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Anisotropic Effect on Elastic Interaction Between Dislocation and General Grain Boundaries in Some Hexagonal Metals: Be,Y, Zn

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Abstract: In this study, we examine the anisotropic effect on elastic interaction between dislocations and general grain boundaries for hexagonal metals; Be Y and Zn. In the setting of the anisotropic linear elasticity in continuous media the calculations of the elastic interaction energy ΔE have been gotten by Head then to be improved by Barnett and Lothe. The dislocations in elastic interaction with a grain boundary in a bicrystal of an elastically anisotropic material are submitted to an image force Fi = -ΔE/d. The results are represented in isoenergy cards on a stereographic projection. The result showed that the interaction energy is inversely depends to the factor of anisotropy H. The maximal energy of interaction is lower then 14 pJ m^{-1} its always weaker compared to the case of the cubic metals where it is of the order of 100 pJ m^{-1}. The image force can be attractive repulsive or null. The proportion of attracted dislocations depends to the disorientation and the factor of anisotropy H.

Key words: Gains boundaries, dislocation, anisotropic elasticity, elastic interaction, image force, metal

INTRODUCTION

The mechanical properties of the polycrystalline materials are greatly affected by the interaction of lattice dislocations with grain boundaries. The objective of this study is to investigate the anisotropic effect on the elastic interaction between dislocation and grain boundaries. The calculation of elastic interaction energy in the hexagonal metals, Be, Y and Zn, completes previously results gotten by Khalfallah and Priester (1999), Priester (2001) and Moulahem (2002). In a bicrystal of elastically anisotropic material the dislocations in elastic interaction with grain boundaries are submitted to image force due to the disorientation between the two crystals (Stroh, 1958; Head, 1965; Tucker, 1969; Willis, 1970; Barnett and Swanger, 1971, Barnett and Lothe, 1975, 1985; Ting and Barnett, 1993; Wu, 1998, 1999). In the setting of the anisotropic linear elasticity theory in continuous media the calculations of the elastic interaction energy have been gotten by Head then by Barnett and Lothe.

Concepts and calculation of the image force: In a bi-crystal of elastically anisotropic material, the forces result exercising on the matrix dislocation near and parallel to an interface comprehend a supplementary term due to the interface presence and qualified as the image force, Fi = - ΔE/d (Priester and Khalfallah, 1994) where ΔE is the elastic interaction energy and d is the distance between dislocation and grain boundary.

Head theorem: In the setting of the anisotropic linear elasticity the calculation of the energy of elastic interaction has been execute by Head (1953) that takes in account $E^{(1)}$ the energy of the dislocation in crystal (1) and $E^{(2)}$ the energy of his image in crystal (2).

$$\Delta E = E^{(2)} - E^{(1)} \quad (1)$$

The Burgers vector is given by:

$$b_{image}/b = E_{(2)} - E_{(1)}/E_{(2)}+E_{(1)} \quad (2)$$

Barnett and Lothe theorem: The elastic interaction energy ΔE has been given by Barnett and Lothe (1974) considering $E^{(1)}$ the dislocation energy in the infinite crystal (1) and $E^{(1/2)}$ the energy of the same dislocation at the interface, Fig. 1. The calculation of the interaction energy ΔE are performed using the integral formalism (Kirchner and Lothe, 1987; Condat and Kirchner, 1987)

$$\Delta E = [E^{(1)} - E^{(1/2)}] \quad (3)$$

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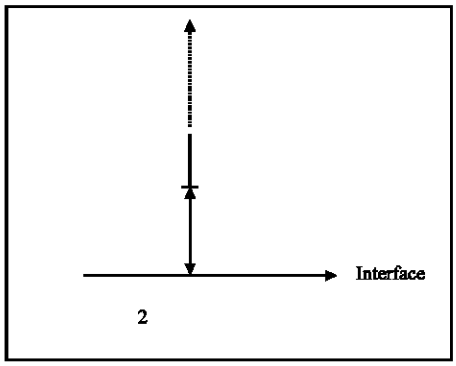

Fig. 1: Geometric configuration used for the calculation of the interaction energy

Table 1: Crystallographic parameters (Å), elastic constants (10^{-11} dyn cm^{-2}), anisotropy factor H (10^{-11} dyn cm^{-2}) and anisotropy ratios Ac and As

Metal	Be	Y	Zn
a	2.29	3.65	2.66
c	3.58	5.12	4.95
c/ a	1.56	1.57	1.86
C_{11}	29.2	7.79	16.4
C_{12}	2.67	2.92	3.64
C_{13}	1.40	2.00	5.30
C_{33}	33.64	7.69	6.35
C_{44}	16.3	2.43	3.88
C_{66}	13.3	2.44	6.38
H	6.07	-0.008	-5
A_c	0.90	1.18	8.00
A_s	1.22	0.99	0.59

Table 2: Burgers vector and line orientations of dislocations

Dislocations	b	t
Screw	a [0001]	[0001]
Edge	a [0001]	<11-20>, <1-100>

The image force depends on several parameters describing the dislocation and grain boundaries configuration: the disorientation of the bicrystal, the line orientation of the dislocation t and the Burgers vector b, the anisotropy of the material characterized by the elastic constants C_{ij}, the factor of anisotropy H, the shear parameter A_s and the compression parameter A_c. The distance d between the dislocation and the grain boundary plane allows to determine the force image intensity. According to these parameters the image force may be attractive repulsive or null.

MATERIALS AND METHODS

Grain boundary configuration: The materials of hexagonal structure are characterized by their crystallographic (a, c, c/a) (Rarey *et al*., 1975) and elastic (C_{ij}, H, A_c, A_s) parameters (Leipfrid and Breuer, 1978), Table 1.

$$H = 2\,C_{44}+C_{12}-C_{11} \quad (4)$$

$$Ac = 2\,C_{44}/C_{11}-C_{12} \quad (5)$$

$$As = C_{11}+C_{12}-2C_{13}/C_{33}-C_{13} \quad (6)$$

The Burgers vector of dislocations is b = a [0001]. The screw dislocation and the edge dislocations are given in Table 2.

The grain boundaries which have been considered are characterized by disorientation axe with simple indices, R = [10-10] and the angle of disorientation varying from 0-180°.

RESULTS AND DISCUSSION

Extremes interaction energies: The Table 3 indicates the values of the extremal interaction energies.

The maximal interaction energy is gotten for the screw dislocations [0001] in the case of Y, however in the case of Be and Zn its gotten for mixed dislocations near of screw ones. The minimal energy interaction in the case of Be is gotten for the edge dislocation.

Disorientations effect: The variation of the maximal and minimal interaction energies according to the disorientation are represented in the Fig. 2 and 3.

The variation of the maximal and minimal interaction energy as function of disorientation is symmetrical to 90° for the three metals considered.

In the case of Zn the maximal interaction energy is always positive. It increases globally with disorientation until 13.5 pJ m^{-1} apart for 90°. The minimal interaction energy is positive for the disorientation varying from 70-120°. The force image is repulsive for all dislocations.

For Yttrium, the interaction energy variation with the disorientation is very weaker. It is always of the order of 1 pJ m^{-1}.

The maximal interaction energy in the case of Be is positive for the disorientations lower then 30°, ΔE = 0.6 pJ m^{-1}. For the disorientation varying from 40-150° the interaction energy is always negative. The image force is attractive for all dislocations.

Anisotropy effect: The variation of the maximal interaction energy as a function of the anisotropy factor is reported in Table 4.

The maximal repulsion is gotten in the case of Zn for which H is negative however, the maximal attraction is gotten in the case of Be for wich H is positive. When H is weak in the case of Y, the interaction is also weak. The interaction energy variation is inversely correlated with the anisotropy factor H.

Table 3: Values of the extremes energy of interaction

Metal	ΔE_{max} (pJ m^{-1})	Dislocations t[uvtw]	Disorientation angle Θ(°)	ΔE_{min} (pJ m^{-1})	Dislocations t [uvtw]	Disorientation angle Θ(°)
Zn	13.5	[-48-41]	80	-3.6	[1-217]	30
Be	0.55	[1-107]	20	-11.05	[1-210]	90
Y	0.95	[0001]	60	-0.75	[-36-32]	60

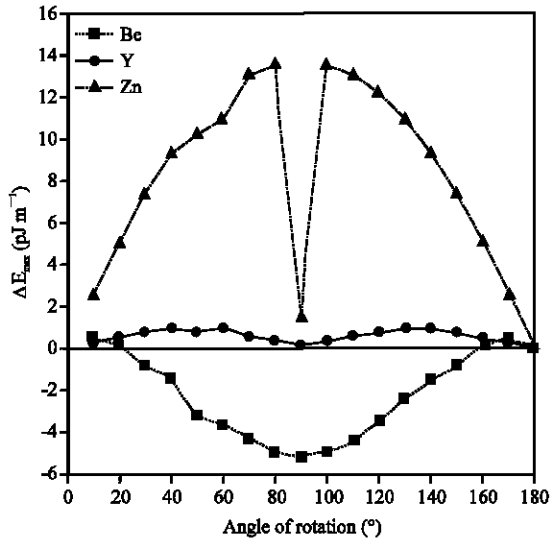

Fig. 2: Maximal energy of interaction

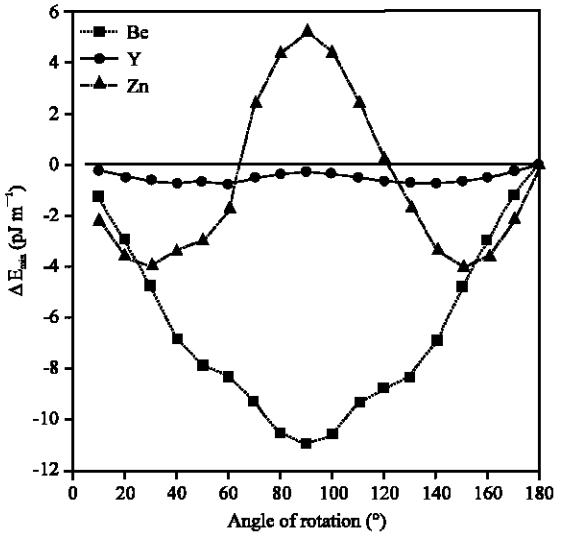

Fig. 3: Minimal energy of interaction

Mobility of dislocations: The movement of the dislocation is controlled by the image force Fi and the Peierls stress τ_p (Hirth and Lothe, 1982) (Table 5).

$$\tau_p = (2\mu b/(1-\nu)) \text{ Sin } 4\pi \alpha \exp(-2\pi w/b) \quad (10)$$

The maximal stress τp is given by:

$$\tau_p = (2\mu b/(1-\nu)) \exp(-2\pi w/b) \quad (11)$$

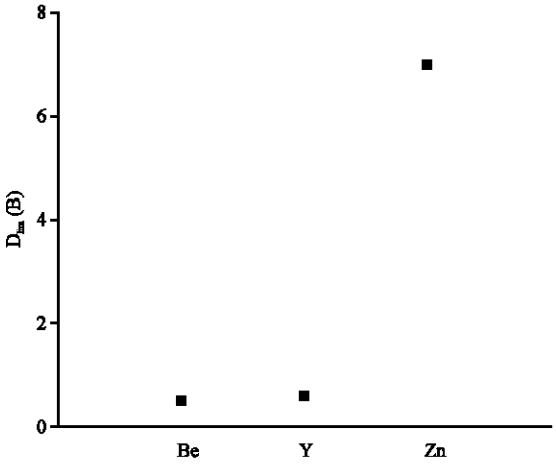

Fig. 4: Distance limit in lengths of burgers vector

Table 4: Anisotropy effect on energy of interaction

Metal	H (10^{-11} dyn cm^{-2})	ΔE (pJ m^{-1})
Be	6.07	-11.05
Y	-0.008	0.95
Zn	-5	13.5

Table 5: The maximal constraint of Peierls

B		[0001]	
Dislocation			
Angle (°)		70	
Metal	Be	Y	Zn
τ_p	15.5	0.85	1.64
μ	14.93	2.54	4.66
λ	1.49	2.42	4.16
ν	0.045	0.24	0.24

The elastic parameters μ and ν of hexagonal metals are gotten by means of Voigt (Saada and Champier, 1967)

$$\mu = 1/30 (7C_{11}-5C_{12}+2C_{33}+12C_{44}-4C_{13}) \quad (12)$$

$$\lambda = 1/15 (C_{11}+C_{33}+5C_{12}+8C_{13}-4C_{44}) \quad (13)$$

$$\nu = \lambda/2(\mu+\lambda) \quad (14)$$

The limit distance D for the setting in movement is the intersection between the curve of the force image and the line of the Peierls stress. This distance is a maximal distance for the mobility of the dislocation Fig. 4.

The limit distance is different from a metal to the other. The limit distance maximal is equal to 7b, it is obtained for Zn (H = -5). The minimal limit distance is equal to 0.5b, it is obtained for Be (H =6.07). The variation

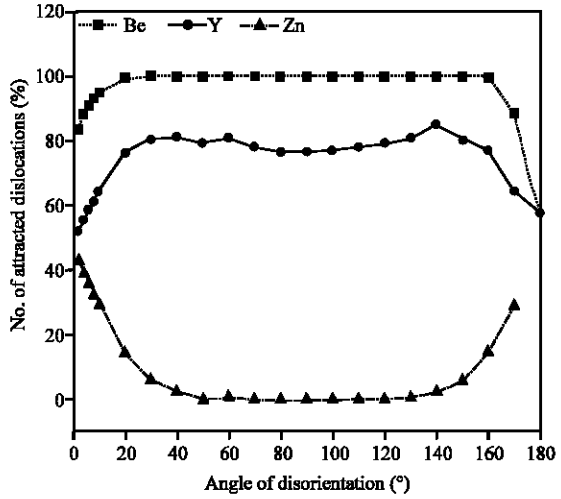

Fig. 5: Numbers of attracted dislocations

of the limit distance from a metal to the other is inversely correlated with the anisotropy factors H of the metals.

Attractive image force: For disorientation lower than 1° the numbers of attracted dislocations is equal to 50% for Zn and Y, in the case of Be it is equal to 80% (Fig. 5).

In the case of Be (H = 6.07) the number of attracted dislocations increases with the disorientation until 100 %. All dislocations are attracted in the interval (30-150°).

In the case of Y (H = -0.008) the number of attracted dislocations increases until 80% for the disorientation superior to 30°.

Conversely in the case of Zn (H = -5) the number of dislocations attracted decrease with disorientation until 0% in the interval (50-130°) all dislocations are repelled.

CONCLUSION

The elastic interaction energy between a dislocation and a grain boundary can be positive negative or null. The intensity of the interaction is the order of the pico joule by meter. It is always very weak compared to the one gotten for the cubic materials that are of the order of 100 pJ m^{-1}. The elastic interaction energy variation versus the disorientation angle is symmetrical in relation to 90°. The maximal repulsion, 13.6 pJ m^{-1}, is gotten for Zn (H = -5), the maximal attraction, -11 pJ m^{-1}, is gotten for Be (H = 6.07). It's inversely correlated with the anisotropy factor H.

The image force can be repulsive, attractive or null. The proportion of dislocations attracted depends on the anisotropy factor H of the metal and the angle of disorientation of the bicrystal.

If H is positive, the number of attracted dislocations increases with disorientation until 100% for the disorientations lower than 170°. It decreases for superior disorientation.

If H is negative, the number of attracted dislocations decreases until 0% for the disorientations lower than 140°. It increases for superior disorientation.

If H is close to zero the number of attracted dislocations is always considerable in the interval of disorientation considered.

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