

Article

Three-Dimensional Singular Stress Fields and Interfacial Crack Path Instability in Bicrystalline Superlattices of Orthorhombic/Tetragonal Symmetries

Reaz A. Chaudhuri [†]

Department of Materials Science & Engineering, 122 S. Central Campus Dr. Room 304, University of Utah, Salt Lake City, UT 84112-0560, USA; r.chaudhuri@utah.edu; Tel.: +1-(801)-581-6282

[†] Retired Faculty.

Abstract: First, a recently developed eigenfunction expansion technique, based in part on the separation of the thickness variable and partly utilizing a modified Frobenius-type series expansion technique in conjunction with the Eshelby–Stroh formalism, is employed to derive three-dimensional singular stress fields in the vicinity of the front of an interfacial crack weakening an infinite bicrystalline superlattice plate, made of orthorhombic (cubic, hexagonal, and tetragonal serving as special cases) phases of finite thickness and subjected to the far-field extension/bending, in-plane shear/twisting, and anti-plane shear loadings, distributed through the thickness. Crack-face boundary and interface contact conditions as well as those that are prescribed on the top and bottom surfaces of the bicrystalline superlattice plate are exactly satisfied. It also extends a recently developed concept of the lattice crack deflection (LCD) barrier to a superlattice, christened superlattice crack deflection (SCD) energy barrier for studying interfacial crack path instability, which can explain crack deflection from a difficult interface to an easier neighboring cleavage system. Additionally, the relationships of the nature (easy/easy, easy/difficult, or difficult/difficult) interfacial cleavage systems based on the present solutions with the structural chemistry aspects of the component phases (such as orthorhombic, tetragonal, hexagonal, as well as FCC (face-centered cubic) transition metals and perovskites) of the superlattice are also investigated. Finally, results pertaining to the through-thickness variations in mode I/II/III stress intensity factors and energy release rates for symmetric hyperbolic sine-distributed loads and their skew-symmetric counterparts that also satisfy the boundary conditions on the top and bottom surfaces of the bicrystalline superlattice plate under investigation also form an important part of the present investigation.

Keywords: three-dimensional; crack; stress singularity; bicrystalline superlattice; orthorhombic; cubic; stress intensity factor; energy release rate



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1. Introduction

Leading technological developments during the last decades relate to advanced materials, which are concerned with the deposition of thin films over substrates through the employment of techniques such as epitaxy, chemical vapor deposition (CVD), and physical vapor deposition (PVD) [1]. Bicrystals made of orthorhombic/cubic crystalline phases are common occurrences in many modern advanced technological applications, such as sensors [2], semiconductors [3], superconductivity [4], and so on. For example, gold nanocrystal superlattices can be formed on silicon nitride substrates with long-range ordering over several microns [2]. Pashley et al. [3] have reported the preparation of mono-crystalline films of gold and silver onto molybdenum disulfide inside an electron microscope that permits the direct observation of the mode of growth [1]. Although considered to be non-conventional for microelectronics, grain boundary junction engineering is frequently employed in metal oxide superconductor (MOS) THz frequency applications [4]. Yin et al. [5] employed the magnetron sputtering technique to deposit superconducting

$\text{Yb}_2\text{Cu}_3\text{O}_{7-\delta}$ (Yttrium barium copper oxide, or in short, YBCO) thin films on four polycrystalline metal substrates, with Yttrium-stabilized zirconia (YSZ) and silver serving as buffer layers.

A brief review of the literature reveals the extensive analytical treatment of singular stress fields at the tips of cracks, anticracks (through slit cracks filled with infinitely rigid lamellas), wedges, and junctions weakening/reinforcing homogeneous/biomaterial/trimaterial isotropic as well as anisotropic plates, from a two-dimensional point of view (see Refs. [6–13] and citations therein). In contrast, the mathematical difficulties posed by three-dimensional stress singularity problems have, until recently [14,15], posed an unsurmountable challenge to the researchers in the field. To start with, the governing PDE's are much more complicated, and the exact satisfaction of the boundary and interface conditions is another matter altogether [16]. Earlier attempts to solve the three-dimensional through-crack problem resulted in controversies that lasted for about a quarter century [15,16]. More specifically, two-dimensional anisotropic fracture mechanics literature is more or less entirely based upon the inplane stress functions-based formulation due to Lekhnitskii [6], which is an extension of its isotropic counterpart due to Kolosov and Mushkhelishvili [17]. In contrast, a three-dimensional anisotropic fracture mechanics formulation cannot by definition employ the Lekhnitskii-pioneered inplane stress functions approach, and must be formulated in terms of displacement functions. More importantly, two-dimensional isotropic/anisotropic fracture mechanics studies, e.g., [8–13], are all based on complex variables. Since the three-dimensional space is too small to accommodate the next higher-dimensional analog of complex variables (for which at least a four-dimensional space will be required), these complex variable-based analyses are not by themselves adequate for the analysis of three-dimensional cracked anisotropic solids [18]. In addition, only an analytical solution can detail the structures of singularities related to the sharpness of a crack or anticrack, while the majority of weighted residual-type methods, e.g., the finite elements, finite difference, and boundary element approaches that are often beset by a lack of convergence, and oscillation (in the absence of the knowledge of the order of the stress singularity) resulting in poor accuracy, can hardly be expected to produce the necessary resolution [19,20]. The primary objective of the present investigation is to analytically solve the crack front stress singularity problems of bicrystalline superlattice plates made of orthorhombic, tetragonal, or cubic phases, subjected to mode I/II/III far-field loading, from a three-dimensional perspective.

During the last three decades, three-dimensional crack/anticrack/notch/antinotch/wedge front stress singularity problems have been solved by introducing a novel eigenfunction expansion technique. Various categories of three-dimensional stress singularity problems include: (i) through-thickness crack/anticrack [15,16,21] as well as their biomaterial and trimaterial interface counterparts [14,22,23], (ii) corresponding wedges/notches [24–28], (iii) biomaterial free/fixed straight edge-face [29–31], (iv) tri-material junction [32], (v) interfacial bond line of a tapered jointed plate [33], (vi) circumferential junction corner line of an island/substrate [1], (vii) fiber–matrix interfacial debond [34–36], (viii) fiber breaks and matrix cracking in composites [37], (v) penny-shaped crack/anticrack [38,39] and their biomaterial interface counterparts [40,41], (vi) through/part-through hole/rigid inclusion [42,43] and their biomaterial counterparts [44,45], as well as elastic inclusion [46,47], among others. Only the penny-shaped crack/anticrack [38] (and their biomaterial counterparts [40]), the hole [42], the biomaterial hole [44], and inclusion problems [46] have previously been adequately addressed in the literature. A unified three-dimensional eigenfunction approach has recently been developed by Chaudhuri and co-workers [1,14–16,21–38,41,43,45,47] to address three-dimensional stress singularity problems covering all the aspects mentioned above. These facts not only lend credence to the validity of the afore-mentioned three-dimensional eigenfunction expansion approach, but also reinforce the afore-mentioned conceptual as well as mathematical similarities of and linkages among the afore-cited classes of three-dimensional stress singularity problems.

The separation of the variables approach above has recently been extended to cubic and orthorhombic/orthotropic and monoclinic/anisotropic materials [48–55]. Cracked/anticracked transversely isotropic (smeared-out composite) [48] as well as cubic/orthorhombic/diamond cubic mono-crystalline plates subjected to mode I/II far-field loadings [49–51] and cubic/orthorhombic/monoclinic/diamond cubic mono/tricrystalline plates under mode III loading [49,51–54] have been solved by a novel three-dimensional eigenfunction expansion technique, based in part on the above-mentioned separation of the thickness variable and partly an affine transformation, which is similar (but not identical) in spirit to that due to Eshelby et al. [56] and Stroh [7]. This eigenfunction expansion approach has also recently been employed to obtain three-dimensional asymptotic stress fields in the vicinity of the front of the kinked carbon fiber–matrix junction [18] (see also Chaudhuri et al. [55] for its two-dimensional counterpart with isotropic glass fibers).

In what follows, the afore-mentioned modified eigenfunction expansion technique [18,48–54], based in part on the separation of the thickness variable and partly utilizing a modified Frobenius-type series expansion technique in conjunction with the Eshelby–Stroh formalism, is employed to derive heretofore unavailable three-dimensional singular stress fields in the vicinity of the front of an interfacial crack weakening an infinite bicrystalline superlattice plate, made of orthorhombic (cubic, hexagonal, and tetragonal serving as special cases) phases of finite thickness and subjected to far-field extension/bending, in-plane shear/twisting, and anti-plane shear loadings, distributed through the thickness. Crack-face boundary and interface contact conditions as well as those that are prescribed on the top and bottom surfaces of the bicrystalline superlattice plate are exactly satisfied. This has applications in semiconductors, photovoltaics, superconductors, and fiber-reinforced composites [18], among many others.

The second and more important objective is to extend a recently led concept of a lattice crack deflection (LCD) barrier [49,57] to a superlattice, christened the superlattice crack deflection (SCD) energy barrier, for studying interfacial crack path instability, which can explain crack deflection from a difficult interface to an easier neighboring cleavage system. What follows is an attempt to fill a gap or address an incompleteness regarding the concept of the sufficient condition for fracture in the contexts of three-dimensionality and a bicrystalline superlattice. That idea was previously explored for a cracked mono-crystalline lattice of orthorhombic symmetry only [57]. The second idea is the relationship of superlattice interfacial crack path stability/instability to the elastic parameter, which was not explored earlier. The present study is an attempt to tie up some of those loose and missing strings of ideas, and extend them to a bicrystalline superlattice. In other words, the present study combines two primary novelties: (i) three-dimensionality, and (ii) crack path stability/instability that satisfies the sufficient condition (non-Griffith/Irwin approach).

Third, the hitherto unexplored relationships of the nature (easy/easy, easy/difficult, or difficult/difficult) interfacial cleavage systems based on the present solutions with the structural chemistry aspects of the component phases (such as orthorhombic, tetragonal, hexagonal, as well as FCC (face-centered cubic) transition metals and perovskites) of the superlattice are also investigated. Finally, results pertaining to the through-thickness variations in mode I/II/III stress intensity factors and energy release rates for symmetric hyperbolic sine distributed loads and their skew-symmetric counterparts that also satisfy the boundary conditions on the top and bottom surfaces of the bicrystalline superlattice plate under investigation also form an important part of the present investigation.

2. Statement of the Problem

The Cartesian coordinate system (x, y, z) is convenient to describe the deformation behavior in the vicinity of the front of an interfacial semi-infinite crack weakening an infinite pie-shaped bicrystalline superlattice plate. The thickness of the bicrystalline superlattice plate is $2h$ (Figure 1). The cylindrical polar coordinate system (r, θ, z) is, however, more convenient to describe the boundary and interfacial contact conditions. The x - y plane serves as the interfacial plane. Here, the z -axis ($|z| \leq h$) is placed along the straight crack

front, while the coordinates r , θ , or x , y are used to define the position of a point in the plane of the plate (see Figure 1). The bicrystalline superlattice interface between materials 1 and 2 is located at $\theta = 0$, i.e., it coincides with the positive x -axis, while the crack-side faces are located at $\theta = \pm\pi$ (Figure 1). Components of the displacement vector in the j^{th} crystal ($j = 1, 2$) in x and y directions are denoted by u_j and v_j , while the component in the z -direction is denoted by w_j , $j = 1, 2$. The displacement components in the radial and tangential directions are represented by u_{rj} and $u_{\theta j}$, respectively.

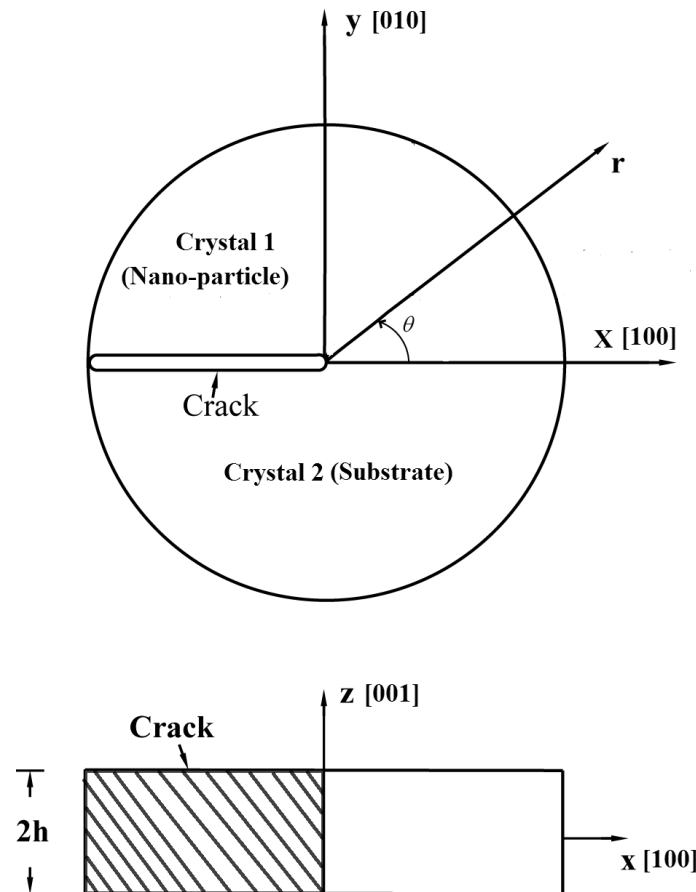


Figure 1. Schematic of a bicrystalline superlattice plate with an interfacial crack.

In what follows, σ_{xj} , σ_{yj} , and σ_{zj} represent the normal stresses, while τ_{yzj} , τ_{xzj} , and τ_{xyj} denote the shear stresses. ε_{xj} , ε_{yj} , and ε_{zj} are the normal strains, while γ_{yzj} , γ_{xzj} , and γ_{xyj} represent shear strains. $c_{il}^{(j)}$, $i, l = 1, \dots, 6$, denotes the elastic stiffness constants of the j^{th} orthorhombic crystal, given in the form:

$$\begin{Bmatrix} \sigma_{xj} \\ \sigma_{yj} \\ \sigma_{zj} \\ \tau_{yzj} \\ \tau_{xzj} \\ \tau_{xyj} \end{Bmatrix} = \begin{bmatrix} c_{11}^{(j)} & c_{12}^{(j)} & c_{13}^{(j)} & 0 & 0 & 0 \\ c_{12}^{(j)} & c_{22}^{(j)} & c_{23}^{(j)} & 0 & 0 & 0 \\ c_{13}^{(j)} & c_{23}^{(j)} & c_{33}^{(j)} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44}^{(j)} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{55}^{(j)} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66}^{(j)} \end{bmatrix} \begin{Bmatrix} \varepsilon_{xj} \\ \varepsilon_{yj} \\ \varepsilon_{zj} \\ \gamma_{yzj} \\ \gamma_{xzj} \\ \gamma_{xyj} \end{Bmatrix} \quad (1)$$

In the absence of body forces, the coupled partial differential equations for a linear elastic crystalline solid in terms of the displacement functions u_j , v_j , and w_j are given as follows:

$$c_{11}^{(j)} \frac{\partial^2 u_j}{\partial x^2} + c_{66}^{(j)} \frac{\partial^2 u_j}{\partial y^2} + c_{55}^{(j)} \frac{\partial^2 u_j}{\partial z^2} + (c_{12}^{(j)} + c_{66}^{(j)}) \frac{\partial^2 v_j}{\partial x \partial y} + (c_{13}^{(j)} + c_{55}^{(j)}) \frac{\partial^2 w_j}{\partial x \partial z} = 0, \quad (2a)$$

$$(c_{12}^{(j)} + c_{66}^{(j)}) \frac{\partial^2 u_j}{\partial x \partial y} + c_{66}^{(j)} \frac{\partial^2 v_j}{\partial x^2} + c_{22}^{(j)} \frac{\partial^2 v_j}{\partial y^2} + c_{44}^{(j)} \frac{\partial^2 v_j}{\partial z^2} + (c_{23}^{(j)} + c_{44}^{(j)}) \frac{\partial^2 w_j}{\partial y \partial z} = 0, \quad (2b)$$

$$(c_{13}^{(j)} + c_{55}^{(j)}) \frac{\partial^2 u_j}{\partial x \partial z} + (c_{23}^{(j)} + c_{44}^{(j)}) \frac{\partial^2 v_j}{\partial y \partial z} + c_{55}^{(j)} \frac{\partial^2 w_j}{\partial x^2} + c_{44}^{(j)} \frac{\partial^2 w_j}{\partial y^2} + c_{33}^{(j)} \frac{\partial^2 w_j}{\partial z^2} = 0, \quad j = 1, 2 \quad (2c)$$

The boundary conditions on the bicrystalline superlattice plate surfaces, $z = \pm h$, are given as follows:

Traction-free (see Section 6 below):

$$\sigma_{zj} = \tau_{xzj} = \tau_{yzj} = 0, \quad j = 1, 2. \quad (3)$$

The interfacial contact conditions as well as boundary conditions at the crack-side surfaces (valid for $r > 0$) are more conveniently expressed in local cylindrical polar coordinates (Figure 1). Assuming that the bicrystalline superlattice interface at $\theta = 0$ is always perfectly bonded, it is easy to establish the continuity conditions of the stresses and displacements along this interface as follows:

$$(i) \theta = 0: u_{\theta 1} = u_{\theta 2}, u_{r1} = u_{r2}, u_{z1} = u_{z2}, \quad (4a)$$

$$\sigma_{\theta 1} = \sigma_{\theta 2}, \tau_{r\theta 1} = \tau_{r\theta 2}, \tau_{\theta z 1} = \tau_{\theta z 2}. \quad (4b)$$

The boundary conditions at the crack-side surfaces, at $\theta = \pm\pi$, are presented below:

$$\sigma_{\theta 1}(\pi) = \tau_{r\theta 1}(\pi) = \tau_{\theta z 1}(\pi) = 0, \quad (5a)$$

$$\sigma_{\theta 2}(-\pi) = \tau_{r\theta 2}(-\pi) = \tau_{\theta z 2}(-\pi) = 0, \quad (5b)$$

where σ_{rj} , $\sigma_{\theta j}$, and σ_{zj} represent the normal stresses, and $\tau_{r\theta j}$, τ_{rzj} , and $\tau_{\theta zj}$ denote the shear stresses in the j^{th} crystal ($j = 1, 2$) in the cylindrical polar coordinate system (r, θ, z) .

3. Singular Stress Fields in the Vicinity of a Crack Front Weakening a Bicrystalline Superlattice with Orthorhombic Phases under General Loading

The assumed displacement functions for the j^{th} crystal ($j = 1, 2$) for the three-dimensional interfacial crack problem under consideration are selected on the basis of the separation of z -variables. These are presented below [18,48–54]:

$$u_j(x, y, z) = e^{i\alpha z} U_j(x, y), \quad (6a)$$

$$v_j(x, y, z) = e^{i\alpha z} V_j(x, y), \quad (6b)$$

$$w_j(x, y, z) = e^{i\alpha z} W_j(x, y), \quad (6c)$$

where α is a constant, called the wave number, required for a Fourier series expansion in the z -direction. It may be noted that, since the separated z -dependent term and its first partial derivative can either be bounded and integrable at most admitting ordinary discontinuities, or the first partial derivative at worst be a square integrable (in the sense of the Lebesgue integration) in its interval, $z \in [-h, h]$, i.e., admitting singularities weaker than a square root (i.e., $z^{(-1/2+\epsilon)}$, $\epsilon > 0$ being a very small number), it can be best represented by the Fourier series [18,48–54]. The latter case is justified by the Parseval theorem [58], and its physical implication is that of satisfying the criterion of finiteness of local strain energy and path independence [59]. The substitution of Equation (6) into Equation (2) yields the following system of coupled partial differential equations (PDEs):

$$c_{11}^{(j)} \frac{\partial^2 U_j}{\partial x_1^2} + c_{66}^{(j)} \frac{\partial^2 U_j}{\partial y_1^2} + c_{55}^{(j)} U_j + (c_{12}^{(j)} + c_{66}^{(j)}) \frac{\partial^2 V_j}{\partial x_1 \partial y_1} + (c_{13}^{(j)} + c_{55}^{(j)}) \frac{\partial W_j}{\partial x_1} = 0, \quad (7a)$$

$$(c_{12}^{(j)} + c_{66}^{(j)}) \frac{\partial^2 U_j}{\partial x_1 \partial y_1} + c_{66}^{(j)} \frac{\partial^2 V_j}{\partial x_1^2} + c_{22}^{(j)} \frac{\partial^2 V_j}{\partial y_1^2} + c_{44}^{(j)} V_j + (c_{23}^{(j)} + c_{44}^{(j)}) \frac{\partial W_j}{\partial y_1} = 0, \quad (7b)$$

$$(c_{13}^{(j)} + c_{55}^{(j)}) \frac{\partial U_j}{\partial x_1} + (c_{23}^{(j)} + c_{44}^{(j)}) \frac{\partial V_j}{\partial y_1} + c_{55}^{(j)} \frac{\partial^2 W_j}{\partial x_1^2} + c_{44}^{(j)} \frac{\partial^2 W_j}{\partial y_1^2} + c_{33}^{(j)} W_j = 0, \quad (7c)$$

where

$$x_1 = i\alpha x, \quad y_1 = i\alpha y. \quad (8a,b)$$

The solution to the system of coupled partial differential Equation (7) subjected to the most general loading can now be sought in the form of the following modified Frobenius-type series in terms of the variable $x_1 + py_1$ as follows:

$$U(x_1, y_1) = \sum_{n=0}^{\infty} a'_{s+n} (x_1 + py_1)^{s+2n+1} + \sum_{n=0}^{\infty} \bar{a}_{s+n} (x_1 + py_1)^{s+2n}, \quad (9a)$$

$$V(x_1, y_1) = \sum_{n=0}^{\infty} b'_{s+n} (x_1 + py_1)^{s+2n+1} + \sum_{n=0}^{\infty} \bar{b}_{s+n} (x_1 + py_1)^{s+2n}, \quad (9b)$$

$$W(x_1, y_1) = \sum_{n=0}^{\infty} c'_{s+n} (x_1 + py_1)^{s+2n} + \sum_{n=0}^{\infty} \bar{c}_{s+n} (x_1 + py_1)^{s+2n+1}. \quad (9c)$$

For an orthorhombic lamina, out of the various combinations presented above, such as $(a'_{sn}, b'_{sn}, c'_{sn})$, $(\bar{a}_{sn}, \bar{b}_{sn}, \bar{c}_{sn})$, $(a'_{sn}, \bar{b}_{sn}, \bar{c}_{sn})$, $(\bar{a}_{sn}, b'_{sn}, \bar{c}_{sn})$, $(\bar{a}_{sn}, \bar{b}_{sn}, c'_{sn})$, $(a'_{sn}, b'_{sn}, \bar{c}_{sn})$, $(a'_{sn}, \bar{b}_{sn}, c'_{sn})$, and $(\bar{a}_{sn}, b'_{sn}, c'_{sn})$, only the first two groupings can produce meaningful solutions for mode III and mode I/II loading cases, respectively. This step permits the separation of mode III from modes I/II for the problem under investigation. The first grouping is described below, while the second one has previously been employed for the anti-plane shear case [49,51–54].

4. Singular Stress Fields in the Vicinity of a (010)[001] Through-Thickness Crack Front Propagating under Mode I (Extension/Bending) and Mode II (Sliding Shear/Twisting) in the [100] Direction

The solution to the system of coupled partial differential Equation (7), subjected to far-field mode I (extension/bending) and mode II (sliding shear/twisting) loading, can now be sought in the form of the following modified Frobenius-type series in terms of the variable $x_1 + py_1$ as follows [48–51], although unlike in the case of isotropic materials [14–16,21–26,29–33], the x_1 and y_1 variables are no longer separable:

$$U_j(x_1, y_1) = \sum_{n=0}^{\infty} \bar{a}_{sj+n} (x_1 + p^{(j)} y_1)^{s+2n}, \quad (10a)$$

$$V_j(x_1, y_1) = \sum_{n=0}^{\infty} \bar{b}_{sj+n} (x_1 + p^{(j)} y_1)^{s+2n}, \quad (10b)$$

$$W_j(x_1, y_1) = \sum_{n=0}^{\infty} \bar{c}_{sj+n} (x_1 + p^{(j)} y_1)^{s+2n+1}. \quad (10c)$$

Here, s represents a fractional exponent, while n denotes an integer in the power series. The combined variable, $x_1 + py_1$, represents an affine transformation in the same spirit as that by Eshelby et al. [56] and Stroh [7], although these latter authors employed completely different techniques. The substitution of Equation (10) into Equation (7) and equating the coefficients of $(x_1 + p^{(j)} y_1)^{s+2n-2}$ yields the following two recurrent relations:

$$\begin{aligned} (s+2n)(s+2n-1)(c_{11}+c_{66}p^{(j)2})\bar{a}_{s+n}+c_{55}\bar{a}_{s+n-1}+ \\ (s+2n)(s+2n-1)(c_{12}+c_{66})p^{(j)}\bar{b}_{s+n}+(s+2n-1)(c_{13}+c_{55})\bar{c}_{s+n-1}=0, \end{aligned} \quad (11a)$$

$$\begin{aligned} (s+2n)(s+2n-1)(c_{12}+c_{66})p^{(j)}\bar{a}_{s+n}+(s+2n)(s+2n-1)(c_{22}+c_{66}p^{(j)2})\bar{b}_{s+n} \\ +c_{44}\bar{b}_{s+n-1}+(s+2n-1)(c_{23}+c_{44})\bar{c}_{s+n-1}=0, \end{aligned} \quad (11b)$$

which, for $n = 0$, reduces to

$$\begin{bmatrix} c_{11}+c_{66}p^{(j)2} & (c_{12}+c_{66})p^{(j)} \\ (c_{12}+c_{66})p^{(j)} & c_{22}p^{(j)2}+c_{66} \end{bmatrix} \begin{Bmatrix} \bar{a}_s \\ \bar{b}_s \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix}, \text{ for } s \neq 0, 1. \quad (12)$$

The characteristic equation for the coupled partial differential Equation (2) or Equation (7) can now be written as follows:

$$p^{(j)4}+2\chi^{(j)}p^{(j)2}+\frac{c_{11}^{(j)}}{c_{22}^{(j)}}=0, j=1,2 \quad (13)$$

where the normalized elastic parameter, $\kappa^{(j)} = 1/\chi^{(j)}$, is given by

$$\kappa^{(j)} = \frac{1}{\chi^{(j)}} = \frac{2c_{22}^{(j)}c_{66}^{(j)}}{(c_{11}^{(j)}c_{22}^{(j)}-c_{12}^{(j)2}-2c_{12}^{(j)}c_{66}^{(j)})}, j=1,2. \quad (14a)$$

It is also sometimes convenient to relate $\kappa = 1/\chi$, as will be seen later, to $A = 1/\lambda$, with A being the planar anisotropic ratio (in the x [100] – y [010] plane), as shown below.

$\kappa^{(j)}, j=1,2$, can also be expressed in terms of the planar anisotropic ratio (in the x - y plane), $A^{(j)}$, as follows:

$$\kappa^{(j)} = \frac{A^{(j)}c_{22}^{(j)}}{\sqrt{c_{11}^{(j)}c_{22}^{(j)}}+c_{12}^{(j)}(1-A^{(j)})}, j=1,2, \quad (14b)$$

where

$$A^{(j)} = \frac{2c_{66}^{(j)}}{\sqrt{c_{11}^{(j)}c_{22}^{(j)}}-c_{12}^{(j)}}, j=1,2, \quad (15)$$

It can easily be seen from Equation (15) that A is higher when the shear stiffness (modulus) and major Poisson's ratio in the x [100], y [010] plane assume larger magnitudes. This simple fact assumes great importance as this investigation aims to solve one Holy Grail issue, in the fracture mechanics of anisotropic media, of coming up with a dimensionless parameter akin to the Reynold's number in fluid flow problems, crossing a critical value that signifies a transition from one regime to another, such as the critical value of the Reynold's number above which the flow is turbulent and below which it is laminar. It is an attendant issue relating to crack deflection in mono-crystalline orthorhombic laminas [57].

Equation (13) has either (a) four complex or (b) four imaginary roots, depending on whether:

$$(a) A^{(j)} > 1 \text{ or equivalently, } |\kappa^{(j)}| > \sqrt{\frac{c_{11}^{(j)}}{c_{22}^{(j)}}}, \quad (16a)$$

$$\text{or (b) } A^{(j)} < 1 \text{ or equivalently, } |\kappa^{(j)}| < \sqrt{\frac{c_{11}^{(j)}}{c_{22}^{(j)}}}, \quad (16b)$$

$A^{(j)} = 1$ or $\kappa^{(j)} = 1$ represents the degenerate isotropic material case, for which the solution is available in Chaudhuri and Xie [15,16].

Case (a): Complex Roots

$$p_{1,2} = \xi^{(j)} \pm i\eta^{(j)}, \quad p_{3,4} = -\xi^{(j)} \pm i\eta^{(j)}, \quad (17a,b)$$

where

$$\xi^{(j)} = \frac{1}{\sqrt{2}} \left[\left(\frac{c_{11}^{(j)}}{c_{22}^{(j)}} \right)^{1/2} - \frac{1}{\kappa^{(j)}} \right]^{1/2}, \quad (18a)$$

$$\eta^{(j)} = \frac{1}{\sqrt{2}} \left[\left(\frac{c_{11}^{(j)}}{c_{22}^{(j)}} \right)^{1/2} + \frac{1}{\kappa^{(j)}} \right]^{1/2}, \quad (18b)$$

$$\text{valid for } |\kappa^{(j)}| > \sqrt{\frac{c_{11}^{(j)}}{c_{22}^{(j)}}}.$$

Case (b): Imaginary Roots

The four imaginary roots of Equation (13) are given by

$$p_{1,2} = \pm i(\xi'^{(j)} + i\eta'^{(j)}), \quad p_{3,4} = \pm i(\xi'^{(j)} - i\eta'^{(j)}), \quad (19a,b)$$

where

$$\xi'^{(j)} = \frac{1}{\sqrt{2}} \left[\left(\frac{c_{11}^{(j)}}{c_{22}^{(j)}} \right)^{1/2} + \frac{1}{\kappa^{(j)}} \right]^{1/2}, \quad (20a)$$

$$\eta'^{(j)} = \frac{1}{\sqrt{2}} \left[-\left(\frac{c_{11}^{(j)}}{c_{22}^{(j)}} \right)^{1/2} + \frac{1}{\kappa^{(j)}} \right]^{1/2}, \quad (20b)$$

$$\text{valid for } |\kappa^{(j)}| < \sqrt{\frac{c_{11}^{(j)}}{c_{22}^{(j)}}}.$$

5. Satisfaction of Crack-Face Boundary and Interfacial Contact Conditions**5.1. Both Crystal Layers with Complex Roots**

For the cases of both crystal layers with complex roots, the substitution of Equations (A2b,c) and (A6a,b) in conjunction with Equation (A7) into the left- and right-hand sides of Equations (4a) and (4b), respectively, would yield four homogeneous equations. In addition, the substitution of Equation (A2b,c), in conjunction with Equation (A7), into the left-hand sides of Equation (5a,b) would yield another set of four homogeneous equations. These can be expressed in the compact form as follows:

$$[\Delta(s)] \{A_{ij}\} = 0. \quad (21a)$$

The existence of a nontrivial solution for A_{ij} requires a vanishing of the coefficient determinant

$$|\Delta(s)| = 0. \quad (21b)$$

$\Delta(s)$ is an 8×8 matrix involving s in a transcendental form. The solution that has physical meaning is given by $0 < \text{Re}(s) < 1$. Here, $s = 0.5 \pm i\varepsilon$, where ε is obtained from the following relationships, obtained by equating the real and imaginary parts:

Real Part:

$$a \cosh^4(\varepsilon\pi) - b \cosh^2(\varepsilon\pi) + c = 0, \quad (22)$$

Equation (22) yields

$$\cosh(\varepsilon\pi) = \left\{ \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \right\}^{1/2}, \quad (23)$$

where

$$a = -(a_1e_1 + b_1f_1)c_2^2d_1f_1, \quad (24a)$$

$$b = c_2f_1\{a_1c_2(a_1c_1 + b_1d_1) - (c_1f_1 - d_1e_1)(b_2(d_1 + d_2) + a_2c_2)\}, \quad (24b)$$

$$c = a_1b_2c_2d_1(c_1f_1 - d_1e_1). \quad (24c)$$

where

$$a_1 = c_{12}^{(1)} + c_{22}^{(1)}(H_{11}\xi^{(1)} - H_{21}\eta^{(1)}), \quad (25a)$$

$$b_1 = c_{22}^{(1)}(H_{11}\xi^{(1)} + H_{21}\eta^{(1)}), \quad (25b)$$

$$c_1 = H_{11} + \xi^{(1)}, \quad (25c)$$

$$d_1 = H_{21} + \eta^{(1)}, \quad (25d)$$

$$a_2 = c_{12}^{(2)} + c_{22}^{(2)}(H_{12}\xi^{(2)} - H_{22}\eta^{(2)}), \quad (26a)$$

$$b_2 = c_{22}^{(2)}(H_{22}\xi^{(2)} + H_{12}\eta^{(2)}), \quad (26b)$$

$$c_2 = H_{12} + \xi^{(2)}, \quad (26c)$$

$$d_2 = H_{22} + \eta^{(2)}, \quad (26d)$$

$$e_1 = \frac{H_{11}(a_2c_2 + b_2d_2) - c_1(H_{12}a_2 - H_{22}b_2)}{H_{22}c_2 + H_{12}d_2}, \quad (27a)$$

$$f_1 = \frac{H_{21}(a_2c_2 + b_2d_2) - d_1(H_{12}a_2 - H_{22}b_2)}{H_{22}c_2 + H_{12}d_2}. \quad (27b)$$

Imaginary Part:

$$a'' \cosh^4(\varepsilon''\pi) + b'' \cosh^2(\varepsilon''\pi) + c'' = 0, \quad (28)$$

where

$$a'' = c + d - e, \quad b'' = e - 2c''. \quad (29)$$

Equation (28) yields

$$\cosh(\delta''\pi) = \left\{ \frac{-(e - 2c'') \pm \sqrt{e^2 - 4dc''}}{2(d - e + c'')} \right\}^{1/2}, \quad (30)$$

where

$$c'' = a_1b_2^2d_1(c_1f_1 - d_1e_1), \quad (31a)$$

$$d = c_2f_1(a_1e_1 + b_1f_1)\{b_2d_2 - c_2(a_1 - a_2)\}, \quad (31b)$$

$$e = a_1b_2c_2d_1(a_1e_1 + b_1f_1) + (c_1f_1 - d_1e_1)(a_2b_2c_2f_1 - b_2^2d_2f_1 - a_1^2b_2c_2). \quad (31c)$$

5.2. Both Crystal Layers with Imaginary Roots

Similarly, for the case of both crystal layers with imaginary roots, the substitution of Equations (A9b,c) and (A12a,b) in conjunction with Equation (A7) into the left- and right-hand sides of Equations (4a) and (4b), respectively, would also yield four homogeneous equations. Additionally, the substitution of Equation (A9b,c), in conjunction with Equation (A7), into the left-hand sides of (5a,b) would yield another set of four homoge-

neous equations. Proceeding in a similar manner, one obtains $s = 0.5 \pm i\varepsilon'\pi$, where ε' is obtained from the relationship:

$$a' \cosh^4(\varepsilon'\pi) + b' \cosh^2(\varepsilon'\pi) + c' = 0. \quad (32)$$

Equation (32) yields

$$\cosh(\varepsilon'\pi) = \left\{ \frac{-b' \pm \sqrt{b'^2 - 4a'c'}}{2a'} \right\}^{1/2}, \quad (33)$$

where

$$a' = f'_1 f'_2 \left(-2a'_1 b'_1 c'_1 d'_1 + a'^2_1 d'^2_1 + e'^2_1 \right) + 2a'^2_1 d'_1 e'_1 e'_2 f'_1 + a'_1 c'_1 e'_2 (a'_2 - b'_2) \left(e'^2_1 + b'^2_1 c'^2_1 + a'^2_1 d'^2_1 \right), \quad (34a)$$

$$b' = f'_1 f'_2 \left(2a'_1 b'_1 c'_1 d'_1 - a'^2_1 d'^2_1 - e'^2_1 \right) + a'_1 e'_1 e'_2 f'_1 (b'_1 c'_1 - 2a'_1 d'_1) + a'_1 c'_1 (a'_1 d'_1 - b'_1 c'_1) (f'_1 g'_2 - f'_2 g'_1) + a'_1 c'_1 (a'_2 - b'_2) \left(c'_1 e'_1 g'_2 - d'_1 e'_1 f'_2 + b'^2_1 c'^2_1 e'_2 - 2e'^2_1 e'_2 - a'^2_1 d'^2_1 e'_2 \right), \quad (34b)$$

$$c' = -a'_1 b'_1 c'_1 d'_1 f'_1 f'_2 + a'_1 c'_1 e'_1 e'_2 (a'_1 g'_1 - b'_1 f'_1) + a'_1 c'_1 (a'_1 d'_1 + b'_1 c'_1) (f'_1 g'_2 + f'_2 g'_1) - a'^2_1 c'^2_1 g'_1 g'_2 + a'_1 c'_1 e'_1 (a'_2 - b'_2) (e'_1 e'_2 - c'_1 g'_2 + d'_1 f'_2), \quad (34c)$$

where

$$a'_1 = c^{(1)}_{12} + c^{(1)}_{22} H'_{11} \left(\xi^{(1)}_1 + \eta^{(1)}_1 \right), \quad (35a)$$

$$b'_1 = c^{(1)}_{12} + c^{(1)}_{22} H'_{21} \left(\xi^{(1)}_1 - \eta^{(1)}_1 \right), \quad (35b)$$

$$c'_1 = H'_{11} - \left(\xi^{(1)}_1 + \eta^{(1)}_1 \right), \quad (35c)$$

$$d'_1 = H'_{21} - \left(\xi^{(1)}_1 - \eta^{(1)}_1 \right), \quad (35d)$$

$$a'_2 = c^{(2)}_{12} + c^{(2)}_{22} H'_{12} \left(\xi^{(2)}_1 + \eta^{(2)}_1 \right), \quad (36a)$$

$$b'_2 = c^{(2)}_{12} + c^{(2)}_{22} H'_{22} \left(\xi^{(2)}_1 - \eta^{(2)}_1 \right), \quad (36b)$$

$$c'_2 = H'_{12} - \left(\xi^{(2)}_1 + \eta^{(2)}_1 \right), \quad (36c)$$

$$d'_2 = H'_{22} - \left(\xi^{(2)}_1 - \eta^{(2)}_1 \right), \quad (36d)$$

$$e'_1 = b'_1 c'_1 - a'_1 d'_1, \quad (37a)$$

$$f'_1 = c'_2 (a'_1 - b'_2) - d'_2 (a'_1 - a'_2), \quad (37b)$$

$$g'_1 = c'_2 (b'_1 - b'_2) - d'_2 (b'_1 - a'_2), \quad (37c)$$

$$e'_2 = H'_{22} c'_2 - H'_{12} d'_2, \quad (38a)$$

$$f'_2 = b'_2 (H'_{12} c'_1 - H'_{11} c'_2) - (H'_{22} a'_1 c'_1 + H'_{11} a'_2 d'_2), \quad (38b)$$

$$g'_2 = H'_{21} (b'_2 c'_2 - a'_2 d'_2) + d'_1 (H'_{22} a'_2 - H'_{12} b'_2). \quad (38c)$$

5.3. Top Crystal (Layer 1) with Complex Roots and Bottom Crystal (Layer 2) with Imaginary Roots

For the case of the top crystal (layer 1) with complex roots and bottom crystal (layer 2) with imaginary roots, the substitutions of Equation (A6a,b) as well as Equation (A2b,c) in conjunction with Equation (A7) into the left-, and those of Equation (A12a,b) as well as Equation (A9b,c) in conjunction with Equation (A7) into the right-hand sides of Equation (4a,b) would yield four homogeneous equations. In addition, the substitution of Equation (A2b,c), in conjunction with Equation (A7), into the left-hand sides of

Equation (5a) would yield another set of two homogeneous equations. Likewise, the substitution of Equation (A9b,c), in conjunction with Equation (A7), into the left-hand sides of (5b) would yield the remaining set of two homogeneous equations. Proceeding in a similar manner as above, one obtains $s = 0.5 \pm i\bar{\varepsilon}\pi$, where $\bar{\varepsilon}$ is obtained from the relationship:

$$\bar{a} \cosh^4(\bar{\varepsilon}\pi) + \bar{b} \cosh^2(\bar{\varepsilon}\pi) + \bar{c} = 0, \quad (39)$$

Equation (39) yields

$$\cosh(\bar{\varepsilon}\pi) = \left\{ \frac{-\bar{b} \pm \sqrt{\bar{b}^2 - 4\bar{a}\bar{c}}}{2\bar{a}} \right\}^{1/2}, \quad (40)$$

where

$$\bar{a} = \bar{d} - \bar{e}\bar{g}, \quad \bar{b} = \bar{d} - \bar{e}\bar{h} - \bar{f}\bar{g}, \quad \bar{c} = -\bar{f}\bar{h}, \quad (41)$$

where

$$\bar{d} = \bar{e}_1^2 (H_{11}\bar{f}_1 + c_1\bar{e}_2 + b_1\bar{f}_2) [a_1(c_2 - d_2) - d_1(a_2 - b_2) - \bar{f}_1], \quad (42a)$$

$$\bar{e} = -\bar{e}_1 (H_{21}\bar{f}_1 + d_1\bar{e}_2 - a_1\bar{f}_2), \quad (42b)$$

$$\bar{f} = -d_1\bar{e}_1 (\bar{f}_1 + \bar{e}_2), \quad (42c)$$

$$\bar{g} = b_1\bar{e}_1 (c_2 - d_2), \quad (42d)$$

$$\bar{h} = b_1 [c_1\bar{f}_1 + \bar{e}_1 (c_2 - d_2)], \quad (42e)$$

where

$$\bar{e}_1 = a_1c_1 + b_1d_1, \quad (43a)$$

$$\bar{f}_1 = b_2c_2 - a_2d_2, \quad (43b)$$

$$\bar{e}_2 = a_2H'_{22} - b_2H'_{12}, \quad (43c)$$

$$\bar{f}_2 = c_2H'_{22} - d_2H'_{12}. \quad (43d)$$

It may be noted that, for a homogeneous solution, such as what is presented above, the seven eigenvector components, $A_{12}(z)$, $A_{21}(z)$, $\dots$, $A_{42}(z)$, cannot be evaluated in absolute terms, but can only be expressed in terms of the eighth component, $A_{11}(z)$, which can be related to the “stress intensity factors”, $K_{Ij}(z)$ and $K_{IIj}(z)$, which can, in turn, be resolved as follows:

$$K_{Ij}(z) = K_{Isj}(z) + K_{Ija}(z) \quad (44a)$$

$$K_{IIj}(z) = K_{IIsj}(z) + K_{IIja}(z) \quad (44b)$$

where $K_{Isj}(z)$ and $K_{IIsj}(z)$, $j = 1, 2$, represent the symmetric (with respect to z) mode I and mode II stress intensity factors, which correspond to in-plane extension and sliding shear, respectively. $K_{Iaj}(z)$ and $K_{IIaj}(z)$, $j = 1, 2$, denote the antisymmetric (with respect to z) mode I and mode II stress intensity factors, which correspond to bending and twisting, respectively.

The stress intensity factors and the energy release rates are found to be as follows:

$$K_{I/IIj}(z) = K_{I/IIj,2D} D_{bj}(z), \quad G_{I/IIj}(z) = G_{I/IIj,2D} [D_{bj}(z)^2], \quad (45a,b)$$

where $K_{I/IIj,2D}$ and $G_{I/IIj,2D}$ are available in the published literature; see e.g., Wu [10] and Wang et al. [12]. In what follows, the primary focus will be on the three-dimensionality and lattice (more specifically super-lattice) aspects of bicrystalline interfacial fracture.

6. Boundary Conditions on the Bicrystalline Superlattice Plate Surfaces and Through-Thickness Distribution of Singular Stress Fields

6.1. General Distributed Far-Field Loading

By using the traction-free boundary conditions at the top and bottom surfaces, $z^* = z/h = \pm 1$, of the plate, given by Equation (3), the general form of $D_{bj}(z)$, defined in Equation (A3), can be obtained. The stress field that satisfies traction-free boundary conditions at $z^* = \pm 1$, in the vicinity of the front of a bicrystalline interface crack under extension/sliding shear, can be recovered if, in Equation (A3):

$$D_{bj}(z) = D_{bsj}(z) = D_{2j} \cos(\alpha z), \quad j = 1, 2 \quad (46)$$

By substituting Equation (A2d) or Equation (A9d) into the boundary condition on the singular stress-free surface of a cracked bicrystalline superlattice plate, given by Equation (3), the general form of $D_{bsj}(z)$ can be obtained as follows:

$$D_{bsj}(z) = \sum_{m=0}^{\pm\infty} D_{1mj} \cos\left(\frac{(2m+1)\pi z^*}{2}\right), \quad j = 1, 2. \quad (47)$$

Hence, $KI = KIs$ and $KII = KIIs$ represent symmetric “stress intensity factors”. If the odd functions are selected from $D_{bj}(z)$ that satisfies traction-free boundary condition at $z^* = \pm 1$, it can yield the out-of-plane bending/twisting case given by

$$D_{bj}(z) = D_{baj}(z) = D_{1j} \sin(\alpha z), \quad j = 1, 2 \quad (48)$$

$D_{baj}(z)$ that satisfies the singular stress-free conditions on the cracked bicrystalline superlattice plate surfaces is given by

$$D_{baj}(z) = \sum_{m=1}^{\pm\infty} D_{2mj} \sin(m\pi z^*), \quad j = 1, 2, \quad (49)$$

Here, $KI = KIa$ and $KII = KIIa$ are anti-symmetric stress intensity factors. Equations (48) and (49) are valid, provided the loading function vanishes at $z^* = 0$, thus eliminating the possibility of discontinuity of the function at $z^* = 0$. In the presence of the discontinuity of the function at $z^* = 0$, $D_{baj}(z)$ can be written as follows:

$$D_{baj}(z) = \left| \sum_{m=0}^{\pm\infty} D_{1mj} \cos\left(\frac{(2m+1)\pi z^*}{2}\right) \right|, \quad j = 1, 2 \quad (50)$$

If the singular stress-free boundary conditions, given by Equation (3), on the cracked bicrystalline superlattice plate surfaces are satisfied, all the displacements also vanish on these surfaces in the vicinity of the front of a bicrystalline interface crack.

6.2. Hyperbolic Sine Distributed Far-Field Loading

Hyperbolic sine distributed far-field loading, which is proportional to $\sinh(z^*)$, $|z^*| < 1$, is applied. The applied antisymmetric loading function and the corresponding stress intensity factors (valid for $|\tilde{z}^*| \leq 1$) are proportional to

$$D_{ba}(z^*) = \sinh(z^*) = \frac{\exp(z^*) - \exp(-z^*)}{2}. \quad (51)$$

The corresponding Fourier series can be derived as follows:

$$D_{ba}(z^*) = \sum_{m=0}^{\infty} \frac{\{e^{-1}(-1)^m - e(-1)^m\}}{\{1 + m^2\pi^2\}} m\pi \sin(m\pi z^*). \quad (52)$$

The applied symmetric loading function (valid for $|z^*| < 1$) and the corresponding stress intensity factors (valid for $|z^*| \leq 1$) are proportional to

$$D_{bs}(z^*) = |\sinh(-z)| = \frac{1}{2} |\exp(z^*) - \exp(-z^*)|. \quad (53)$$

The corresponding Fourier series can be obtained as given below:

$$D_{bs}(z^*) = \left| \sum_{m=0}^{\infty} \frac{\{e^{-1}(-1)^m - e(-1)^m\}}{\{1 + m^2\pi^2\}} m\pi \sin(m\pi z^*) \right|. \quad (54)$$

Alternatively, since $D_{bs}(z^*)$ has no discontinuity at $z^* = 0$, it can also be derived as given below:

$$D_{bs}(z^*) = \sum_{m=0}^{\infty} \frac{\{e^{-1}(-1)^m - e(-1)^m\}}{\left\{1 + \left(m + \frac{1}{2}\right)^2 \pi^2\right\}} \left(m + \frac{1}{2}\right) \pi \cos\left(\left(\frac{2m+1}{2}\right) \pi z^*\right). \quad (55)$$

7. Singular Stress Fields in the Vicinity of a Through-Crack Front Propagating under Mode III (Anti-Plane Shear) in the [100] Direction

Yoon and Chaudhuri [54] have already addressed the problem of a cracked tricrystal plate subjected to mode III (anti-plane shear loading). The present problem is a special case of that, and can be obtained by substituting $\theta_1 = \pi$ (refer to Figure 1 of Yoon and Chaudhuri [54]).

8. Crack Path Stability/Instability Criteria

8.1. Necessary Condition—Griffith–Irwin Theory-Based Crack Deflection Criterion

The important issue of a cleavage plane being deemed easy or difficult can be related to a crack deflection criterion, which is based on the relative fracture energy (or the energy release rate) available for possible fracture pathways [13]. The deflection or kinking of a crack from cleavage system 1 to cleavage system 2 is favored if (however, not iff, i.e., if and only if):

$$\frac{G_1}{(2\Gamma_1)} < 1 < \frac{G_2}{(2\Gamma_2)} \Rightarrow \frac{G_2}{G_1} > \frac{\Gamma_2}{\Gamma_1}, \quad (56)$$

where G_j and Γ_j , $j = 1, 2$, are the energy release rate (fracture energy) and surface energy, respectively, of the j^{th} cleavage system.

It may be noted here that an experimental determination of the critical surface energy, Γ_j , $j = 1, 2$, of the component phase or the corresponding interfacial energy, Γ_{int} , of a bicrystalline superlattice can sometimes be notoriously challenging, due to the presence of micro-to-nanoscale defects, such as porosity, dislocation, twin boundaries, misalignment of bonds with respect to the loading axis, and the like. In contrast, the bond shear strain at superlattice crack deflection, γ_{bd}^s , and superlattice crack deflection (SCD) barrier, ΔK^{s*} , to be discussed below, are, relatively speaking, much easier to determine in comparison to the critical surface or interfacial energy.

8.2. Sufficient Condition

The above Griffith–Irwin theory-based crack deflection criterion (albeit being still very useful and widely employed) is not accepted as a sufficient condition for a cleavage system deemed to be easy or difficult for crack propagation in single crystals [60], the most enigmatic being the {100} cleavage of BCC transition metals, especially macroscopically isotropic tungsten (W). Although the close-packed {110} surface has a lower surface energy, the preferred cleavage plane has experimentally been observed by Hull et al. [61] to be {100} (see also Riedle et al. [60]). For W, {100}<001> ({crack plane}<crack front>) is deemed to be

the preferred cleavage system for the reason of having d^2sp^3 hybridized orbitals, while $\{-110\}\langle 001 \rangle$ is considered to be difficult for crack propagation.

Atomistic scale modeling of cracks requires the consideration of both long-range elastic interactions and short-range chemical reactions. The Griffith theory does not take the latter into account [49]. Secondly, and more importantly, fracture criteria derived from equilibrium theories, such as the Griffith (thermodynamics-based) energy balance criterion, are not equipped to meet the sufficiency condition because of prevailing non-equilibrium conditions, such as physico-chemical reactions during crack propagation. Hence, such criteria can only be regarded as necessary conditions for fractures, but not as sufficient [60,62]. The effect of short-range chemical reactions can obviously be encapsulated by atomic-scale simulations, such as the investigation of low-speed propagation instabilities in silicon using quantum-mechanical hybrid multi-scale modeling due to Kermode et al. [63], which, however, entails extensive computational and other resources. Alternatively, and more importantly, such short-range interactions can also be captured by elastic property-based parameters (with a few exceptions), such as the planar anisotropic ratio, A_j , or equivalently, the normalized elastic parameter, κ_j , $j = 1, 2$ [49]. The general theory behind these characteristics pertaining to the structural chemistry of crystals is available in well-known treatises (see, e.g., [64–66]). More specifically, the elastic properties of superconducting $YBa_2Cu_3O_{7-\delta}$ are strongly influenced by oxygen non-stoichiometry (as well as various structural defects).

A single dimensionless parameter, such as the planar anisotropic ratio, A_j , or equivalently, the normalized elastic parameter, κ_j , $j = 1, 2$, can serve as the Holy Grail quantity for an *a priori* determination of the status of a cleavage system to be easy or difficult, very much akin to the Reynold's number for fluid flow problems, crossing a critical value that signifies the transition from one regime to another. Here, the planar anisotropic ratio, A_j , or equivalently, the normalized elastic parameter, κ_j , $j = 1, 2$, for a $(010)[001] \times [100]$ cleavage system, crossing the critical value of 1 or $\sqrt{c_{22}^{(j)} / c_{11}^{(j)}}$, $j = 1, 2$, respectively, signifies transitioning from self-similar crack growth or propagation to crack deflection or turning from a difficult cleavage system onto a nearby easy one. This is a significant qualitative as well as quantitative improvement over a two-parameter-based model, introduced by Wang et al. [12], in the context of two-dimensional anisotropic fracture mechanics.

Finally, just as the introduction of the Reynold's number facilitated the design and setting up of experiments in addition to the experimental verification of analytical and computational solutions in fluid dynamics, the accuracy and efficacy of the available experimental results on elastic constants of mono-crystalline superconducting $YBa_2Cu_3O_{7-\delta}$, measured by modern experimental techniques with resolutions at the atomic scale or nearly so, such as X-ray diffraction [67], ultrasound technique [68–70], neutron diffraction [71]/scattering [72], Brillouin spectroscopy [73,74]/scattering [75], resonant ultrasound spectroscopy [76,77], and the like, in a way best suited to preserve the characteristics associated with short-range interactions [57], are assessed with a powerful theoretical analysis of crack path stability/instability, in part based on a single dimensionless parameter, such as the planar anisotropic ratio, A_j , or equivalently, the normalized elastic parameter, κ_j , $j = 1, 2$.

9. Numerical Results and Discussions (Tables 1–49)

9.1. Structure–Fracture Property Relations for Certain Model Bicrystalline Superlattices

In what follows, 22 model bicrystal (superlattice) cleavage systems, each comprising a nano-film deposited on a substrate, are investigated. Table 1 lists the structures and elastic stiffness constants (with respect to $\langle 100 \rangle$ axes) of these mono-crystalline materials. Tables 2–23 list the cleavage systems, (crack plane)[crack front] $\times$ [initial propagation direction], and elastic stiffness constants (with respect to suitably rotated coordinates) of the component phases of bicrystalline superlattice systems 1–22. For example, the hexagonal substrate or material 2 is rotated such that $\{11\bar{2}0\}$ (a prism plane) is parallel to the crack face. It may be noted that the rotated crystal displays tetragonal-type symmetry.

The bicrystalline superlattice systems investigated here are namely as follows: (i) Au (gold), nano-layer/film or material 1 deposited on Si_3N_4 (silicon nitride), substrate or material 2 (Tables 2–5); (ii) Au (nano-layer/film) deposited on substrate MgO (magnesium oxide) (Tables 6–9); (iii) $\text{YBa}_2\text{Cu}_3\text{O}_7$ (tetragonal/fully oxidized or non-superconducting $\text{YBa}_2\text{Cu}_3\text{O}_7$, in short YBCO^T) nano-layer/film, deposited on substrate Si_3N_4 (Table 10); (iv) $\text{YBa}_2\text{Cu}_3\text{O}_7$ (nano-layer/film) deposited on substrate SrTiO_3 (Tables 11–14); (v) $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (superconducting YBCO, in short YBCO) nano-layer/film, deposited on substrate Si_3N_4 (Table 15); (vi) $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$, nano-layer/film deposited on substrate MgO (Tables 16 and 17); and (vii) $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (nano-layer/film) deposited on substrate SrTiO_3 (strontium titanate) (Tables 18–23). For the bicrystalline superlattice systems under investigation, the computed mode I, II, or mixed-mode I/II order-of-stress singularity, $\lambda_i = 1 - s_i$, $i = 1, 2$, is found to be $0.5 \pm i\varepsilon$ or 0.5. In contrast, the computed mode III order-of-stress singularity, $\lambda_3 = 1 - s_3$, is always equal to 0.5.

Table 1. Structures and elastic properties of various single crystals.

Single Crystal	Bravais Lattice	Structure	c_{11} (GPa)	c_{22} (GPa)	c_{33} (GPa)	c_{12} (GPa)	c_{13} (GPa)	c_{23} (GPa)	c_{44} (GPa)	c_{55} (GPa)	c_{66} (GPa)
Au [78]	FCC	FCC	192.9	192.9	192.9	163.8	163.8	163.8	41.5	41.5	41.5
MgO [78]	FCC	Rock Salt	289.3	289.3	289.3	87.70	87.70	87.70	154.77	154.77	154.77
SrTiO_3 [78]	Simple Cubic	Perovskite	348.17	348.17	348.17	100.64	100.64	100.64	454.55	454.55	454.55
Si_3N_4	HCP	HCP	343.0	343.0	600.0	136.0	120.0	120.0	124.0	124.0	103.5
$\text{YBa}_2\text{Cu}_3\text{O}_7$ [72] *	Tetragonal	Perovskite	230.0	230.0	150.0	100.0	100.0	100.0	50.0	50.0	85.0
$\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ [57,70,76] †	Orthorhombic	Perovskite	231.0	268.0	186.0	66.0	71.0	95.0	49.0	37.0	82.0

* All values measured by neutron scattering by Reichardt et al. [72]; † all values measured by resonant ultrasound spectroscopy by Lei et al. [76], except c_{12} and c_{66} measured by ultrasound by Saint-Paul and Henry [70].

Table 2. Cleavage system: (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 1.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	Au (FCC)	(010)[001]×[100]	192.9	192.9	192.9	163.8	163.8	163.8	41.5	41.5	41.5
2 *	Si_3N_4 (HCP)	(001)[0 $\bar{1}$ 0]×[$\bar{1}$ 00]	343.0	600.0	343.0	120.0	136.0	120.0	124.0	103.5	124.0

* Rotated about the z-axis by 90° , then rotated about the new x-axis by -90° .

Table 3. Cleavage system: (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 2.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	Au (FCC)	(010)[001]×[100]	192.9	192.9	192.9	163.8	163.8	163.8	41.5	41.5	41.5
2 *	Si_3N_4 (HCP)	($\bar{1}$ 00)[0 $\bar{1}$ 0]×[001]	600.0	343.0	343.0	120.0	120.0	136.0	103.5	124.0	124.0

* Rotated first about the y-axis by -90° , then rotated about the new x-axis by 90° .

Table 4. Cleavage system: (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 3.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	Au (FCC)	($\bar{1}$ 10)[001]×[110]	219.85	219.85	192.9	136.85	163.8	163.8	41.5	41.5	14.5
2 *	Si_3N_4 (HCP)	(001)[0 $\bar{1}$ 0]×[$\bar{1}$ 00]	343.0	600.0	343.0	120.0	136.0	120.0	124.0	103.5	124.0

* Rotated about the z-axis by 90° , then rotated about the new x-axis by -90° .

Table 5. Cleavage system: (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 4.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	Au (FCC)	($\bar{1}10$)[001]×[110]	219.85	219.85	192.9	136.85	163.8	163.8	41.5	41.5	14.5
2 *	Si ₃ N ₄ (HCP)	($\bar{1}00$)[0 $\bar{1}0$]×[001]	600.0	343.0	343.0	120.0	120.0	136.0	103.5	124.0	124.0

* Rotated first about the y -axis by -90° , then rotated about the new x -axis by 90° .

Table 6. Cleavage system: (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 5.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	Au (FCC)	(010)[001]×[100]	192.9	192.9	192.9	163.8	163.8	163.8	41.5	41.5	41.5
2	MgO (FCC)	(010)[001]×[100]	289.3	289.3	289.3	87.7	87.7	87.7	154.77	154.77	154.77

Table 7. Cleavage system: (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 6.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	Au (FCC)	(010)[001]×[100]	192.9	192.9	192.9	163.8	163.8	163.8	41.5	41.5	41.5
2	MgO (FCC)	($\bar{1}10$)[001]×[110]	343.27	343.27	289.3	33.73	87.7	87.7	154.77	154.77	100.8

Table 8. Cleavage system: (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 7.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	Au (FCC)	($\bar{1}10$)[001]×[110]	219.85	219.85	192.9	136.85	163.8	163.8	41.5	41.5	14.5
2	MgO (FCC)	(010)[001]×[100]	289.3	289.3	289.3	87.7	87.7	87.7	154.77	154.77	154.77

Table 9. Cleavage system: (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 8.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	Au (FCC)	($\bar{1}10$)[001]×[110]	219.85	219.85	192.9	136.85	163.8	163.8	41.5	41.5	14.5
2	MgO (FCC)	($\bar{1}10$)[001]×[110]	343.27	343.27	289.3	33.73	87.7	87.7	154.77	154.77	100.8

In the FCC metal nano-film, Au, listed in Tables 2–9 and 24–31, all the orbitals belong to the d-block with partially filled d-shells [66]. In a mono-crystalline FCC metal, the bonds are oriented along the face diagonals, $\langle 110 \rangle$. Such a metal contains linear chains of near-neighbor bonds in these directions, resulting in higher elastic stiffness constants along them. As shown in Tables 20, 25, 28 and 29, $A = 2.8522 > 1$ and $\kappa = 4.9777 > \sqrt{c'_{22}/c'_{11}} = 1$ for Au, giving rise to complex roots for a $\{010\}\langle 001 \rangle \times \langle 100 \rangle$ through-crack. Similar calculations yield $A' = 0.3494 < 1$ and $\kappa' = 0.2487 < \sqrt{c'_{22}/c'_{11}} = 1$ for Au, giving rise to imaginary roots for the $\{\bar{1}10\}\langle 001 \rangle \times \langle 110 \rangle$ through-crack [49], as can be seen in Tables 26, 27, 30 and 31. It can then be inferred that $\{\bar{1}10\}\langle 001 \rangle \times \langle 110 \rangle$ would constitute an easy cleavage system, while $\{010\}\langle 001 \rangle \times \langle 100 \rangle$ would be deemed difficult.

Table 10. Cleavage system (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 9.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	YBa ₂ C ₃ O ₇ (Tetragonal)	(010)[001]×[100]	230.0	230.0	150.0	100.0	100.0	100.0	50.0	50.0	85.0
2 *	Si ₃ N ₄ (HCP)	($\bar{1}00$)[0 $\bar{1}0$]×[001]	600.0	343.0	343.0	120.0	120.0	136.0	103.5	124.0	124.0

* Rotated first about the y -axis by -90° , then rotated about the new x -axis by 90° .

Table 11. Cleavage system (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 10.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	YBa ₂ C ₃ O ₇ (Tetragonal)	(010)[001]×[100]	230.0	230.0	150.0	100.0	100.0	100.0	50.0	50.0	85.0
2	SrTiO ₃ (Simple Cubic)	(010)[001]×[100]	348.17	348.17	348.17	100.64	100.64	100.64	454.55	454.55	454.55

Table 12. Cleavage system (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 11.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	YBa ₂ C ₃ O ₇ (Tetragonal)	(010)[001]×[100]	230.0	230.0	150.0	100.0	100.0	100.0	50.0	50.0	85.0
2	SrTiO ₃ (Simple Cubic)	($\bar{1}10$)[001]×[110]	678.96	678.96	348.17	−230.15	100.64	100.64	454.55	454.55	123.77

Table 13. Cleavage system (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 12.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	YBa ₂ C ₃ O ₇ (Tetragonal)	($\bar{1}10$)[001]×[110]	250.0	250.0	150.0	80.0	100.0	100.0	50.0	50.0	65.0
2	SrTiO ₃ (Simple Cubic)	($\bar{1}10$)[001]×[110]	678.96	678.96	348.17	−230.15	100.64	100.64	454.55	454.55	123.77

Table 14. Cleavage system (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 13.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	YBa ₂ C ₃ O ₇ (Tetragonal)	($\bar{1}10$)[001]×[110]	250.0	250.0	150.0	80.0	100.0	100.0	50.0	50.0	65.0
2	SrTiO ₃ (Simple Cubic)	(010)[001]×[100]	348.17	348.17	348.17	100.64	100.64	100.64	454.55	454.55	454.55

The ionic crystal MgO (an alkaline earth metal oxide), used as a substrate, which is listed in Tables 6–9, 16 and 17, in addition to in Tables 28–31, 38 and 39, is structurally of the rock salt type, but is an exception to the general rule for ionic crystals, such as alkali halides (e.g., NaCl and KCl) with a rock salt structure [49,64]. The reason is, as explained by Newnham [64], due to Mg²⁺ (and also Li⁺) having small cations, which permit the anions to be in contact with one another and, consequently, restrict bending actions. As a

result, elastic stiffness coefficients in the $\langle 110 \rangle$ and $\langle 111 \rangle$ directions become larger than their $\langle 100 \rangle$ counterparts. This is in contrast to NaCl and KCl, wherein Cl[−] anions are not in contact. Additionally, the importance of anion–anion forces were pointed out by Weidner and Simmons [79]. These researchers found, in connection with the computation of elastic properties of several alkali halides from a two-body central force model, the necessity to include anion–anion interactions in addition to cation–anion forces. As shown in Tables 29, 31 and 39, $A' = 0.6513$ and $\kappa' = 0.6297$ are both less than unity ($A' < 1$, $\kappa' < \sqrt{c'_{22}/c'_{11}} = 1$), giving rise to imaginary roots for the $(\bar{1}10)[001] \times [110]$ through-crack. This is in contrast to $A = 1.5354$ and $\kappa = 1.8329$ being both larger than unity ($A > 1$, $\kappa > \sqrt{c_{22}/c_{11}} = 1$), giving rise to complex roots for the $(010)[001] \times [100]$ through-crack, as shown in Tables 28, 30 and 38. It can then be inferred that $\{\bar{1}10\}\langle 001 \rangle \times \langle 110 \rangle$ would constitute an easy cleavage system, while $\{010\}\langle 001 \rangle \times \langle 100 \rangle$ would be deemed difficult.

Table 15. Cleavage system: (crack plane)[crack front] $\times$ [initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 14.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	(001)[100] $\times$ [010]	268.0	186.0	231.0	95.0	66.0	71.0	37.0	82.0	49.0
2 *	Si ₃ N ₄ (HCP)	(001)[0 $\bar{1}0$] $\times$ [$\bar{1}00$]	343.0	600.0	343.0	120.0	136.0	120.0	124.0	103.5	124.0

* Rotated about the z-axis by 90°, then rotated about the new x-axis by −90°.

Table 16. Cleavage system: (crack plane)[crack front] $\times$ [initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 15.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	(001)[100] $\times$ [010]	268.0	186.0	231.0	95.0	66.0	71.0	37.0	82.0	49.0
2	MgO (FCC)	(010)[001] $\times$ [100]	289.3	289.3	289.3	87.7	87.7	87.7	154.77	154.77	154.77

Table 17. Cleavage system: (crack plane)[crack front] $\times$ [initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 16.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	(001)[100] $\times$ [010]	268.0	186.0	231.0	95.0	66.0	71.0	37.0	82.0	49.0
2	MgO (FCC)	($\bar{1}10$)[001] $\times$ [110]	343.27	343.27	289.3	33.73	87.7	87.7	154.77	154.77	100.8

Table 18. Cleavage system (crack plane)[crack front] $\times$ [initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 17.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	(001)[100] $\times$ [010]	268.0	186.0	231.0	95.0	66.0	71.0	37.0	82.0	49.0
2	SrTiO ₃ (Simple Cubic)	(010)[001] $\times$ [100]	348.17	348.17	348.17	100.64	100.64	100.64	454.55	454.55	454.55

Table 19. Cleavage system (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 18.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	(001)[100]×[010]	268.0	186.0	231.0	95.0	66.0	71.0	37.0	82.0	49.0
2	SrTiO ₃ (Simple Cubic)	($\bar{1}10$)[001]×[110]	678.96	678.96	348.17	−230.15	100.64	100.64	454.55	454.55	123.77

Table 20. Cleavage system (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 19.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	(010)[001]×[100]	231.0	268.0	186.0	66.0	71.0	95.0	49.0	37.0	82.0
2	SrTiO ₃ (Simple Cubic)	(010)[001]×[100]	348.17	348.17	348.17	100.64	100.64	100.64	454.55	454.55	454.55

Table 21. Cleavage system (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 20.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	(010)[001]×[100]	231.0	268.0	186.0	66.0	71.0	95.0	49.0	37.0	82.0
2	SrTiO ₃ (Simple Cubic)	($\bar{1}10$)[001]×[110]	678.96	678.96	348.17	−230.15	100.64	100.64	454.55	454.55	123.77

Table 22. Cleavage system (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 21.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	($\bar{1}00$)[001]×[010]	268.0	231.0	186.0	66.0	95.0	71.0	37.0	49.0	82.0
2	SrTiO ₃ (Simple Cubic)	(010)[001]×[100]	348.17	348.17	348.17	100.64	100.64	100.64	454.55	454.55	454.55

Table 23. Cleavage system (crack plane)[crack front]×[initial propagation direction] and elastic stiffness constants of the component phases of bicrystalline superlattice system 22.

Material (j) #	Single Crystal Phase	Cleavage System	c'_{11} (GPa)	c'_{22} (GPa)	c'_{33} (GPa)	c'_{12} (GPa)	c'_{13} (GPa)	c'_{23} (GPa)	c'_{44} (GPa)	c'_{55} (GPa)	c'_{66} (GPa)
1	YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	($\bar{1}00$)[001]×[010]	268.0	231.0	186.0	66.0	95.0	71.0	37.0	49.0	82.0
2	SrTiO ₃ (Simple Cubic)	($\bar{1}10$)[001]×[110]	678.96	678.96	348.17	−230.15	100.64	100.64	454.55	454.55	123.77

The next substrate, Strontium titanate (SrTiO₃), which is a perovskite, is listed in Tables 11–14 and 18–23 as well as in Tables 33–36 and 40–45. SrTiO₃ has at room temperature, an ideal cubic perovskite structure with TiO₆ octahedra being connected by straight chains [63]. Tables 34, 36 and 41 show that $A' = 0.2723$ and $\kappa' = 0.3614$ are both less than unity ($A' < 1$, $\kappa' < \sqrt{c_{11}/c'_{11}} = 1$), giving rise to imaginary roots for the ($\bar{1}10$)[001]×[110] through-crack. This is in contrast to $A = 3.6727$ and $\kappa = 16.1473$ being both larger than unity

($A > 1$, $\kappa > \sqrt{c_{22}/c_{11}} = 1$), giving rise to complex roots for the (010)[001] $\times$ [100] through-crack, as shown in Tables 33, 35 and 40. It can then be inferred that $\{\bar{1}10\}\langle 001 \rangle \times \langle 110 \rangle$ would constitute an easy cleavage system, while $\{010\}\langle 001 \rangle \times \langle 100 \rangle$ would be deemed difficult.

The third and last substrate studied here is hexagonal close-packed (HCP) Si_3N_4 , which is listed in Tables 2–5, 10 and 15 as well as in Tables 24–27, 32 and 37. Tables 24, 26 and 32 show that $A' = 0.7433 < 1$ and $\kappa' = 0.9206 < \sqrt{c'_{22}/c'_{11}} = 1.3226$, giving rise to imaginary roots for the (001)[0 $\bar{1}0$] $\times$ [$\bar{1}00$] through-crack. In a similar vein, $A' = 0.7433 < 1$ and $\kappa' = 0.5263 < \sqrt{c'_{22}/c'_{11}} = 0.5717$, giving rise to imaginary roots for the ($\bar{1}00$)[0 $\bar{1}0$] $\times$ [001] through-crack, as shown in Tables 25, 27 and 37. It can then be inferred that $\{001\}\langle 0\bar{1}0 \rangle \times \langle \bar{1}00 \rangle$ and $\{\bar{1}00\}\langle 0\bar{1}0 \rangle \times \langle 001 \rangle$ would both constitute easy cleavage systems.

Fully oxidized (non-superconducting) tetragonal $\text{YBa}_2\text{C}_3\text{O}_7$, the second nano-film investigated here, is listed in Tables 10–14 and also in Tables 32–36. Granozio and di Uccio [80] have also presented approximate theoretical results of fully oxidized YBCO's ($\delta = 0, 1$), and concluded that the three lowest surface energies follow the inequality: $\gamma(001) < \gamma(100) < \gamma(010)$. Furthermore, based on the experimental results from transmission electron microscopy [81], X-ray photo-emission microscopy [82], low-energy ion scattering spectroscopy [83], and surface polarity [84] analyses performed on fully oxidized $\text{YBa}_2\text{C}_3\text{O}_7$ crystals, these authors [80] have shown that the low energy cut is between the Ba=O and Cu=O planes. Tables 32–34 show that $A = 1.9077$ and $\kappa = 3.1514$ are both larger than unity ($A > 1$, $\kappa > \sqrt{c_{22}/c_{11}} = 1$), giving rise to complex roots for the (010)[001] $\times$ [100] through-crack. This is in contrast to $A' = 0.7647$ and $\kappa' = 0.7112$ being both less than unity ($A' < 1$, $\kappa' < \sqrt{c'_{11}/c'_{11}} = 1$), giving rise to imaginary roots for the ($\bar{1}10$)[001] $\times$ [110] through-crack, as shown in Tables 35 and 36. It can then be inferred that $\{\bar{1}10\}\langle 001 \rangle \times \langle 110 \rangle$ would constitute an easy cleavage system, while $\{010\}\langle 001 \rangle \times \langle 100 \rangle$ would be deemed difficult.

Finally, the third nano-film, $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}$ (orthorhombic), investigated here is a high TC superconductor, and is listed in Tables 15–23 in addition to Tables 37–45. As can be seen in Tables 2–7 of Chaudhuri [57], all the cleavage systems are predicted to be easy, which are in agreement with the experimentally observed fracture characteristics of $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}$ due to Cook et al. [85], Raynes et al. [86], and Goyal et al. [87], among others; see also Granozio and di Uccio [80] for a summary of the available experimental results. Here, $A' = 0.764 < 1$ and $\kappa' = 0.5784 < \sqrt{c'_{22}/c'_{11}} = 0.8331$, giving rise to imaginary roots for the (001)[100] $\times$ [010] through-crack, as shown in Tables 37–41; see also Table 6 of Chaudhuri [57]. Similarly, $A = 0.8971 < 1$ and $\kappa = 0.9406 < \sqrt{c'_{22}/c'_{11}} = 1.0771$, giving rise to imaginary roots for the (010)[001] $\times$ [100] through-crack, as shown in Tables 42 and 43; see also Table 2 of Chaudhuri [57]. Likewise, $A' = 0.8971 < 1$ and $\kappa' = 0.817 < \sqrt{c'_{22}/c'_{11}} = 0.9284$, giving rise to imaginary roots for the ($\bar{1}00$)[001] $\times$ [010] through-crack, as shown in Tables 44 and 45; see also Table 4 of Chaudhuri [57]. It can then be inferred that $\{001\}\langle 100 \rangle \times \langle 010 \rangle$ would constitute an easy cleavage system.

Table 24. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 1.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
Au (FCC)	(010)[001] $\times$ [100]	2.8522	1.0	4.9777	Complex	Difficult
Si_3N_4 (HCP)	(001)[0 $\bar{1}0$] $\times$ [$\bar{1}00$]	0.7433	1.3226	0.9206	Imaginary	Easy

Table 25. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 2.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
Au (FCC)	(010)[001]×[100]	2.8522	1.0	4.9777	Complex	Difficult
Si ₃ N ₄ (HCP)	($\bar{1}00$)[0 $\bar{1}0$]×[001]	0.7433	0.5717	0.5263	Imaginary	Easy

Table 26. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 3.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
Au (FCC)	($\bar{1}10$)[001]×[110]	0.3494	1.0	0.2487	Imaginary	Easy
Si ₃ N ₄ (HCP)	(001)[0 $\bar{1}0$]×($\bar{1}00$)	0.7433	1.3226	0.9206	Imaginary	Easy

Table 27. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 4.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
Au (FCC)	($\bar{1}10$)[001]×[110]	0.3494	1.0	0.2487	Imaginary	Easy
Si ₃ N ₄ (HCP)	($\bar{1}00$)[0 $\bar{1}0$]×[001]	0.7433	0.5717	0.5263	Imaginary	Easy

Table 28. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 5.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
Au (FCC)	(010)[001]×[100]	2.8522	1.0	4.9777	Complex	Difficult
MgO (FCC)	(010)[001]×[100]	1.5354	1.0	1.8329	Complex	Difficult

Table 29. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 6.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
Au (FCC)	(010)[001]×[100]	2.8522	1.0	4.9777	Complex	Difficult
MgO (FCC)	($\bar{1}10$)[001]×[110]	0.6513	1.0	0.6297	Imaginary	Easy

Table 30. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 7.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
Au (FCC)	($\bar{1}10$)[001]×[110]	0.3494	1.0	0.2487	Imaginary	Easy
MgO (FCC)	(010)[001]×[100]	1.5354	1.0	1.8329	Complex	Difficult

Table 31. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 8.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
Au (FCC)	$(\bar{1}10)[001] \times [110]$	0.3494	1.0	0.2487	Imaginary	Easy
MgO (FCC)	$(\bar{1}10)[001] \times [110]$	0.6513	1.0	0.6297	Imaginary	Easy

Table 32. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 9.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
YBa ₂ C ₃ O ₇ (Tetragonal)	$(010)[001] \times [100]$	1.9077	1.0	3.1514	Complex	Difficult
Si ₃ N ₄ (HCP)	$(\bar{1}00)[0\bar{1}0] \times [001]$	0.7433	0.5717	0.9206	Imaginary	Easy

Table 33. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 10.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
YBa ₂ C ₃ O ₇ (Tetragonal)	$(010)[001] \times [100]$	1.9077	1.0	3.1514	Complex	Difficult
SrTiO ₃ (Simple Cubic)	$(010)[001] \times [100]$	3.6727	1.0	16.1473	Complex	Difficult

Table 34. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 11.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
YBa ₂ C ₃ O ₇ (Tetragonal)	$(010)[001] \times [100]$	1.9077	1.0	3.1514	Complex	Difficult
SrTiO ₃ (Simple Cubic)	$(\bar{1}10)[001] \times [110]$	0.2723	1.0	0.3614	Imaginary	Easy

Table 35. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 12.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
YBa ₂ C ₃ O ₇ (Tetragonal)	$(\bar{1}10)[001] \times [110]$	0.7647	1.0	0.7112	Imaginary	Easy
SrTiO ₃ (Simple Cubic)	$(010)[001] \times [100]$	3.6727	1.0	16.1473	Complex	Difficult

Table 36. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 13.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
YBa ₂ C ₃ O ₇ (Tetragonal)	($\bar{1}10$)[001] × [110]	0.7647	1.0	0.7112	Imaginary	Easy
SrTiO ₃ (Simple Cubic)	($\bar{1}10$)[001] × [110]	0.2723	1.0	0.3614	Imaginary	Easy

Table 37. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 14.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	(001)[100] × [010]	0.764	0.8331	0.5784	Imaginary	Easy
Si ₃ N ₄ (HCP)	(001)[0 $\bar{1}0$] × [$\bar{1}00$]	0.7433	1.3226	0.9206	Imaginary	Easy

Table 38. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 15.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	(001)[100] × [010]	0.764	0.8331	0.5784	Imaginary	Easy
MgO (FCC)	(010)[001] × [100]	1.5354	1.0	1.8329	Complex	Difficult

Table 39. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 16.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	(001)[100] × [010]	0.764	0.8331	0.5784	Imaginary	Easy
MgO (FCC)	($\bar{1}10$)[001] × [110]	0.6513	1.0	0.6297	Imaginary	Easy

Table 40. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 17.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	(001)[100] × [010]	0.764	0.8331	0.5784	Imaginary	Easy
SrTiO ₃ (Simple Cubic)	(010)[001] × [100]	3.6727	1.0	16.1473	Complex	Difficult

Table 41. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 18.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	(001)[100] × [010]	0.764	0.8331	0.5784	Imaginary	Easy
SrTiO ₃ (Simple Cubic)	($\bar{1}10$)[001] × [110]	0.2723	1.0	0.3614	Imaginary	Easy

Table 42. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 19.

Material (j) #	Cleavage System	A	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	(010)[001] × [100]	0.8971	1.0771	0.9406	Imaginary	Easy
SrTiO ₃ (Simple Cubic)	(010)[001] × [100]	3.6727	1.0	16.1473	Complex	Difficult

Table 43. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 20.

Material (j) #	Cleavage System	A	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	(010)[001] × [100]	0.8971	1.0771	0.9406	Imaginary	Easy
SrTiO ₃ (Simple Cubic)	($\bar{1}10$)[001] × [110]	0.2723	1.0	0.3614	Imaginary	Easy

Table 44. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 21.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	($\bar{1}00$)[001] × [010]	0.8971	0.9284	0.817	Imaginary	Easy
SrTiO ₃ (Simple Cubic)	(010)[001] × [100]	3.6727	1.0	16.1473	Complex	Difficult

Table 45. Normalized elastic parameter, roots of characteristic equation, and the nature (easy or difficult) of the through-thickness cleavage system of bicrystalline superlattice system 22.

Material (j) #	Cleavage System	A'	$\sqrt{\frac{c'_{22}}{c'_{11}}}$	κ'	Roots	Cleavage System: Easy or Difficult
YBa ₂ C ₃ O _{7-δ} (Orthorhombic)	($\bar{1}00$)[001] × [010]	0.8971	0.9284	0.817	Imaginary	Easy
SrTiO ₃ (Simple Cubic)	($\bar{1}10$)[0 $\bar{1}01$] × [110]	0.2723	1.0	0.3614	Imaginary	Easy

Table 46 summarizes the nature (easy or difficult) of the cleavage system in component phases of the afore-mentioned bicrystalline superlattice systems. It also lists the real or

complex eigenvalues, $s = 0.5 \pm i\epsilon$, of these bicrystalline superlattices. These results suggest that the interfacial cracks would propagate in the mixed (I/II) mode, primarily when both the component phases are characterized by difficult cleavage systems (complex roots), the exception being perovskite SrTiO_3 serving as the substrate (for $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}$ or $\text{YBa}_2\text{C}_3\text{O}_7$ nano-films). A plausible reason for this exceptional behavior of SrTiO_3 may lie in its unusually high shear stiffness, c_{66} , which is substantially greater than its longitudinal stiffness, c_{11} , in combination with easiest cleavage system of $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}$ (or $\text{YBa}_2\text{C}_3\text{O}_7$). This is in contrast with other cubic mono-crystals, such as FCC rock salt MgO . This fact results in a negative Poisson's ratio effect, when rotated about the $[001]$ axis by 45° , which is not generally encountered in cubic crystal elasticity. Additionally, this behavior is also in contrast with other easy cleavage systems of $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}$ deposited on the same 45° rotated SrTiO_3 , as shown in Tables 43, 45 and 46.

Table 46. Real or complex eigenvalues of the bicrystalline superlattice systems with through interfacial cracks.

Bicrystal System #	Nano-Film/Substrate	Cleavage Systems	Roots	Cleavage System: Easy or Difficult	$s = 0.5$ or $s = 0.5 \pm i\epsilon$
1	Au/ Si_3N_4	$(010)[001] \times [100] / (001)[0\bar{1}0] \times [\bar{1}00]$	Complex/Imaginary	Difficult/Easy	0.5
2	Au/ Si_3N_4	$(010)[001] \times [100] / (\bar{1}00)[0\bar{1}0] \times [001]$	Complex/Imaginary	Difficult/Easy	0.5
3	Au/ Si_3N_4	$(\bar{1}10)[001] \times [110] / (001)[00] \times [\bar{1}00]$	Imaginary/Imaginary	Easy/Easy	0.5
4	Au/ Si_3N_4	$(\bar{1}10)[001] \times [110] / (\bar{1}00)[0\bar{1}0] \times [001]$	Imaginary/Imaginary	Easy/Easy	0.5
5	Au/ MgO	$(010)[001] \times [100] / (010)[001] \times [100]$	Complex/Complex	Difficult/Difficult	$0.5 \pm 0.3814i$ $0.5 \pm 0.2108i$
6	Au/ MgO	$(010)[001] \times [100] / (10)[001] \times [110]$	Complex/Imaginary	Difficult/Easy	0.5
7	Au/ MgO	$(\bar{1}10)[001] \times [110] / (010)[001] \times [100]$	Imaginary/Complex	Easy/Easy	0.5
8	Au/ MgO	$(\bar{1}10)[001] \times [110] / (\bar{1}10)[001] \times [110]$	Imaginary/Imaginary	Easy/Easy	0.5
9	$\text{YBa}_2\text{C}_3\text{O}_7/\text{Si}_3\text{N}_4$	$(010)[001] \times [100] / (\bar{1}00)[0\bar{1}0] \times [001]$	Complex/Imaginary	Difficult/Easy	0.5
10	$\text{YBa}_2\text{C}_3\text{O}_7/\text{SrTiO}_3$	$(010)[001] \times [100] / (010)[001] \times [100]$	Complex/Complex	Difficult/Difficult	$0.5 \pm 0.7636i$
11	$\text{YBa}_2\text{C}_3\text{O}_7/\text{SrTiO}_3$	$(010)[001] \times [100] / (\bar{1}10)[001] \times [110]$	Complex/Imaginary	Difficult/Easy	0.5
12	$\text{YBa}_2\text{C}_3\text{O}_7/\text{SrTiO}_3$	$(\bar{1}10)[001] \times [110] / (010)[001] \times [100]$	Imaginary/Complex	Easy/Difficult	0.5
13	$\text{YBa}_2\text{C}_3\text{O}_7/\text{SrTiO}_3$	$(\bar{1}10)[001] \times [110] / (\bar{1}10)[001] \times [110]$	Imaginary/Imaginary	Easy/Easy	$0.5 \pm 0.0580i$
14	$\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{Si}_3\text{N}_4$	$(001)[100] \times [010] / (001)[0\bar{1}0] \times [\bar{1}00]$	Imaginary/Imaginary	Easy/Easy	0.5
15	$\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{MgO}$	$(001)[100] \times [010] / (010)[001] \times [100]$	Imaginary/Complex	Easy/Difficult	0.5
16	$\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{MgO}$	$(001)[100] \times [010] / (\bar{1}10)[001] \times [110]$	Imaginary/Imaginary	Easy/Easy	0.5
17	$\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{SrTiO}_3$	$(001)[100] \times [010] / (010)[001] \times [100]$	Imaginary/Complex	Easy/Difficult	0.5
18	$\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{SrTiO}_3$	$(001)[100] \times [010] / (10)[001] \times [110]$	Imaginary/Imaginary	Easy/Easy	$0.5 \pm 0.1757i$
19	$\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{SrTiO}_3$	$(010)[001] \times [100] / (010)[001] \times [100]$	Imaginary/Imaginary	Easy/Easy	0
20	$\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{SrTiO}_3$	$(010)[001] \times [100] / (\bar{1}10)[001] \times [110]$	Imaginary/Imaginary	Easy/Easy	0
21	$\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{SrTiO}_3$	$(\bar{1}00)[001] \times [010] / (010)[001] \times [100]$	Imaginary/Imaginary	Easy/Easy	0
22	$\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{SrTiO}_3$	$(\bar{1}00)[001] \times [010] / (\bar{1}10)[001] \times [110]$	Imaginary/Imaginary	Easy/Easy	0

9.2. Superlattice Trapping and Superlattice Crack Deflection (SCD)

The theory of lattice crack deflection (LCD) is discussed in Chaudhuri [49]. Table 47 displays the structures and elastic compliance constants of mono-crystalline FCC transition metal Au, FCC rock salt MgO , cubic perovskite SrTiO_3 , HCP ceramic Si_3N_4 , fully oxidized tetragonal $\text{YBa}_2\text{C}_3\text{O}_7$, and orthorhombic (superconducting) $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}$ [49,57,78]. Table 48 shows the results for computed lattice crack deflection (LCD) parameters (energy barrier) and associated bond shear strains at crack deflection from a difficult cleavage system to an easy one, and their correlations with the anisotropic ratios relating to the difficult cleavage system along with Bravais lattice and structure. Only two crack systems are considered: $\{010\}\langle 001 \rangle \times \langle 100 \rangle$ and $\{\bar{1}10\}\langle 001 \rangle \times \langle 110 \rangle$.

Table 47. Structures and elastic compliance constants of selected single crystals [49,78].

Single Crystal	Bravais Lattice	Structure	s_{11} (10^{-2} GPa $^{-1}$)	s_{22} (10^{-2} GPa $^{-1}$)	s_{33} (10^{-2} GPa $^{-1}$)	s_{12} (10^{-2} GPa $^{-1}$)	s_{13} (10^{-2} GPa $^{-1}$)	s_{23} (10^{-2} GPa $^{-1}$)	s_{44} (10^{-2} GPa $^{-1}$)	s_{55} (10^{-2} GPa $^{-1}$)	s_{66} (10^{-2} GPa $^{-1}$)
Au [79,88]	FCC	FCC	2.355	2.355	2.355	−1.081	−1.081	−1.081	2.4096	2.4096	2.4096
MgO [79]	FCC	Rock Salt	0.4024	0.4024	0.4024	−0.0936	−0.0936	−0.0936	0.6461	0.6461	0.6461
SrTiO ₃ [79]	Simple Cubic	Perovskite	0.33	0.33	0.33	−0.074	−0.074	−0.074	0.22	0.22	0.22
Si ₃ N ₄	HCP	HCP	0.3576	0.3576	0.1852	−0.1255	−0.0464	−0.0464	0.8065	0.8065	0.9662
YBa ₂ C ₃ O ₇	Tetragonal	Perovskite	0.6389	0.6389	1.1186	−0.1304	−0.339	−0.339	2.0	2.0	1.1765
Y Ba ₂ C ₃ O _{7−δ}	Orthorhombic	Perovskite	0.5003	0.4648	0.7054	−0.0678	−0.1564	−0.2115	2.0408	2.7027	1.2195

For mono-crystalline FCC transition metals, $\{010\}\langle 001 \rangle \times \langle 100 \rangle$ is deemed to be a difficult cleavage system for the reasons explained above, while $\{\bar{1}10\}\langle 001 \rangle \times \langle 110 \rangle$ is considered to be the preferred one for crack propagation. This is illustrated in Figure 26a in Chaudhuri [49]. A nonvanishing lattice crack deflection (LCD) energy barrier implies that a $\{010\}\langle 001 \rangle \times \langle 100 \rangle$ through-crack in such single crystals would not deflect right at the appropriate Griffith/Irwin critical stress intensity factor (K_c) for mixed-mode propagation because of the lattice effect, but would require additional bond shear strains for Au (Table 48). In the case of the nonvanishing lattice crack deflection (LCD) barrier, e.g., in Au with a moderately high anisotropic ratio, $A = 2.8481 > 1$, the difficult $\{010\}\langle 001 \rangle \times \langle 100 \rangle$ crack may initially become lattice-trapped and/or propagate in a “difficult” manner till an applied load somewhat higher than its Griffith mixed-mode counterpart is reached, and then only deflect into the easy cleavage system, $\{\bar{1}10\}\langle 001 \rangle \times \langle 110 \rangle$. In addition, bond breaking would not be continuous, but abrupt. In contrast, for the same crystal with a very low modified anisotropic ratio, $A' = 0.3494 < 1$, the lattice crack deflection (LCD) barrier vanishes and the easy $\{\bar{1}10\}\langle 001 \rangle \times \langle 110 \rangle$ crack would begin to propagate right at the Griffith/Irwin critical stress intensity factor. There would be no crack turning.

Table 48. Easy/difficult cleavage system, lattice crack deflection (LCD) barrier, and associated bond shear strains in selected single crystals.

Crystal	Easy Cleavage System (ECS)	Difficult Cleavage System (DCS)	Aniso. Ratio, A, at DCS	Bond Shear Strain at Lattice Crack Deflection (γ_{bd})	Lattice Crack Deviation LCD Parameter in DCS (ΔK^*)
Au [88]	$\{\bar{1}10\}\langle 001 \rangle \times \langle 110 \rangle$	$\{010\}\langle 001 \rangle \times \langle 110 \rangle$	2.8522	0.6438	0.8364
MgO	$\{\bar{1}10\}\langle 001 \rangle \times \langle 110 \rangle$	$\{010\}\langle 001 \rangle \times \langle 100 \rangle$	1.5354	0.5353	0.6414
SrTiO ₃	$\{\bar{1}10\}\langle 001 \rangle \times \langle 110 \rangle$	$\{010\}\langle 001 \rangle \times \langle 100 \rangle$	3.6727	0.6075	0.5114
Si ₃ N ₄	$(\bar{1}00)[0\bar{1}0] \times [001]^*$	-----			
YBa ₂ C ₃ O ₇	$\{\bar{1}10\}\langle 001 \rangle \times \langle 110 \rangle$	$\{010\}\langle 001 \rangle \times \langle 100 \rangle$	1.9077	0.5055	0.6071
YBa ₂ C ₃ O _{7−δ}	$\{001\}\langle 100 \rangle \times \langle 010 \rangle$	-----			

* Rotated about the z-axis by 90°, then rotated about the new x-axis by −90°.

Bicrystals form superlattices have not been discussed, to the author’s knowledge, in anisotropic fracture mechanics literature [88]. However, the geometric mean of the two constituent phases would serve as a reasonably accurate procedure for the computation of the bond shear strain at the superlattice crack deviation, γ_{bd}^s , and superlattice crack deflection (SCD) barrier, ΔK^{s*} ; see also Chaudhuri [88]. Rigorous proof of this is currently being worked out and will be presented in the near future. The numerical results are shown in Table 49. For a bicrystalline superlattice, e.g., Au/MgO (respectively, YBa₂C₃O₇/SrTiO₃), with both difficult cleavage systems, $(010)[001] \times [100]/(010)[001] \times [100]$, serving as the interface, with the SCD barrier, ΔK^{s*} , value of 0.7324 (resp., 0.6240), the interfacial crack would encounter a tough interface and would initially be superlattice-trapped and/or experience a mixed-mode propagation in a “difficult” manner till an applied load somewhat higher than its Griffith/Irwin mixed-mode interfacial fracture toughness counter-

part — quantified by ΔK^{S*} — is reached, and thence deflect into the available easier cleavage system, $\{\bar{1}10\}\langle 001\rangle \times \langle 110\rangle$, of the component phase with the lower LCD barrier, $\Delta K^* = 0.6414$ for MgO (resp. 0.5114 for SrTiO₃). In addition, bond breaking would not be continuous, but abrupt. In contrast, for the same bicrystalline superlattice, Au/MgO, with both easy $(\bar{1}10)[001] \times [110]/(\bar{1}10)[001] \times [110]$ cleavage systems serving as the interface, the SCD barrier, ΔK^{S*} , vanishes, and the easy interfacial crack would begin to propagate (in the absence of mode mixity) in a self-similar manner right at the Griffith/Irwin critical stress intensity factor. The bond breaking would be smooth and continuous. Interestingly, for the Au/MgO or YBa₂C₃O₇/SrTiO₃ superlattice, with one easy and the second one difficult, either $(010)[001] \times [100]/(\bar{1}10)[001] \times [110]$ or $(\bar{1}10)[001] \times [110]/(010)[001] \times [100]$ cleavage systems serving as the interface, the SCD barrier, ΔK^{S*} , also vanishes, and the interfacial crack would begin to propagate (in the absence of mode mixity) on the easier side of and parallel to the interface at the Griffith/Irwin critical stress intensity factor. Bond breaking would be smooth and continuous on the easier side, but discontinuous and abrupt on the tougher side of the interface.

Table 49. Cleavage system, lattice crack deflection barrier, and associated bond shear strains in selected bicrystalline superlattice systems.

Bicrystal System #	Nano-film/Substrate	Cleavage Systems	Cleavage System: Easy or Difficult	Bond Shear Strain at Superlattice Crack Deflection (γ_{bd}^s)	Superlattice Crack Deviation (SCD) Parameter in DCS (ΔK^{S*})
1	Au/Si ₃ N ₄	(010)[001] × [100]/(001)[0 $\bar{1}$ 0] × [$\bar{1}$ 00]	Difficult/Easy	0	0
2	Au/Si ₃ N ₄	(010)[001] × [100]/($\bar{1}$ 00)[0 $\bar{1}$ 0] × [001]	Difficult/Easy	0	0
3	Au/Si ₃ N ₄	($\bar{1}$ 10)[001] × [110]/(001)[00] × [$\bar{1}$ 00]	Easy/Easy	0	0
4	Au/Si ₃ N ₄	($\bar{1}$ 10)[001] × [110]/($\bar{1}$ 00)[0 $\bar{1}$ 0] × [001]	Easy/Easy	0	0
5	Au/MgO	(010)[001] × [100]/(010)[001] × [100]	Difficult/Difficult	0.4710	0.7324
6	Au/MgO	(010)[001] × [100]/(10)[001] × [110]	Difficult/Easy	0	0
7	Au/MgO	($\bar{1}$ 10)[001] × [110]/(010)[001] × [100]	Easy/Difficult	0	0
8	Au/MgO	($\bar{1}$ 10)[001] × [110]/($\bar{1}$ 10)[001] × [110]	Easy/Easy	0	0
9	YBa ₂ C ₃ O ₇ /Si ₃ N ₄	(010)[001] × [100]/($\bar{1}$ 00)[0 $\bar{1}$ 0] × [001]	Difficult/Easy	0	0
10	YBa ₂ C ₃ O ₇ /SrTiO ₃	(010)[001] × [100]/(010)[001] × [100]	Difficult/Difficult	0.5202	0.6240
11	YBa ₂ C ₃ O ₇ /SrTiO ₃	(010)[001] × [100]/($\bar{1}$ 10)[001] × [110]	Difficult/Easy	0	0
12	YBa ₂ C ₃ O ₇ /SrTiO ₃	($\bar{1}$ 10)[001] × [110]/(010)[001] × [100]	Easy/Difficult	0	0
13	YBa ₂ C ₃ O ₇ /SrTiO ₃	($\bar{1}$ 10)[001] × [110]/($\bar{1}$ 10)[001] × [110]	Easy/Easy	0	0
14	YBa ₂ C ₃ O _{7-δ} /Si ₃ N ₄	(001)[100] × [010]/(001)[0 $\bar{1}$ 0] × [$\bar{1}$ 00]	Easy/Easy	0	0
15	YBa ₂ C ₃ O _{7-δ} /MgO	(001)[100] × [010]/(010)[001] × [100]	Easy/Difficult	0	0
16	YBa ₂ C ₃ O _{7-δ} /MgO	(001)[100] × [010]/($\bar{1}$ 10)[001] × [110]	Easy/Easy	0	0
17	YBa ₂ C ₃ O _{7-δ} /SrTiO ₃	(001)[100] × [010]/(010)[001] × [100]	Easy/Difficult	0	0
18	YBa ₂ C ₃ O _{7-δ} /SrTiO ₃	(001)[100] × [010]/(10)[001] × [110]	Easy/Easy	0	0
19	YBa ₂ C ₃ O _{7-δ} /SrTiO ₃	(010)[001] × [100]/(010)[001] × [100]	Easy/Difficult	0	0
20	YBa ₂ C ₃ O _{7-δ} /SrTiO ₃	(010)[001] × [100]/($\bar{1}$ 10)[001] × [110]	Easy/Easy	0	0
21	YBa ₂ C ₃ O _{7-δ} /SrTiO ₃	($\bar{1}$ 00)[001] × [010]/(010)[001] × [100]	Easy/Difficult	0	0
22	YBa ₂ C ₃ O _{7-δ} /SrTiO ₃	($\bar{1}$ 00)[001] × [010]/($\bar{1}$ 10)[001] × [110]	Easy/Easy	0	0

For the Au/Si₃N₄ superlattice, with both easy cleavage systems, either $(\bar{1}10)[001] \times [110]/(001)[0\bar{1}0] \times [\bar{1}00]$ or $(\bar{1}10)[001] \times [110]/(\bar{1}00)[0\bar{1}0] \times [001]$, serving as the interface, the SCD barrier, ΔK^{S*} , again vanishes, and the easy interfacial crack would begin to propagate (in the absence of mode mixity) in a self-similar manner right at the Griffith/Irwin critical stress intensity factor. Bond breaking would be smooth and continuous. As before, the same super-

lattice, with one easy and the second one difficult, either $(010)[001] \times [100] / (001)[0\bar{1}0] \times [\bar{1}00]$ or $(010)[001] \times [100] / (\bar{1}00)[0\bar{1}0] \times [001]$ cleavage systems serving as the interface, ΔK^{S*} , also vanishes, and the interfacial crack would begin to propagate (in the absence of mode mixity) on the easier side of and parallel to the interface at the Griffith/Irwin critical stress intensity factor. Bond breaking would be smooth and continuous on the easier side, but discontinuous and abrupt on the tougher side of the interface. A similar situation prevails for the $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{Si}_3\text{N}_4$ superlattice, with one difficult and the second one easy, $(010)[001] \times [100] / (\bar{1}00)[0\bar{1}0] \times [001]$, serving as the interface.

For the orthorhombic perovskite/HCP $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{Si}_3\text{N}_4$ superlattice, with both easy $(001)[100] \times [010] / (001)[0\bar{1}0] \times [\bar{1}00]$ cleavage systems serving as the interface, the SCD barrier, ΔK^{S*} , again vanishes, and the easy interfacial crack would begin to propagate (in the absence of mode mixity) in a self-similar manner right at the Griffith/Irwin critical stress intensity factor. Similar results follow for the orthorhombic perovskite/FCC rock salt $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{MgO}$ superlattice, with both easy $(001)[100] \times [010] / (\bar{1}10)[001] \times [110]$ cleavage systems serving as the interface.

For the perovskite orthorhombic/FCC rock salt MgO bicrystalline superlattice, with both easy $(001)[100] \times [010] / (\bar{1}10)[001] \times [110]$ cleavage systems serving as the interface, ΔK^{S*} would again vanish, and the resulting easy interfacial crack would begin to propagate (in the absence of mode mixity) in a self-similar manner right at the Griffith/Irwin critical stress intensity factor. Bond breaking would be smooth and continuous. As before for ΔK^{S*} for the same superlattice, with one easy and the second one difficult, $(001)[100] \times [010] / (010)[001] \times [100]$ would also vanish, and the interfacial crack would begin to propagate (in the absence of mode mixity) on the easier side of and parallel to the interface at the Griffith/Irwin critical stress intensity factor. Bond breaking would be smooth and continuous on the easier side, but discontinuous and abrupt on the tougher side of the interface.

Finally, for the perovskite orthorhombic/cubic perovskite $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{SrTiO}_3$ (respectively, $\text{YBa}_2\text{C}_3\text{O}_7/\text{SrTiO}_3$) bicrystalline superlattice, with both easy $(001)[100] \times [010] / (\bar{1}10)[001] \times [110]$ (respectively, $(\bar{1}10)[001] \times [110] / (\bar{1}10)[001] \times [110]$) cleavage systems serving as the interface, ΔK^{S*} would again vanish, and the resulting easy interfacial crack would experience a mixed-mode propagation/growth right at the Griffith/Irwin critical complex stress intensity factor. Rice [9] has discussed the computation and interpretation of the resulting complex stress intensity factor (S.I.F.) for an isotropic bimaterial interface crack; see Section 9.3 below. Bond breaking is expected to be smooth and continuous. The reason for this exceptional behavior of SrTiO_3 lies, as has been explained above, in its unusually high shear stiffness, c_{66} , which is substantially greater than its longitudinal stiffness, c_{11} . However, ΔK^{S*} for the same superlattices, with one easy and the second one difficult, $(001)[100] \times [010] / (010)[001] \times [100]$ for $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{SrTiO}_3$, or $(\bar{1}10)[001] \times [110] / (010)[001] \times [100]$ and $(010)[001] \times [100] / (\bar{1}10)[001] \times [110]$ for $\text{YBa}_2\text{C}_3\text{O}_7/\text{SrTiO}_3$ also vanish, and the interfacial crack would begin to propagate (in the absence of mode mixity) on the easier side of and parallel to the interface at the Griffith/Irwin critical stress intensity factor. Bond breaking would be smooth and continuous on the easier side, but discontinuous and abrupt on the tougher side of the interface.

9.3. Complex Stress Intensity Factor (S.I.F.) and Raman Spectroscopic Surface Measurement

9.3.1. Complex Stress Intensity Factor (S.I.F.)

Rice [9] has discussed the validity of the complex stress intensity factor, $K = K_I + iK_{II}$, as a characterizing parameter in the context of a two-dimensional bimaterial interface crack for material systems (of isotropic phases), for small-scale yielding and small-scale contact zones at the crack tip. The proportion of opening and shearing modes at the interfacial crack tip is characterized by means of the phase angle, given by $\psi = \text{Arctan}(K_{II}/K_I)$. Wang et al. [12] and Wu [10] have extended Rice's [9] analysis, and presented corresponding relations for interface cracks in monoclinic composites.

9.3.2. Raman Spectroscopic Surface Measurement of Carbon/Graphite Fiber–Epoxy Interfacial Bond

It has been argued by Chaudhuri et al. [36] that, in connection with a Raman spectroscopic study of a carbon fiber–epoxy interfacial debond, in real-life composite materials, the fiber–matrix interface (a sharp material discontinuity) is replaced by an interphase region (of the order of 0.5 μm thickness), which permits us to ignore the contact of the Comninou [89] type ($\varepsilon = 0$). Various factors that contribute to the formation of this interphase region are molecular entanglement following interdiffusion, electrostatic attraction, cationic groups at the ends of molecules attracted to an anionic surface that result in polymer matrix orientation at the fiber surface, chemical reaction, mechanical keying, etc. [90]. Additionally, the residual stress and coupling agents (e.g., silanes on glass fibers) applied to the fiber's surface have pronounced effects on the interfacial bond strength. Under these circumstances, the macroscopic (mean field, e.g., linear elasticity) analysis presented above may be considered to be only a first approximation to the detailed microscopic (fluctuating) state of stress at the carbon fiber–epoxy debond tip. It may further be noted that the oscillatory behavior characterizing the interpenetration of the component phases is not that unrealistic after all, but is rather a first-order approximation of the interdiffusion followed by molecular entanglement, chemical bonding, and other similar microscopic (kinetic) phenomena studied by materials scientists.

A close scrutiny of two asymptotic solutions for bimetals involving (i) the complex eigenvalues ($\varepsilon > 0$) and (ii) their real counterpart ($\varepsilon = 0$), in light of the Raman spectroscopic measurements, reveals that they represent two extreme cases of the interfacial (interphase) region of the carbon/graphite fibers with a polymeric matrix, such as epoxy [36]. While case (i) corresponds to an idealized carbon fiber with the surface layer(s) being comprised of completely disordered (amorphous) carbon resembling activated charcoal ($R = I_{A1g}/I_{E2g} = 1$), case (ii) represents an idealized version of graphite fiber with the surface layer(s) consisting of a completely ordered (crystalline) carbon lattice resembling stress-annealed pyrolytic graphite ($R = 0$). Actual carbon/graphite fibers, both commercial and experimental (experimentally investigated by Chaudhuri et al. [36]), fall somewhere in between the two idealized extremes with $0 < R < 1$. Therefore, the interfacial debond nucleation and propagation in an actual carbon/graphite fiber/epoxy matrix composite will be governed by the solution with ε replaced by [36]:

$$\bar{\varepsilon} = \varepsilon R = \varepsilon(I_{A1g}/I_{E2g}), \quad (57)$$

where I_{A1g} and I_{E2g} represent the relative (Raman) intensities of the peaks corresponding to the A_{1g} (weak) and E_{2g} (strong) modes, respectively. R represents the degree of chemical functionality (potential for strong or covalent bond formation). R ranges from 0.22 (Morganite I) to 0.85 (Thornel 10), with the industry standard AS4 being 0.811, as reported by Tuinstra and Koenig [91]. For the experimental fibers (grown in a carefully controlled environment to mimic their commercial counterparts) investigated by Chaudhuri et al. [36], R ranges from 0.279 to 0.785.

9.4. Through-Thickness Distribution of Stress Intensity Factors (Fracture Toughness) and Energy Release Rates (Fracture Energy)

Figure 2a,b show variations in the normalized stress intensity factor, $K_{ij}^*(z) = K_{ij}(z)/K_{ij,\max}$, $i = \text{I, II, III}$, $j = 1, 2$, through the thickness of a bicrystalline superlattice plate, weakened by the through-crack investigated here. Figure 2a shows the through-thickness variation in the stress intensity factor for a far-field symmetrically distributed hyperbolic sine (modes I, II, and III) load, while its antisymmetric counterpart, not encountered in two-dimensional analyses can be deemed associated with the singular residual stress field [92] and is displayed in Figure 2b. Figure 3 shows the corresponding variation in the energy release rate, G^* , through the top half of the plate thickness. For through-thickness symmetric far-field loading, the crack is expected to grow through thickness in a stable manner till the stress intensity factor or the energy release rate reaches its critical

value at the maximum location (just below the top and bottom surfaces). With a further increase in the magnitude of the far-field loading, unstable crack growth is expected to progressively spread throughout the plate thickness. For skew-symmetric loading, as reported on earlier occasions [16], the bottom half will experience crack closure. Such types of results describing the three-dimensional distribution of stress intensity factors and energy release rates have only recently become available in fracture mechanics literature.

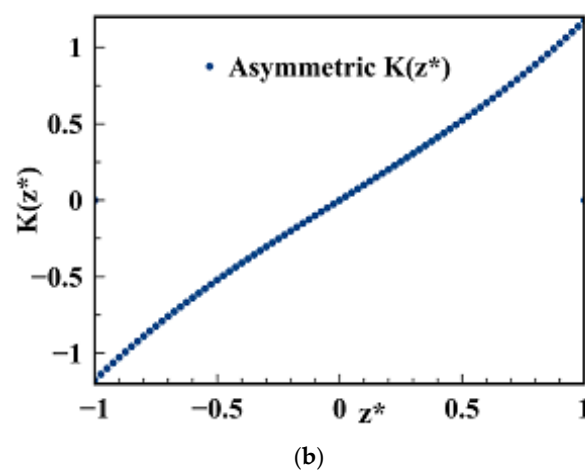
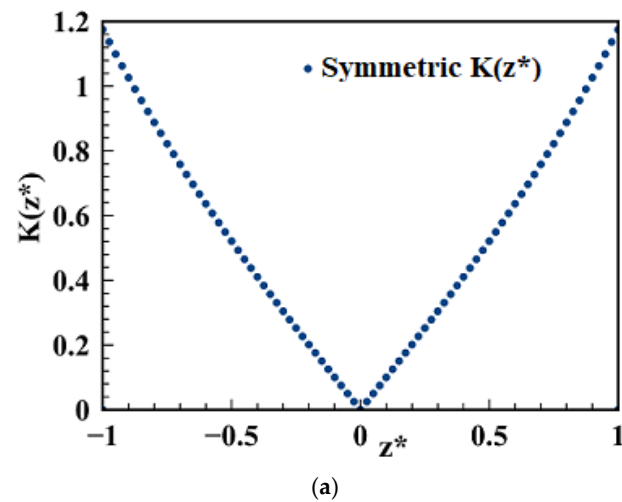


Figure 2. Variation in stress intensity factors through thickness for sine hyperbolic load: (a) symmetric and (b) skew-symmetric.

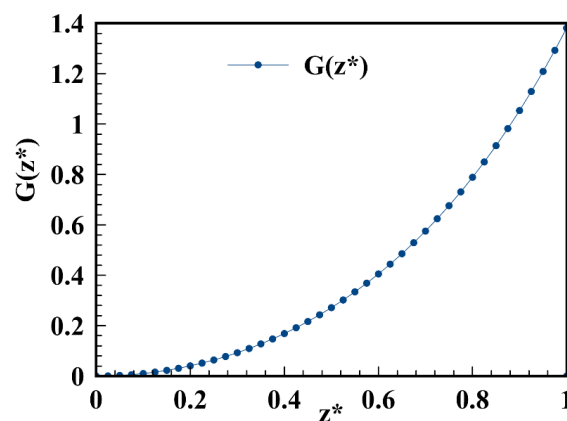


Figure 3. Variation in (modes I, II, or III) energy release rate through thickness due to far-field sine hyperbolic load.

10. Summary and Conclusions

A recently developed eigenfunction expansion method, based in part on the separation of the thickness variable and partly utilizing a modified Frobenius-type series expansion in terms of affine-transformed x-y coordinate variables of the Eshelby–Stroh type, is employed for obtaining three-dimensional asymptotic displacement and stress fields in the vicinity of the front of an interfacial crack weakening an infinite pie-shaped bicrystalline superlattice plate, of finite thickness, formed as a result of a mono-crystalline metal or superconductor film deposited over a substrate. The bicrystalline superlattice is made of orthorhombic (tetragonal, hexagonal, and cubic as special cases) phases, and is subjected to the far-field extension/bending, in-plane shear/twisting, and anti-plane shear loadings distributed through the thickness. Crack-face boundary and interface contact conditions as well as those that are prescribed on the top and bottom surfaces of the bicrystalline superlattice plate are exactly satisfied.

It also extends a recently developed concept of the lattice crack deflection (LCD) barrier to its superlattice counterpart, christened the superlattice crack deflection (SCD) energy barrier, for studying interfacial crack path instability, which can explain crack deflection from a difficult interface to an easier neighboring cleavage system. Additionally, the relationships of the nature (easy/easy, easy/difficult, or difficult/difficult) of interfacial cleavage systems based on the present solutions with the structural chemistry aspects of the component phases (such as orthorhombic, tetragonal, hexagonal, as well as FCC (face-centered cubic) transition metals and perovskites) of the superlattice are also investigated.

Important conclusions drawn from this study can be listed as follows:

(i) Atomistic-scale modeling of interfacial cracks requires a consideration of both long-range elastic interactions and short-range chemical reactions. The Griffith thermodynamic-based theory does not take the latter into account, and hence must be regarded as only a necessary condition (albeit being still very useful and widely employed), but not as sufficient.

(ii) The effect of short-range chemical reactions can be adequately captured by elastic properties-based parameters, such as the planar anisotropic ratio, A_j , or equivalently, the normalized elastic parameter, κ_j , $j = 1, 2$. This is because the elastic properties are controlled by various aspects of the underlying structural chemistry of single crystals, such as the Bravais lattice type, bonding (covalent, ionic, and metallic), bonding (including hybridized) orbitals, electro-negativity of constituent atoms in a compound, polarity, etc. More specifically, the elastic properties of superconducting $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ are strongly influenced by oxygen non-stoichiometry (as well as various structural defects).

(iii) A single dimensionless parameter, such as the planar anisotropic ratio, A_j , or equivalently, the normalized elastic parameter, κ_j , $j = 1, 2$, can serve as the Holy Grail quantity for an *a priori* determination of the status of a cleavage system to be easy or difficult, very much akin to the Reynold's number for fluid flow problems, crossing a critical value that signifies transition from one regime to another. Here, the planar anisotropic ratio, A_j , or equivalently, the normalized elastic parameter, κ_j , $j = 1, 2$, for a (010)[001] $\times$ [100] cleavage system, crossing the critical value of 1 or $\sqrt{c_{22}^{(j)}/c_{11}^{(j)}}$, $j = 1, 2$, respectively, signifies transitioning from self-similar crack growth or propagation to crack deflection or turning from a difficult cleavage system onto a nearby easy one. This is a significant qualitative as well as quantitative improvement over two-parameter-based models, suggested by previous researchers, e.g., [13], in the context of two-dimensional anisotropic fracture mechanics.

(iv) Just as the introduction of the Reynold's number facilitated the design and setting up of experiments in addition to experimental verification of analytical and computational solutions in fluid dynamics, the accuracy and efficacy of the available test results on elastic constants of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ single crystals, measured by modern experimental techniques with resolutions at the atomic scale or nearly so, such as X-ray diffraction, ultrasound technique, neutron diffraction/scattering, Brillouin spectroscopy/scattering, resonant ultrasound spectroscopy, and the like, are assessed with a powerful theoretical analysis of crack path stability/instability, in part based on a single dimensionless parameter, such as the planar anisotropic ratio, A_j , $j = 1, 2$.

(v) Experimental determination of the surface energy, Γ_j , $j = 1, 2$, of the component phases or the corresponding interfacial energy, Γ_{int} , of a bicrystalline superlattice can sometimes be notoriously challenging, due to the presence of micro-to-nanoscale defects, such as porosity, dislocation, twin boundaries, misalignment of bonds with respect to the loading axis, and the like. In contrast, the above-derived bond shear strain at superlattice crack deflection, γ_{bd}^s , and superlattice crack deflection (SCD) barrier, ΔK^{s*} , are, relatively speaking, much easier in comparison to the determination of surface or interfacial energy.

(vi) Computed complex eigenvalues, $s = 0.5 \pm i\varepsilon$, for Au/MgO, and $\text{YBa}_2\text{C}_3\text{O}_7/\text{SrTiO}_3$, bicrystalline superlattices, with $(010)[001] \times [100]/(010)[001] \times [100]$ serving as the interface suggest that the corresponding interfacial cracks would propagate in a mixed (I/II) mode. Likewise, for the bicrystalline superlattice, $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{SrTiO}_3$ (respectively, $\text{YBa}_2\text{C}_3\text{O}_7/\text{SrTiO}_3$) with $(001)[100] \times [010]/(\bar{1}10)[001] \times [110]$ (respectively, $(\bar{1}10)[001] \times [110]/(\bar{1}10)[001] \times [110]$) cleavage systems serving as the interface, the computed eigenvalues are also complex, resulting in a mixed (I/II)-mode interfacial crack growth.

(vii) For the bicrystalline superlattice, Au/MgO (respectively, $\text{YBa}_2\text{C}_3\text{O}_7/\text{SrTiO}_3$), with both difficult cleavage systems, $(010)[001] \times [100]/(010)[001] \times [100]$, serving as the interface, with the bond shear strain at superlattice crack deflection, γ_{bd}^s , value of 0.4710 (respectively, 0.5202) and superlattice crack deflection (SCD) barrier, ΔK^{s*} , value of 0.7324 (resp., 0.6240), the interfacial crack would encounter a tough interface, and would initially be superlattice-trapped and/or experience a mixed-mode propagation in a “difficult” manner till an applied load somewhat higher than its Griffith/Irwin mixed-mode interfacial fracture toughness counterpart—quantified by ΔK^{s*} —is reached, and thence deflect onto the available easier cleavage system, $\{\bar{1}10\}\langle 001 \rangle \times \langle 110 \rangle$, of the component phase with the lower LCD barrier, $\Delta K^* = 0.6414$ for MgO (0.5114 for SrTiO_3). In addition, bond breaking would not be continuous, but abrupt.

(viii) In contrast, for the perovskite orthorhombic/cubic perovskite $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{SrTiO}_3$ (respectively, $\text{YBa}_2\text{C}_3\text{O}_7/\text{SrTiO}_3$) bicrystalline superlattice, with both easy $(001)[100] \times [010]/(\bar{1}10)[001] \times [110]$ (respectively, $(\bar{1}10)[001] \times [110]/(\bar{1}10)[001] \times [110]$) cleavage systems serving as the interface, both bond shear strain at superlattice crack deflection, γ_{bd}^s , and superlattice crack deflection (SCD) barrier, ΔK^{s*} , vanish, and the resulting easy interfacial crack would experience a mixed-mode propagation/growth right at the Griffith/Irwin-based critical complex stress intensity factor (S.I.F.), the computation and interpretation of which is expounded by Rice’s [9] extension from a two-dimensional isotropic bimaterial interface crack to its anisotropic counterpart. Bond breaking is expected to be smooth and continuous.

(ix) For the Au/ Si_3N_4 or $\text{YBa}_2\text{C}_3\text{O}_7/\text{Si}_3\text{N}_4$ superlattice, with both easy cleavage systems, either $(\bar{1}10)[001] \times [110]/(001)[0\bar{1}0] \times [\bar{1}00]$ or $(\bar{1}10)[001] \times [110]/(\bar{1}00)[0\bar{1}0] \times [001]$, serving as the interface, both bond shear strain at superlattice crack deflection, γ_{bd}^s , and superlattice crack deflection (SCD) barrier, ΔK^{s*} , vanish, and the easy interfacial crack would begin to propagate (in the absence of mode mixity) in a self-similar manner right at the Griffith/Irwin critical stress intensity factor. Likewise, a $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{Si}_3\text{N}_4$ superlattice, with both easy cleavage systems, either $\{001\}\langle 100 \rangle \times \langle 010 \rangle/(001)[0\bar{1}0] \times [\bar{1}00]$ or $\{001\}\langle 100 \rangle \times \langle 010 \rangle/(\bar{1}00)[0\bar{1}0] \times [001]$, serving as the interface, would elicit a similar behavior. Bond breaking would be smooth and continuous.

(x) Other examples of superlattices, with both easy cleavage systems, include the Au/MgO (respectively, $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{MgO}$) bicrystalline superlattice with $(\bar{1}10)[001] \times [110]/(\bar{1}10)[001] \times [110]$ (respectively, $\{001\}\langle 100 \rangle \times \langle 010 \rangle/(\bar{1}10)[001] \times [110]$) cleavage systems serving as the interface. A similar response also ensues for the $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{SrTiO}_3$ bicrystalline superlattice with $(010)[001] \times [100]/(\bar{1}10)[001] \times [110]$ or $(\bar{1}00)[001] \times [010]/(\bar{1}10)[001] \times [110]$ cleavage systems serving as the interface. Again, bond breaking would be smooth and continuous.

(xi) Interestingly, for the Au/MgO or $\text{YBa}_2\text{C}_3\text{O}_7/\text{SrTiO}_3$ superlattice, with one easy and the second one difficult, either $(010)[001] \times [100]/(\bar{1}10)[001] \times [110]$ or $(\bar{1}10)[001] \times [110]/(010)[001] \times [100]$ cleavage systems serving as the interface, the SCD barrier, ΔK^{s*} , also

vanishes, and the interfacial crack would begin to propagate (in the absence of mode mixity) on the easier side of and parallel to the interface at the Griffith/Irwin critical stress intensity factor. Bond breaking is expected to be smooth and continuous on the easier side, but discontinuous and abrupt on the tougher side of the interface.

(xii) Response similar to item (xi) ensues for the $\text{YBa}_2\text{C}_3\text{O}_{7-\delta}/\text{SrTiO}_3$ bicrystalline superlattice with $\{001\}\langle 100 \rangle \times \langle 010 \rangle / (010)[001] \times [100]$ cleavage systems serving as the interface. Likewise, the $\text{Au}/\text{Si}_3\text{N}_4$ or $\text{YBa}_2\text{C}_3\text{O}_7/\text{Si}_3\text{N}_4$ superlattice with one easy and the second one difficult, either $(010)[001] \times [100] / (001)[0\bar{1}0] \times [\bar{1}00]$ or $(010)[001] \times [100] / (\bar{1}00)[0\bar{1}0] \times [001]$ cleavage systems serving as the interface, produces the same outcome. Again, bond breaking is expected to be smooth and continuous on the easier side, but discontinuous and abrupt on the tougher side of the interface.

(xiii) Finally, the hitherto unavailable results, pertaining to the through-thickness variations in normalized stress intensity factors for a symmetrically distributed hyperbolic sine load and its skew-symmetric counterpart that also satisfy the boundary conditions on the top and bottom surfaces of the bicrystalline superlattice plate, in the vicinity of an interfacial crack front under investigation, bridge a longstanding gap in interfacial stress singularity/fracture mechanics literature.

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Appendix A Details of the Derivation of the Solution Involving Complex Roots for a $(010)[001] \times [100]$ Crack (Mode I/II Loading)

Some of the details of the mathematical derivation of the solution, involving complex roots, for an orthorhombic crystal plate, reinforced by $(010)[001]$ through-anticrack and subjected to mode I/II loading (Section 4, case (a)), are presented here. The components of displacement that satisfy the equilibrium Equation (1) can be expressed in the following form:

$$u_j(r, \theta, z) = r^s D_{bj}(z) (ik)^s \left[\left\{ (\cos(\theta) + \xi^{(j)} \sin(\theta))^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{s/2} \{ A_{1j} \cos(s\psi_j) + A_{2j} \sin(s\psi_j) \} \right. \\ \left. + \left\{ (\cos(\theta) - \xi^{(j)} \sin(\theta))^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{s/2} \{ A_{3j} \cos(s\psi'_j) + A_{4j} \sin(s\psi'_j) \} + O(r^{s+2}), \right. \quad (\text{A1a})$$

$$v_j(r, \theta, z) = r^s D_{bj}(z) (ik)^s \left[\left\{ \cos^2(\theta) + (\xi^{(j)} + \eta^{(j)})^2 \sin^2(\theta) \right\}^{s/2} \{ (H_{1j}A_{1j} + H_{2j}A_{2j}) \cos(s\psi_j) \right. \\ \left. + (H_{1j}A_{2j} - H_{2j}A_{1j}) \sin(s\psi_j) \} + \left\{ (\cos(\theta) - \xi^{(j)} \sin(\theta))^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{s/2} \{ -(H_{1j}A_{3j} \right. \\ \left. + H_{2j}A_{4j}) \cos(s\psi'_j) - (H_{1j}A_{4j} - H_{2j}A_{3j}) \sin(s\psi'_j) \} + O(r^{s+2}), \right. \quad (\text{A1b})$$

$$w_j(r, \theta, z) = O(r^{s+2}), \quad (\text{A1c})$$

and

$$\sigma_{xj}(r, \theta, z) = r^{s-1} D_{bj}(z) (ik)^s \left\langle \left\{ (\cos(\theta) + \xi^{(j)} \sin(\theta))^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{(s-1)/2} [(A_{1j} \{ c_{11}^{(j)} \right. \right. \\ \left. + (\xi^{(j)} H_{1j} - \eta^{(j)} H_{2j}) c_{12}^{(j)} \} + A_{2j} \{ (\eta^{(j)} H_{1j} + \xi^{(j)} H_{2j}) c_{12}^{(j)} \}) \cos((s-1)\psi_j) + (-A_{1j} \{ (\eta^{(j)} H_{1j} + \xi^{(j)} H_{2j}) c_{12}^{(j)} \} \right. \\ \left. + A_{2j} \{ c_{11}^{(j)} + (\xi^{(j)} H_{1j} - \eta^{(j)} H_{2j}) c_{12}^{(j)} \}) \sin((s-1)\psi_j)] + \left\{ (\cos(\theta) - \xi^{(j)} \sin(\theta))^2 \right. \\ \left. + \eta^{(j)2} \sin^2(\theta) \right\}^{(s-1)/2} [(A_{3j} \{ c_{11}^{(j)} + (\xi^{(j)} H_{1j} - \eta^{(j)} H_{2j}) c_{12}^{(j)} \} + A_{4j} \{ (\eta^{(j)} H_{1j} + \xi^{(j)} H_{2j}) c_{12}^{(j)} \}) \cos((s-1)\psi'_j) \right. \\ \left. + (-A_{3j} \{ (\eta^{(j)} H_{1j} + \xi^{(j)} H_{2j}) c_{12}^{(j)} \} + A_{4j} \{ c_{11}^{(j)} + (\xi^{(j)} H_{1j} - \eta^{(j)} H_{2j}) c_{12}^{(j)} \}) \sin((s-1)\psi'_j)] \right\rangle \quad (\text{A2a})$$

$$\begin{aligned} \sigma_{yj}(r, \theta, z) = r^{s-1} D_{bj}(z) (ik)^s s \left\langle \left\{ \left(\cos(\theta) + \xi^{(j)} \sin(\theta) \right)^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{(s-1)/2} \right. & \left[(A_{1j} \{ c_{12}^{(j)} \right. \\ & + \left(\xi^{(j)} H_{1j} - \eta^{(j)} H_{2j} \} c_{22}^{(j)} \} + A_{2j} \{ \left(\eta^{(j)} H_{1j} + \xi^{(j)} H_{2j} \} c_{22}^{(j)} \} \right) \cos((s-1)\psi_j) + (-A_{1j} \{ \left(\eta^{(j)} H_{1j} + \xi^{(j)} H_{2j} \} c_{22}^{(j)} \} \right. \\ & + A_{2j} \{ c_{12}^{(j)} + \left(\xi^{(j)} H_{1j} - \eta^{(j)} H_{2j} \} c_{22}^{(j)} \} \} \sin((s-1)\psi_j) \right] + \left\{ \left(\cos(\theta) - \xi^{(j)} \sin(\theta) \right)^2 \right. \\ & + \eta^{(j)2} \sin^2(\theta) \}^{(s-1)/2} \left[(A_{3j} \{ c_{12}^{(j)} + \left(\xi^{(j)} H_{1j} - \eta^{(j)} H_{2j} \} c_{22}^{(j)} \} + A_{4j} \{ \left(\eta^{(j)} H_{1j} + \xi^{(j)} H_{2j} \} c_{22}^{(j)} \} \right) \cos((s-1)\psi'_j) \right. \\ & \left. \left. + (-A_{3j} \{ \left(\eta^{(j)} H_{1j} + \xi^{(j)} H_{2j} \} c_{22}^{(j)} \} + A_{4j} \{ c_{12}^{(j)} + \left(\xi^{(j)} H_{1j} - \eta^{(j)} H_{2j} \} c_{22}^{(j)} \} \} \sin((s-1)\psi'_j) \right] \right] \right\rangle \end{aligned} \quad (A2b)$$

$$\begin{aligned} \tau_{xyj}(r, \theta, z) = r^{s-1} D_{b1}(z) (ik)^s s c_{66}^{(j)} \left\langle \left\{ \left(\cos(\theta) + \xi^{(j)} \sin(\theta) \right)^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{(s-1)/2} \right. & \left[\{ A_{1j} (\xi^{(j)} + H_{1j}) \right. \\ & + A_{2j} (\eta^{(j)} + H_{2j}) \} \cos((s-1)\psi_j) + \{ -A_{1j} (\eta^{(j)} + H_{2j}) + A_{2j} (\xi^{(j)} + H_{1j}) \} \sin((s-1)\psi_j) \right] \\ & + \left\{ \left(\cos(\theta) - \xi^{(j)} \sin(\theta) \right)^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{(s-1)/2} \left[\{ -A_{3j} (\xi^{(j)} + H_{1j}) - A_{4j} (\eta^{(j)} + H_{2j}) \} \cos((s-1)\psi'_j) \right. \\ & \left. + \{ A_{3j} (\eta^{(j)} + H_{2j}) - A_{4j} (\xi^{(j)} + H_{1j}) \} \sin((s-1)\psi'_j) \right] \right\rangle + O(r^{s+1}), \end{aligned} \quad (A2c)$$

$$\begin{aligned} \sigma_{zj}(r, \theta, z) = r^{s-1} D_{bj}(z) (ik)^s s \left\langle \left\{ \left(\cos(\theta) + \xi^{(j)} \sin(\theta) \right)^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{(s-1)/2} \right. & \left[(A_{1j} \{ c_{12}^{(j)} \right. \\ & + \left(\xi^{(j)} H_{1j} - \eta^{(j)} H_{2j} \} c_{23}^{(j)} \} + A_{2j} \{ \left(\eta^{(j)} H_{1j} + \xi^{(j)} H_{2j} \} c_{23}^{(j)} \} \right) \cos((s-1)\psi_j) + (-A_{1j} \{ \left(\eta^{(j)} H_{1j} + \xi^{(j)} H_{2j} \} c_{23}^{(j)} \} \right. \\ & + A_{2j} \{ c_{12}^{(j)} + \left(\xi^{(j)} H_{1j} - \eta^{(j)} H_{2j} \} c_{23}^{(j)} \} \} \sin((s-1)\psi_j) \right] + \left\{ \left(\cos(\theta) - \xi^{(j)} \sin(\theta) \right)^2 \right. \\ & + \eta^{(j)2} \sin^2(\theta) \}^{(s-1)/2} \left[(A_{3j} \{ c_{12}^{(j)} + \left(\xi^{(j)} H_{1j} - \eta^{(j)} H_{2j} \} c_{23}^{(j)} \} + A_{4j} \{ \left(\eta^{(j)} H_{1j} + \xi^{(j)} H_{2j} \} c_{23}^{(j)} \} \right) \cos((s-1)\psi'_j) \right. \\ & \left. \left. + (-A_{3j} \{ \left(\eta^{(j)} H_{1j} + \xi^{(j)} H_{2j} \} c_{23}^{(j)} \} + A_{4j} \{ c_{12}^{(j)} + \left(\xi^{(j)} H_{1j} - \eta^{(j)} H_{2j} \} c_{23}^{(j)} \} \} \sin((s-1)\psi'_j) \right] \right] \right\rangle \end{aligned} \quad (A2d)$$

$$\tau_{xzj}(r, \theta, z) = O(r^s), \quad \tau_{yzj}(r, \theta, z) = O(r^s). \quad (A2e,f)$$

$$\tau_{xzj}(r, \theta, z) = O(r^s), \quad \tau_{yzj}(r, \theta, z) = O(r^s).$$

where $s = 1 - \lambda$, λ being the strength or order of the stress singularity, and

$$D_{bj}(z) = D_{1j} \sin(\alpha z) + D_{2j} \cos(\alpha z), \quad j = 1, 2 \quad (A3)$$

$$H_{1j} = -\frac{\xi^{(j)} (\sqrt{c_{11}^{(j)} c_{22}^{(j)}} + c_{66}^{(j)})}{(c_{12}^{(j)} + c_{66}^{(j)})}, \quad H_{2j} = \frac{\eta^{(j)} (\sqrt{c_{11}^{(j)} c_{22}^{(j)}} - c_{66}^{(j)})}{(c_{12}^{(j)} + c_{66}^{(j)})}. \quad (A4a,b)$$

$$\cos(\psi_j(\theta)) = \frac{\cos(\theta) + \xi^{(j)} \sin(\theta)}{\left\{ (\cos(\theta) + \xi^{(j)} \sin(\theta))^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{1/2}}, \quad (A5a)$$

$$\sin(\psi_j(\theta)) = \frac{\eta^{(j)} \sin(\theta)}{\left\{ (\cos(\theta) + \xi^{(j)} \sin(\theta))^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{1/2}}, \quad (A5b)$$

$$\cos(\psi'_j(\theta)) = \frac{\cos(\theta) - \xi^{(j)} \sin(\theta)}{\left\{ (\cos(\theta) - \xi^{(j)} \sin(\theta))^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{1/2}}, \quad (A5c)$$

$$\sin(\psi'(\bar{\theta})) = \frac{-\eta \sin(\bar{\theta})}{\left\{ (\cos(\bar{\theta}) - \xi \sin(\bar{\theta}))^2 + \eta^2 \sin^2(\bar{\theta}) \right\}^{1/2}}, \quad (A5d)$$

A_{ij} , $i = 1, \dots, 4$, $j = 1, 2$, are undetermined coefficients (i.e., eigenvectors related to “stress intensity factors”). It may be noted that, since s or $\text{Re } s$ (when s is complex) is positive, all the higher-order terms in Equation (A2) vanish as $r \rightarrow 0$. The components of displacement can now be expressed in the cylindrical polar coordinate system as follows:

$$\begin{aligned}
u_{rj}(r, \theta, z) = r^s D_{bj}(z) (ik)^s & \left\langle \left\{ \left(\cos(\theta) + \zeta^{(j)} \sin(\theta) \right)^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{s/2} \left[\{ A_{1j} \cos(\theta) + \right. \right. \\
& (H_{1j}A_{1j} + H_{2j}A_{2j}) \sin(\theta) \} \cos(s\psi_j) + \{ A_{2j} \cos(\theta) + (H_{1j}A_{2j} - H_{2j}A_{1j}) \sin(\theta) \} \sin(s\psi_j) \Big] \\
& + \left\{ \left(\cos(\theta) - \zeta^{(j)} \sin(\theta) \right)^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{s/2} \left[\{ A_{3j} \cos(\theta) + (-H_{1j}A_{3j} + H_{2j}A_{4j}) \sin(\theta) \} \cos(s\psi'_j) \right. \\
& \left. \left. + \{ A_{4j} \cos(\theta) - (H_{1j}A_{4j} - H_{2j}A_{3j}) \sin(\theta) \} \sin(s\psi'_j) \right] \right\rangle + O(r^{s+2}),
\end{aligned} \tag{A6a}$$

$$\begin{aligned}
u_{\theta j}(r, \theta, z) = r^s D_{bj}(z) (ik)^s & \left\langle \left\{ \left(\cos(\theta) + \zeta^{(j)} \sin(\theta) \right)^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{s/2} \left[\{-A_{1j} \sin(\theta) + \right. \right. \\
& (H_{1j}A_{1j} + H_{2j}A_{2j}) \cos(\theta) \} \cos(s\psi_j) + \{-A_{2j} \sin(\theta) + (H_{1j}A_{2j} - H_{2j}A_{1j}) \cos(\theta) \} \sin(s\psi_j) \Big] \\
& + \left\{ \left(\cos(\theta) - \zeta^{(j)} \sin(\theta) \right)^2 + \eta^{(j)2} \sin^2(\theta) \right\}^{s/2} \left[-\{ A_{3j} \sin(\theta) + (H_{1j}A_{3j} - \right. \\
& \left. H_{2j}A_{4j}) \cos(\theta) \} \cos(s\psi'_j) - \{ A_{4j} \sin(\theta) + (H_{1j}A_{4j} + H_{2j}A_{3j}) \cos(\theta) \} \sin(s\psi'_j) \right] \Big] + O(r^{s+2}),
\end{aligned} \tag{A6b}$$

$$w_j(r, \theta, z) = O(r^{s+1}). \tag{A6c}$$

Similarly, the components of the asymptotic stress field can be conveniently expressed by using the standard transformation rule:

$$\begin{Bmatrix} \sigma_{rj} \\ \sigma_{\theta j} \\ \tau_{r\theta j} \end{Bmatrix} = \begin{bmatrix} \cos^2(\theta) & \sin^2(\theta) & \sin(2\theta) \\ \sin^2(\theta) & \cos^2(\theta) & -\sin(2\theta) \\ -\frac{1}{2} \sin(2\theta) & \frac{1}{2} \sin(2\theta) & \cos(2\theta) \end{bmatrix} \begin{Bmatrix} \sigma_{xj} \\ \sigma_{yj} \\ \tau_{xyj} \end{Bmatrix}, \tag{A7a}$$

$$\begin{Bmatrix} \tau_{rzj} \\ \tau_{\theta zj} \end{Bmatrix} = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix} \begin{Bmatrix} \tau_{xzj} \\ \tau_{yzj} \end{Bmatrix}. \tag{A7b}$$

The stress component, σ_{zj} , is as presented in (A2d).

Appendix B Details of the Derivation of the Solution Involving Imaginary Roots for a (010)[001]×[100] Crack (Mode I/II Loading)

This appendix provides some of the details of the mathematical derivation of the solution, involving imaginary roots, for an orthorhombic crystal plate, weakened by (010)[001] through-crack and subjected to mode I/II loading (Section 4, case (b)). The components of displacement that satisfy the equilibrium Equation (1) can be expressed in the following form:

$$\begin{aligned}
u_j(r, \theta, z) = r^s D_{bj}(z) (ik)^s & \left[\left\{ \cos^2(\theta) + \left(\zeta'^{(j)} + \eta'^{(j)} \right)^2 \sin^2(\theta) \right\}^{s/2} \{ A_{1j} \cos(s\psi_{1j}) + A_{2j} \sin(s\psi_{1j}) \} \right. \\
& \left. + \left\{ \cos^2(\bar{\theta}) + \left(\zeta'^{(j)} - \eta'^{(j)} \right)^2 \sin^2(\theta) \right\}^{s/2} \{ A_{3j} \cos(s\psi'_{1j}) + A_{4j} \sin(s\psi'_{1j}) \} \right] + O(r^{s+2}),
\end{aligned} \tag{A8a}$$

$$\begin{aligned}
v_j(r, \theta, z) = r^s D_{bj}(z) (ik)^s & \left[\left\{ \cos^2(\theta) + \left(\zeta'^{(j)} + \eta'^{(j)} \right)^2 \sin^2(\theta) \right\}^{s/2} \{ -H'_{1j}A_{2j} \cos(s\psi_{1j}) + H'_{1j}A_{1j} \sin(s\psi_{1j}) \} \right. \\
& \left. + \left\{ \cos^2(\theta) + \left(\zeta'^{(j)} - \eta'^{(j)} \right)^2 \sin^2(\theta) \right\}^{s/2} \{ -H'_{2j}A_{4j} \cos(s\psi'_{1j}) + H'_{2j}A_{3j} \sin(s\psi'_{1j}) \} \right] + O(r^{s+2}),
\end{aligned} \tag{A8b}$$

$$w_j(r, \theta, z) = O(r^{s+1}). \tag{A8c}$$

and

$$\begin{aligned} \sigma_{xj}(r, \theta, z) = r^{s-1} D_{bj}(z) (ik)^s \left\langle \left\{ \cos^2(\theta) + (\xi'^{(j)} + \eta'^{(j)})^2 \sin^2(\theta) \right\}^{(s-1)/2} \left\{ c_{11}^{(j)} + \right. \right. \\ \left. \left. H'_{1j}(\xi' + \eta') c_{12}^{(j)} \right\} \left\{ A_{1j} \cos((s-1)\psi_{1j}) + A_{2j} \sin((s-1)\psi_{1j}) \right\} + \left\{ \cos^2(\theta) + \right. \right. \\ \left. \left. (\xi'^{(j)} - \eta'^{(j)})^2 \sin^2(\theta) \right\}^{(s-1)/2} \left\{ c_{11}^{(j)} + H'_{2j}(\xi'^{(j)} - \eta'^{(j)}) c_{12}^{(j)} \right\} \left\{ A_{3j} \cos((s-1)\psi'_{1j}) + A_{4j} \sin((s-1)\psi'_{1j}) \right\} \right\rangle \end{aligned} \quad (\text{A9a})$$

$$\begin{aligned} \sigma_{yj}(r, \theta, z) = r^{s-1} D_{bj}(z) (ik)^s \left\langle \left\{ \cos^2(\theta) + (\xi' + \eta')^2 \sin^2(\theta) \right\}^{(s-1)/2} \left\{ c_{12}^{(j)} + \right. \right. \\ \left. \left. H'_{1j}(\xi'^{(j)} + \eta'^{(j)}) c_{22}^{(j)} \right\} \left\{ A_{1j} \cos((s-1)\psi_{1j}) + A_{2j} \sin((s-1)\psi_{1j}) \right\} + \left\{ \cos^2(\theta) + \right. \right. \\ \left. \left. (\xi'^{(j)} - \eta'^{(j)})^2 \sin^2(\theta) \right\}^{(s-1)/2} \left\{ c_{12}^{(j)} + H'_{2j}(\xi'^{(j)} - \eta'^{(j)}) c_{22}^{(j)} \right\} \left\{ A_{3j} \cos((s-1)\psi'_{1j}) + A_{4j} \sin((s-1)\psi'_{1j}) \right\} \right\rangle \end{aligned} \quad (\text{A9b})$$

$$\begin{aligned} \tau_{xyj}(r, \theta, z) = r^{s-1} D_{bj}(z) (ik)^s c_{66}^{(j)} \left\langle \left\{ \cos^2(\theta) + (\xi'^{(j)} + \eta'^{(j)})^2 \sin^2(\theta) \right\}^{(s-1)/2} \left\{ H'_{1j} \right. \right. \\ \left. \left. - (\xi'^{(j)} + \eta'^{(j)}) \right\} \left\{ -A_{2j} \cos((s-1)\psi_{1j}) + A_{1j} \sin((s-1)\psi_{1j}) \right\} + \left\{ \cos^2(\theta) + \right. \right. \\ \left. \left. (\xi'^{(j)} - \eta'^{(j)})^2 \sin^2(\theta) \right\}^{(s-1)/2} \left\{ H'_{2j} - (\xi'^{(j)} - \eta'^{(j)}) \right\} \left\{ -A_{4j} \cos((s-1)\psi_{1j}) + A_{3j} \sin((s-1)\psi_{1j}) \right\} \right\rangle \end{aligned} \quad (\text{A9c})$$

$$\begin{aligned} \sigma_{zj}(r, \theta, z) = r^{s-1} D_{bj}(z) (ik)^s \left\langle \left\{ \cos^2(\theta) + (\xi'^{(j)} + \eta'^{(j)})^2 \sin^2(\theta) \right\}^{(s-1)/2} \left\{ c_{12}^{(j)} + \right. \right. \\ \left. \left. H'_{1j}(\xi'^{(j)} + \eta'^{(j)}) c_{23}^{(j)} \right\} \left\{ A_{1j} \cos((s-1)\psi_{1j}) + A_{2j} \sin((s-1)\psi_{1j}) \right\} + \left\{ \cos^2(\theta) + \right. \right. \\ \left. \left. (\xi'^{(j)} - \eta'^{(j)})^2 \sin^2(\theta) \right\}^{(s-1)/2} \left\{ c_{12}^{(j)} + H'_{2j}(\xi'^{(j)} - \eta'^{(j)}) c_{23}^{(j)} \right\} \left\{ A_{3j} \cos((s-1)\psi'_{1j}) + A_{4j} \sin((s-1)\psi'_{1j}) \right\} \right\rangle \end{aligned} \quad (\text{A9d})$$

$$\tau_{xzj}(r, \theta, z) = O(r^s), \quad \tau_{yzj}(r, \theta, z) = O(r^s). \quad (\text{A9e,f})$$

where

$$H'_{1j} = -\frac{\left\{ \sqrt{c_{11}^{(j)} c_{22}^{(j)}} - c_{66}^{(j)} (\xi'^{(j)} + \eta'^{(j)})^2 \right\}}{(c_{12}^{(j)} + c_{66}^{(j)}) (\xi'^{(j)} + \eta'^{(j)})}, \quad H'_{2j} = \frac{\left\{ \sqrt{c_{11}^{(j)} c_{22}^{(j)}} - c_{66}^{(j)} (\xi'^{(j)} - \eta'^{(j)})^2 \right\}}{(c_{12}^{(j)} + c_{66}^{(j)}) (\xi'^{(j)} - \eta'^{(j)})}. \quad (\text{A10a,b})$$

and

$$\cos(\psi_{1j}(\theta)) = \frac{\cos(\theta)}{\left\{ \cos^2(\theta) + (\xi'^{(j)} + \eta'^{(j)})^2 \sin^2(\theta) \right\}^{1/2}}, \quad (\text{A11a})$$

$$\sin(\psi_{1j}(\theta)) = \frac{(\xi'^{(j)} + \eta'^{(j)}) \sin(\theta)}{\left\{ \cos^2(\theta) + (\xi'^{(j)} + \eta'^{(j)})^2 \sin^2(\theta) \right\}^{1/2}}, \quad (\text{A11b})$$

$$\cos(\psi'_{1j}(\theta)) = \frac{\cos(\theta)}{\left\{ \cos^2(\theta) + (\xi'^{(j)} - \eta'^{(j)})^2 \sin^2(\theta) \right\}^{1/2}}, \quad (\text{A11c})$$

$$\sin(\psi'_{1j}(\theta)) = \frac{(\xi'^{(j)} - \eta'^{(j)}) \sin(\theta)}{\left\{ \cos^2(\theta) + (\xi'^{(j)} - \eta'^{(j)})^2 \sin^2(\theta) \right\}^{1/2}}, \quad (\text{A11d})$$

It may be noted that, since s or $\text{Re } s$ (when s is complex) is positive, all the higher-order terms in Equation (A9) vanish as $r \rightarrow 0$. The components of displacement can now be expressed in the cylindrical polar coordinate system as follows:

$$u_{rj}(r, \theta, z) = r^s D_{bj}(z) (ik)^s \left\langle \left\{ \cos^2(\theta) + \left(\zeta'^{(j)} + \eta'^{(j)} \right)^2 \sin^2(\theta) \right\}^{s/2} \left[\{ A_{1j} \cos(\theta) - H'_{1j} A_{2j} \sin(\theta) \} \cos(s\psi_{1j}) \right. \right. \right. \\ \left. \left. \left. + \{ A_{2j} \cos(\theta) + H'_{1j} A_{1j} \sin(\theta) \} \sin(s\psi_{1j}) \right] + \left\{ \cos^2(\theta) + \left(\zeta'^{(j)} - \eta'^{(j)} \right)^2 \sin^2(\theta) \right\}^{s/2} \left[\{ A_{3j} \cos(\theta) \right. \right. \right. \\ \left. \left. \left. - H'_{2j} A_{4j} \sin(\theta) \} \cos(s\psi'_{1j}) + \{ A_{4j} \cos(\theta) + H'_{2j} A_{3j} \sin(\theta) \} \sin(s\psi'_{1j}) \right] \right\rangle + O(r^{s+2}), \quad (A12a)$$

$$u_{\theta j}(r, \theta, z) = r^s D_{bj}(z) (ik)^s \left\langle \left\{ \cos^2(\theta) + \left(\zeta'^{(j)} + \eta'^{(j)} \right)^2 \sin^2(\theta) \right\}^{s/2} \left[-\{ A_{1j} \sin(\theta) + H'_{1j} A_{2j} \cos(\theta) \} \cos(s\psi_{1j}) \right. \right. \right. \\ \left. \left. \left. + \{ -A_{2j} \sin(\theta) + H'_{1j} A_{1j} \cos(\theta) \} \sin(s\psi_{1j}) \right] + \left\{ \cos^2(\theta) + \left(\zeta'^{(j)} - \eta'^{(j)} \right)^2 \sin^2(\theta) \right\}^{s/2} \left[-\{ A_{3j} \sin(\theta) \right. \right. \right. \\ \left. \left. \left. + H'_{2j} A_{4j} \cos(\theta) \} \cos(s\psi'_{1j}) + \{ -A_{4j} \sin(\theta) + H'_{2j} A_{3j} \cos(\theta) \} \sin(s\psi'_{1j}) \right] \right\rangle + O(r^{s+2}), \quad (A12b)$$

$$w_j(r, \theta, z) = O(r^{s+1}). \quad (A12c)$$

Similarly, the components of the asymptotic stress field can be conveniently expressed by using the standard transformation rule, provided earlier in Equation (A7). The stress component, σ_z , is presented in Equation (A9d).

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