⁽⁵⁾, and the possible glide planes of $a+c$ dislocations have been shown to be $\{11\bar{2}2\}$ and $\{10\bar{1}1\}$ by the simulation of core structures⁽⁶⁾⁻⁽⁸⁾. The preference of the glide planes of $a+c$ dislocations in real metals has not been understood yet.

Yoo and Loh⁽⁹⁾ developed a general method to calculate elastic fields of dislocations in anisotropic media, and suggested that such calculations would give

Table 1 Slip planes of common h.c.p. metals*.

Metal	c/a	Slip planes	
		a slip	$a+c$ slip
Be	1.568	(0002)	$\{11\bar{2}2\}$
Mg	1.624	(0002)	$\{11\bar{2}2\}$
Y	1.572	$\{10\bar{1}0\}$	Unknown
Ti	1.587	$\{10\bar{1}0\}$	$\{10\bar{1}1\}$
Zr	1.593	$\{10\bar{1}0\}$	$\{10\bar{1}1\}$
Hf	1.581	$\{10\bar{1}0\}$	Unknown
Co	1.623	(0002)	$\{11\bar{2}2\}$
Zn	1.856	(0002)	$\{11\bar{2}2\}$
Cd	1.886	(0002)	$\{11\bar{2}2\}$

* For the sources of the data, see Ref. (24) for a slip and Ref. (25) for $a+c$ slip.

useful information on the properties of dislocations. In the present study we examine $a+c$ dislocations in h.c.p. metals in terms of anisotropic elasticity theory. It seems worthwhile to see whether elastic anisotropy influences the glide behaviour, in particular, the choice of the glide plane of $a+c$ dislocations.

II. Elastic Anisotropy of H.C.P. Metals

The elastic properties of nine h.c.p. metals studied are shown in Table 2. Hexagonal crystals possess six elastic stiffness constants, among which five being independent. The shear anisotropy factor A is defined as C_{44}/C_{66} , where C_{44} and C_{66} are the shear moduli on the basal plane and on the prismatic plane in the a axis direction, respectively. Elastic property of Be is anomalous in that C_{12} and C_{13} are much smaller than the shear moduli, resulting in a small Poisson's ratio of 0.045.

[†] Graduate Student, Kyoto University.

Table 2 Elastic constants at room temperature⁽²⁶⁾. A is the shear anisotropy factor. μ and ν are the shear modulus and the Poisson's ratio calculated by the Voigt average.

Metal	Elastic stiffness constants/GPa						A ($=C_{44}/C_{66}$)	μ /GPa	ν
	C_{11}	C_{33}	C_{12}	C_{13}	C_{44}	C_{66}^*			
Be	292.3	336.4	26.7	14.0	162.5	132.8	1.22	149.3	0.045
Mg	59.4	61.6	25.6	21.4	16.4	16.9	0.97	17.4	0.288
Y	77.9	76.9	28.5	21.0	24.3	24.7	0.98	25.5	0.245
Ti	162.4	180.7	92.0	69.0	46.7	35.2	1.33	44.1	0.319
Zr	143.4	164.8	72.8	65.3	32.0	35.3	0.91	36.4	0.331
Hf	181.1	196.9	77.2	66.1	55.7	51.9	1.07	56.0	0.280
Co	306.3	357.4	165.1	101.9	75.3	70.6	1.07	84.3	0.306
Zn	163.7	63.5	36.4	53.0	38.8	63.6	0.61	44.8	0.251
Cd	113.8	50.6	39.2	40.0	20.0	37.3	0.54	26.1	0.303

* $C_{66} = (C_{11} - C_{12})/2$

Fig. 1 Diagrams showing relative elastic anisotropy of hexagonal crystals.

Relative elastic anisotropy is shown graphically for some selected metals in Fig. 1. The six stiffness constants are normalized to the corresponding quantities for isotropy, i.e. C_{11} and C_{33} to $\lambda + 2\mu$, C_{12} and C_{13} to λ , C_{44} and C_{66} to μ , where λ and μ are Lamé constants obtained by the Voigt average, and the companion constants are plotted along the same axis in the opposite directions. From this diagram it can readily be seen that Zn is strongly anisotropic. Similar features are also found for Cd (not shown). On the other hand, elastic anisotropy is relatively weak in Mg, and in Y and Hf (not shown).

III. Calculation Procedure and Results

In terms of anisotropic elasticity theory, the favourable glide plane of a dislocation for a given Burgers vector should be either the plane on which the self-energy of the dislocation is the lowest, or the plane on which the stress required for the glide motion is the lowest. We first calculate parameters relevant to these two aspects for $a+c$ dislocations, as in the previous considerations on a slip systems⁽¹⁾⁽³⁾.

1. Self-energy

The total energy of a dislocation is the sum of the core

Table 3 Calculated parameters for the glide of $a+c$ edge dislocations. a is the lattice parameter in the basal plane.

Metal	b/a	Slip plane	d/a	K/GPa	$10^{-12}s'_{66}/\text{Pa}^{-1}$	ζ/b	$\tau_p^{\text{an}}/\text{GPa}$
Be	1.860	$\{10\bar{1}0\}$	0.866	162.6	6.55	0.248	14
		$\{10\bar{1}1\}$	0.758	162.3	6.59	0.218	21
		$\{11\bar{2}2\}$	0.422	162.2	6.60	0.121	71
		(Screw)		(152.5)			
Mg	1.907	$\{10\bar{1}0\}$	0.866	24.2	60.5	0.333	0.74
		$\{10\bar{1}1\}$	0.764	24.8	54.7	0.272	1.6
		$\{11\bar{2}2\}$	0.426	25.0	53.2	0.148	7.8
		(Screw)		(17.7)			
Y	1.863	$\{10\bar{1}0\}$	0.866	33.1	41.0	0.315	1.3
		$\{10\bar{1}1\}$	0.759	33.9	37.4	0.258	2.6
		$\{11\bar{2}2\}$	0.422	34.1	36.5	0.141	12
		(Screw)		(25.9)			
Ti	1.876	$\{10\bar{1}0\}$	0.866	65.9	23.4	0.356	1.5
		$\{10\bar{1}1\}$	0.760	69.4	20.6	0.290	3.6
		$\{11\bar{2}2\}$	0.423	70.3	19.9	0.158	19
		(Screw)		(46.1)			
Zr	1.881	$\{10\bar{1}0\}$	0.866	54.1	30.4	0.379	0.93
		$\{10\bar{1}1\}$	0.761	56.2	25.6	0.290	2.9
		$\{11\bar{2}2\}$	0.424	56.7	24.3	0.155	16
		(Screw)		(37.2)			
Hf	1.871	$\{10\bar{1}0\}$	0.866	78.4	18.3	0.333	2.4
		$\{10\bar{1}1\}$	0.760	80.4	17.0	0.277	5.0
		$\{11\bar{2}2\}$	0.423	80.9	16.6	0.152	24
		(Screw)		(57.3)			
Co	1.906	$\{10\bar{1}0\}$	0.866	120.4	13.5	0.370	2.3
		$\{10\bar{1}1\}$	0.764	129.3	10.5	0.272	8.4
		$\{11\bar{2}2\}$	0.426	131.7	9.67	0.142	44
		(Screw)		(87.8)			
Zn	2.108	$\{10\bar{1}0\}$	0.866	47.3	23.5	0.228	5.4
		$\{10\bar{1}1\}$	0.785	41.0	36.5	0.278	2.5
		$\{11\bar{2}2\}$	0.440	39.3	38.4	0.158	11
		(Screw)		(36.8)			
Cd	2.135	$\{10\bar{1}0\}$	0.866	29.1	44.9	0.266	2.1
		$\{10\bar{1}1\}$	0.787	26.5	54.2	0.265	1.9
		$\{11\bar{2}2\}$	0.442	25.9	56.0	0.150	7.9
		(Screw)		(21.4)			

energy, E_c , and the elastic energy stored in its stress field, E_{el} . The elastic energy per unit length of a dislocation in an anisotropic medium is given by

$$E_{\text{el}} = \frac{Kb^2}{4\pi} \log \frac{R}{r_0}, \quad (1)$$

where K is the energy factor, which is a function of elastic constants and the orientation of the dislocation, b is the magnitude of the Burgers vector, R is the radius of the stress field of the dislocation, and r_0 is the core radius. Since the core energy is relatively small and the factor $\log(R/r_0)$ in the elastic energy is not sensitive to elastic anisotropy, the variation of the self-energy comes primarily through the orientation dependence of K . Expressions of K for hexagonal crystals have been given by Teutonico⁽¹⁰⁾⁽¹¹⁾.

The values of the energy factor of an $a+c$ edge dislocation, K_e , on $\{10\bar{1}0\}$, $\{10\bar{1}1\}$, and $\{11\bar{2}2\}$ planes are given in Table 3. Those of a screw dislocation, K_s , are also shown for comparison. As reported by Fisher and Alfred⁽¹²⁾, K_e is lower on $\{11\bar{2}2\}$ than on $\{10\bar{1}1\}$ in Zn and Cd, which is in agreement with the fact that the slip plane

is $\{11\bar{2}2\}$ in these metals. This is also the case for Be, although the differences in K_e among the three orientations are small. In all the other metals, K_e is the lowest on the prismatic plane, on which glide of $a+c$ dislocations is geometrically possible but has never been observed as the slip plane in real metals.

2. Peierls stress

According to the Peierls-Nabarro model of a dislocation core, the stress necessary to move an edge dislocation in an isotropic medium is

$$\tau_p^i = \frac{2\mu}{1-\nu} \exp\left(-\frac{2\pi}{1-\nu} \frac{d}{b}\right), \quad (2)$$

where d is the interplanar spacing of the slip plane^{(13)†}. The corresponding expression for an elastically anisotropic medium is⁽¹⁴⁾⁽¹⁵⁾

$$\tau_p^{\text{an}} = 2K_e \exp\left(-4\pi \frac{\zeta}{b}\right), \quad (3a)$$

$$\zeta = \frac{1}{2} K_e s'_{66} d, \quad (3b)$$

where s'_{66} is the reduced compliance for the plane strain condition relevant to the shear on the slip plane in the direction of the Burgers vector⁽¹⁶⁾, and ζ is a measure of the width of the dislocation core⁽¹⁴⁾. Since Peierls stress is an exponential function of ζ/b , the magnitude of Peierls stress is primarily determined by this parameter. Eshelby⁽¹⁴⁾ suggested that ζ/b would serve as a measure of the ease of glide motion.

The reduced compliance, the ease of glide parameter, and the Peierls stress of $a+c$ edge dislocations on $\{10\bar{1}0\}$, $\{10\bar{1}1\}$, and $\{11\bar{2}2\}$ planes for nine h.c.p. metals are given in Table 3. The values of Peierls stress is plotted against the interplanar spacing for Ti and Zn in Fig. 2. Those with an isotropic approximation, obtained from eq. (2), are plotted together for comparison. In all the metals except Zn and Cd, the Peierls stress is the lowest on the prismatic plane. In the exponent of eq. (3a), the relative variation of the quantity $K_e s'_{66}$ with the orientation is within 30%, whereas the geometrical parameter d/b differs by a factor of 2 between $\{10\bar{1}0\}$ and $\{11\bar{2}2\}$ planes. Thus the Peierls stress is the lowest on the prismatic plane, which has the widest interplanar spacing among the three planes. In Zn and Cd, on the other hand, $K_e s'_{66}$ increases in the order $\{10\bar{1}0\}$, $\{10\bar{1}1\}$, $\{11\bar{2}2\}$; the Peierls stresses on the pyramidal planes are decreased significantly by the elastic anisotropy. However, the plane of the lowest Peierls stress is not the observed slip plane, $\{11\bar{2}2\}$, but $\{10\bar{1}1\}$.

3. Displacement field around a screw dislocation

A screw dislocation in an isotropic elastic medium possesses only the displacement parallel to the dislocation line, which is a linear function of the polar angle. In

† There exist several modifications of the original model, giving different expressions for the Peierls stress (see, e.g. Ref. (23)).

Fig. 2 Calculated Peierls stress of $a+c$ edge dislocations in Ti (a) and Zn (b).

elastically anisotropic media, there exist displacements normal to the dislocation, and the screw displacement versus the polar angle curve bears modulation due to the elastic anisotropy. The modulation occurs in such a way that the screw displacement varies with the polar angle more rapidly at a certain direction corresponding to a plane of high symmetry, which means that the screw displacement is concentrated in that direction. Such a feature can be interpreted as the screw dislocation being extended over the plane. The plane on which a screw dislocation is extended is considered to be favoured as the glide plane of the dislocation. Thus, the preference of the glide plane may be predicted by examining the nonuniform displacement distribution around a screw dislocation.

Determination of the displacement field of a dislocation in an anisotropic medium can be reduced to solving a sextic equation. In hexagonal crystals, the sextic equation can be solved analytically for any dislocation, owing to the symmetry about the c axis⁽¹⁰⁾. Since dislocations in h.c.p. metals have not yet been studied from this viewpoint, it seems pertinent to examine a dislocations first.

(1) a screw dislocation

We define a coordinate system $\{x_i\}$ for an a screw dislocation in which x_1 , x_2 , and x_3 axes are taken parallel

Fig. 3 Coordinate system for an a screw dislocation.

Fig. 4 Displacement profiles around an a screw dislocation for hypothetical cases of $\sqrt{A}=0.5$ and $\sqrt{A}=2$.

to the $[0001]$, $[10\bar{1}0]$, and $[\bar{1}2\bar{1}0]$ directions, respectively, as illustrated in Fig. 3. The dislocation line and the Burgers vector are parallel to the x_3 axis. The displacement field of this dislocation consists only of the screw component; normal components do not exist even in elastically anisotropic crystals because of the high geometrical symmetry. The screw component is given by⁽¹⁰⁾

$$u_3 = \frac{b}{2\pi} \tan^{-1}(\sqrt{A} \tan \phi), \quad (4)$$

where ϕ is the polar angle and $\tan \phi = x_2/x_1$. The profile of the distribution of the screw displacement is therefore determined by the shear anisotropy factor A .

Figure 4 shows illustrious examples of u_3 versus ϕ curves for $\sqrt{A}=0.5$ and $\sqrt{A}=2$. When $A < 1$, the slope of the curve is the largest at $\phi=90^\circ$ and 270° ; the displacement varies most rapidly on crossing the basal plane. Such a profile suggests spreading of the dislocation core over the basal plane. When $A > 1$, the steepest slope

Fig. 5. Coordinate system for an $a+c$ screw dislocation.

appears at $\phi=0^\circ$ and 180° , which correspond to the prismatic plane. Therefore, the basal slip is expected for metals with $A < 1$: Mg, Y, Zr, Zn, and Cd (see Table 2), whereas the slip along the prismatic plane is expected for metals with $A > 1$: Be, Ti, Hf, and Co. These predictions agree with the experimental observations for the five metals, Mg, Zn, Cd, Ti, and Hf, including those possessing considerable shear anisotropy (Cd, Zn, Ti), but not for the other four metals, Be, Y, Zr, and Co. Although the shear anisotropy takes a part in the slip plane preference, stacking fault energies have been shown to be more important⁽⁵⁾. The basal slip of Co must be attributed to the extension of the dislocation over the basal plane due to the low basal stacking fault energy⁽¹⁷⁾.

(2) $a+c$ screw dislocation

Figure 5 shows the coordinate system adopted for this dislocation. The displacement field of a screw dislocation parallel to the x_3 axis is given by

$$u_1 = \frac{b}{2\pi} [\alpha_{13}(\theta_1 + \theta_2) + \beta_{13}\theta_3 + \gamma_{13}v], \quad (5a)$$

$$u_2 = \frac{b}{2\pi} [\alpha_{23} \log r_1 r_2 + \beta_{23} \log r_3 + \gamma_{23}t], \quad (5b)$$

$$u_3 = \frac{b}{2\pi} [\alpha_{33}(\theta_1 + \theta_2) + \beta_{33}\theta_3 + \gamma_{33}v], \quad (5c)$$

where the notations used by Teutonico⁽¹⁰⁾ are followed; α_{ij} , β_{ij} , and γ_{ij} are coefficients dependent on elastic constants and the dislocation line direction, $\theta_1 + \theta_2$, θ_3 , v , and t are functions of the polar angle ϕ . The definitions of these coefficients and functions are given in the original paper of Teutonico. The components u_1 and u_3 are functions of ϕ , whereas u_2 depends explicitly on the distance r

Fig. 6. Displacement field around an $a+c$ screw dislocation in Ti. (a) Normal components, u_1 and u_2 . (b) Modulation in the screw component, $u_3 - u_3^i$.

from the origin as well as on ϕ through the logarithmic terms, as described in Appendix. The logarithmic terms can be further separated into those dependent only of r and only of ϕ . Here we neglect r -dependent terms in u_2 so as to examine the angular dependence of the displacement field. (See Appendix for details.)

The calculated displacement components for Ti and Zn are shown in Figs. 6 and 7, respectively. The normal components, u_1 and u_2 , which represent bending of (1122) and (1100) planes, may have important effects on interactions with other dislocations or with point defects, but will not be discussed here. To emphasize the effect of anisotropy, the screw displacement for an isotropic material, $u_3^i = (b/2\pi)\phi$, has been subtracted from u_3 . The profile of the screw displacement in Ti (Fig. 6(b)) suggests spreading of the dislocation over the prismatic plane, which is not the actual slip plane of $a+c$ dislocations in this metal. For the case of Zn (Fig. 7(b)), the screw displacement spreads over (1122), in agreement with the experimental observation. The maximum amplitude of the modulation, $u_3 - u_3^i$, is $0.005b$ in Ti and is $0.015b$ in Zn.

The shapes of the screw displacement curves of the other metals can be classified into the two types, Ti-like or Zn-like. The spreading occurs along either of the two planes, the horizontal plane, (1100), or the vertical plane, (1122). In no case is found an indication of spreading over (1011). The plane of spreading and the modulation

Fig. 7. Displacement field around an $a+c$ screw dislocation in Zn. (a) Normal components, u_1 and u_2 . (b) Modulation in the screw component, $u_3 - u_3^i$.

amplitude of the nine metals are summarized in Table 4. From the anisotropic modulation of the screw displacements, the favourable glide plane is expected to be $\{11\bar{2}2\}$ in Be, Zn, and Cd (though Be is marginal), and $\{10\bar{1}0\}$ in the others. In particular, the modulation of the screw displacement is significant in Co; spreading of the dislocation over $\{10\bar{1}0\}$ is strongly suggested. However, the slip plane has been reported to be $\{11\bar{2}2\}$.

In the table are listed the shear moduli c_{44} and c_{55} , and their ratio A' . Here the suffixes refer to the coordinate system of Fig. 5; the transformed elastic constants are

denoted by small letters. In contrast to the case of a screw dislocation, it is difficult to see how the modulation occurs directly from the analytic expression for u_3 because of its complicated form. However, by analogy with the case of a dislocation, where the shear anisotropy factor A determines the modulation, the screw displacement of an $a+c$ screw dislocation may be characterized by a pertinent shear anisotropy parameter; in the present case this should be the ratio of the shear moduli in the $[\bar{1}\bar{1}23]$ direction on $(1\bar{1}00)$ and $(11\bar{2}2)$ planes, i.e. c_{44} and c_{55} . As seen from the table, the screw displacement spreads along $(11\bar{2}2)$ in metals in which their ratio, A' is greater than unity, and along $(1\bar{1}00)$ in those in which A' is less than unity. The relation between A' and the modulation amplitude is approximately linear if the amplitude of either of the two groups are taken to be negative. The general trend of the screw displacement can therefore be found from the shear anisotropy relevant to the dislocation.

IV. Discussion

The magnitudes of the theoretical Peierls stress of a perfect edge dislocation are not correlated well with experimental observations even if elastic anisotropy is taken into account. In all of the metals examined except Zn and Cd, the geometrical parameter d/b prevails over elastic anisotropy; the Peierls stress is the lowest on the plane of the widest spacing, $\{10\bar{1}0\}$. Even in Zn and Cd, where the elastic anisotropy makes the glide easier as the plane normal becomes closer to the c axis, the Peierls stress on $\{11\bar{2}2\}$, which is the actual glide plane, is still higher than on the others because of the smaller interplanar spacing.

Both the variation of the self-energy of an edge dislocation with orientation and the modulation of displacements of a screw dislocation stem solely from elastic anisotropy. It is therefore reasonable that the conclusions reached from the two aspects are essentially the same. In Zn and Cd, the predicted glide planes of a dislocations and of $a+c$ dislocations are those observed experimentally. The strong elastic anisotropy of these metals is considered to have an effect, which can be

Table 4 Modulation in the screw component of the displacement field of a and $a+c$ screw dislocations. c_{44} and c_{55} are shear moduli in the $\langle\bar{1}\bar{1}23\rangle$ direction on $\{1\bar{1}00\}$ and $\{11\bar{2}2\}$ planes, respectively.

Metal	a screw dislocation			$a+c$ screw dislocation			
	Plane of spreading	Amplitude / $10^{-3}b$	c_{44} /GPa	c_{55} /GPa	A' ($=c_{44}/c_{55}$)	Plane of spreading	Amplitude / $10^{-3}b$
Be	$\{10\bar{1}0\}$	8.3	153.9	152.3	1.01	$\{11\bar{2}2\}$	0.5
Mg	$\{0002\}$	0.8	16.5	18.9	0.87	$\{10\bar{1}0\}$	5.3
Y	$\{0002\}$	0.8	24.4	27.5	0.89	$\{10\bar{1}0\}$	4.6
Ti	$\{10\bar{1}0\}$	11.1	43.4	50.4	0.86	$\{10\bar{1}0\}$	5.2
Zr	$\{0002\}$	4.1	32.9	42.1	0.78	$\{10\bar{1}0\}$	9.7
Hf	$\{10\bar{1}0\}$	3.1	54.6	60.4	0.90	$\{10\bar{1}0\}$	3.9
Co	$\{10\bar{1}0\}$	2.4	74.0	107.0	0.69	$\{10\bar{1}0\}$	13.6
Zn	$\{0002\}$	19.7	44.4	32.9	1.35	$\{11\bar{2}2\}$	14.9
Cd	$\{0002\}$	24.9	23.8	20.7	1.15	$\{11\bar{2}2\}$	8.8

evaluated by the anisotropy factors A and A' , on the glide behaviour. For the other metals, the agreement between the theory and experiment is rather poor. The predicted glide plane of $a+c$ dislocations is $\{10\bar{1}0\}$ for the six metals in which the actual glide plane is either $\{10\bar{1}1\}$ or $\{11\bar{2}2\}$.

Previous computer simulation studies showed that it was possible for an $a+c$ dislocation to extend over $\{11\bar{2}2\}$ and/or $\{10\bar{1}1\}$ planes⁽¹⁸⁾⁽¹⁹⁾. Although the dissociation was not always definite, the core structures obtained by the simulation were reasonably interpreted in terms of stacking faults on these planes. Spreading of the core over the prismatic plane, on the other hand, seems to be difficult because of the lack of appropriate stacking faults⁽⁴⁾⁽²⁰⁾; $a+c$ slip on the prismatic plane can be ruled out from an atomistic point of view. For the choice of glide planes of $a+c$ dislocations between $\{11\bar{2}2\}$ and $\{10\bar{1}1\}$ planes, relative magnitudes of the stacking fault energies on these planes must be important. If the dislocation is extended over either of the planes by virtue of the presence of a low energy stacking fault, the Peierls stress is significantly lower than that for a perfect dislocation because of an increase of the width of the dislocation core. While the theoretical core width, 2ζ , of a perfect $a+c$ dislocation is about $0.4\text{--}0.6b$ (see Table 3), it was found in the simulation studies that the core region extended to a distance of $2\text{--}3b$ ⁽¹⁸⁾⁽¹⁹⁾⁽²¹⁾. In this respect, reliable estimates of the stacking fault energies are most essential to a better understanding of the slip behaviour.

Finally, we shall examine the effect of normal stresses on the dislocation motion, which arises from elastic anisotropy and can be evaluated in terms of the Peierls stress⁽²²⁾. Deformation experiments with attention to $a+c$ slip or twinning are usually done with a single crystal specimen by tension or compression along the c axis. Under such conditions, stress components other than the glide stress exist if glide occurs along either of the pyramidal planes, and the non-glide stresses also contribute to the glide strain through elastic anisotropy. This effect, the anisotropic coupling effect of non-glide stresses, on the Peierls stress may be estimated by multiplying $K_{\text{e}}s'_{66}$ (for the case of an edge dislocation) in the exponent of the expression for the Peierls stress by $1+\alpha$, where α is a numerical parameter defined as

$$\alpha = \frac{s'_{16} \sigma_{11}}{s'_{66} \sigma_{12}} + \frac{s'_{26} \sigma_{22}}{s'_{66} \sigma_{12}}, \quad (6)$$

where σ_{12} is the glide stress for the edge dislocation and σ_{11} and σ_{22} are non-glide stresses⁽²²⁾. We list some values of α for the glide of $a+c$ edge dislocations on $\{10\bar{1}1\}$ and $\{11\bar{2}2\}$ planes under c axis loading:

	Be	Ti	Zn	Cd
$\{10\bar{1}1\}$	-0.03	<u>-0.06</u>	0.55	0.34
$\{11\bar{2}2\}$	<u>-0.03</u>	-0.06	<u>0.49</u>	<u>0.32</u>

where underlines denote observed slip systems. In Be and Ti, the effect of non-glide stresses on the mobility of dislocations is expected to be small. In contrast, the large

positive values of α for Zn and Cd indicate that the non-glide stresses facilitate significantly the dislocation motion on the pyramidal planes. This effect may be important in actual deformation experiments.

V. Conclusions

The glide planes of $a+c$ dislocations in the h.c.p. metals cannot be explained satisfactorily by anisotropic elasticity theory. While some aspects arising purely from elastic anisotropy, i.e. the orientation-dependent elastic energy of an edge dislocation and the modulation of the displacement of a screw dislocation, are in agreement with the favourable slip planes in the metals which show strong elastic anisotropy (Zn and Cd), the theoretical Peierls stress shows little correlation with the experimental observations. The discrepancy in turn suggests that factors other than those considered in the framework of elasticity theory (crystal symmetry, geometry of the dislocation as well as elastic anisotropy) have strong influence on the dislocation properties; the core structure must be one of such factors. Dissociation of the dislocation at an atomic level, or extension of the core, may be more important than the elastic anisotropy in determining the slip plane and the slip mechanism.

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Appendix

On the r -dependent terms in the displacement component u_2 .

The arguments of the logarithmic terms, $r_1 r_2$ and r_3 , in eq. (5b) are defined as⁽¹⁰⁾

$$r_1^2 r_2^2 = x_1^4 + \delta_2 x_1^2 x_2^2 + \delta_1^2 x_2^4, \quad (\text{A1})$$

$$r_3^2 = x_1^2 + \delta_3^2 x_2^2, \quad (\text{A2})$$

where δ_1 , δ_2 , and δ_3 are coefficients dependent on the elastic constants and the orientation of the dislocation. The logarithmic terms in eq. (5b) can be written as follows by using the two-dimensional polar coordinates (r , ϕ) instead of Cartesian coordinates (x_1 , x_2):

$$\begin{aligned} \log r_1 r_2 &= \frac{1}{2} \log (x_1^4 + \delta_2 x_1^2 x_2^2 + \delta_1^2 x_2^4) \\ &= 2 \log r + \frac{1}{2} \log (\cos^4 \phi + \delta_2 \cos^2 \phi \sin^2 \phi + \delta_1^2 \sin^4 \phi), \end{aligned} \quad (\text{A3})$$

$$\begin{aligned} \log r_3 &= \frac{1}{2} \log (x_1^2 + \delta_3^2 x_2^2) \\ &= \log r + \frac{1}{2} \log (\cos^2 \phi + \delta_3^2 \sin^2 \phi). \end{aligned} \quad (\text{A4})$$

We have dropped the $\log r$ terms in calculating u_2 . The magnitude of u_2 corresponds to the displacement at the unit distance from the dislocation centre.

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