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Stress Fields Generated by Surface Triple-grain Junctions

(i.e., at the intersection of a grain boundary and a stress-free edge in a columnar polycrystal)

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Discovery at the Interface of Science and Engineering: Science Matters!

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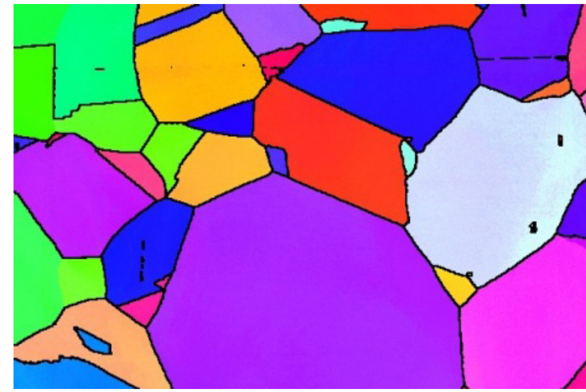
LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

What is the nature of the singular stress field at the intersection of a grain boundary and a stress-free edge in a columnar polycrystal?

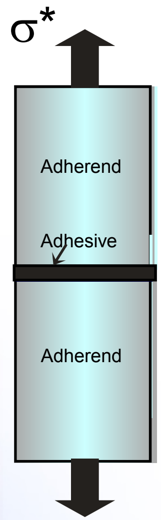
- Well known that material and geometric discontinuities can generate power-law singularities.
  - typically much weaker than a crack tip singularity.
- Do some combinations of crystal and grain boundary orientations generate stress levels that are significantly higher than the nominal value?
- If so, does and elevated stress occurs over an appreciable region?
- Dependence of singular fields on
  - crystal orientations
  - crystal properties
  - grain boundary orientation
  - grain geometry and length scale

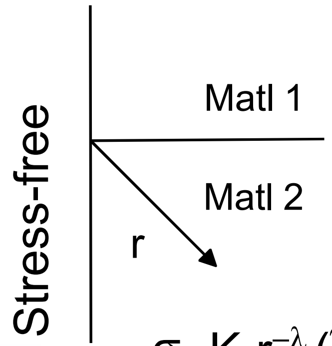


Some notable previous work on triple-grain junctions:

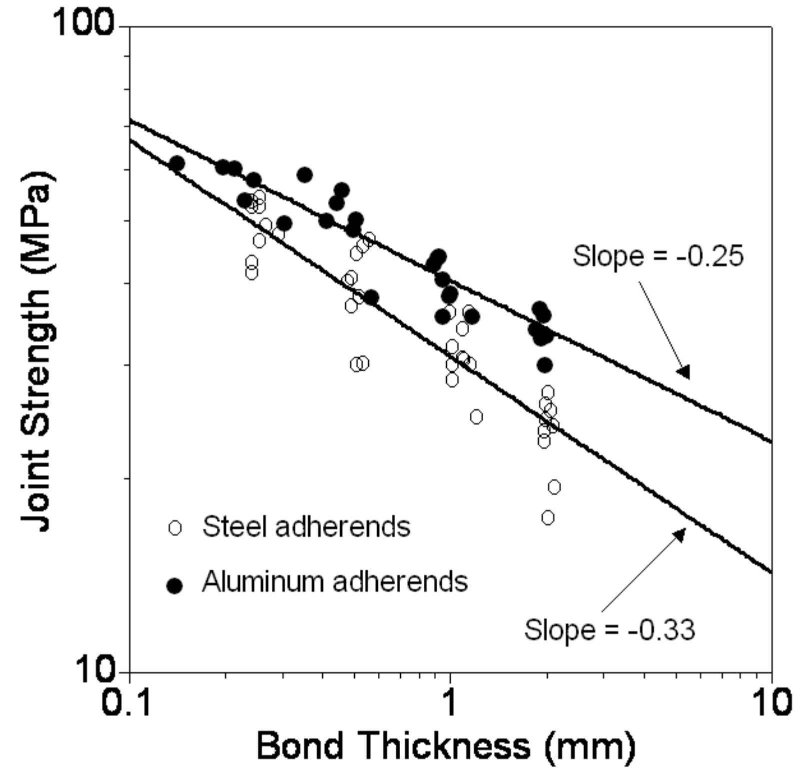
1. R. C. Picu, and V. Gupta: JAM 63, p295 (1996). Focused on determining strength of singularity as a function GB angles and crystal orientations.
2. V. Tvergaard, and J. W. Hutchinson: J Am Ceram Soc 71, p157 (1988). Considered certain special cases with a focus on grain boundary cracking.

Test results for when edge discontinuity dominates





$\sigma \sim K_a r^{-\lambda}$ (λ>0)



- Edge discontinuity

$$K_a = \sigma^* h^\lambda A_p(\alpha, \beta)$$

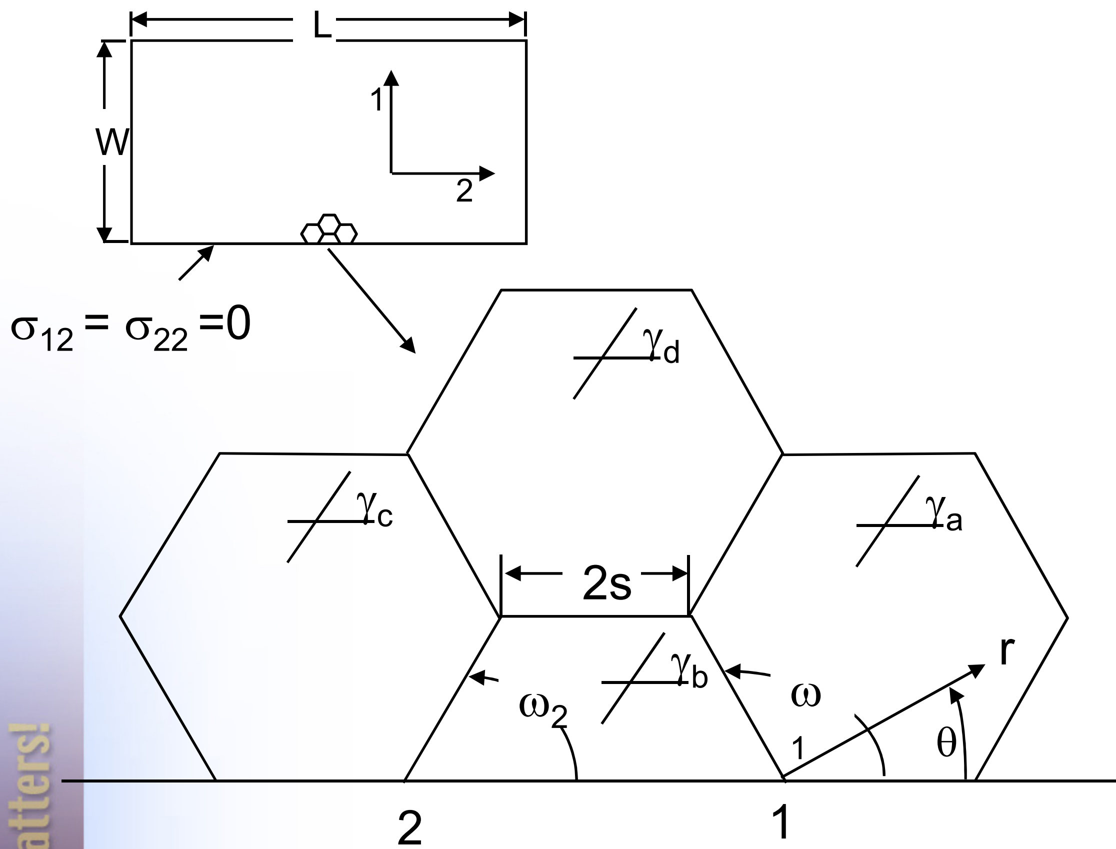
- Failure initiated at the edge
- Slope of log(strength) vs. log(bond thickness) is reasonably consistent with theoretical expectation for when an edge discontinuity dominates

  -0.27 aluminum/epoxy
  -0.30 for steel/epoxy

Reedy, E. D., Jr. and T. R. Guess (1993). "Comparison of Butt Tensile Strength Data with Interface Corner Stress Intensity Factor Prediction." International Journal of Solids and Structures 30: 2929-2936.

Reedy, E. D., Jr. and T. R. Guess (1997). "Interface Corner Failure Analysis of Joint Strength: Effect of Adherend Stiffness." International Journal of Fracture 88: 305-314.

Analyzed highly idealized problem



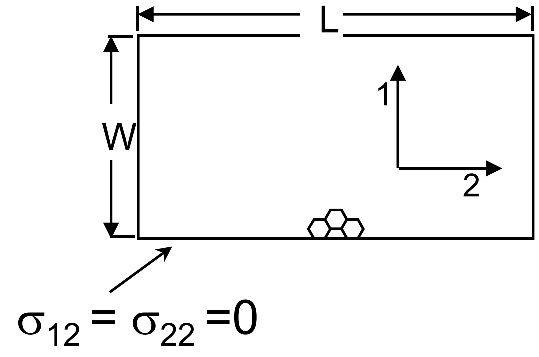
- Current work focused on an idealized columnar polycrystalline 2D, plane strain geometry.
- Explicitly modeled 4 cubic crystals that have one axis of material symmetry perpendicular to the top surface.
- Embed crystals in an effective isotropic material.
- Loaded in uniaxial tension parallel to the stress-free surface.

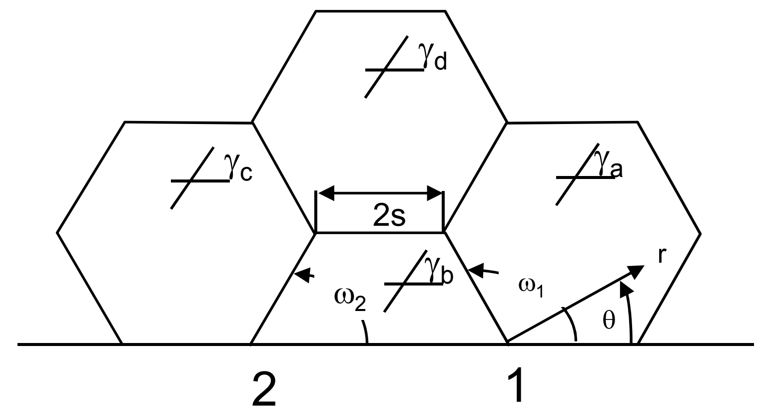
Meshed so can resolve nature of stress singularities

- 21 logarithmically spaced rings surrounding points 1 and 2
- radius of adjacent rings increase by a factor of 1.33
- inner ring at r/s=0.001

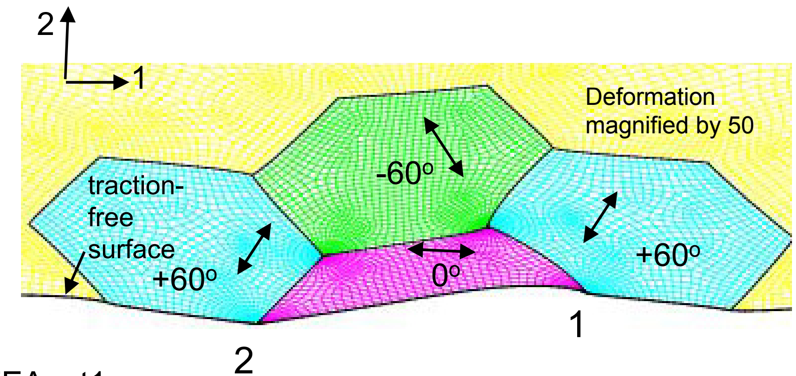
Baseline Configuration

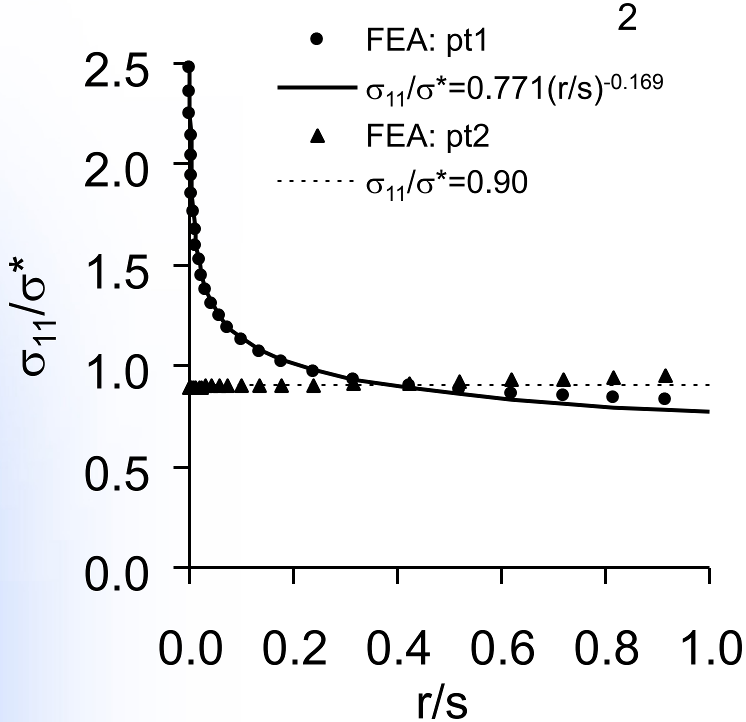
- L=2W=80s
  - L or W have negligible effect on local stress
- Regular hexagon with angle between side edges =120^o with side length 2s = 10 μm
- $\gamma_a = \gamma_c = -\gamma_d$ = 60^o, γ_b = 0^o.
- Cu with
  - C_{11} = 168 GPa,
  - C_{12} = 122 GPa
  - C_{66} = 76 GPa
- Effective isotropic properties for columnar Cu are E =115 GPa and ν = 0.354.



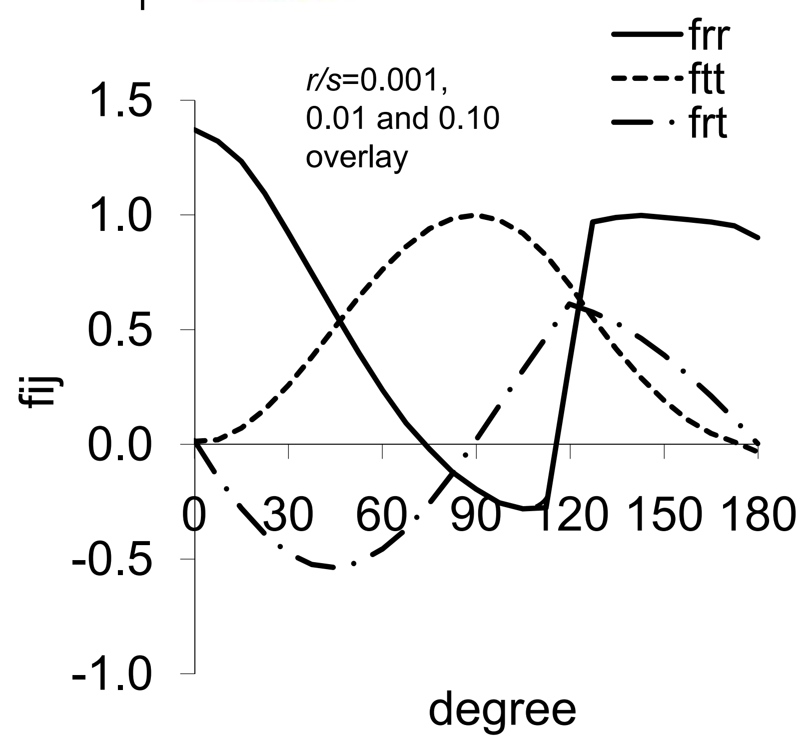


Results for baseline material and geometry





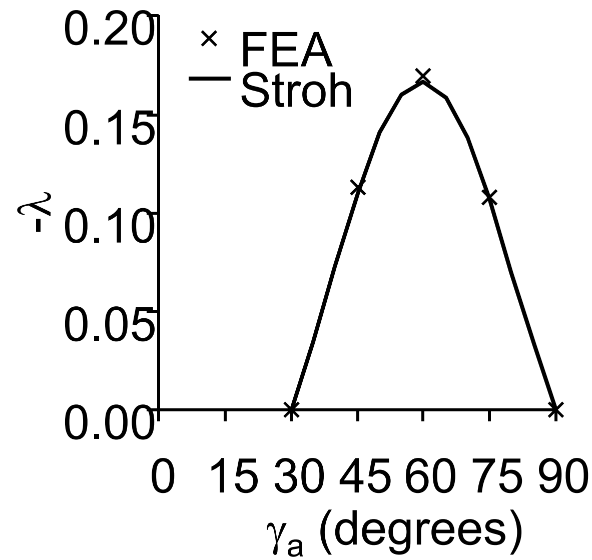
radial stress dependence of pt1 and pt2



angular stress dependence for pt1

Effect of crystal orientation on strength of singularity at pt1

- Baseline configuration, but $\gamma_a = \gamma_c = -\gamma_d$, $\gamma_b = 0$,
- FEA results for γ_a =0, 15, 30, 45, 60, 75 deg
- Only some γ_a generate stress singularities.
- When singular, only 1 power law term.
- Accuracy of FEA method is verified by comparison with asymptotic λ values determined using the Stroh formalism for anisotropic elasticity.



When the stress is singular

$$\sigma_{ij} = K_a r^{\lambda} f_{ij}(\theta, \text{grain boundary angle, crystal properties and oreintation})$$

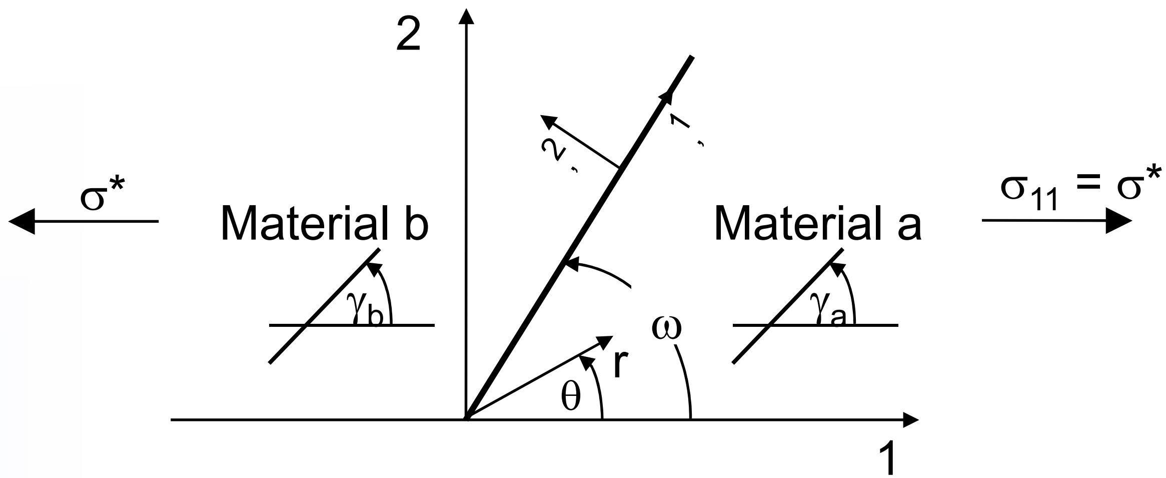
where

$$K_a = \sigma^* s^{-\lambda} A(\text{geometry,material properties})$$

"geometry" includes overall global geometry as well as the local microstructure and the f_{ij} functions have been normalized by setting $f_{tt}(\theta=90^o) = 1$.

Demarcation between singular and non-singular stress states

- Associated with grain boundary and crystal orientation combinations that generate a fully continuous stress state across the interface.
- Derive equation for stress continuity across the interface in terms of γ_a, γ_b, and ω.



Governing equation is independent of crystal compliances.

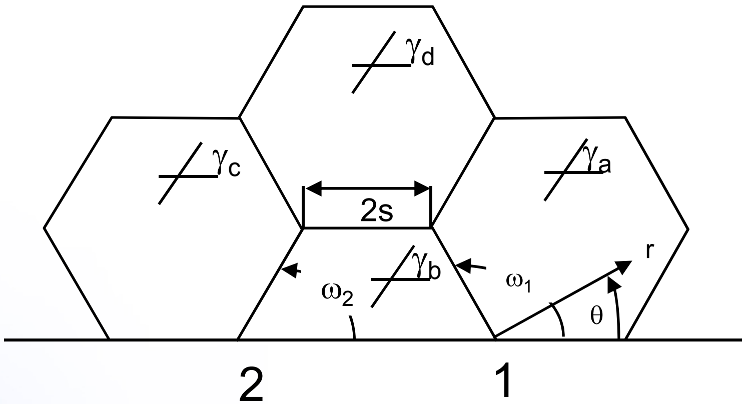
$$\cos(4\gamma_a - 2\omega) - \cos(4\gamma_b - 2\omega) = 0$$

Solutions:

$$\gamma_a = \gamma_b + n\frac{\pi}{2} \quad \text{where } n = \text{integer}$$

$$\omega = \gamma_a + \gamma_b + n\frac{\pi}{2} \quad \text{where } n = \text{integer}$$

Effect of crystal orientation on pt1 singular stress state



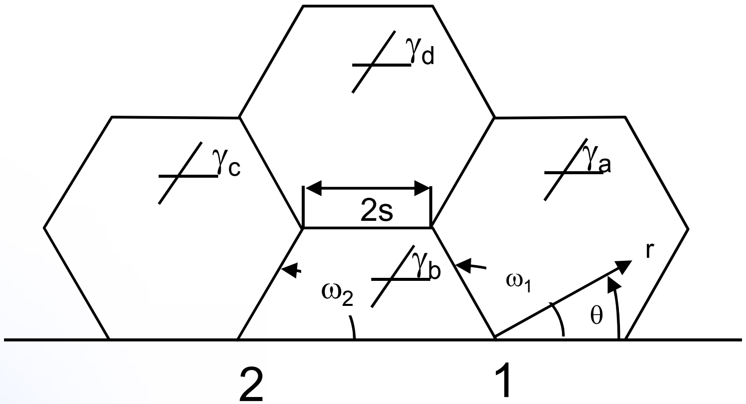
$$\sigma_{ij} = K_a r^{\lambda} f_{ij}(\theta, \text{etc.})$$

$$K_a = \sigma^* s^{-\lambda} A(\text{geometry}, \text{material properties})$$

γ_a (o)	γ_b (o)	γ_c (o)	γ_d (o)	A	λ	r_d/s	$\sigma_{rr}(\theta=0^o)/\sigma^*$ r/s=0.01	$\sigma_{rr}(\theta=0^o)/\sigma^*$ r/s=0.10
0	0	0	0	-	-	-	0.78	0.78
15	0	15	-15	-	-	-	0.66	0.75
30	0	30	-30	-	-	-	0.90	0.90
45	0	45	-45	0.708	-0.113	0.62	1.55	1.19
60	0	60	-60	0.562	-0.169	0.52	1.68	1.13
75	0	75	-75	0.606	-0.108	0.52	1.20	0.93
60	0	60	0	0.726	-0.168	0.18	2.16	1.48
60	45	30	-45	1.091	-0.078	0.08	1.73	1.41
60	75	15	-15	0.850	-0.077	0.82	1.38	1.16

r_d is distance beyond which the power-law singularity and the FEA analysis values for σ_{rr} differ by more than 2% (along the ray directed away from the central crystal).

Stress intensity factor can be affected by grains other than those at the singular point.



$$\sigma_{ij} = K_a r^{\lambda} f_{ij}(\theta, \text{etc.})$$

$$K_a = \sigma^* s^{-\lambda} A(\text{geometry,material properties})$$

γ_a (°)	γ_b (°)	γ_c (°)	γ_d (°)	A	λ	r_d/s	$\sigma_{rr}(\theta=0°)/\sigma^*$ r/s=0.01	$\sigma_{rr}(\theta=0°)/\sigma^*$ r/s=0.10
0	0	0	0	-	-	-	0.78	0.78
15	0	15	-15	-	-	-	0.66	0.75
30	0	30	-30	-	-	-	0.90	0.90
45	0	45	-45	0.708	-0.113	0.62	1.55	1.19
60	0	60	-60	0.562	-0.169	0.52	1.68	1.13
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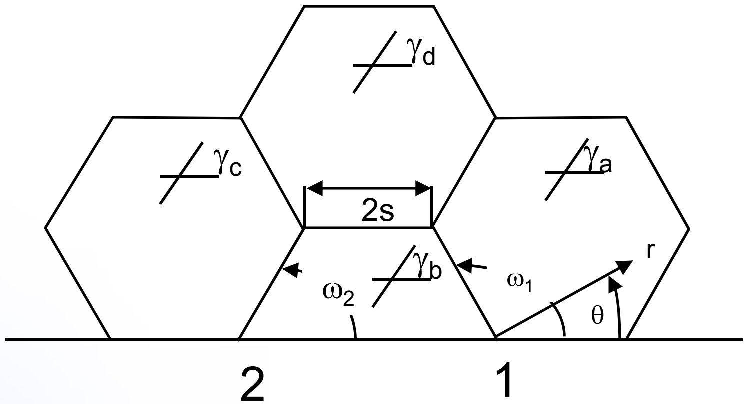
60	45	30	-45	1.091	-0.078	0.08	1.73	1.41
60	75	15	-15	0.850	-0.077	0.82	1.38	1.16

Effect of crystal orientation on pt2 singular stress state

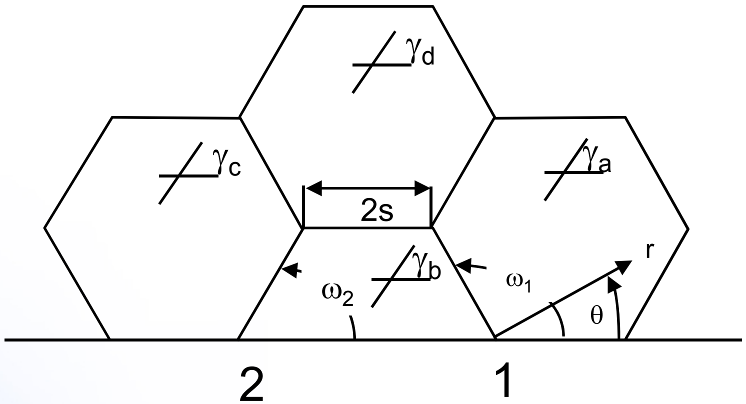


$$\sigma_{ij} = K_a r^{\lambda} f_{ij}(\theta, \text{etc.})$$

$$K_a = \sigma^* s^{-\lambda} A(\text{geometry,material properties})$$

γ_a (°)	γ_b (°)	γ_c (°)	γ_d (°)	A	λ	r_d/s	$\sigma_{rr}(\theta=180°)/\sigma^*$ r/s=0.01	$\sigma_{rr}(\theta=180°)/\sigma^*$ r/s=0.10
0	0	0	0	-	-	-	0.78	0.78
15	0	15	-15	0.606	-0.108	0.52	1.20	0.93
30	0	30	-30	0.562	-0.169	0.52	1.68	1.13
45	0	45	-45	0.708	-0.113	0.62	1.55	1.19
60	0	60	-60	-	-	-	0.90	0.90
75	0	75	-75	-	-	-	0.66	0.75
60	0	60	0	-	-	-	0.96	0.98
60	45	30	-45	1.091	-0.078	0.08	1.73	1.41
60	75	15	-15	0.883	-0.139	0.10	2.10	1.50

Combination with strongest singularity does not necessarily generate highest stress at *r/s* = 0.1



$$\sigma_{ij} = K_a r^{\lambda} f_{ij}(\theta, \text{etc.})$$

$$K_a = \sigma^* s^{-\lambda} A(\text{geometry,material properties})$$

γ_a (°)	γ_b (°)	γ_c (°)	γ_d (°)	A	λ	r_d/s	$\sigma_{rr}(\theta=180°)/\sigma^*$ r/s=0.01	$\sigma_{rr}(\theta=180°)/\sigma^*$ r/s=0.10
0	0	0	0	-	-	-	0.78	0.78
15	0	15	-15	0.606	-0.108	0.52	1.20	0.93
30	0	30	-30	0.562	-0.169	0.52	1.68	1.13
45	0	45	-45	0.708	-0.113	0.62	1.55	1.19
60	0	60	-60	-	-	-	0.90	0.90
75	0	75	-75	-	-	-	0.66	0.75
60	0	60	0	-	-	-	0.96	0.98
60	45	30	-45	1.091	-0.078	0.08	1.73	1.41
60	75	15	-15	0.883	-0.139	0.10	2.10	1.50

Effect of crystal properties on pt1 singular stress state

Baseline case, but vary crystal material.

- Ni has C_{11} = 248 GPa, C_{12} = 155 GPa, and C_{66} = 124 GPa
  - effective isotropic properties of E = 201 and ν = 0.310.
- Si has C_{11} = 166 GPa, C_{12} = 64 GPa, and C_{66} = 80 GPa
  - effective isotropic properties of E = 156 and ν = 0.222.
- Note R and Q are measures on anisotropy.
  - $R = (C_{12} + 2\,C_{66})/C_{11}$ and $Q = C_{66}/C_{12}$
  - R=1 for an isotropic material.

	R	Q	A	λ	r_d/s	$\sigma_{rr}(\theta=0^o)/\sigma^*$ r/s=0.01	$\sigma_{rr}(\theta=0^o)/\sigma^*$ r/s=0.10
Si	1.35	1.25	0.84	-0.058	0.72	1.21	1.06
Ni	1.63	0.80	0.64	-0.133	0.52	1.53	1.12
Cu	1.63	0.62	0.56	-0.169	0.52	1.68	1.13

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Size effects

- As is linear elastic fracture mechanics, there is an intrinsic size effect, with side length playing the role of crack length.
  - a uniform increase in the size of all crystals results in K_a value that scales has $s^{-\lambda}$
  - for baseline configuration, increasing s by a factor of 2 increases stress at a fixed distance r from the singular point by a factor of 1.12, (i.e. $2^{0.169} = 1.12$).
- The effect of increasing the size of only some of the crystals is less obvious.
- Examined case where the center crystal geometry is the same as that of the baseline, but the size of the surrounding crystals is increased.
- A limited set of results indicated no consistent trend.

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Conclusions

- There are combinations of grain boundary and crystal orientations that generate elevated stress of more than 1.4s^* for $r/s < 0.1$.
- The region dominated by a singularity can be relatively large.
- The magnitude of the elevated stress can be affected by grains other than those at the singular point.
- Orientation combinations with a more negative λ do not necessarily generate a higher stress at $r/s = 0.1$.
- There may be relatively few special triple-grain junctions along a surface that dominate behavior and possibly influence initial yielding or failure.

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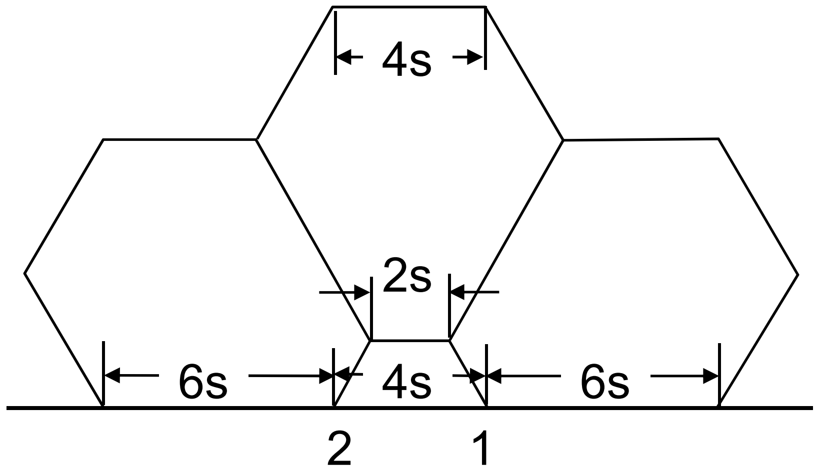
Additional results

Center crystal is surrounded by larger crystals



pt1 singular stress state for $\gamma_a = \gamma_c = -\gamma_d,\ \gamma_b = 0$ *and* $s = 5\ \mu m$

geometry	γ_a (°)	A	λ	r_d/s	$\sigma_{rr}(\theta=0°)/\sigma^*$ r/s=0.01	$\sigma_{rr}(\theta=0°)/\sigma^*$ r/s=0.10
baseline	60	0.562	-0.169	0.52	1.68	1.13
larger crystals	60	0.515	-0.170	0.13	1.54	1.03
baseline	45	0.708	-0.113	0.62	1.55	1.19
larger crystals	45	0.735	-0.113	0.62	1.61	1.24

- Share same ω_1 so have same λ.
- This limited set of results indicate that there is no consistent trend.

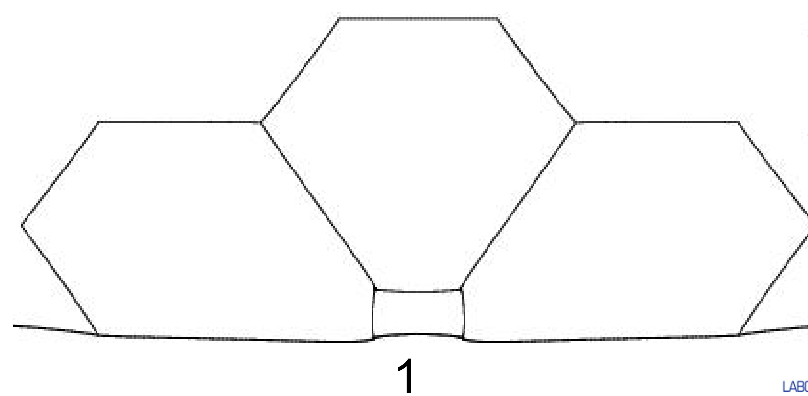
Effect of grain boundary angle on pt1 stress state

- Performed a few calculations to examine the effect of grain boundary angle.
- Used same “big grains around small grain” geometry, except move point 1 (2) to change the grain boundary angle ω_1 (ω_2) from 120° (60°) to 90° (90°) or 150° (30°).

ω_1 (°)	Γ_a (°)	γ_b (°)	γ_c (°)	γ_d (°)	A	λ	r_d/s	$\sigma_{rr}(\theta=0)/\sigma^*$ r/s=0.01	$\sigma_{rr}(\theta=0)/\sigma^*$ r/s=0.10
90	45	0	45	-45	-	0.050	-	1.57	1.60
90	0	45	0	-15	-	0.087	-	0.65	0.77
90	0	15	0	0	-	0.002	-	0.80	0.81
150	45	0	45	-45	-	0.146	-	0.42	0.59
150	75	0	75	-75	0.690	-0.040	0.24	0.83	0.77
150	75	15	75	-75	0.694	-0.142	0.13	1.40	1.02

Deformed geometry (highly deformed) for case where ω_1=90° and with γ_a = 45, γ_b = 0, γ_c = 45, γ_d= -45.

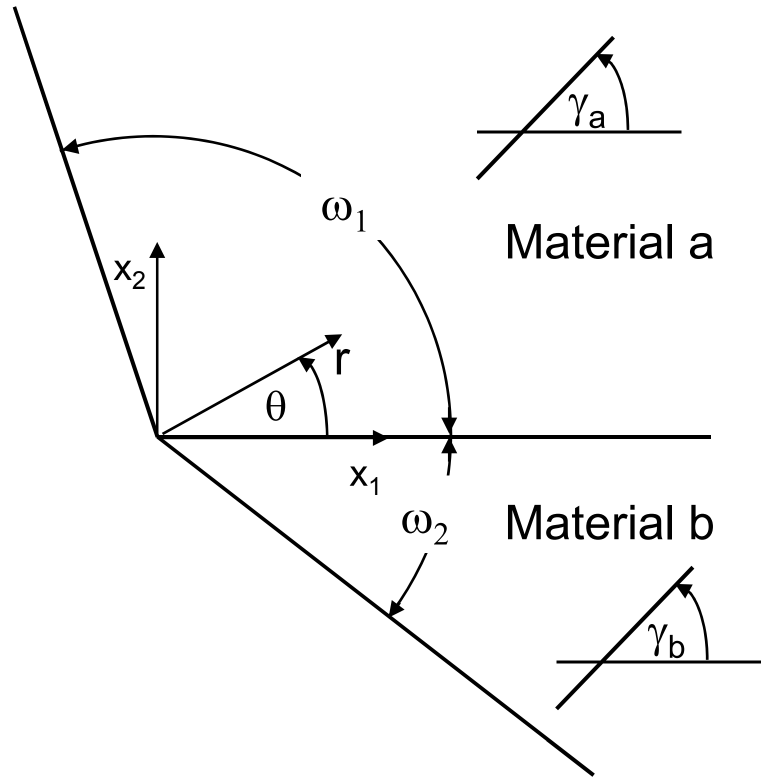
Peak stress at r/s=0.042



Asymptotic solution using Stroh's formalism for anisotropic elasticity

Asymptotic solution using Stroh's formalism for anisotropic elasticity

- Material a and b are the same cubic material, but with different orientations γ_a and γ_b wrt the x_1-axis.
- The out-of-plane x_3-axis of the crystals are aligned so in-plane and anti-plane deformations are uncoupled.
- Solve for in-plane deformations that are function only of in-plane coordinates, x_1 and x_2.
- Use contracted notation ($\sigma_1=\sigma_{11}$, $\sigma_2=\sigma_{22}$, $\sigma_6=\sigma_{12}$)
- Cubic stiffness components C_{ij}, i,j=1,2,6 for material a and b are transformed into the x_1-x_2 coordinate system.



Asymptotic Solution using Stroh's formalism for anisotropic elasticity

The in-plane displacement vector ***u*** and the surface traction vector ***t*** near the vertex of an anisotropic elastic wedge can be expressed as (see T.C.T. Ting, IJSS, 1986)

$$u(\theta) = \sum_{\omega=1}^{2} \left(q_\omega a_\omega z_\omega^{\delta+1} + h_\omega \bar{a}_\omega \bar{z}_\omega^{\delta+1} \right) / (\delta + 1) \qquad (1)$$

$$t(\theta) = \sum_{\omega=1}^{2} \frac{1}{r} \left(q_\omega b_\omega z_\omega^{\delta+1} + h_\omega \bar{b}_\omega \bar{z}_\omega^{\delta+1} \right) \qquad (2)$$

where q_w and h_w are arbitrary complex constants and $z_\omega = x_1 + p_\omega x_2 = r(\cos(\theta) + p_\omega \sin(\theta))$. The scalars p_ω and the vectors $\boldsymbol{a}_\omega$ and $\boldsymbol{b}_\omega$ are the eigenvalues and the associated eigenvectors determined by solving the linear eigenvalue problem

$$\begin{bmatrix} \mathbf{N}_1 & \mathbf{N}_2 \\ \mathbf{N}_3 & \mathbf{N}_1^T \end{bmatrix} \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix} = p \begin{Bmatrix} \mathbf{a} \\ \mathbf{b} \end{Bmatrix} \qquad (3)$$

where

$$\mathbf{N}_1 = -\mathbf{T}^{-1}\mathbf{R}^T, \quad \mathbf{N}_2 = \mathbf{T}^{-1}, \quad \mathbf{N}_3 = -\mathbf{Q} + \mathbf{R}\mathbf{T}^{-1}\mathbf{R}^T \qquad (4)$$

and

$$\mathbf{Q} = \begin{bmatrix} C_{11} & C_{16} \\ C_{16} & C_{66} \end{bmatrix} \quad \mathbf{R} = \begin{bmatrix} C_{16} & C_{12} \\ C_{66} & C_{26} \end{bmatrix} \quad \mathbf{T} = \begin{bmatrix} C_{66} & C_{26} \\ C_{26} & C_{22} \end{bmatrix} \qquad (5)$$

Note: there are two pairs of complex conjugates when the p_ω are distinct.

Asymptotic Solution using Stroh's formalism for anisotropic elasticity

Eq. 1 and 2 can be rewritten in matrix form as (H-P Chen, IJSS, 1998)

$$u(\theta) = r^{\delta+1}\left(AE(\theta)q + \overline{A}\hat{E}(\theta)h\right)/(\delta+1) \qquad (6)$$

$$t(\theta) = r^{\delta}\left(BE(\theta)q + \overline{B}\hat{E}(\theta)h\right) \qquad (7)$$

where q_ω and h_ω are the components of vectors $\boldsymbol{q}$ and $\boldsymbol{h}$, respectively; $\boldsymbol{a}_\omega$ and $\boldsymbol{b}_\omega$, are the columns of matrix **A** and **B**, respectively; and the diagonal matrices $E(\theta), \hat{E}(\theta)$ are

$$E(\theta) = \mathrm{Diag}(\eta_1^{\delta+1}, \eta_2^{\delta+1}, \eta_3^{\delta+1}) \quad \text{and} \quad \hat{E}(\theta) = \mathrm{Diag}(\overline{\eta}_1^{\delta+1}, \overline{\eta}_2^{\delta+1}, \overline{\eta}_3^{\delta+1}) \qquad (8)$$

where $\eta_\omega = \cos(\theta) + p_\omega \sin(\theta)$, $\omega = 1,2$

Note that when $\theta = 0$, the location of the interface in the problem considered here, $E(\theta), \hat{E}(\theta)$ are simply the identify matrix.

Asymptotic Solution using Stroh's formalism for anisotropic elasticity

For the problem of interest, the boundary conditions define eight homogeneous equations

$$B_a E_a(\omega_1) q_a + \overline{B}_a \hat{E}_a(\omega_1) h_a = 0$$
$$B_b E_b(\omega_2) q_b + \overline{B}_b \hat{E}_b(\omega_2) h_b = 0$$
$$A_a q_a + \overline{A}_a h_a - A_b q_b - \overline{A}_b h_b = 0$$
$$B_a q_a + \overline{B}_a h_a - B_b q_b - \overline{B}_b h_b = 0$$

where the subscript defines the material, either material a or b.

The determinant of this set of equations defines the characteristic equation for the strength of the singularity δ.