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Elastic Interaction between Dislocation and Interface in Elastically Anisotropic Ceramic Bimaterials Al_2O_3-AlN: Image Force Effect

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Abstract The Al_2O_3 and AlN materials are often used as electrical insulators (electronic substrates) also the case of pressure sensors where the aluminum nitride (AlN) is selected as the piezoelectric layer and the alumina (Al_2O_3) as a solid substrate insulating. This study aims to investigate the mobility of dislocations near the heterophase interface of bimaterials based alumina (Al_2O_3) under the effect of the image force, without the effect of temperature, deformation and external stress These dislocations having a Burgers vector b = $1/3\,[11\bar{2}0]$, they are located in Al_2O_3. The interface is defined by its plane parallel to the dislocation line and disorientation varies between 0 and 180° around the axis $[10\bar{1}0]$. Usually, the image force calculated in the context of the anisotropic linear elasticity using Barnett and Lothe theory with Stroh formalism, Fi = ΔE / d, where ΔE is the elastic interaction energy. The results show that dislocation motion under the image force effect depends on the elastic and crystallographic properties of the materials constituting the bicrystals and even disorientation of the interface which has an effect on the intensity of the elastic interaction energy. The dislocations are repelled to the interface if the difference in shear modulus between the two materials is positive ($\Delta\mu = \mu_2 - \mu_1 > 0$), they are attracted to the interface in the opposite case ($\Delta\mu = \mu_2 - \mu_1 < 0$).

Keywords Dislocations, Image Force, Peierls Stress, Elastic Anisotropy

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1. Introduction

Ceramic materials have a very important defect, which is their greater or less fragility. However, it is primarily due to structural defects or impurities in the molecular networks and is made more resistant by improving the purity of the base materials and by better controlling the manufacturing processes. In general, mechanical properties are modified by the interactions between the defects in the crystal. The elastic interactions between a specific defect and a dislocation and between dislocations have established the basis of mono-crystalline homophase behavior. The interaction between dislocations and grain boundaries allow us to understand the polycrystalline homophase properties, while the interactions between dislocations and interphase boundaries allow us to approach the properties of multiphase alloys that are well known. Anisotropic elasticity with applications to dislocation theory, the movement of a dislocation requires prior knowledge of the effective force to which it was submitted. A dislocation located proximate of an interface will undergo additional force, called image force.

Image force is due to the discontinuity of the elastic properties in passing of the interface, it is modeled by the stress field of a symmetrical virtual dislocation of the first with respect to the interface. Depending on the direction and intensity of the image force the dislocation is attracted or repelled.

Several factors are related to image force, the boundary plane and disorientation, the dislocations characteristics (direction and Burgers vector), the different shear modulus of the materials constituting the bicrystals; and the distance of dislocation associated to the interphase boundaries.

The expression of image force was established by Barnett and Lothe [1] in the case of an arbitrary Burgers vector in an anisotropic half-space. In the single-phase bicrystals Khalfallah and al. [2-4] was studied image force according to disorientation of the grain boundaries case the CC structural materials and hexagonal structure. Priester and al. [5] have dealt with the case of CFC structural materials and interactions between the matrix dislocations and grain boundaries during plastic deformation [6]. Koning et al. [7] and Dewald et al. [8-10] have used simulations to better understand these interactions.

The image forces is comparable in magnitude with other forces acting on the dislocation and cannot be neglected, this force describes the behavior of the dislocations near an interface and explains observations of ***in situ*** TEM in several studies [11-14].

The objective of our work is the study of the setting in motion of the dislocations, near and parallel to an interphase boundary, under the effect of the image force in ceramic bicrystals Al_2O_3-AlN.

2. Materials and Technical Study

In this study a bicrystal formed by two metal ceramics Al_2O_3 / AlN with same structure and different nature. We chose these type ceramic materials complement the results obtained for the CFC, CC and HC structural metal bicrystals [2-5]. Ceramics offer exceptional properties, although superior to those of plastics or metals, dimensional stability at high temperatures, electrical insulating, dielectric properties and resistance to mechanical wear.

These ceramics having a hexagonal structure and a tensor of the elastic constants are characterized by five independent constants (C_{11}, C_{12}, C_{13}, C_{33}, C_{44}) and $C_{66} = ½ (C_{11}-C_{12})$ [15, 16]. Different sets elastic constants of two ceramic phases Al_2O_3 and AlN have been used for the calculations.

The elastic parameters μ and ν are obtained by the mean of Voigt for the materials of hexagonal structure [17].

$\lambda + 2\mu = 1 / 15\ (8C_{11} + 4C_{13} + 3C_{33} + 8C_{44})$

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

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

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

The elastic interaction between a dislocation and interphase boundaries was performed for the Al_2O_3-AlN. Tables 1 and 2 present their elastic and crystallographic parameters.

Table 1. Elastic parameters of the ceramics studied in 10^{10} Pa [18, 19]

Materials	Al_2O_3	AlN
C11	49.70	39.60
C12	16.30	13.70
C13	11.10	10.80
C33	49.80	37.30
C44	14.70	11.60
C66	16.70	12.95
μ	16.60	12.64
ν	0.229	0.247

Table 2. Structural parameters a and c in [Å], and their ratio c / a [20]

Materials	a	c	c/a
Al_2O_3	4.758	12.991	2.730
AlN	3.112	4.982	1.600

The calculation of elastic interaction energies between dislocation and the interface conducted under of the theory of linear anisotropic elasticity, are based on the theorem of Barnett and Lothe [1] using Stroh formalism [21]

The elastic interaction energies **ΔE** is equal to the difference between, the pre-logarithmic energy factor for a dislocation located in an infinite crystal (Al_2O_3) , $E_{(1)}$, and the pre-logarithmic energy factor , $E_{(1/2)}$, of the same dislocation located at the interface (Al_2O_3/AlN).

$$\Delta E = -\ [E_{(1/2)} - E_{(1)}].$$

The image force is obtained by dividing ΔE by the distance d between the dislocation and the interface. The negative sign of ΔE corresponds to an attraction of the dislocation to the interface and vice versa.

$$F_i = \frac{\Delta E}{d} \tag{1}$$

We are interested in this work to study the mobility of screw and edge dislocations [0001] close to the hetrointerfaceAl_2O_3 / AlN under the effect of the image force (Figure 1). These dislocation having a Burgers vector $b = 1/3\,[11\bar{2}0]$, they are located in Al_2O_3. The interface is defined by its plane parallel to the dislocation line and disorientation varies between 0 and 180° around the axis$[10\bar{1}0]$.

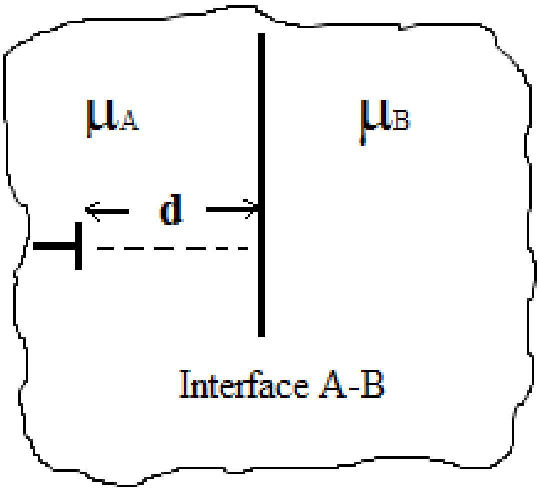


Figure 1. Geometric configuration used for the calculation of the interaction between a dislocation and an interface that is parallel to it. The interface between the anisotropic media (A) and (B) of a bicrystal

3. Results and Discussion

A. Disorientation Effect in elastic Interaction Energies

The variation of interaction elastic energies with disorientation of dislocation shows in Figure 2.

The interaction energies of the screw dislocation increasing with disorientation from 0° to 60° and then they decrease until θ = 90°. In the case of the edge dislocation, the interaction energies decrease with disorientation from 0° to 45° and then it increases to θ = 90°. In both case, their variation is symmetrical to the range [90°, 180°].

The values of the interaction energy depend on the elastic parameters of the two materials constituting the bicrystals.

In terms of intensity, elastic interaction energies depend on the dislocation character. Interaction Energy of the screw dislocation with the interface is still less than that of the edge dislocation with the same interface.

The results show that the values of the elastic interaction energy is always negative, they depend on the difference of shear modulus between the two crystals, which $\Delta\mu < 0$ [22-23], the second crystal is softer than Al_2O_3, the image force is attractive, all dislocations located in Al_2O_3 are attracted to the Al_2O_3 / AlN interface.

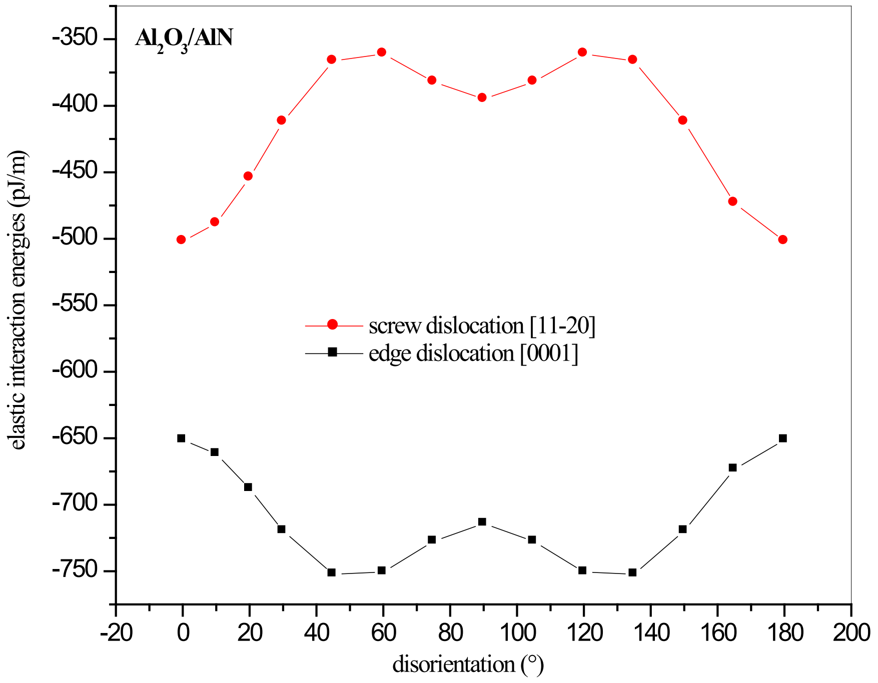
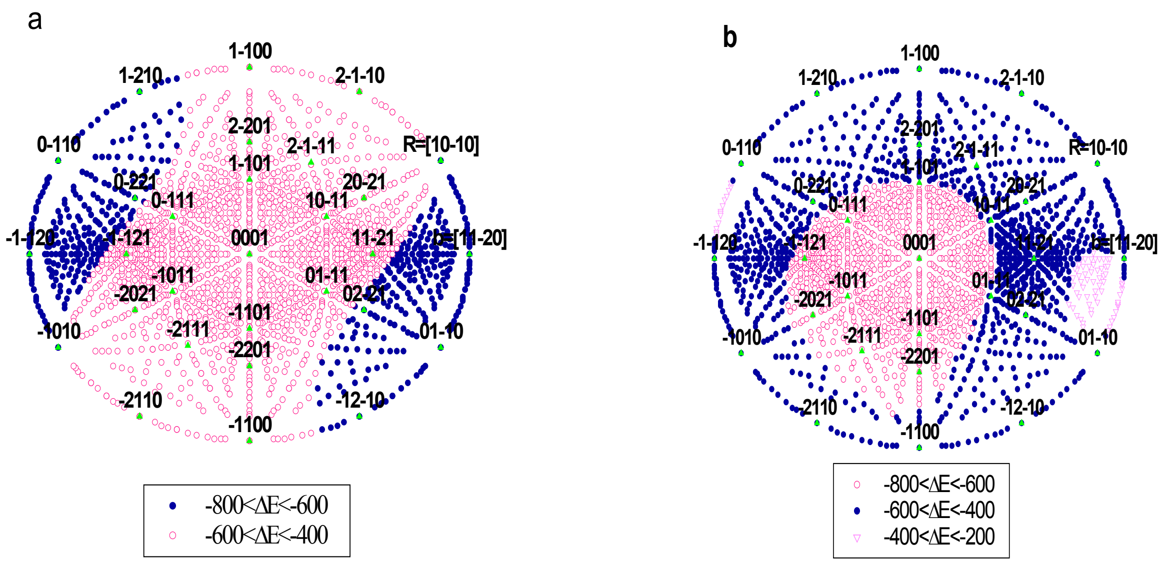
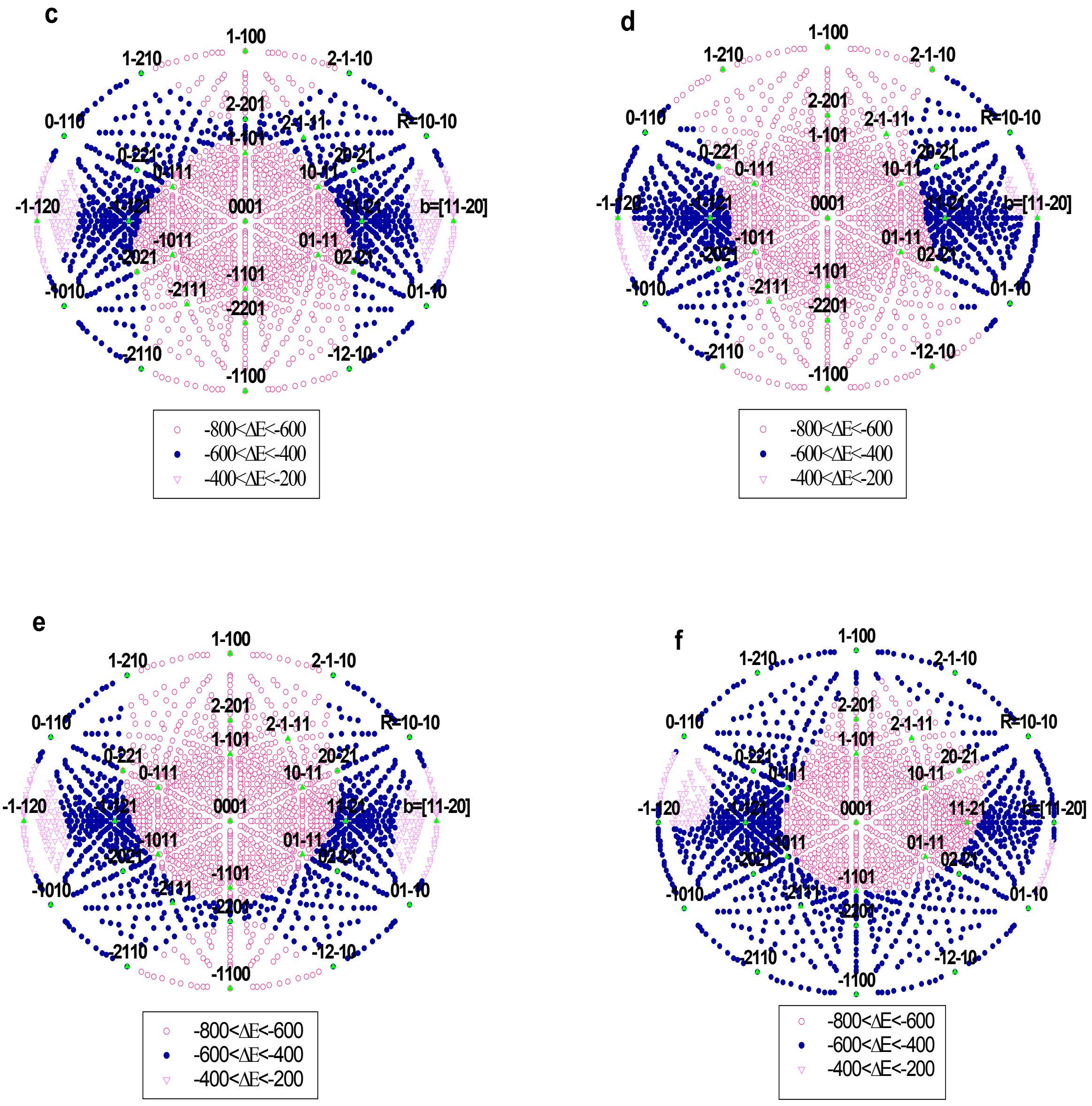


Figure 2. Elastic interaction energy as a function of disorientation for screw [11-20] and the edge [0001] dislocations in the bicrystal Al_2O_3- AlN

B. Isoenergy Cards: Figure 3





Disorientation: a) 0°, b) 30°, c) 60°, d) 90°, e) 120° and f) 150°.

Figure 3. The isoenergy cards for a bicrystals Al_2O_3-AlN

The isoenergy cards represent the elastic interaction energy in the orientation of dislocations, for data configurations:

- Disorientation θ of bicrystals around an axis **R** = $[10\bar{1}0]$
- Burgers vector dislocations b // $[11\bar{2}0]$
- Projections of dislocation lines are of the same color for each interval of the elastic interaction energies.

On the Figures 3:

For the bicrystal Al_2O_3-AlN having a difference shear modulus ($\Delta\mu$ = -39.6 GPa) present high energy intervals, negative and are not symmetrical.

The sets of directions of dislocations belonging to the same interval ΔE are not comparable in terms of disorientation of a bicrystal.

In terms of elastic interaction energy intensity:

- At 0°, the maximum interaction energies are obtained for the dislocations near the edge dislocation [0001] in the center of the map. The minimum interaction energies are obtained around the screw and mixed dislocations.
- Depending on the disorientation (30°, 60°, 90°, 120° and 150°), it appears energy interval [-400 - -200] pJ / m, and the maximum interaction energies are for dislocations near the edge dislocation [0001] in the center of the map. The minimum elastic interaction

energies are obtained around the screw and mixed dislocations. the configuration is inverted with respect to the null disorientation

The isoenergy maps where areas with high and low energy and for disorientation 30° and 60° are located symmetrically compared to those at 150° and 120° respectively.

The review of isoenergy cards obtained show that disorientation bicrystal affects the intensity of the interaction.

C. The Mobility of Dislocations under the effect of image force: The effectiveness distance of the image force in Al_2O_3-AlN

The setting in motion is effective if the intensity of the image force exceeds the constraint Peierls. The dislocation is attracted or repelled by the sense of image force. A critical distance dc is defined when the image force is equal to the force of Peierls (friction force) [24]. We consider that this distance is a maximum distance to the mobility of the dislocation.

$$\mathrm{Fi = FPN:} \qquad \frac{|\Delta E|}{d_c}\square\mathrm{PN}\square b \Rightarrow \mathrm{dc} = \frac{|\Delta E|}{\sigma_{\mathrm{PN}}.\mathrm{b}} \qquad (2)$$

$$\sigma_{PN} = \frac{2\pi}{K}\, e^{\left(\frac{-2\pi w}{b}\right)}$$

$$\text{where } K = \frac{1-\nu}{1-(cos^2\rho)}$$

K=1 for screw dislocations (ρ=0°) and K=1-ν for edge dislocations (ρ=90°).

w is the core width of the dislocation: *w*=b/ (1-ν)

Table 3 shows the friction force is obtained for Al_2O_3 and AlN in the case of screw dislocations, and edge.

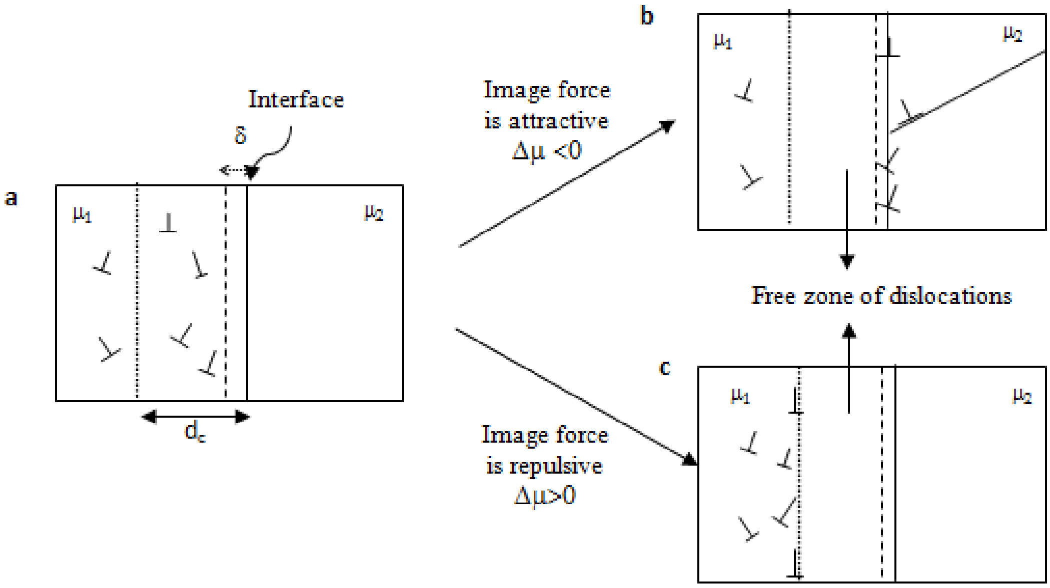
Table 3. Peierls-Nabarro stress $\sigma_{P\text{-}N}$ and network braking force $F_{P\text{-}N}$ in Al_2O_3

Metal	Al_2O_3	AlN
$\sigma_{P\text{-}N}$(Mpa) screw dislocation	96.3	60.3
$F_{P\text{-}N}$ screw10^{-3}(N/m)	45.8	18.7
$\sigma_{P\text{-}N}$(Mpa) edge dislocation	124.0	80.0
$F_{P\text{-}N}$ edge 10^{-3}(N/m)	58.9	24.8

The results show that for a null disorientation around the axis of the interphase boundaries, the effectiveness distance of image force dc for screw and edge dislocations having the same values of dc, it is of the order of 12 nm≈ 23 b. This "long reach" of the image force indicate its effectiveness in nanostructures materials (thin film) in thin layers they are in two layers or multilayer.

Other studies show [25, 26] that this distance (the width of the zone free of dislocations) increases with the absolute value of the difference shear modulus Δμ (Figure 4).

When the image force is attractive, the mobile dislocation reaches the interface; it can integrate the structure of the interface after dissociation or not or else pass through the second crystal if the crystallographic configuration is favorable to sliding in the second crystal.



a) dislocations in interaction with an interface b) image force is attractive and c) image force is repulsive

In the zone of width δ =2b the linear elasticity of the continuous media is not valid.

Figure 4. Creation of a free zone of dislocations with a width dc under the effect of the image force

In this study, based on the Frank and Van der Merwe model [27], where the epitaxy dislocations are located at the interface, we cannot take into account the epitaxial dislocations that exist just to control the difference of two lattice parameters of the two crystals forming the bicrystal, and according to the work J.W .Matthews, in dislocation in solid, [28] and W. Mader [29] The epitaxy dislocations do not possess a long-range stress field. Consequently, they do not induce an interaction force on a matrix dislocation close to an interface.

4. Conclusions

The curves of variation of the elastic interaction energy according to disorientation and the isoenergy cards, present as disorientation of the interface in the bicrystals plays an important role on the intensity of the elastic interaction energy between a dislocation and the interface. The isoenergy cards show that the maximum interaction energies are obtained for the dislocations near the edge dislocation [0001] in the center of the map and the lowest interaction energy is obtained around the screw and mixed dislocations.

All the dislocations located in the area of the image force efficiencies are repelled or attracted to the interface it depends on the difference of shear modulus between the two materials. In the case of Al_2O_3-AlN bicrystal with negative $\Delta\mu$, all the dislocations located in Al_2O_3 at the distance d inferior to dc are attracted to the interface. Under the effect of the image force there appears a free zone of dislocations whose width Equal to 12 nm in Al_2O_3, for the screw and the edge dislocations in interaction with Al_2O_3/AlN interface, it remains to confirm this distance with the aid of electron microscopy at high resolution.

Finally emphasize that the interaction between matrix dislocation and interface for bicrystals of hexagonal structure of materials depends not only crystallography of bicrystals, disorientation and plane of the interface and the character of dislocation, but also the elastic properties of the constituent phase's bicrystal.

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