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DISLOCATIONS MOBILITY UNDER THE IMAGE FORCE EFFECT IN BICRYSTALS OF CFC MATERIALS: CU-X, X = PB, AL, AU, AG AND NI

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Abstract

The image force undergone by a matrix dislocations close and parallel to an interphase boundary is studied in Cu-X bicrystals (with X = Pb, Al, Au, Ag, Ni) for disorientations ranging between 0° and 90°. Dislocations have a Burgers vector = a/2 [110]. The elastic energy of dislocation-boundary interaction is calculated within the framework of anisotropic linear elasticity. The elastic energy is related to the difference of the two metals shear moduli. It is about a few hundred pico Joule per meter. The image force can be repulsive or attractive according to the sign and the intensity of shear moduli difference. The isoenergy maps have various symmetries according to the disorientation.

Keywords: *Interphase Boundary; Dislocation; Elastic Interaction; Image Force; Anisotropic Elasticity; FCC Structure.*

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I. INTRODUCTION

The mechanical properties of materials are determined by the interactions between defects found in the crystal [1-5]. The elastic interactions between a specific defect and a dislocation and between dislocations themselves made it possible to establish the base of the monophased monocrystal behaviour. The interaction between dislocations and grain boundaries enable us to understand the monophased polycrystal properties, whereas the interactions between dislocations and inter-phase boundaries enable us to approach the polyphased alloys properties which are well-known.

In a bicrystal of bimaterials, the result forces exercising on the matrix dislocation near and parallel to an interface comprehend a term due to the interface presence and qualified by "image force ". The image force expression for screw dislocations has been given by Head [6]. A similar expression for an arbitrary Burgers vector in an anisotropic half space has been established by Barnett and Lothe [7]. In mono-phased bicrystals the image force is due to the elastic anisotropy.

It was studied according to the grain boundary disorientation in the iron of CC structure by Khalfallah et al.[8], works was extended to other CC structural materials by Khalfallah et al.[9], Priester et al. [10] was treated the case of CFC structural materials. The case of hexagonal structural materials was approached by Khalfallah et al. [11]. The interactions between matrix dislocations and the grain boundaries are treated by Priester [12]. Koning et al. [13] and Dewald et al. [14 -16] used some simulations for better understanding these interactions. Some cases of interaction between dislocations and interphase boundaries are studied by Jin et al. [17,18] and Liu et al. [19,20].

II. IMAGE FORCE CALCULATION

In the setting of the anisotropic linear elasticity theory in continuous middles and the theorem of Barnet and Loth [7], the image force **F** on a dislocation whose **t** line parallel to an inter-phase boundary is calculate using an integral method [21] :

$$F = \frac{[E^{(1)} - E^{(1/2)}]}{d} = \frac{\Delta E}{d}$$

Where d is the distance between the dislocation and the interface, figure 1, □E is the elastic interaction energy between dislocation and the interface, it is calculated like the difference between $E^{(1)}$, the pre-logarithmic factor of the dislocation elastic energy which is in the infinite crystal (1) and $E^{(1/2)}$, the pre-logarithmic factor of even dislocation located at the interface. For a given Burgers vector **b** and a (**R**, □) disorientation between the twocrystals, the $E^{(1/2)}$ term depends only on the dislocation line orientation

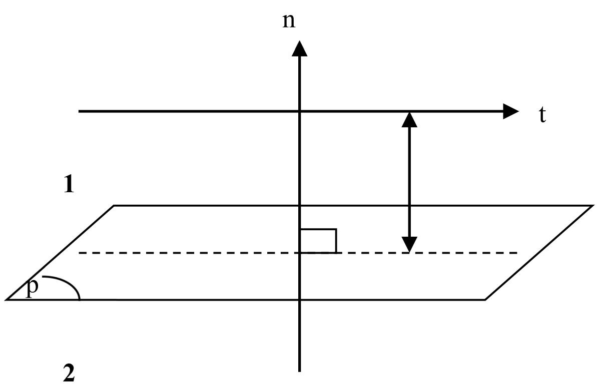


Figure 1: Geometric configuration used for the calculation of the interaction between a dislocation and an interface that is parallel

The image force F, by its sign and its intensity, makes it possible to predict the behaviour of dislocation. It can be attracted or repulsed more or less intensely. If the image force is negative, dislocations are attracted to the interface, if this force is positive, dislocations are repulsed far away from the interface, if it is null dislocations don't undergo any image force.

III. CONFIGURATIONS

Metals

We consider six metals of cubic faces centred structure, Pb, Al, Au, Ag, Cu and Ni. These elements are characterized by their structural parameters **a** [22] and their elastic parameters, table 1 [23]:

Elastic constants C_{11}, C_{12}, C_{44}.

Anisotropic factor $\mathbf{H} = 2C_{44} + C_{12} - C_{11}$.

Shear module $\boldsymbol{\mu} = C_{44} - \frac{1}{5}\,\mathbf{H}$.

Anisotropic ratio $\mathbf{A} = \frac{2C_{44}}{C_{11} - C_{12}}$

Metal	a (A°)	C_{11} (10^{10} Pa)	C_{12} (10^{10} Pa)	C_{44} (10^{10} Pa)	H (10^{10} Pa)	A	μ (10^{10} Pa)
Pb	4.95	4.66	3.92	1.44	2.14	3.90	1.01
Al	4.05	10.82	6.13	2.85	1.01	1.21	2.65
Au	4.08	18.60	15.70	4.20	5.50	2.90	3.10
Ag	4.09	12.40	9.34	4.61	6.16	3.01	3.38
Cu	3.61	16.84	12.14	7.54	10.38	3.21	5.46
Ni	3.52	24.65	14.73	12.47	15.02	2.52	9.47

Table 1: Structural and elastic parameters of studied metals

Bicrystal	Δμ (10^{10} Pa)	ΔE_{max} (pJ/m)	t	θ (°)	ΔE_{min} (pJ/m)	t	θ (°)
Cu-Pb	-4.45	-183	[-221]	90	-397	[-110]	90
Cu-Al	-2.81	-64			-186		
Cu-Au	-2.36	-39	[001]		-172	[010]	
Cu-Ag	-2.08	-37			-175	[-110]	
Cu-Ni	4.01	151			45	[100]	

Table 2: Extreme interaction energies and corresponding lines dislocations.

Dislocations and interphase boundaries

The considered dislocations have <uvw> indices understood between -10 and +10, Burgers vectors are those of the perfect dislocation $\vec{b}$ =a/2[110] and interphase boundaries are characterized by (R□□□) disorientation with R= [110] and □ is included in [0°, 90°] interval, varying by step of 10°. With the various pairs of metals we form Cu-X bicrystals, with X = Pb, Al, Au, Ag and Ni.

IV. RESULTS

The elastic interaction energies are calculated for biphased bicrystals of CFC metals between dislocations and interphase boundaries Cu-X.

Extremes Values

The extremes values of the interaction energies calculated and the corresponding dislocation lines, for the Cu-X studied bicrystals are represented in table 2.

ΔE_{max} : maximum energy (pJ/m),

ΔE_{min} : minimal energy (pJ/m), $\Delta\mu = \mu_2 - \mu_1$ (Pa).

Table 2 shows that the elastic interaction energy, □E, can reach a few hundred pico joule per meter. It varies from -397 to 151 pJ/m.

Extremes energies (maximal or minimal) are obtained for 90° disorientation.

The highest values of the interaction energies, maximal ΔE_{max}, and minimal ΔE_{min}, are obtained for bicrystals having Ni as second crystal and corresponding to the biggest value of Δμ. Whereas The lowest values, are obtained for bicrystals containing Pb as second crystal and corresponding to the weakest value of Δμ.

Shear module effect

In this study we have tow case of bicrystals. Bicrystals with a crystal (1) harder than the crystal (2), □□□<□□ in this case the interaction energies are always negatives for all disorientations. The image forces are always attractive so all dislocations are attracted to the interphase boundary watever the second crystal.

Maximal attraction is obtained for Cu-Pb bicrystal which have the weakest shear moduli difference and minimal attraction is obtained for Cu-Ag which has the greatest shear moduli difference (in this case)

The second case is Cu-Ni bicrystals whith a crystal (2) harder than the crystal (1), □□□□□□ the interaction energies are positive for all disorientations: The image forces are always repulsive and dislocations are repulsed far away from the interface

The interaction energies □E are correlated with □□ in sign and intensity, figure 2.

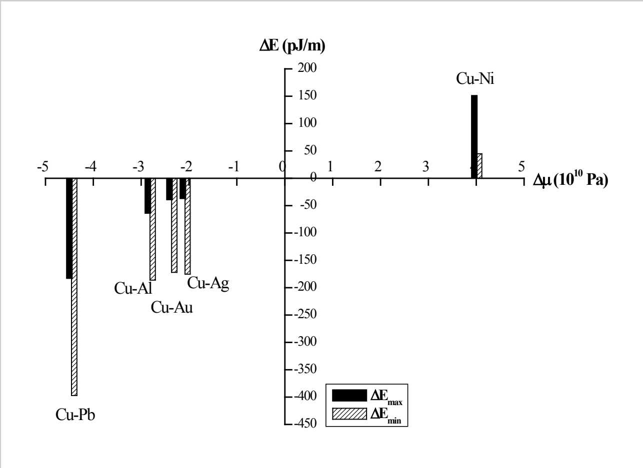


Figure 2: Extreme energy of elastic interaction according to the bicrystals shear moduli difference

Disorientation effect

The interaction energy depends of the disorientation angle. It differently varies with disorientation from one bicrystal to another, figure 3.

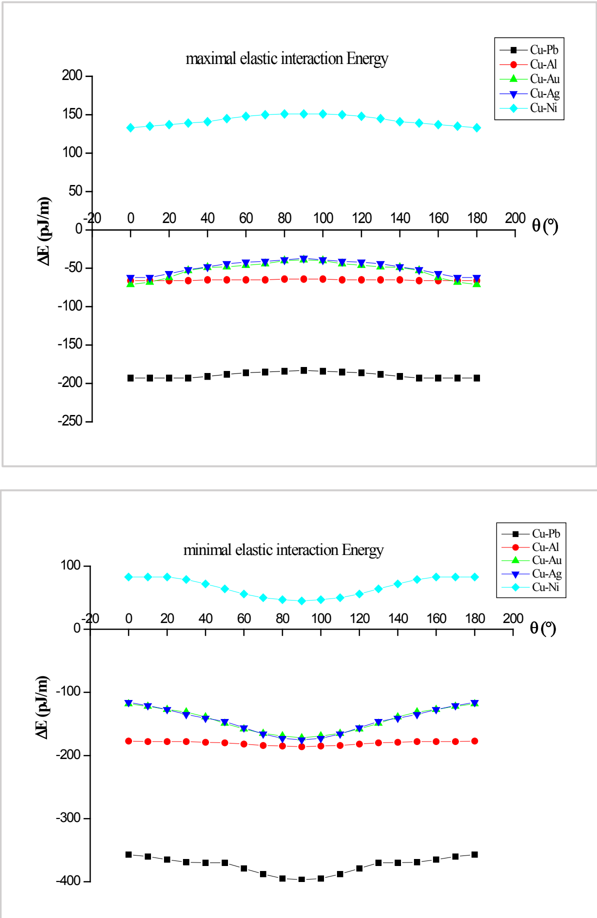


Figure 3: Extreme energies of elastic interaction:

(a) maximal and (b) minimal according to the disorientation angle

When the disorientation increases, the maximal interaction energy increases and the minimal interaction energy decreases for all bicrystals. For each bicrystal, the maximal energies variation is very weak,

few tens of pico joule per meter, from the figure 3 we can say that the energy interval is widened when θ increases. Figure 3 shows also that the variation of interaction energy with θ, present a symmetry at 90°

Crystalline symmetry effect

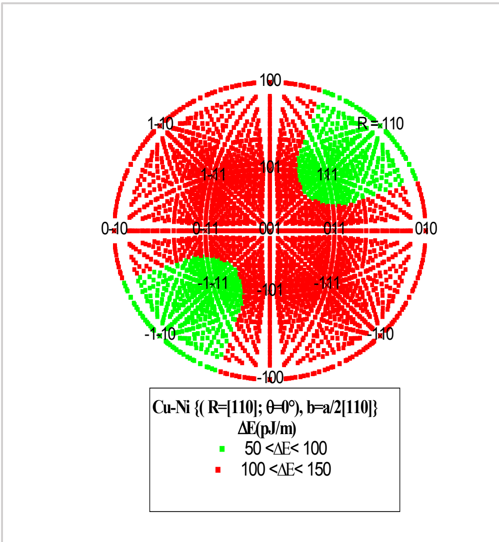
The elastic interaction energies distribution according to the dislocations lines direction is represented in isoenergy maps, figure 4. The maps are stereographic projection of the dislocations directions which are represented by different symbols according to the interaction energies ranges. The lines separating the intervals are the isoenergy lines of the elastic interaction.

For a given grain boundary disorientation (R,□□) and for a given Burgers vector b of the dislocation, the shape of the isoenergy maps and thus general features of the maps are similar for all the CFC materials investigated

The isoenergy maps present a two binary symmetries one compared to the plane trace (110) and the other compared to the plane trace (1-10), which is orthogonal with the precedent one, for the two disorientation □=0° and □=90° Whereas, for disorientations between 10° and 80°, the maps present only one binary symmetry compared to the plane trace (110).

V. CONCLUSION

In biphased bicrystals constituted by cubic faces centred structure metals, Cu-X, the elastic interaction energy between dislocations, Burgers vectors $\vec{b}$ = a/2[110], and the interphase boundaries can reaches a few tens pico joule par meter.



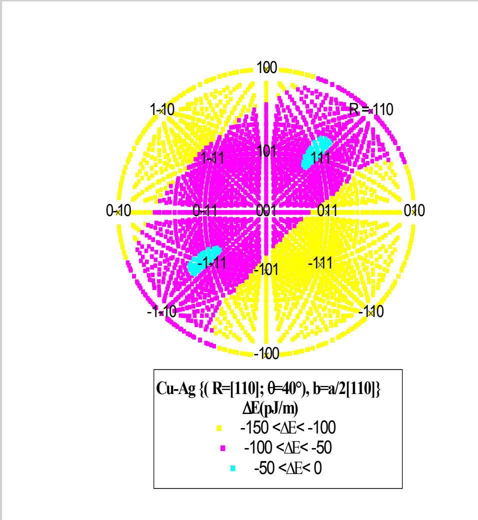


Figure 4: The maps are representative of the observed situations for all bicrystals: two binary symmetries for 0° and 90°.

The elastic interaction energy is related to the shear modules difference of crystals (1) and (2) in sign and in intensity. Two classes of bicrystals according to the Δμ value appear :

- **Δμ>0 :** the elastic interaction energies are positive, the image forces are repulsive some is the bicrystal disorientation, case of Cu-Ni, bicrystal .

- **Δμ<0:** the elastic interaction energies are negative, the image forces are attractive thus the dislocations located in Cu are always repelled far away from the interphase boundary watever the bicrystal disorientation, restful cases of bicrystals.

When the disorientation increases, the maximal interaction energy increases and the minimal interaction energy decreases for all bicrystals. The extreme energies interval widens with the disorientation.

The maximal interaction energy (151pJ/m) is obtained for Cu-Ni bicrystal which presents the greatest difference of shear moduli, for 90° disorientation. The minimal interaction (-397pJ/m) is obtained for Cu-Pb bicrystal which have the weakest shear moduli difference and for the same disorientation.

The dislocations which undergo the strongest attraction are the mixte one [-221]. The edge dislocations [-110] and [001] are attracted with the weakest force.

The dislocations which undergo the strongest repulsion are the edge one [001]. The mixte dislocations [100] are repulsed with the weakest force.

The maximal interaction energy corresponding dislocation, change its character when □ increase.

The isoenergy maps have two binary symmetries one compared to the plane trace (110) and the other compared to the plane trace (1-10) for the two disorientations □□=0° and □□= 90°.

In the range of disorientations (10°- 80°) the maps have only, one binary symmetry compared to the plane trace (110).

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