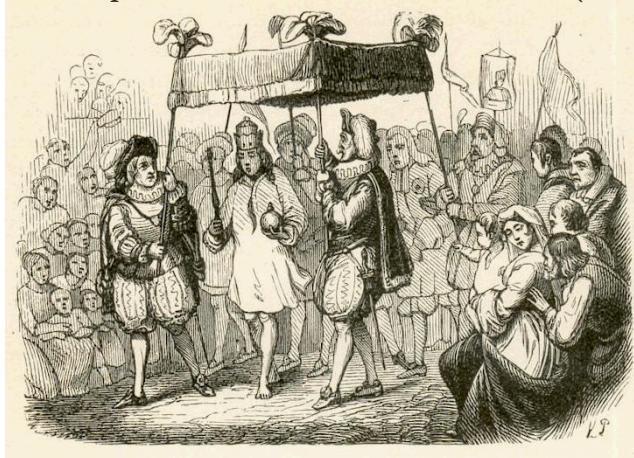


Exceptional service in the national interest



Mechanics of Finite (Interfacial) Cracks: Does the Emperor Have Any Clothes?

The Emperor's New Clothes, H.C. Andersen (1837)



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SAND201-XXX



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A perspective from two length scales demonstrating challenges when modeling interfacial cracks

1. An atomistic view

- Deconvoluting deformation mechanisms from interface structure
- Upscaling observations for fracture analysis

2. A continuum view

- Capturing interface (discrete) structure in a continuum setting
- Singular and oscillatory nature of mechanical fields

Continuum fracture mechanics: A mature field of theoretical mechanics

Dislocations and Cracks in Anisotropic Elasticity†

By A. N. STROH

Department of Physics, University of Sheffield

[Received March 13, 1958]

ABSTRACT

The solution of the elastic equations is considered for the case in which the state of the solid is independent of one of the three Cartesian coordinates. The stresses due to a dislocation, a wall of parallel dislocations, and a crack in an arbitrary non-uniform stress field are obtained. The results hold for the most general anisotropy in which no symmetry elements of the crystal are assumed.

§ 1. INTRODUCTION

ESHELBY *et al.* (1953) have developed the theory of anisotropic elasticity for a three dimensional state of stress in which the stress is independent of one of the Cartesian coordinates, and have applied this to find the stress field of a dislocation. In the present paper, which follows their treatment, the stresses due to a dislocation are treated more fully, and the interactions of dislocations considered; also, the stresses round a crack subjected to an arbitrary non-uniform applied stress are obtained. The object will be to present the results in a form which is, analytically, as simple as possible. It is hoped that, in applications of the theory, this will often allow of the properties of the system studied to be deduced without the need for numerical computation, and that when such computation is unavoidable, as when definite numerical values are required, the labour involved will be reduced to a minimum. For this purpose, the properties of a number of constants introduced in the theory and which are related to the elastic constants are investigated in some detail (§ 3). In § 2 some

Journal of Elasticity 26: 169–195, 1991.
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169 *Proc. R. Soc. Lond. A* 427, 331–358 (1990)
Printed in Great Britain

Interfacial dislocation and its applications to interface cracks in anisotropic bimaterials

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Received 3 April 1989; in revised form 20 June 1990

Abstract. Interfacial dislocations and cracks in anisotropic bimaterials are considered. The displacement and stress fields due to an interfacial dislocation are obtained in a real and simple form. Explicit solutions to the traction along the interface and the crack opening displacement for a Griffith interface crack are derived. Possible definitions of stress intensity factors are given which reduce to the classical definition for a crack in a homogeneous medium. It is found that a planar interface between dissimilar anisotropic solids is completely characterized by no more than 9 independent parameters. Some invariant properties of the dislocation and crack solutions under coordinate transformation are also discussed.

1. Introduction

Dislocations on grain boundaries and cracks along bimaterial interfaces are common interfacial phenomena in polycrystal alloys and composite materials. A dislocation in an isotropic bimaterial has been studied by Dundurs and Mura [1]. Explicit expressions of the traction on the interface due to an interfacial dislocation have been obtained by Comninou [2]. The two-dimensional problem of a crack in isotropic bimaterials has been studied extensively

Singularities, interfaces and cracks
in dissimilar anisotropic media

BY ZHIGANG SUO†

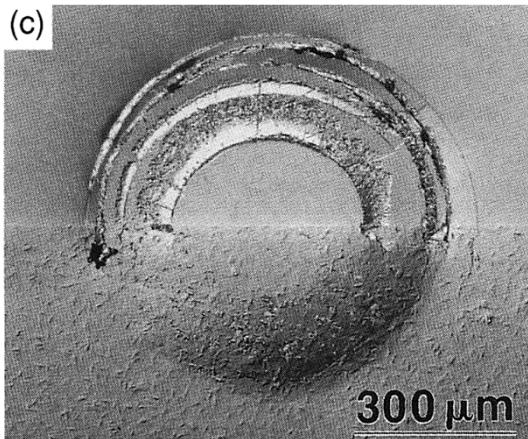
*Division of Applied Sciences, Harvard University, Cambridge,
Massachusetts 02138, U.S.A.*

(Communicated by Rodney Hill, F.R.S. – Received 5 April 1989)

For a non-pathological bimaterial in which an interface crack displays no oscillatory behaviour, it is observed that, apart possibly from the stress intensity factors, the structure of the near-tip field in each of the two blocks is independent of the elastic moduli of the other block. Collinear interface cracks are analysed under this non-oscillatory condition, and a simple rule is formulated that allows one to construct the complete solutions from mode III solutions in an isotropic, homogeneous medium. The general interfacial crack-tip field is found to consist of a two-dimensional oscillatory singularity and a one-dimensional square root singularity. A complex and a real stress intensity factors are proposed to scale the two singularities respectively. Owing to anisotropy, a peculiar fact is that the complex stress intensity factor scaling the oscillatory fields, however defined, does not recover the classical stress intensity factors as the bimaterial degenerates to be non-pathological. Collinear crack problems are also formulated in this context, and a strikingly simple mathematical structure is identified. Interactive solutions for singularity-interface and singularity-interface-crack are obtained. The general results are specialized to decoupled antiplane and in-plane deformations. For this important case, it is found that if a material pair is non-pathological for one set of relative orientations of the interface and the two solids, it is non-pathological for any set of orientations. For

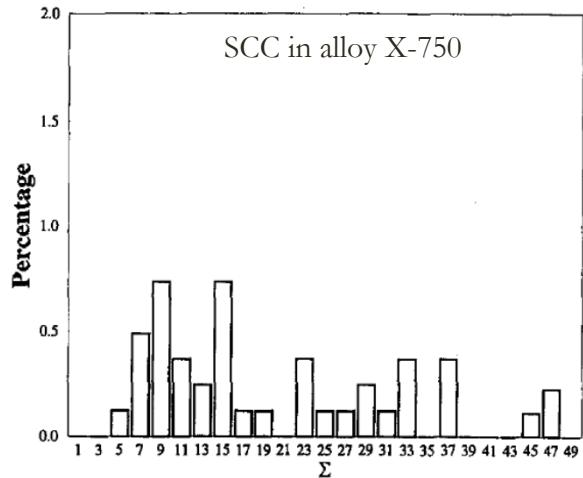
...But from a physical point of view, interfacial structure matters

Crack resistant glass/ceramic



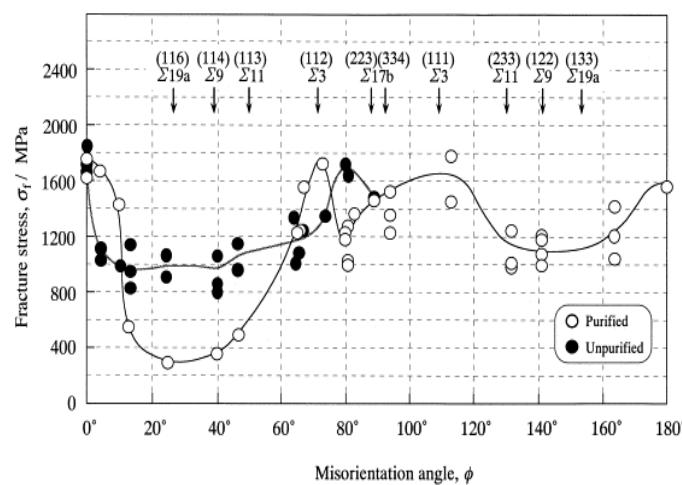
[Wuttiphaphan, 1996, JAmCeramSoc]

GB effects on intergranular SCC



[Pan, 1996, ActaMater]

Fracture stress in Mo bicrystals

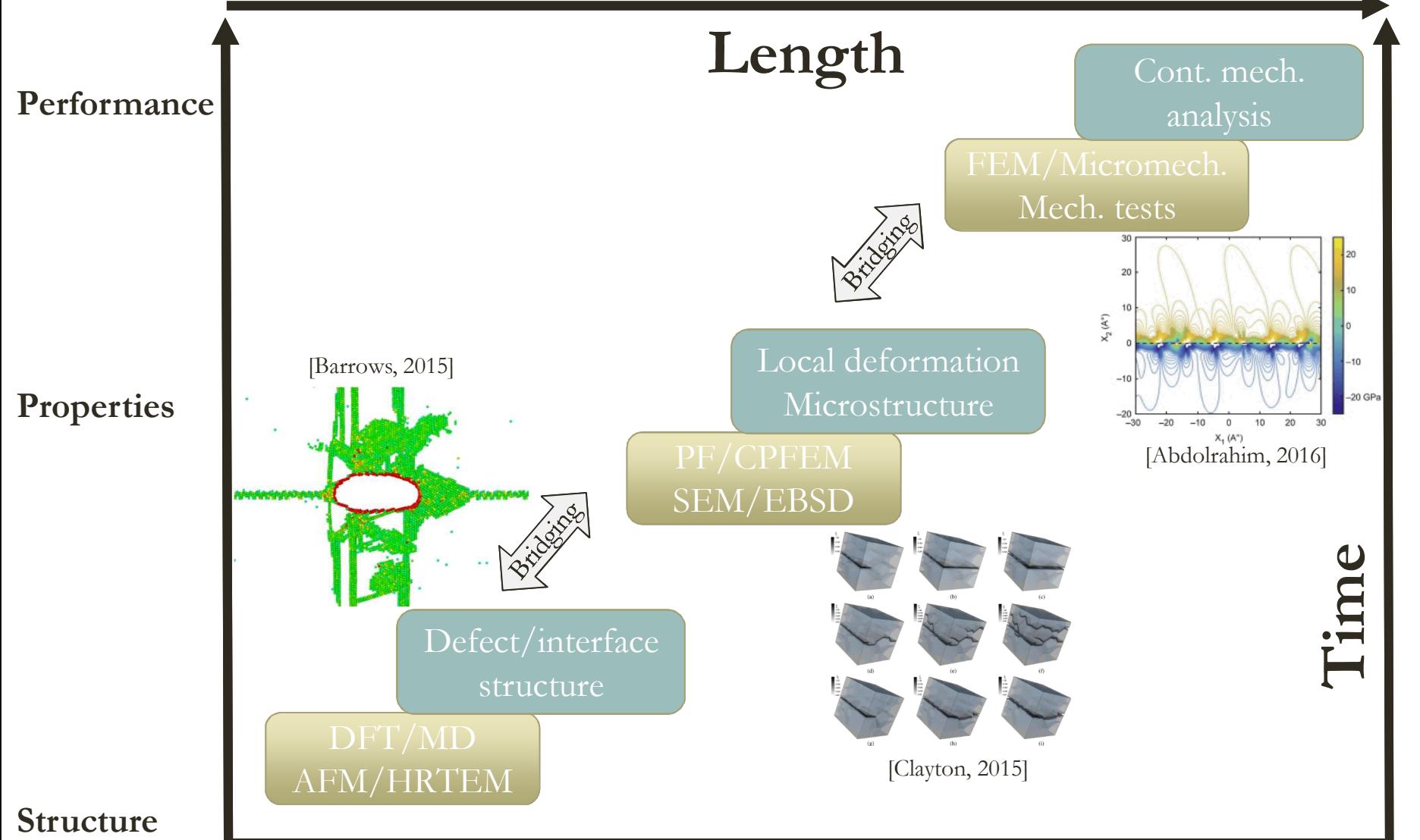


[Watanabe, 1999, ActaMater]

■ Interfacial attributes of importance:

- Elastic mismatch
- Degree of symmetry
- State of interfacial coherency (structure)
(physical and the chemical nature between both phases)

Capturing interfacial structure : an epic journey



Atomic scale
(10^{-11} - 10^{-8} m; 10^{-16} - 10^{-9} s)

Single crystal scale
(10^{-9} - 10^{-6} m; 10^{-10} - 10^{-1} s)

Polycrystal scale
(10^{-6} - 10^{-2} m; 10^{-3} - 10^2 s)

Component scale
(10^{-3} - 1 m; 10^{-3} - 10^2 s)

Some of the concerns associated with modeling the mechanics of interfacial cracks

1. **Fidelity** of the interface behavior representation

(usually where all the effort goes)

- Active mechanisms to include / appropriate constitutive behavior
- Accurate representation needed (2D vs. 3D for example)

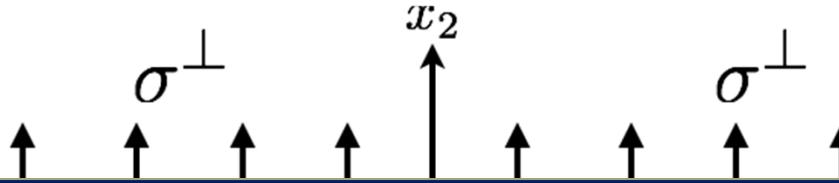
2. **Appropriate length scale** associated with interface mechanical behavior?

- Geometric consideration: Surface to volume ratio
- Type of analysis: atomistic vs. continuum (discrete vs. continuous)

3. **Boundary conditions:** load transfer across the boundary and its computational representation?

- Avoid artifacts from modeling methodology

Griffith crack problem



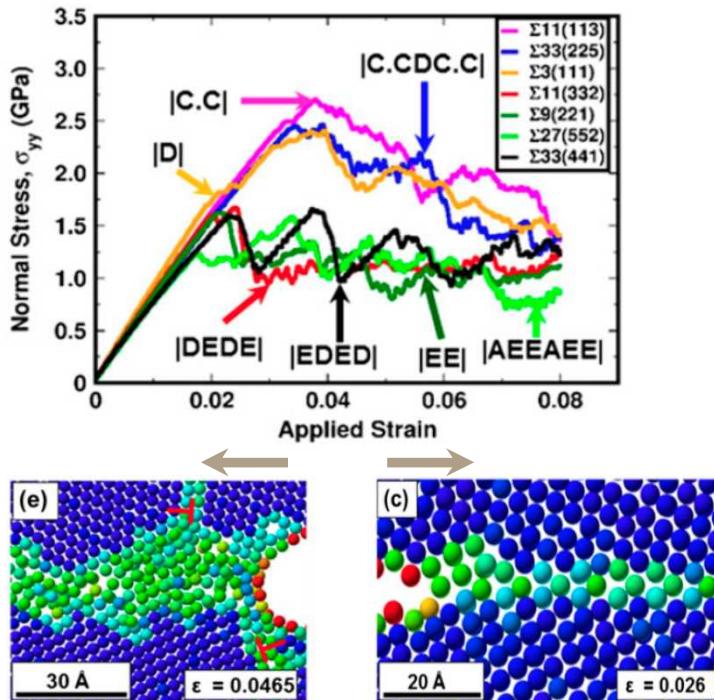
Scientific questions to be addressed

- Are there interfaces more susceptible to fracture?
 - Can we elucidate the coupling between structure and mechanical behavior?
 - If so, what are the characteristic structural features of interest?
- Can we “design” (in the sense of GB engineering) the microstructure to mitigate fracture?

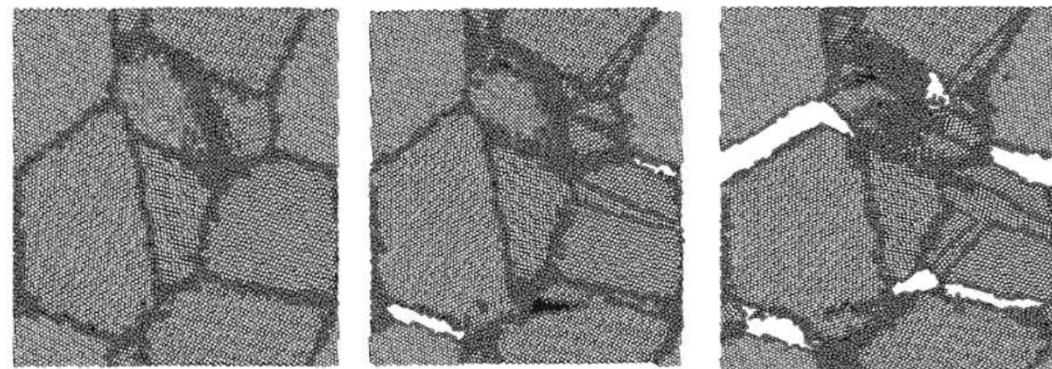


What is the most direct way of incorporating the interface structure into a modeling strategy?

Atomistic simulations is a “natural” tool to study fracture in metals



Strain rate driven fracture asymmetry in Al
(Adlakha et al., 2014)



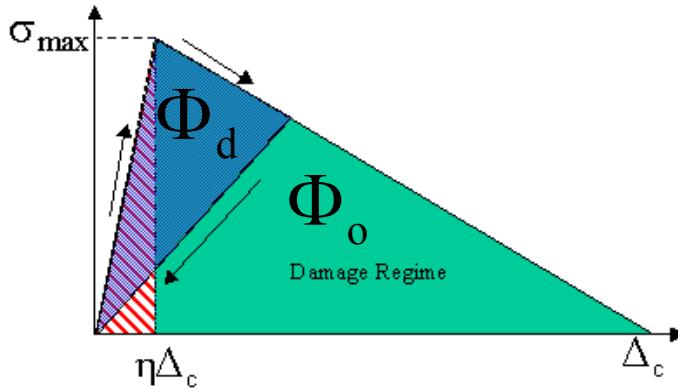
Strain rate driven fracture in nanocrystalline Mo
[Frederiksen et al., 2006]

- **Intrinsic tradeoffs from atomistics:**
 - Rate dependence (10^5 - 10^8 s $^{-1}$)
 - Reliable interatomic potential

Atomistic data needs to be upscaled

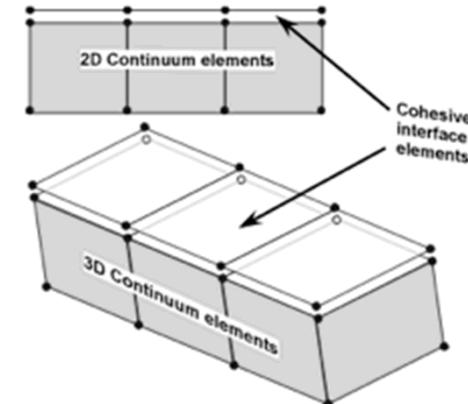
To simulate fracture at the mesoscale and continuum scale, traction-separation potentials are often considered

$$\mathbf{T} = -\frac{\partial \Phi}{\partial \Delta}$$



[Needleman, 1987]

[Zhou and Zhai, 1999]



[Scheider, 2008]

Atomistic simulation can provide structural level details:

- Account for dissipative mechanisms, such as dislocation nucleation and structural rearrangement at the interface during separation
- Distinguish interfaces with various degrees of coherency, misorientation, impurities

Simulating steady-state fracture

Step 1

Build grain boundary structure

Step 2

Equilibrate system under pre-tension

Step 3

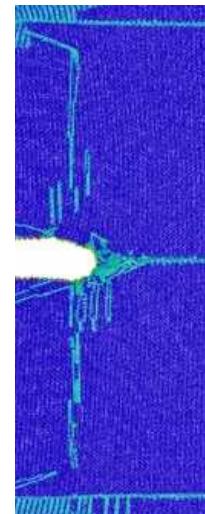
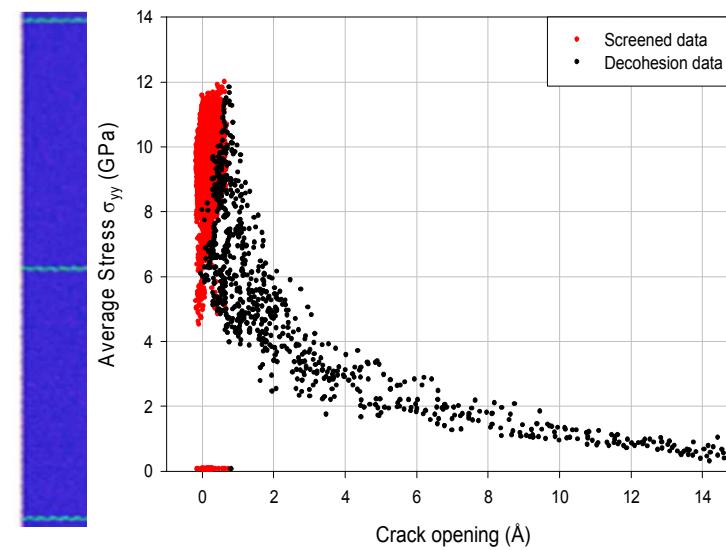
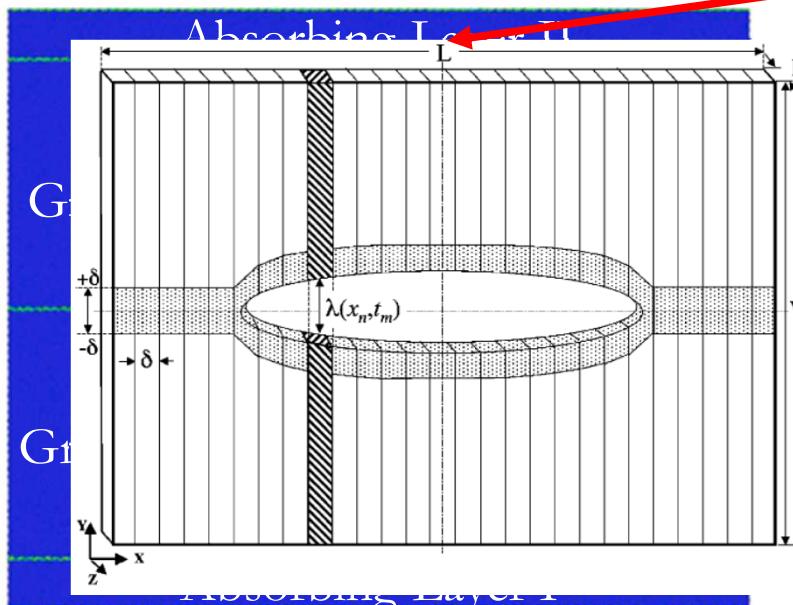
Introduce atomically sharp crack

Step 4

Allow crack growth under pre-tension

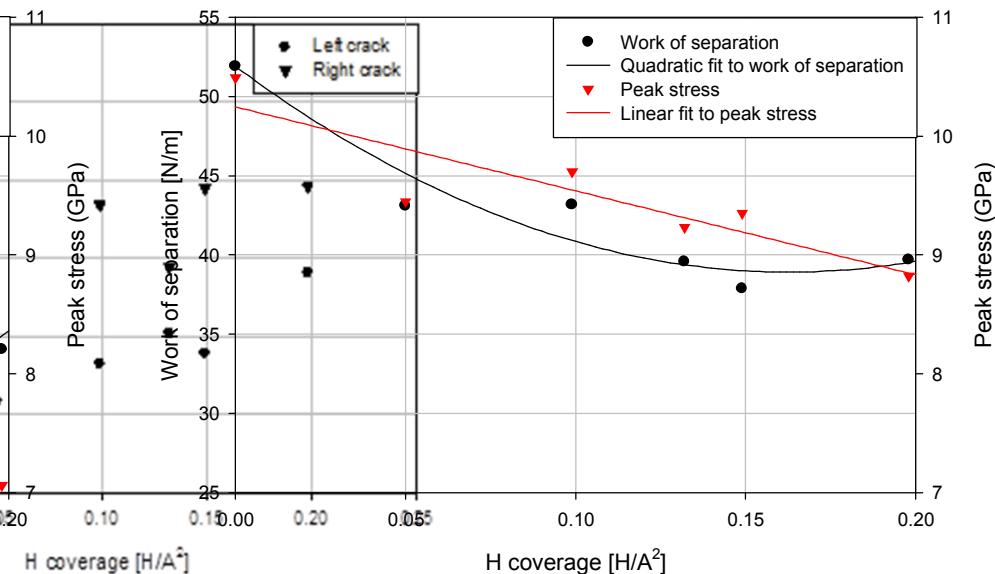
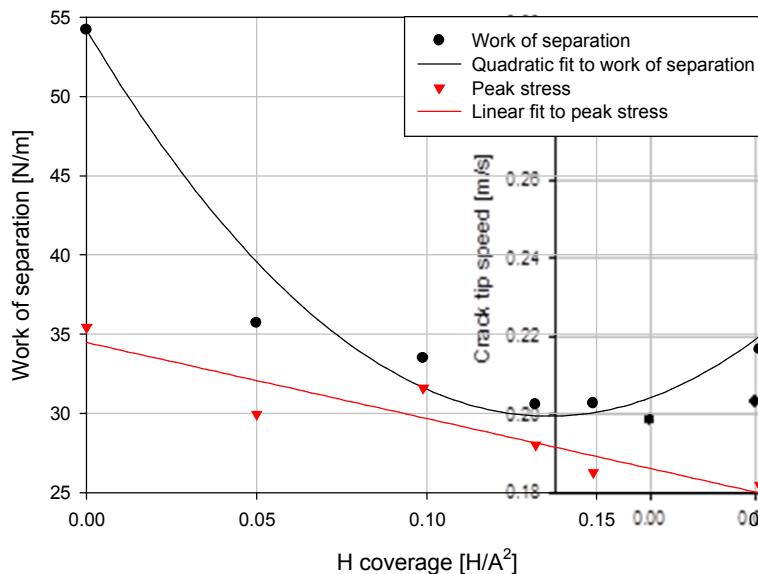
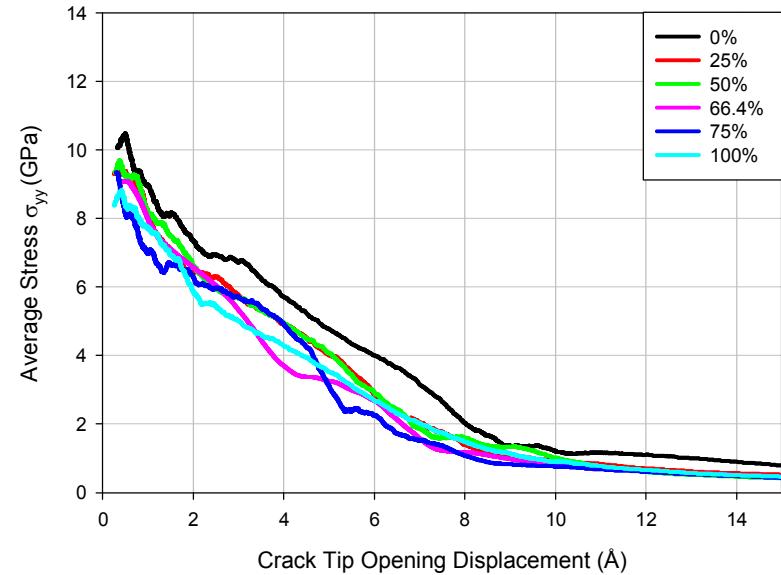
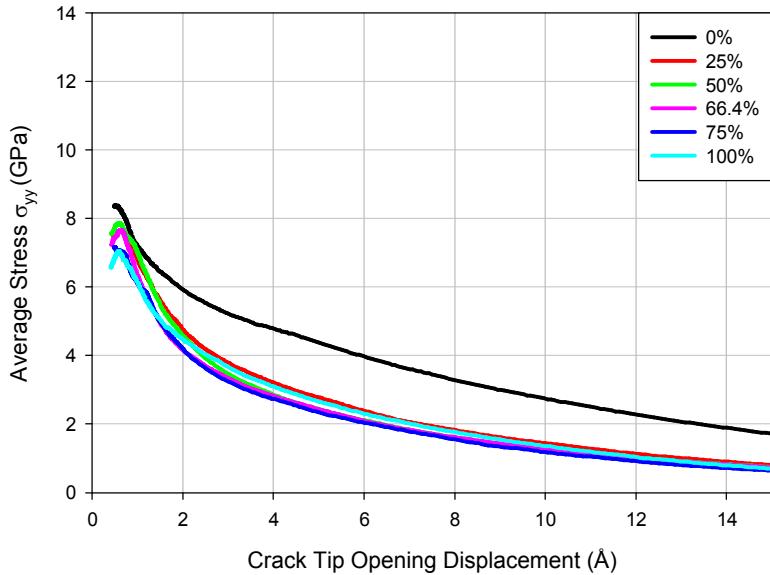
Step 5

Averaging to extract decohesion form



- Statistical driving characteristics imposed to mid-size cavity approach

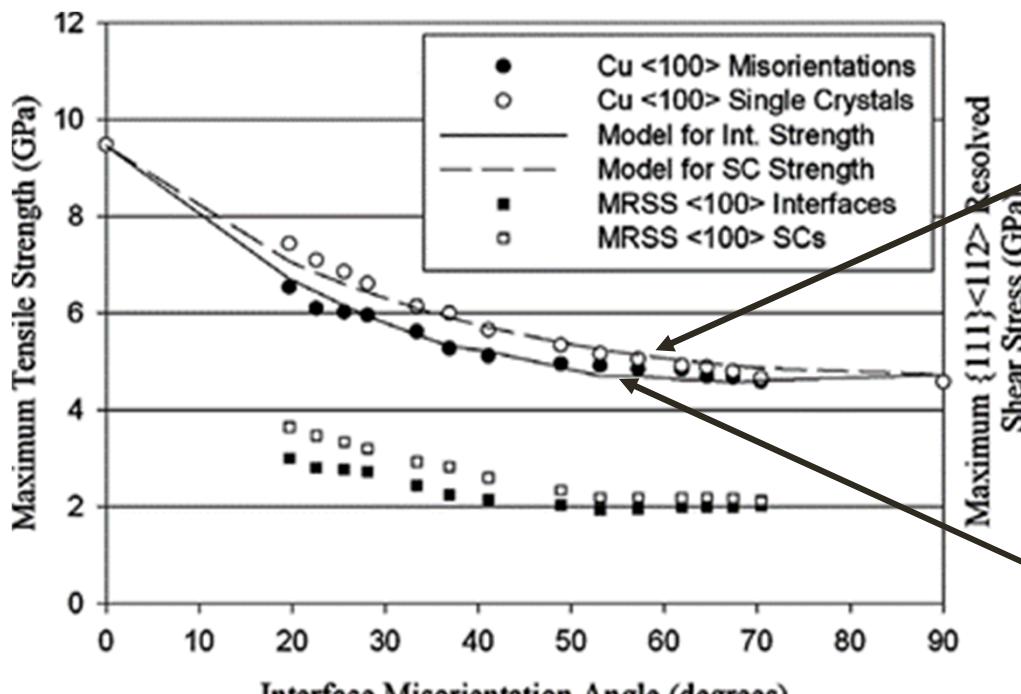
An example on H embrittlement of GB



Can we isolate the role of the interface structure when comparing various boundaries?



How can we deconvolute the role of interface structure from other factor?



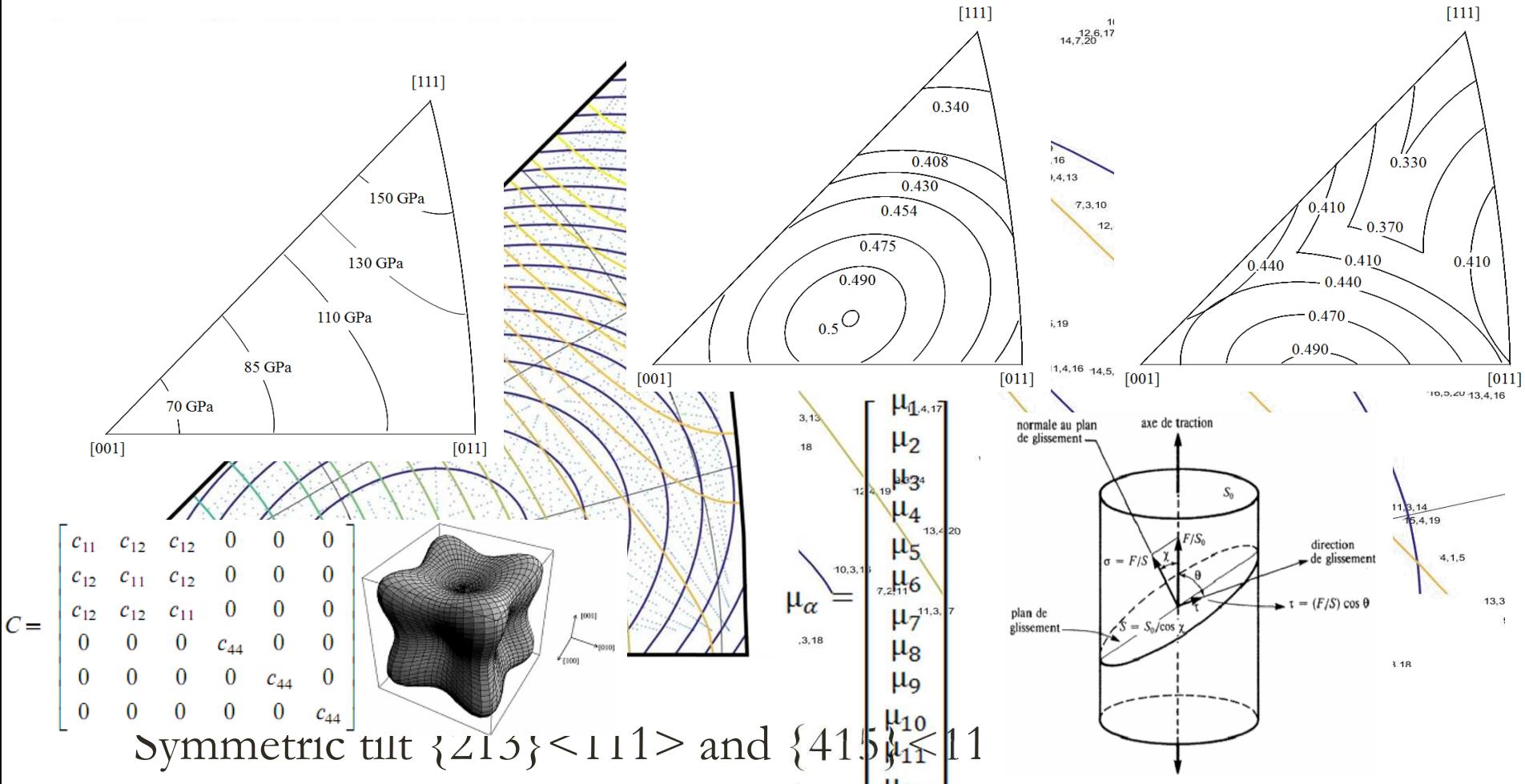
[Spearot, 2007]

Tensile stress necessary for homogeneous dislocation nucleation in single crystal models

Tensile stress necessary for heterogeneous dislocation nucleation from grain boundaries

Selecting grain boundary sets based on their mechanical attributes

- Matching plastic impedance and skip systems of sliding directions



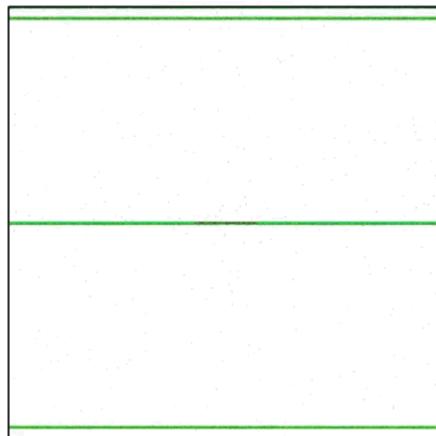
Symmetric tilt $\{115\} <111>$ and $\{415\} <111>$

$\{213\}$: SF = 0.46657, E = 232.6 GPa $\{415\}$: SF = 0.46657, E = 232.6 GPa

Isolating the role of the interface structure (1/3)

Crack propagation:

$$\{213\} \text{ STGB} + 0.198 \text{ H/nm}^2$$



Crack propagation:

$$\{415\} \text{ STGB} + 0.198 \text{ H/nm}^2$$

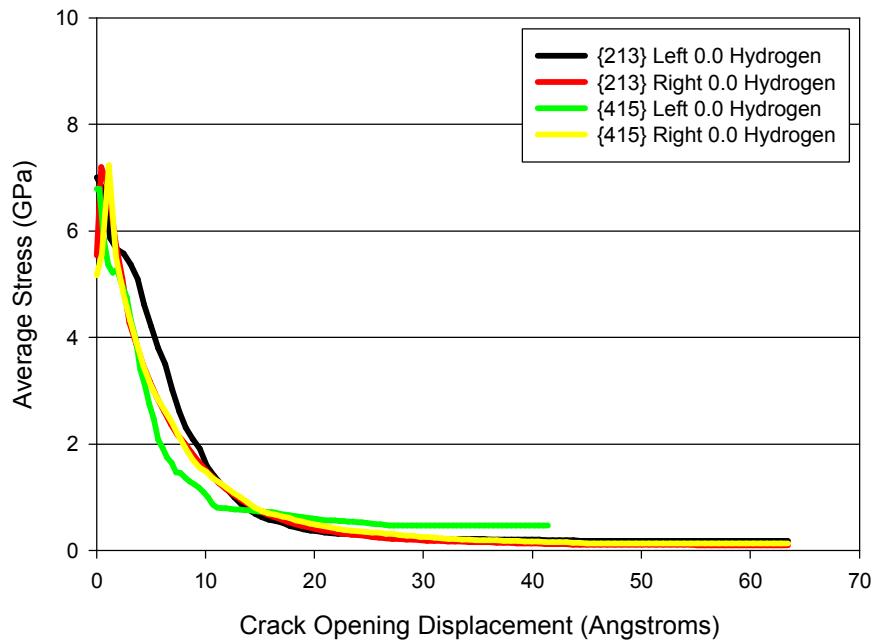


Plasticity similar for
both $\{213\}$ and $\{415\}$
as generally expected
from Schmid Factor

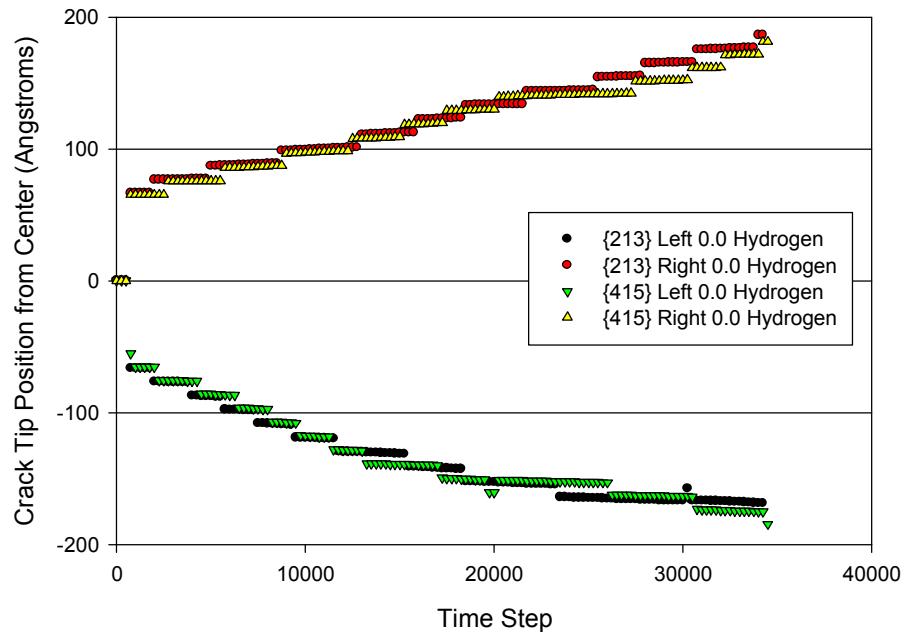
[Dingreville et al., Acta Mater, 2017]

Isolating the role of the interface structure (2/3)

▪ Hydrogen-free grain boundary decohesion



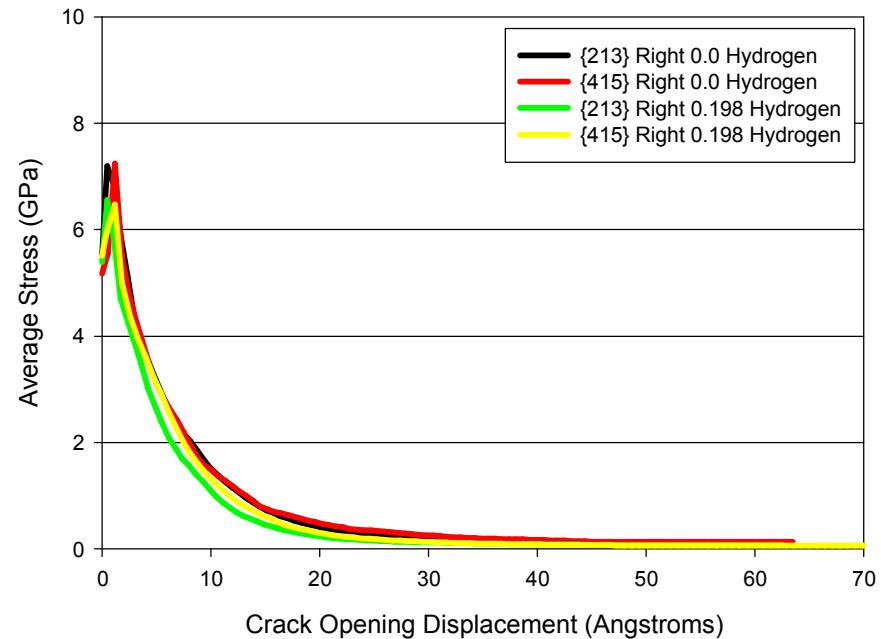
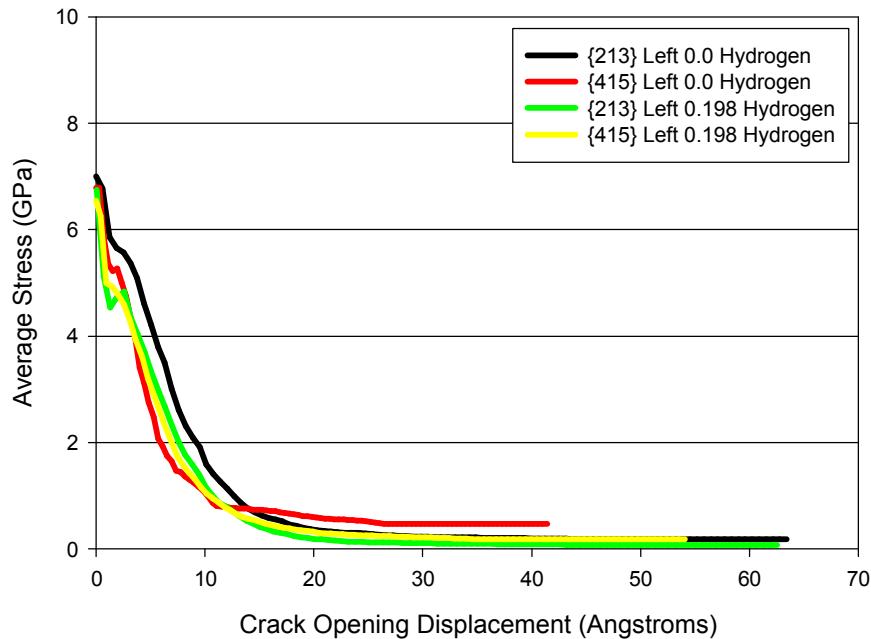
Some asymmetry of the decohesion response is apparent – role of grain boundary structure



Crack propagation rates are steady state within the first ~ 20000 time steps and not significantly different for $\{213\}$ and $\{415\}$ GBs – likely due to matching of lattice attributes

Isolating the role of the interface structure (3/3)

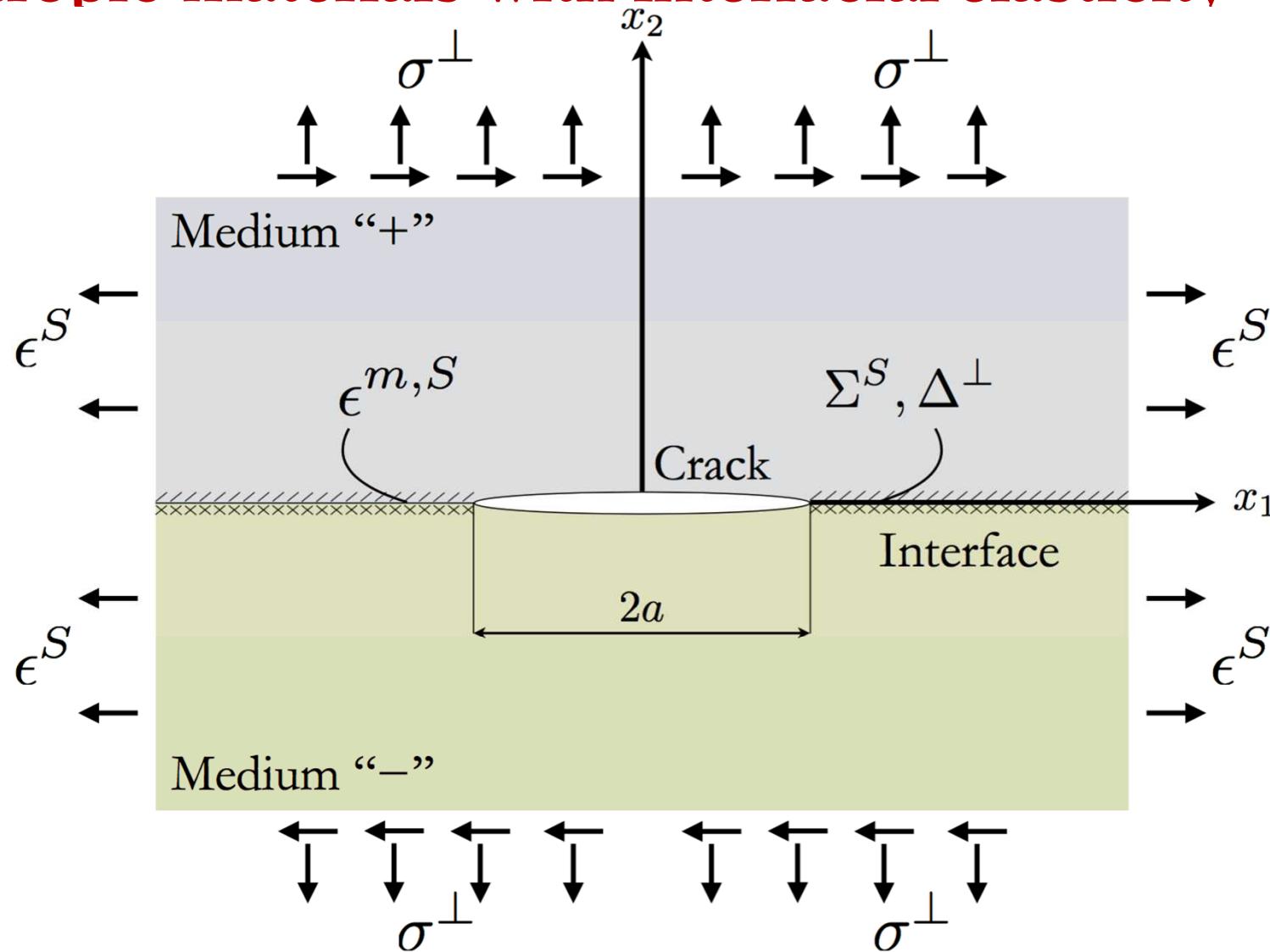
- Hydrogen-induced grain boundary decohesion



- Hydrogen appears to influence the decohesion response of the {415} GB more significantly than the {213} GB

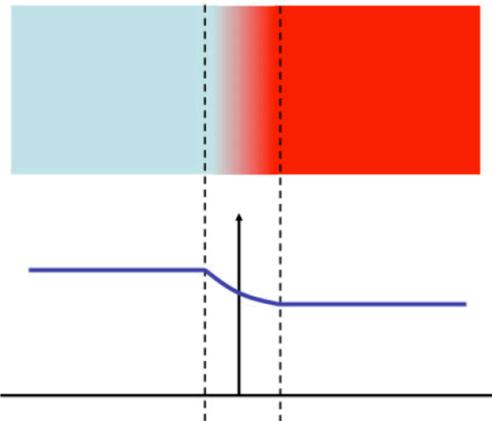
Can we incorporate the discrete
interface structure into a continuum
formulation?

A Griffith crack between two dissimilar anisotropic materials with interfacial elasticity



A generalized interfacial elasticity formulation considering interface structure

Interphase model



Dividing surface model



Surface stress: $\Sigma^S \frac{\partial \Gamma}{\partial \epsilon}$

Interfacial thermodynamic formulation: $\sigma^\perp \cdot \mathbb{H}^S$

$$\Gamma = \hat{\Gamma}(\epsilon^S, \epsilon^m, \sigma^\perp) = \int_0^\infty \Sigma_0^S [\Psi(\Phi^S) - \Psi(\epsilon^m)] dx + \oint_{-\infty}^0 :[\Phi^S(x) \sigma^\perp] \mathbb{H}^S dx$$

$$\frac{d\Gamma}{dt} \text{ Interfacial strain: } \epsilon \Delta^\perp \mathbb{D}^\perp \frac{\partial \Gamma}{\partial \sigma^\perp} + \mathbb{H}^S : \epsilon^m + \Lambda_0^\perp *$$

$$[\text{Dingreville et al., JMPS, 2014}] \quad * = \Lambda_0^\perp + \mathbb{K}^S : \epsilon^{m,S} + \Lambda^\perp \cdot \sigma^\perp - \mathbb{H}^S : \epsilon^S$$

Interface formalism introduces “seemingly imperfect” boundary conditions

$$[\![\mathbf{u}]\!] = \Delta^\perp$$

Displacement jump

$$\mathbf{n} \cdot [\![\boldsymbol{\sigma}]\!] \cdot \mathbf{n} = -\boldsymbol{\Sigma}^S : \boldsymbol{\kappa}$$

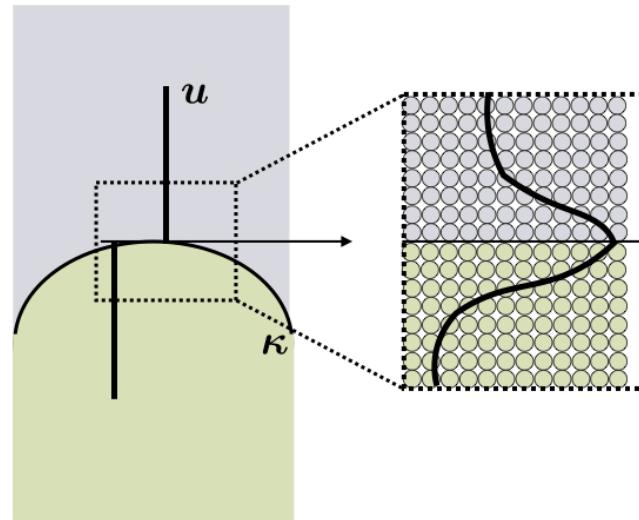
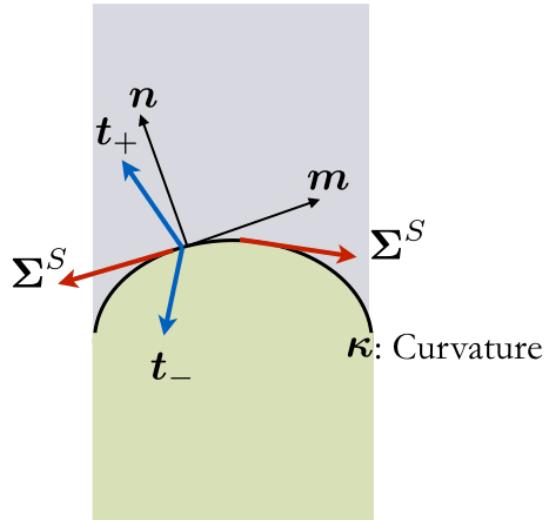
Transverse stress continuity condition

$$\mathbf{P}^S \cdot [\![\boldsymbol{\sigma}]\!] \cdot \mathbf{n} = -\nabla^S \boldsymbol{\Sigma}^S$$

In-plane stress continuity condition

$$[\![\boldsymbol{\epsilon}^S]\!] = 0$$

In-plane strain compatibility condition



Stress function for anisotropic prbs

2D Navier-type equation:

$$Q \frac{\partial^2 \mathbf{u}}{\partial x_1^2} (x_1, x_2) + [\mathbf{R} + \mathbf{R}^T] \frac{\partial^2 \mathbf{u}}{\partial x_1 \partial x_2} (x_1, x_2) + \mathbf{T} \frac{\partial^2 \mathbf{u}}{\partial x_2^2} (x_1, x_2) = \mathbb{C} \nabla \epsilon^{*,S} (x_1, x_2)$$

Starting assumption: $\mathbf{u}_0 (x_1, x_2) = \mathbf{a} \mathbf{f} (z)$ with $z = x_1 + p x_2$
 [Stroh, PhilMag, 1958]

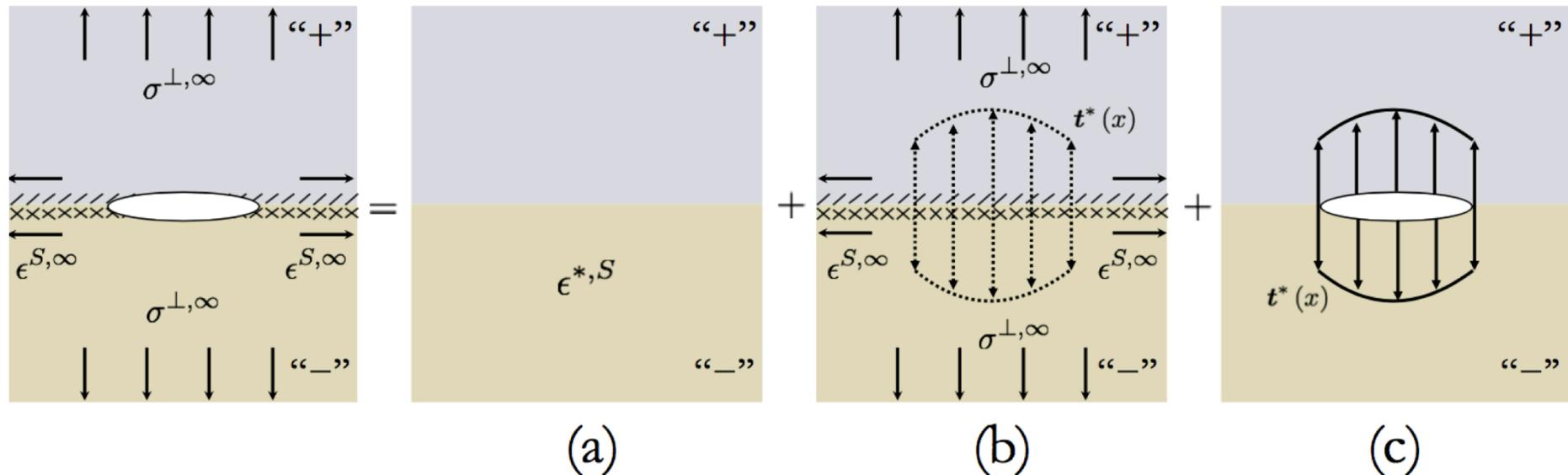
General solution for the displacement and stress fields:

$$u_i^0 = 2\Re e \left(\sum_{j=1}^3 A_{ij} f_j (z_j) \right) \quad \sigma_i^S \equiv \sigma_{i2} = 2\Re e \left(\sum_{j=1}^3 B_{ij} f'_j (z_j) \right)$$

$$\Phi_i^0 = 2\Re e \left(\sum_{j=1}^3 B_{ij} f_j (z_j) \right) \quad \sigma_i^L \equiv \sigma_{i1} = -2\Re e \left(\sum_{j=1}^3 B_{ij} p_j f'_j (z_j) \right)$$

Solving the function vector \mathbf{f} by considering the proper boundary conditions (accounting for interfacial elasticity)

Superposition of three simpler problems

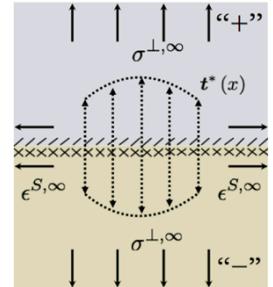


- Problem (a): unloaded bimaterial with a **misfit eigenstrain** tensor prescribed in “–”
- Problem (b): two **seemingly imperfectly bonded** anisotropic materials with transverse stresses and in-plane strains applied at infinity
- Problem (c): finite **Griffith crack lying between two perfectly bonded anisotropic materials** with traction forces applied on the crack’s faces

Seemingly imperfectly bonded bimaterial

Main assumptions:

- Constant transverse stresses and in-plane strains applied at infinity
- Imperfect interface characterized by interfacial elasticity BCs



Mathematical concepts used:

- Analytic complex potential, method of analytical continuation, Liouville's theorem.

Traction continuity: $B_+ f'_+ (x_1) - \overline{B_-} \overline{f'_-} (x_1) = B_- f'_- (x_1) - \overline{B_+} \overline{f'_+} (x_1)$

Equivalent displacement jump condition:

$$H B_+ f''_+ (x_1) + \left[\mathbb{H}_{II}^S M_+ - i \Lambda^\perp \right] B_+ f'''_+ (x_1) = \overline{H} B_- f''_- (x_1) + \left[\mathbb{H}_{II}^S \overline{M}_+ + i \Lambda^\perp \right] B_- f'''_- (x_1)$$

Equivalent eigenvalue problem:

$$\zeta'_m (z) + \mathbb{M}_m \zeta_m (z) = 0 , \quad m = \{+, -\}$$

$$\mathbb{M}_+ = \left[\mathbb{H}_{II}^S M_+ - i \Lambda^\perp \right]^{-1} H$$

$$\mathbb{M}_- = \left[\mathbb{H}_{II}^S \overline{M}_+ + i \Lambda^\perp \right]^{-1} \overline{H} = \overline{\mathbb{M}_+}$$

with, $\zeta_m (z) = B_m f''_m (z)$

\mathbb{M}_m : interfacial coupling

Elastic fields

- Elastic fields for an “imperfect interface” depend on the coupling between interface elastic behavior and bimaterial behavior
- Solutions consistent with classical formulation and interface BCs

Elastic fields solutions:

$$\boldsymbol{\sigma}_+^\perp = 2\Re e (\mathbf{K}_{\sigma_+}) - 2\Re e \left(\mathbf{U} \langle \frac{e^{-\lambda_* z_{*+}}}{\lambda_*} \rangle \mathbf{K}_\Psi \right), \quad \boldsymbol{\sigma}_-^\perp = 2\Re e (\mathbf{K}_{\sigma_-}) - 2\Re e \left(\overline{\mathbf{U}} \langle \frac{e^{-\bar{\lambda}_* z_{*-}}}{\bar{\lambda}_*} \rangle \overline{\mathbf{K}}_\Psi \right)$$

$$\begin{aligned} \mathbf{u}_+ &= 2\Re e \left(\mathbf{A}_+ \mathbf{B}_+^{-1} \mathbf{U} \langle \frac{e^{-\lambda_* z_{*+}}}{\lambda_*^2} \rangle \mathbf{K}_\Psi + \mathbf{A}_+ \langle z_{*+} \rangle \left[\mathbf{A}_+^T \mathbf{g}_\sigma + \mathbf{B}_+^T \mathbf{h}_\epsilon \right] + \mathbf{K}_{u_+} \right) \\ \mathbf{u}_- &= 2\Re e \left(\mathbf{A}_- \mathbf{B}_-^{-1} \overline{\mathbf{U}} \langle \frac{e^{-\bar{\lambda}_* z_{*-}}}{\bar{\lambda}_*^2} \rangle \overline{\mathbf{K}}_\Psi + \mathbf{A}_- \langle z_{*-} \rangle \left[\mathbf{A}_-^T \mathbf{g}_\sigma + \mathbf{B}_-^T \mathbf{h}_\epsilon \right] + \mathbf{K}_{u_-} \right) \end{aligned}$$

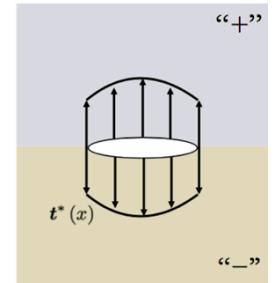
Using boundary conditions to solve for integration constants:

- Stress BC at infinity, $2\Re e (\mathbf{K}_\sigma) \equiv \boldsymbol{\sigma}^{\perp, \infty} = 2\Re e \left(\mathbf{B} \left[\mathbf{A}^T \mathbf{g}_\sigma + \mathbf{B}^T \mathbf{h}_\epsilon \right] \right)$
- In-plane strain compatibility condition, $\mathbf{K}_\Psi = \langle \lambda_* \rangle \mathbf{U}^{-1} \mathbf{H}^{-1} [\mathbf{M}_+ - \mathbf{M}_-] \mathbf{K}_\sigma$
- Displacement jump equation, $\mathbf{K}_{u_+} - \mathbf{K}_{u_-} = \frac{1}{2} \left[\mathbf{\Lambda}_0^\perp + \mathbb{K}^S : \boldsymbol{\epsilon}^{m,S} \right] + i \mathbf{H} \mathbb{M}_+^{-1} \mathbf{K}_\sigma$

Griffith crack problem

Main assumptions:

- Continuity of both traction and displacement across the bonded region
- Loading of the crack faces by the self-equilibrated traction vector obtained from the solution to the imperfectly bonded bimaterial problem



$$\mathbf{t}^*(x_1) = \boldsymbol{\sigma}^{\perp, \infty} - 2\Re e (\mathbf{U} \langle e^{-\lambda_* x_1} \rangle \mathbf{U}^{-1} \mathbf{H}^{-1} [\mathbf{M}_+ - \mathbf{M}_-] \mathbf{K}_\sigma)$$

➤ Traction depends on both interface and bimaterial properties

Classical formulation for stress fields in crack vicinity

$$\gamma(z) = \mathbf{B}_+ \mathbf{f}'_+(z) = \mathbf{H}^{-1} \bar{\mathbf{H}} \mathbf{B}_- \mathbf{f}'_-(z), \quad z \notin C$$

Displacement and traction BCs Heterogeneous Hilbert problem

Traction condition on crack face:

$$\gamma_+(x_1) + \bar{\mathbf{H}}^{-1} \mathbf{H} \gamma_-(x_1) = \mathbf{t}^*(x_1)$$

Displacement jump:

$$\mathbf{H} [\gamma_+(x_1) - \gamma_-(x_1)] = 0$$

Solution to the finite Griffith crack problem

- Solution to the heterogeneous Hilbert problem:

$$\boldsymbol{\gamma}(z) = \boldsymbol{\gamma}_1(z) \mathbf{w} + \boldsymbol{\gamma}_2(z) \bar{\mathbf{w}} + \boldsymbol{\gamma}_3(z) \mathbf{w}_3 \quad (\text{Suo, Proc Roy Soc, 1990})$$

where \mathbf{w} , $\bar{\mathbf{w}}$ and \mathbf{w}_3 are the eigenvectors of $\bar{\mathbf{H}}\mathbf{w} = e^{2\pi\varepsilon} \mathbf{H}\mathbf{w}$

➤ Fields projected along \mathbf{w}_3 and plane spanned by $\Re(\mathbf{w})$ and $\Im(\mathbf{w})$

- Stress elastic fields:

$$\boldsymbol{\sigma}^\perp \propto \boldsymbol{\gamma}_1(z) \quad \text{such that}$$

$$\boldsymbol{\gamma}_1(z) = \frac{(z^2 - a^2)^{-\frac{1}{2}}}{2\pi} \left(\frac{z-a}{z+a} \right)^{i\varepsilon} \int_{-a}^a \frac{(a+x)^{i\varepsilon} (a^2 - x^2)^{\frac{1}{2}}}{(a-x)^{i\varepsilon} (x-z)} t_0 [1 - \delta t(x)] dx$$

Transverse stresses

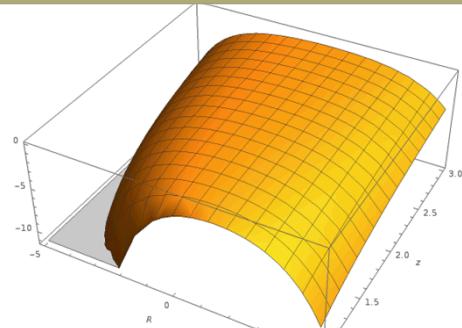
= classical singular & oscillatory term
+ new singular & oscillatory term coupling
interface and bimaterial elastic properties

Are there coupling effects beneficial to reducing “stressers” at the crack tip ?

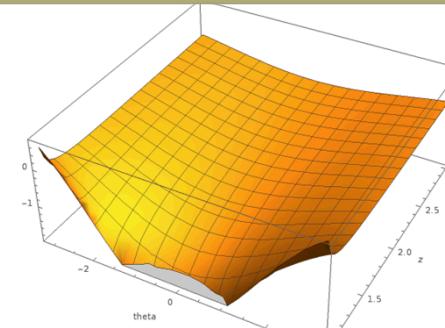


On the singular and oscillatory nature of elastic fields

- Introduction of new destructive/constructive interference terms

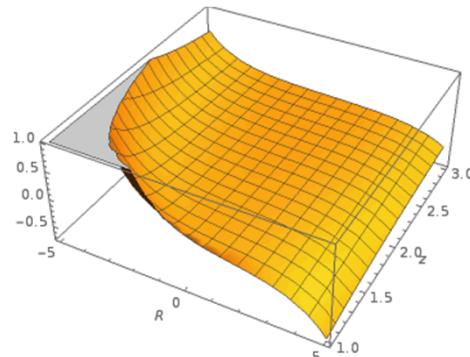


$$\Re(\delta\gamma) \mid \Re(\lambda) \neq 0 ; \Im m(\lambda) = 0$$

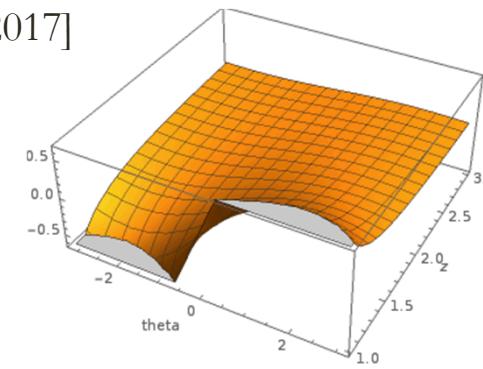


$$\Re(\delta\gamma) \mid \Re(\lambda) = 0 ; \Im m(\lambda) \neq 0$$

Juan & Dingreville, JMPS, 2017]



$$\Im m(\delta\gamma) \mid \Re(\lambda) = 0 ; \Im m(\lambda) \neq 0$$



$$\Im m(\delta\gamma) \mid \Re(\lambda) \neq 0 ; \Im m(\lambda) = 0$$

Direct impact of the real part of the eigenvalues on the osc. magnitude

Influence of the imaginary part of the eigenvalues on the oscillatory behavior

Modeling interfacial fracture: Does the emperor have any clothes?

- Do we need to get everything right?

- That's a tall order!

Yogi Berra: “In theory there is no difference between theory and practice...In practice there is.”

comparative order of magnitudes

- Faith in qualitative trends?