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RESEARCH ARTICLE OPEN ACCESS

SIMULATION OF THE ELASTIC FIELD OF AN INTERFACIAL DISLOCATION IN AN ANISOTROPIC MEDIUM: FOURIER SERIES APPROACH

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ABSTRACT

Interfacial dislocation networks, located at the interface between two crystals, significantly influence the mechanical, thermal and electrical behaviors of materials. Despite their importance, these phenomena have received relatively little attention in the scientific literature. This gap can be mainly explained by the difficulty of analyzing these complex systems under realistic experimental conditions, particularly using advanced techniques, which take into account the anisotropy of materials. This study focuses on the simulation of the elastic field (stresses and displacements) of a dislocation located at the interface of two infinite anisotropic media. Based on previous work in anisotropic elasticity, an analytical formulation based on Fourier series was used to numerically solve a system of 12 equations with 12 unknowns. The results obtained show the equistress curves for different crystalline systems (Al/Al, Cu/Cu and Al/Cu) considering both anisotropic and quasi-isotropic cases. The study highlights more pronounced stress dispersion in copper due to its hardness, as well as notable differences between isotropic and anisotropic cases, especially for heterogeneous materials such as Al/Cu. The conclusions highlight the importance of material heterogeneity in stress distribution and the relevance of the results for modeling crystal interfaces. This work offers promising perspectives for the optimization of materials in industrial fields such as aeronautics, electronics and renewable energies. It also provides a robust methodological framework for the study of complex crystalline materials.

I. INTRODUCTION

The fundamental problem of a rectilinear dislocation in an anisotropic medium was solved by [1] and [2]. In [3] was the first to express, within the framework of anisotropic elasticity, the field of displacements of a rectilinear dislocation on a plane joint. Subsequently, [4] correct certain typographical errors in formula (27) of [3] and verify the validity of their expressions by simulating the contrast of such a dislocation.

To solve the problem of a rectilinear dislocation at the interface of two anisotropic media of different nature, [5], and starting from an analysis different from that of [3], manage to obtain an equivalent analytical expression to that of [4].

According to [6] used static Field Dislocation Mechanics theory to obtain clear closed-form solutions for the misorientation and network stress fields in the broad framework of heterogeneous anisotropic elasticity.

For a nanometric three-layer material, in [7] assessed the effects of elastic fields at the crystalline interface level when bidirectional networks of unidirectional dislocations were present.

In [8] used a numerical method similar to that of Wagoner to calculate the equilibrium positions and stress fields of dislocation stacks in an anisotropic heterogeneous medium.

Under uniaxial pressure [9] investigated the stress condition at a grain boundary perpendicular to a maximum incompatibility stress in an infinitely stretched elastic bicrystal.

The purpose of this article is to simulate the elastic field (stress and displacement) in the scenario of anisotropic elasticity for a dislocation situated at the interface of two infinite media, in accordance with the previously mentioned work. The analytical method used is a Fourier series formulation in which the analytical expressions of its coefficients have been determined numerically with a precision that has been verified against the convergence of the series.

For this, a program has been created that allows a system of 12 equations with 12 unknowns to be numerically inverted. The equistress curves ± 0.30 GPa and ± 0.15 GPa for the infinite *Al/Al* and *Cu/Cu* single crystals as well as for the infinite *Al/Cu* bicrystal in the anisotropic and quasi-isotropic cases are presented. These systems are representative of materials of interest in various industrial and technological contexts, where interfaces play a determining role in material performance.

Ultimately, this study makes a significant contribution to the modeling of the elastic properties of crystalline interfaces, taking into account the anisotropy of materials. It also opens the way to further investigations on the role of interfacial dislocations in other crystallographic configurations and under various experimental conditions.

II. PROBLEM STATEMENT

Figure 1 illustrates the geometric configuration of a dislocation positioned within the interface plane between two infinite media, denoted as (+) and (-). The dislocation, characterized as a corner dislocation, has a Burgers vector b = (1/2) <110> in aluminum (Al). For visualization purposes, the representation is confined to a finite thickness h. The dislocation core is located at x_1 = -2h/3. These two media are distinct in nature and exhibit elastic anisotropy.

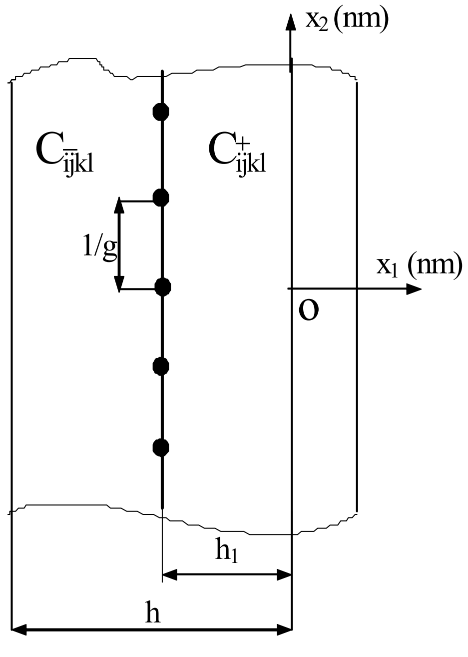

Figure 1: Infinite medium +/-, with an interface unidirectional network of dislocations, the two media's elastic constants are C^{+}_{ijkl} and C^{-}_{ijkl}.
Source: Authors, (2025).

They are distinguished by the period $\Lambda = 1/g$ and the constants C^{+}_{ijkl} and C^{-}_{ijkl}, respectively

III. THE DISPLACEMENT AND STRESS FIELD'S GENERAL FORM

III.1 DISPLACEMENT FIELD

The deformation can be developed in Fourier series at any point in the two media outside of the discontinuity zones, since it is considered to be periodic along the Ox_2 axis [10]:

$$\varepsilon_{ij}(x_1,x_2)=\sum_G \varepsilon_{ij}^{(G)}(x_1).\exp\left(\frac{2.i.\pi.n}{\Lambda}.x_2\right) \quad (1)$$

The integration of (1) gives the displacement field:

$$u_k=u_k^0+v_{k1}^0.x_1+v_{k2}^0.x_2 + \sum_{n\neq 0} u_k^{(n)}(x_1).\exp(2.i\pi.g.n.x_2) \quad k=1,2,3 \quad (2)$$

With $1/g = \Lambda$

Therefore the expression for the displacement field is also written [11]:

$$u_k=\sum_{n\neq 0} u_k^{(n)}(x_1).\exp(2.i\pi.g.n.x_2) \quad k=1,2,3 \quad (3)$$

This field of displacements u_k must satisfy generalized Hooke's law, linking stresses and deformations:

$$\sigma_{ij}=C_{ijkl}.u_{k,l} \quad (4)$$

The state of equilibrium of the stresses in the distortion region is written:

$$\frac{\partial \sigma_{ij}}{\partial x_j}=0 \quad \Rightarrow \quad C_{ijkl}\frac{\partial^2 u_k}{\partial x_j \partial x_l}=0 \quad (5)$$

By replacing (3) in (5), three differential equations that can be expressed as follows are obtained:

$$C_{j1k1}\left(-4\pi^2 g^2 n^2\right)u_k^n+\left(C_{j1k2}+C_{j2k1}\right)(2i\pi ng)u_{k,2}^n + C_{j2k2}u_{k,22}^n=0 \quad (6)$$

This equation's general solution is expressed as follows:

$$u_k^{(n)}(x_1)=\lambda'_{\alpha k}.\exp(2i\pi.g.n.p_\alpha.x_1) \quad (7)$$

Where $\lambda'_{\alpha k}$ and p_α are complex constants that must be found using the three linear equation system that results from substituting (7) in (6):

$$\left[C_{j1k1}+\left(C_{j1k2}+C_{j2k1}\right).p_\alpha+C_{j2k2}.p_\alpha^2\right]\lambda'_{\alpha k}=0 \quad (8)$$

This is written:

$$A_{jk}\lambda'_{\alpha k}=0 \tag{9}$$

Or $A_{jk} = \left[C_{j1k1}+\left(C_{j1k2}+C_{j2k1}\right).p_\alpha + C_{j2k2}.p_\alpha^2\right]$

In the case of a rectilinear dislocation situated within a homogeneous medium exhibiting anisotropic elasticity, the system is analogous to that described by [1]. It admits for each p_α non-trivial solution $\lambda'_{\alpha k}$ if the determinant of A_{jk} is equal to zero:

$$\begin{aligned} det\left(A_{jk}\right) &= \left| C_{j1k1}+\left(C_{j1k2}+C_{j2k1}\right)p_\alpha + C_{j2k2}p_\alpha^2 \right| \\ det\left(A_{jk}\right) &= 0 \end{aligned} \tag{10}$$

We thus obtain a sixth degree equation in p_α (α=1,....,6) In order to facilitate problem solving and improve numerical efficiency, the displacement field's final expression can be expressed as follows: ($u_k^0 = 0$):

$$\begin{aligned} u_k = &\sum_{n\succ 0}\left(\frac{1}{\pi.n}\right)\sum_{\alpha=1}^{3}[\{\cos[n.\omega(x_2+r_\alpha.x_1)] \\ &\times \mathrm{Re}[(-i.X_\alpha^{(n)}.l_{ak}).\exp(-n.\omega.s_\alpha.x_1) \\ &+(-i.Y_\alpha^{(n)}.\bar{\lambda}_{\alpha k}).\exp(n.\omega.s_a.x_1)]\} \\ &+\{\sin[n.\omega(x_2+r_\alpha.x_1)]\times \mathrm{Re}[(X_\alpha^{(n)}.\lambda_{\alpha k}).\exp(-n.\omega.s_\alpha.x_1) \\ &+(Y_\alpha^{(n)}.\bar{\lambda}_{\alpha k}).\exp(n.\omega.s_\alpha.x_1)]\} \\ &(k=1,2,3) \end{aligned} \tag{11}$$

With $\omega = 2.\pi.g$

III.2 STRESS FIELD

By replacing (11) in Hooke's law, we can obtain the expression for the stress field.

$$\begin{aligned} \sigma_{ij} = 2.g &\sum_{n\succ 0}\sum_{\alpha=1}^{3}[\{\cos[n.\omega\ (x_2+r_\alpha x_1)] \\ &\times \mathrm{Re}[X_\alpha^{(n)}.L_{\alpha ij}.\exp(-n.\omega.s_\alpha.x_1) \\ &+Y_\alpha^{(n)}.\bar{L}_{\alpha ij}.\exp(n.\omega.s_\alpha.x_1)\}+\{\sin[n.\omega(x_2+r_\alpha x_1)] \\ &\times \mathrm{Re}[i.X_\alpha^{(n)}.L_{\alpha ij}.\exp(-n.\omega.s_\alpha.x_1)+i.Y_\alpha^{(n)}.\bar{L}_{\alpha ij}.\exp(n.\omega.s_\alpha.x_1)\} \end{aligned} \tag{12}$$

With $L_{\alpha kl}=\lambda_{\alpha j}\left[C_{klj1}+p_\alpha C_{klj2}\right]$

i, j=1,2,3 , l=1,2

The complex constants X_α, Y_α (α = 1, 3) depend on the boundary conditions.

IV. BOUNDARY CONDITIONS OF THE PROBLEM

IV.1 DISPLACEMENT CONDITIONS

It is possible to express the displacement's linearity with respect to the interface using equations (10a, 10c) [11]:

$$\left[u_k^+ - u_k^-\right]_{X_1=-\frac{2}{3}h} = -\frac{b_k}{\pi}\sum_{n=1}^{\infty}(1/n)\sin\left(n\omega x_2\right) \tag{13}$$

Where the upper and bottom crystals are denoted by (+) and (-), respectively.

IV.2 STRESS CONDITIONS

The relationship imposed by the continuity of constraints at the interface is given by:

$$\left[\sigma_{2k}^+\right]_{X_1=-\frac{2}{3}h} = \left[\sigma_{2k}^-\right]_{X_1=-\frac{2}{3}h} \tag{14}$$

At the interface, this condition represents equilibrium.

In the limiting case of two infinite media, the complex constants X_α^-, Y_α^+ (α=1, 3) are chosen to be zero to ensure the convergence of the strain field far from the interface.

The boundary conditions result in the numerical inversion of a system of 12 equations with 12 real unknowns, enabling the calculation of both the stress field and the displacement field within the two crystals.

V. APPLICATION

The equistress curves presented in Figures 2-7 illustrate the evolution of σ_{22} stresses at ±0.15 GPa and ±0.30 GPa around a corner dislocation, for two orientations of the Burgers vector b (b//O$x_1$and b//Ox_2), in *Al/Al*, *Cu/Cu*, and *Al/Cu* crystals. The study considers two scenarios: anisotropic and quasi-isotropic. These curves highlight the stress distribution around the dislocation at the interface of two infinite media. Many studies based on the isotropic elasticity approximation have studied this model, including those of [12],[13]. In each scenario, the core of the dislocation is positioned at x_1=-2h/3.

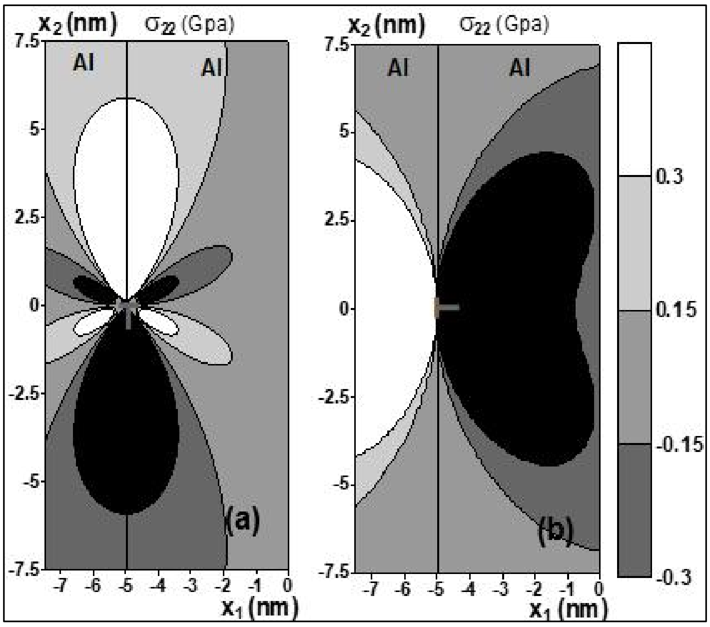

Figure 2: Normal equistresses curves σ_{22} = ± 0.15 GPa and ± 0.3 GPa for a dislocation placed at the interface of an infinite medium *Al/Al* , C_{ij} anisotropics, *(a) b//Ox1* , *(b) b//Ox2.*
Source: Authors, (2025).

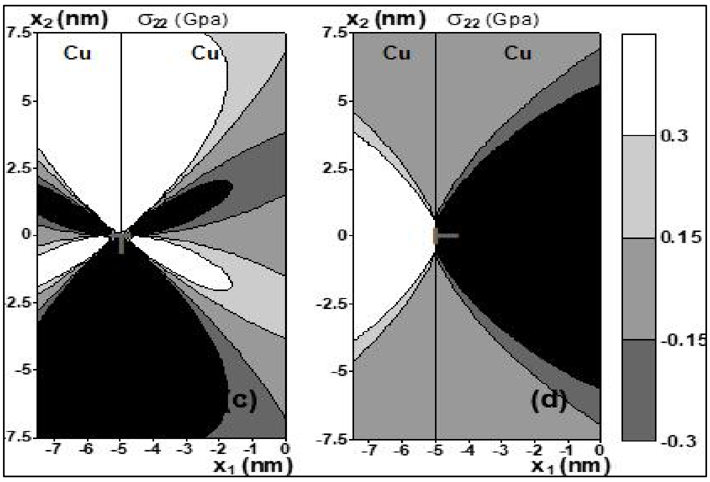

Figure 3: Normal equistresses curves $\sigma_{22} = \pm$ 0.15 GPa and $\pm$ 0.3 GPa for a dislocation placed at the interface of an infinite medium *Cu/Cu* , C_{ij} anisotropics, *(c) b//Ox₁* , *(d) b//Ox₂.*
Source: Authors, (2025).

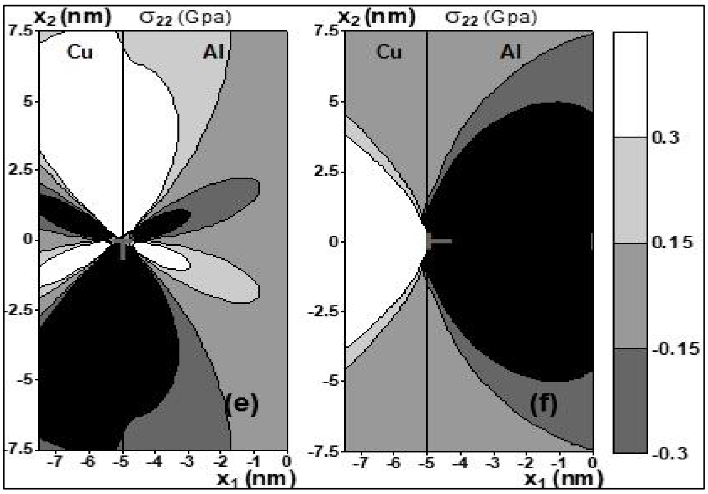

Figure 4: Normal equistresses curves $\sigma_{22} = \pm$ 0.15 GPa and $\pm$ 0.3 GPa for a dislocation placed at the interface of an infinite medium *Al/Cu* , C_{ij} anisotropics, *(e) b//Ox₁* , *(f) b//Ox₂.*
Source: Authors, (2025).

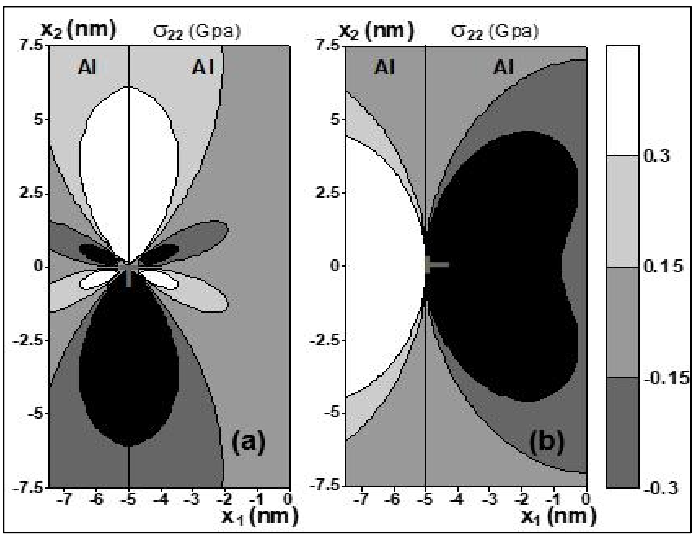

Figure 5: Normal equistresses curves $\sigma_{22} = \pm$ 0.15 GPa and $\pm$ 0.3 GPa for a dislocation placed at the interface of an infinite medium *Al/Al* , C_{ij} quasi-isotropics, *(a) b//Ox₁* , *(b) b//Ox₂.*
Source: Authors, (2025).

Table 1 presents the crystal parameters, elastic moduli, and isotropic and anisotropic elastic constants for Al and Cu utilized in our computations [14]. The values of the constants for aluminum and copper show that these materials differ not only in their isotropic properties (with lower C_{11}, C_{12}, and C_{44} constants for Al) but also in their anisotropic versions, where the constants are adjusted to account for the directionality of the mechanical properties.

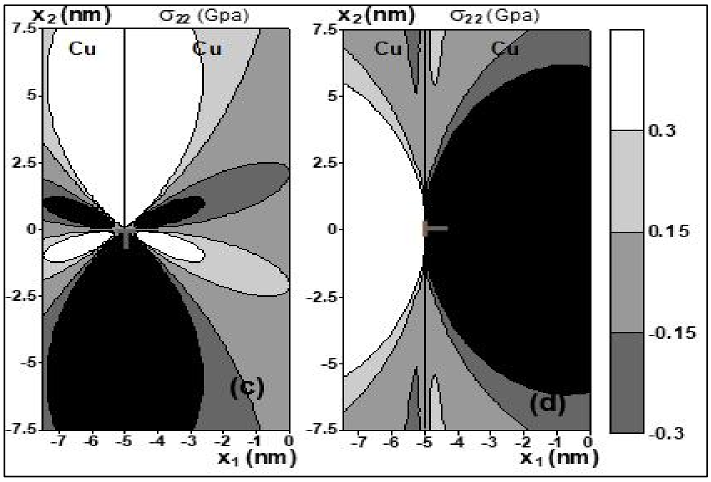

Figure 6: Normal equistresses curves $\sigma_{22} = \pm$ 0.15 GPa and $\pm$ 0.3 GPa for a dislocation placed at the interface of an infinite medium *Cu/Cu* , C_{ij} quasi-isotropics, *(c) b//Ox₁* , *(d) b//Ox₂*
Source: Authors, (2025).

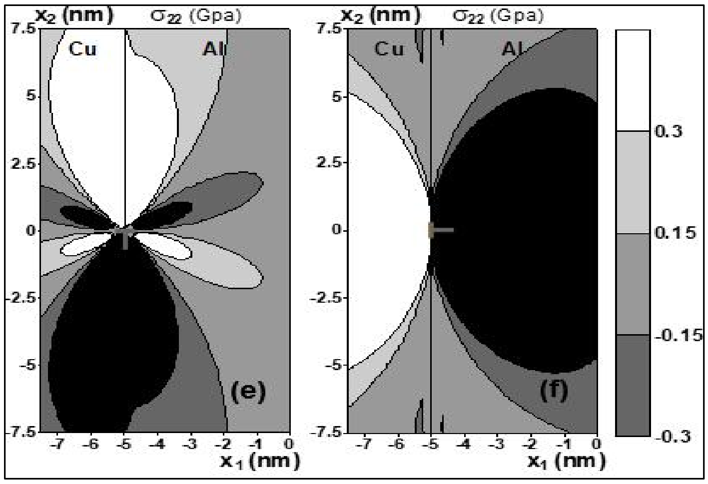

Figure 7: Normal equistresses curves $\sigma_{22} = \pm$ 0.15 GPa and $\pm$ 0.3 GPa for a dislocation placed at the interface of an infinite medium *Al/Cu* , C_{ij} quasi-isotropics, *(e) b//Ox₁* , *(f) b//Ox₂.*
Source: Authors, (2025).

Table 1: Crystal parameters, elastic moduli, elastic constants for *Al* and *Cu.*

	Parameters	***Al***	***Cu***
Isotropic elastic constants	*a* (nm)	0.405	0.405
	μ (GPa)	26.50	46.32
	ν	0.347	0.360
	C_{11} (GPa)	113.1	211.748
	C_{12} (GPa)	60.10	119.1
	C_{44} (GPa)	26.50	46.32
Anisotropic elastic constants	C_{11} (GPa)	108.2	168.4
	C_{12} (GPa)	61.30	121.4
	C_{44} (GPa)	28.50	75.4

Source: [15].

To validate our approach, we conducted convergence tests to ensure the reliability of our program, particularly its ability to function in a quasi-isotropic regime. By replacing the anisotropic elastic constants C_{ij} with their quasi-isotropic counterparts, we obtained results for roots close to the purely imaginary number iG that are consistent with those reported in isotropic elasticity by [12],[13].

The conventional elasticity formulas are used to get the isotropic elastic constants [15].

$$C_{11} = \lambda + 2\mu \; ; \; C_{12} = \lambda \; ; \; C_{44} = \mu \text{ and } \lambda = \frac{2\upsilon\mu}{1-2\upsilon} \quad (15)$$

Where v is Poisson's ratio and λ and μ are the Lamé coefficients.

In the quasi-isotropic case, the constants C_{11} and C_{12} are set to their isotropic counterparts derived from equation (15), while C_{44} is defined as ($\mu - \mu/1000$).

VI. CONCLUSIONS

This work investigates the behavior of a dislocation at the interface of two elastically anisotropic infinite media. It describes the geometric configuration in which a dislocation, with Burgers vector b = 1/2⟨110⟩ in aluminum (*Al*), is positioned at the interface between two media denoted by (+) and (-). The study focuses on the displacement and stress fields associated with this dislocation, which are modulated by the elastic properties of the materials involved.

Key results show how the displacement and stress fields are governed by differential equations derived from generalized Hooke's law and equilibrium conditions. Boundary conditions at the interface, including displacement and stress continuity, are used to solve for the stress and displacement fields in both media. The system of equations is numerically inverted to calculate these fields, leading to a model for stress distribution and deformation near the dislocation.

The stress curves in the anisotropic case (Figures 2-4) show the stress distribution in materials with directional properties, which differs from isotropic materials where the properties are uniform in all directions. Al and Cu materials are characterized by different elastic constants that affect the shape and intensity of the stresses.

The results obtained for the quasi-isotropic case (Figures 5-7) show that the curves are practically superimposable to those from the analytical expression of [15], obtained by [16] in the case of an infinite bicrystal. Moreover, the results obtained in the quasi-isotropic case closely match those of the isotropic examples derived by [17] using the analytical formulations of [18]. This agreement is particularly notable for aluminum, whose characteristics are close to isotropy. This similarity confirms the reliability of our program in anisotropic elasticity. For this same crystal, the differences between the anisotropic and isotropic cases remain negligible.

Regarding the effect of anisotropy, copper exhibits a greater stress dispersion, which can be attributed to its higher hardness compared to aluminum. This characteristic results in steeper stress gradients near the dislocation interface. In contrast, aluminum, being more isotropic, exhibits less complex and more regular stress curves, with limited differences between the anisotropic and isotropic cases.

The study of equistress curves shows the impact of the interface between the materials, in particular for the Al/Cu bicrystal, where the stress lobes are located between those of the two homogeneous crystals (Al/Al and Cu/Cu). The stress transition between the two materials is influenced by the heterogeneity of the materials and the specific anisotropic properties of each phase.

This modeling is useful to understand and predict the behaviors of heterogeneous materials, such as alloys or interfaces in electronic devices, where anisotropic elastic properties play a key role in the mechanical and thermal performance of the materials.

VII. AUTHOR'S CONTRIBUTION

Conceptualization: Allaoua Kherraf, Rachid Benbouta and Mourad Brioua.
Methodology: Rachid Benbouta and Mourad Brioua.
Investigation: Allaoua Kherraf and Mourad Brioua.
Discussion of results: Allaoua Kherraf, Rachid Benbouta and Mourad Brioua.
Writing – Original Draft: Rachid Benbouta.
Writing – Review and Editing: Allaoua Kherraf, Rachid Benbouta and Mourad Brioua.
Resources: Allaoua Kherraf, Rachid Benbouta.
Supervision: Rachid Benbouta.
Approval of the final text: Allaoua Kherraf, Rachid Benbouta and Mourad Brioua.

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