Graph Theory Model for Fatigue Crack Path Modeling

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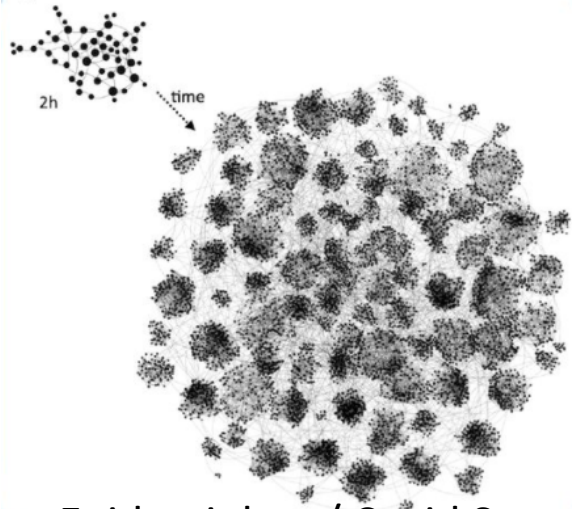
Exciting new developments in networks science and computational graph-theory

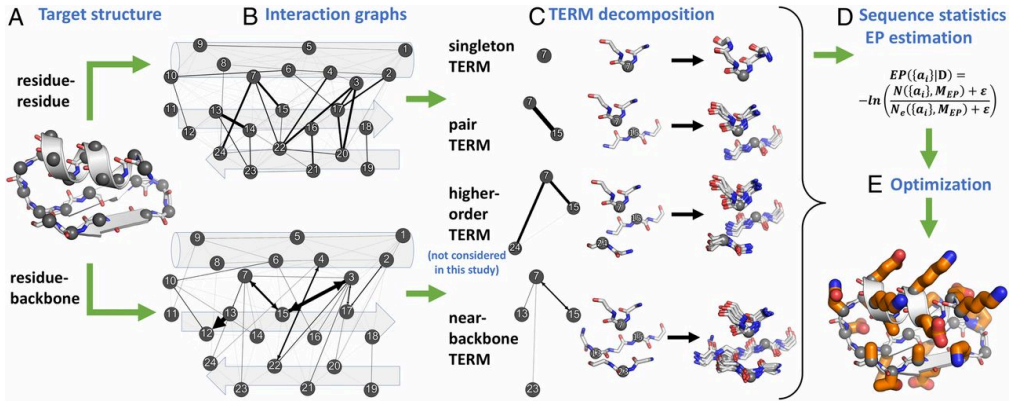
Social networks

(source: medium.com)



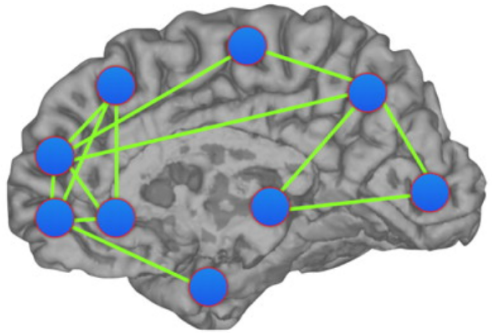
Epidemiology/ Covid Spread

(source: Goldenbogen et.al medRxiv. 2020)



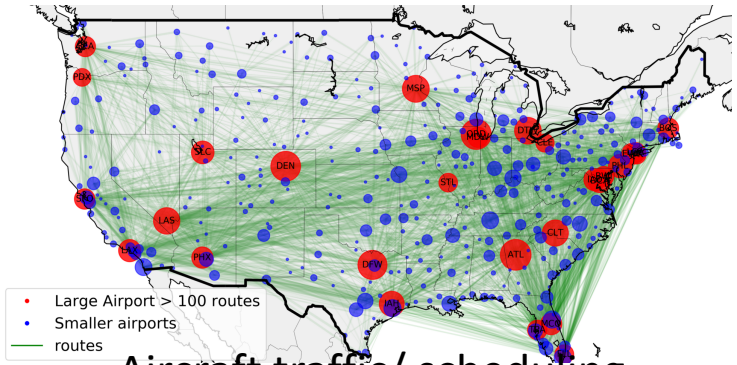
Protein Folding

(source: Zhou et.al. PNAS 2020)



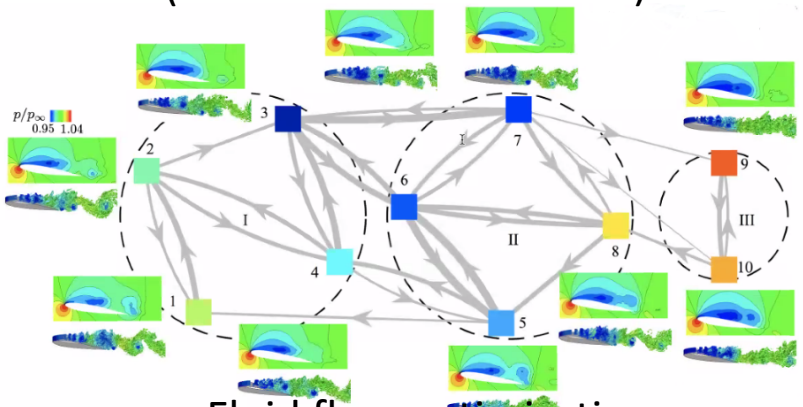
Brain network

(source: Heuvel et.al. Journal of Neuroscience 2010)



Aircraft traffic/ scheduling

(source: towardsdatascience,com)

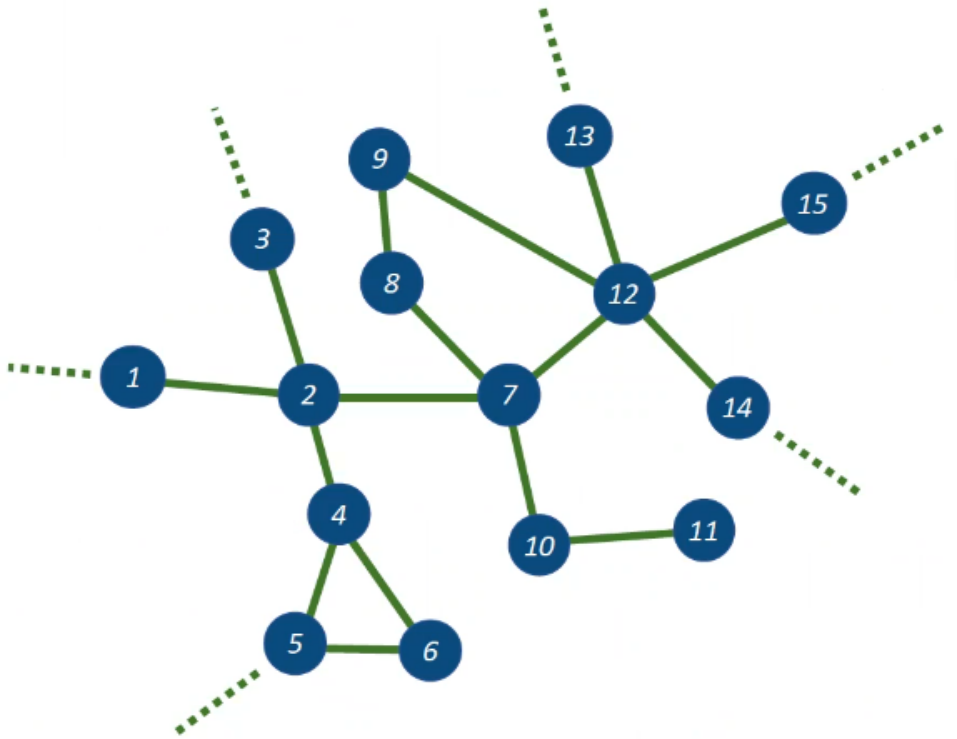


Fluid flow optimization

(source: Nair et.al JFM 2019)

What is a graph?

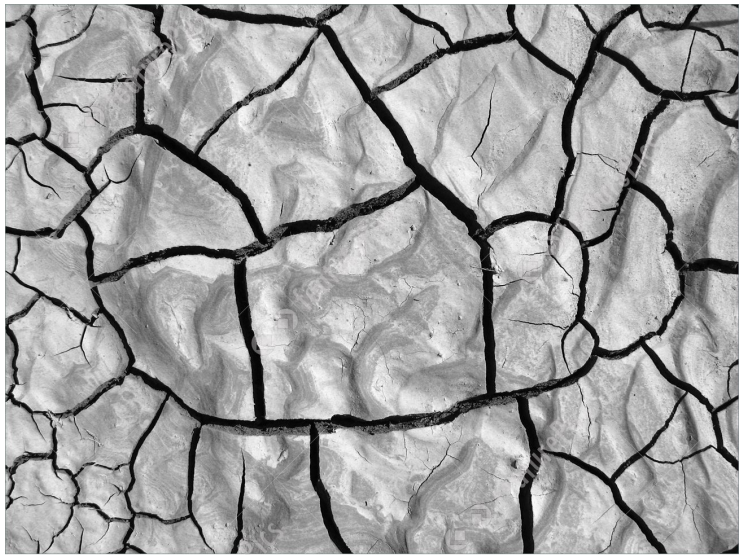
- Graph is a collection of Vertices (blue) and Edges (green). Mathematically summarized as $G(V, E)$



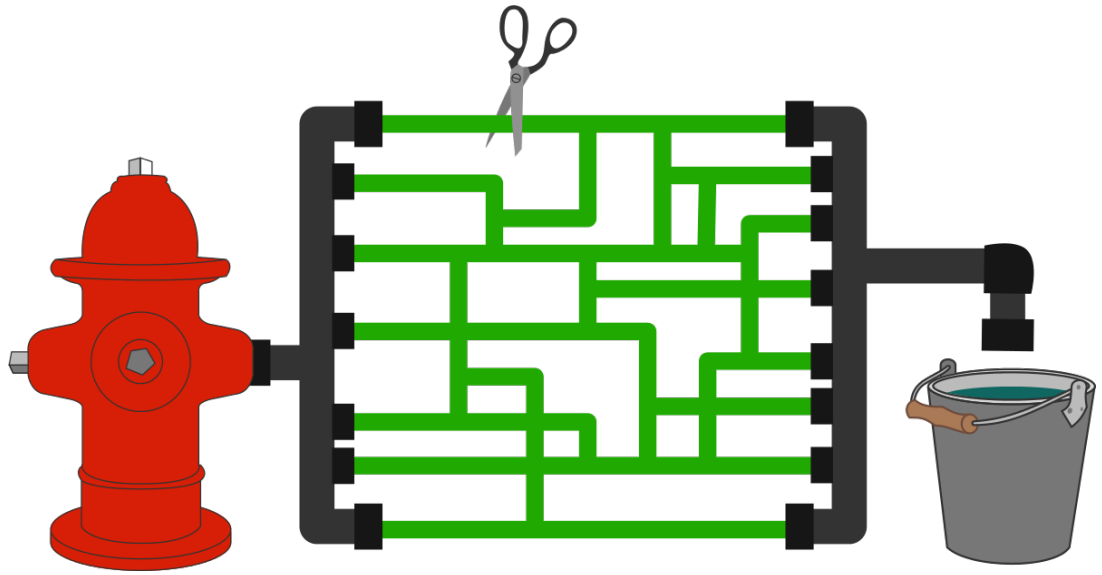
Fracture mechanics as clustering

A cluster of nodes has similar properties – like spatial locations etc.

A completely “Fractured-surface” partitions an object into smaller object.



Duality of cut and flow



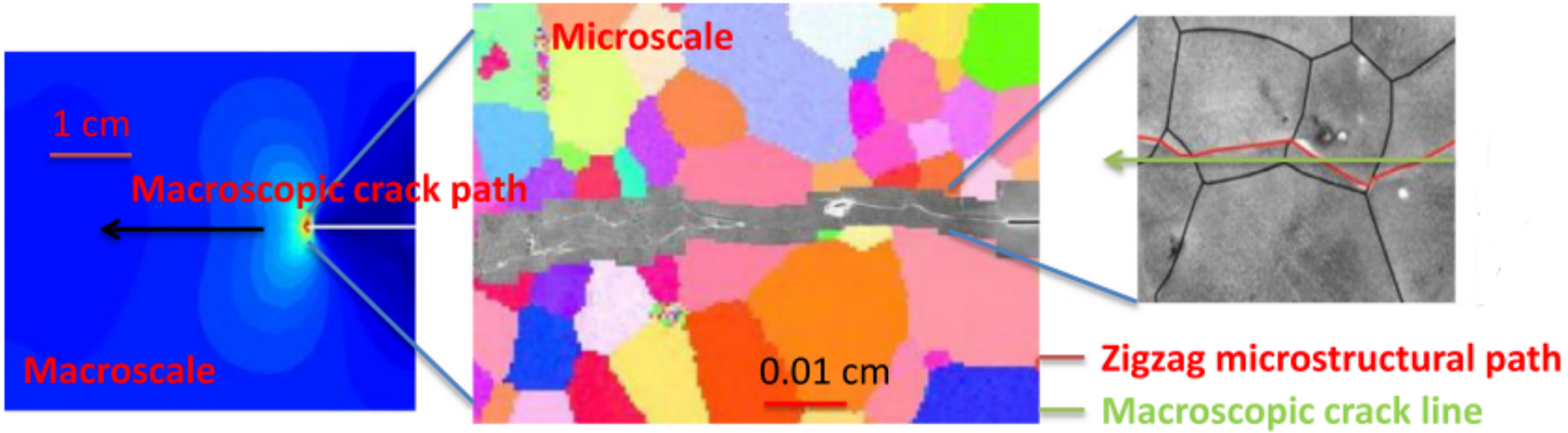
Max-Flow Min-Cut theorem

For any network graph and a selected source and sink node, the max-flow from source to sink = the min-cut necessary to separate source from sink

- Well established numerical methods:
  - (1955) Ford-Fulkerson's Augmenting Path
  - (1970) Edmonds-Karp's Shortest Path and Max capacity
  - (1983) Sleator-Tarjan's Dynamic Trees
  - (1997) Goldberg-Rao's Length Function
  - (2001) Boykov's Graphcut
  - (2010) Quantum Annealing

- **Key idea of this work: "Griffith's energy minimizing problems for fracture can be posed as a min-cut problem"**

Crack propagation in multiple length scales



Can we inform macro-scale continuum constitutive models with statistical information produced at microscale ?

- Formalize multiscale fracture in Ising energy form
- Energy form amenable to classical computation
- Captures rich physics

Representative Paper:

Srivastava S, Yaghoobi M and Sundararaghavan V(2020). “A graph-theoretic approach for multiscale modeling and prediction of crack propagation in polycrystalline materials.” Engineering Fracture Mechanics, 107406

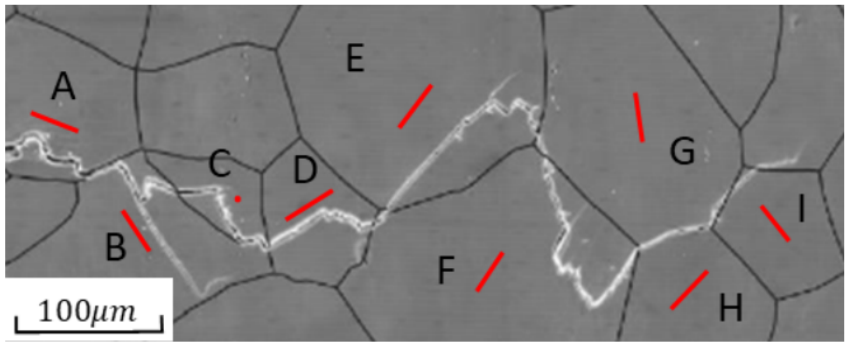
Fractures at microstructure scale

At microscale, inhomogeneities play an important role in deciding fracture paths.

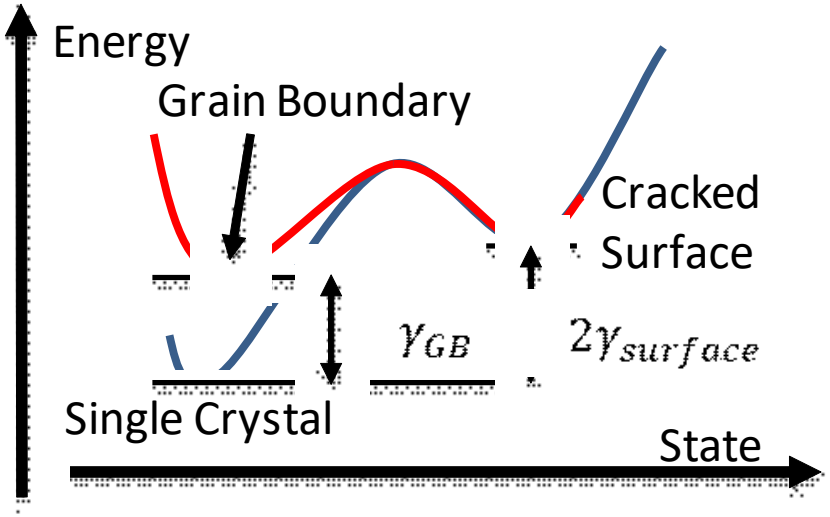
Transgranular fracture: Withing the grains, fracture follows preferred cleavage planes.

Intergranular fracture: The energy of a grain boundary depends on the relative orientations of neighboring grains.

The final crack path is decided by the interplay between different surface energies and change in train energy



Microscopic crack paths in WE43 alloy
red line = Basal trace



Brittle fractures

A mixed mode fracture can be studied as a tensile test of an inclined crack.

Question: What is the angle α, for a given:

(i) Material properties: E, ν

(ii) Loading condition: σ_T

(iii) Main crack parameters: a, β

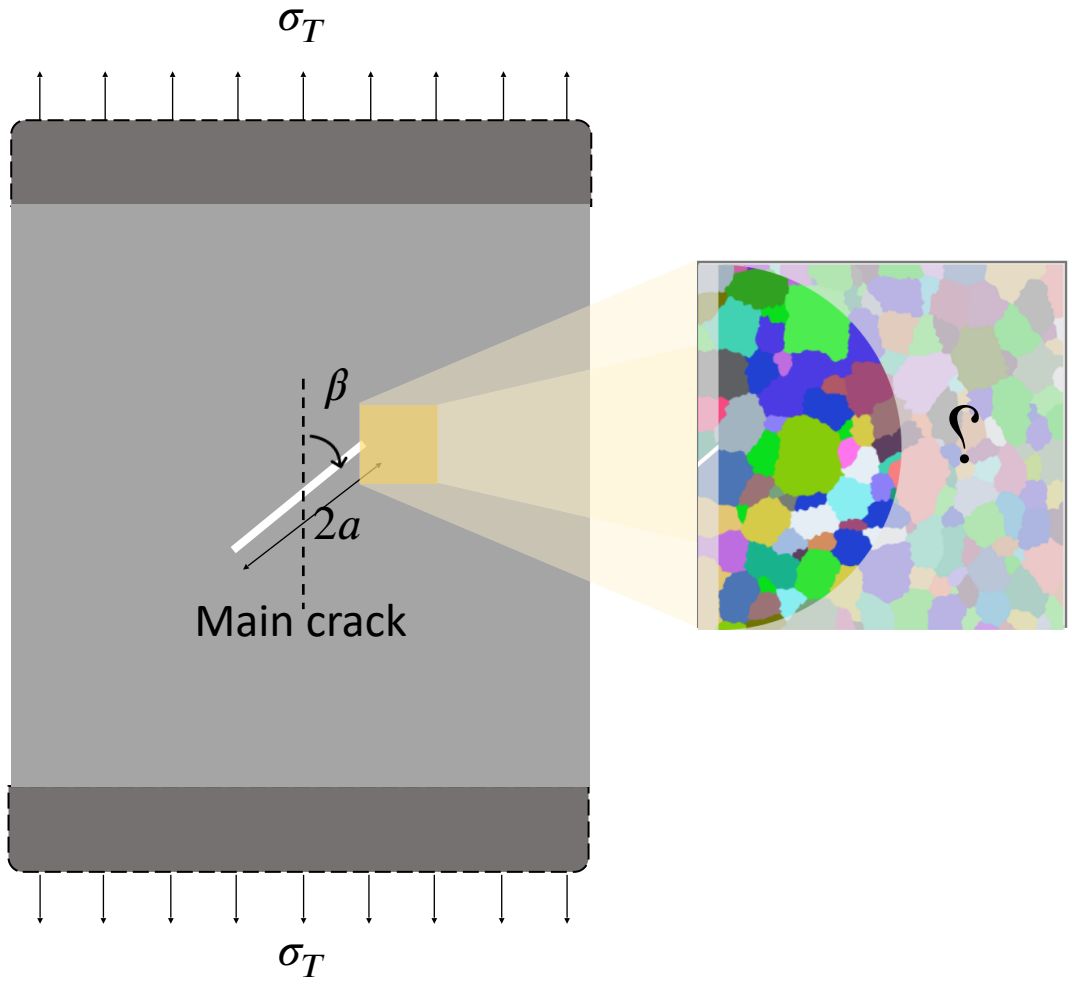
Answer: θ minimizes the energy of the system

For a unit length branched crack:

$$E = 2\gamma - G(\alpha)$$

First term is surface energy due to new surfaces

Second term is the release of strain energy



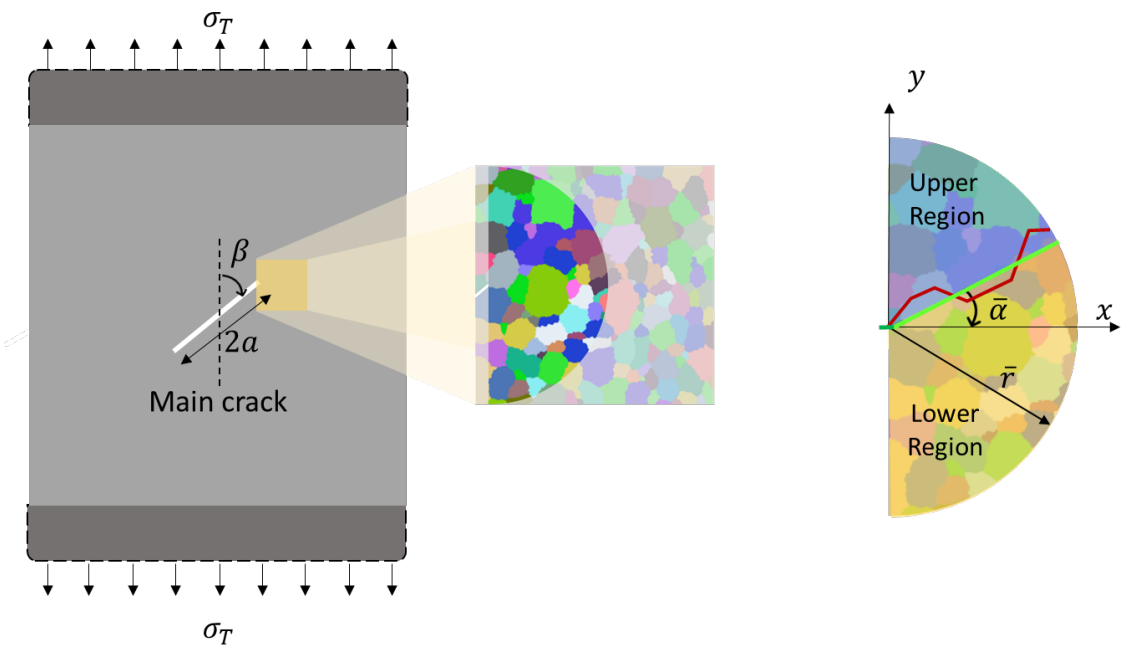
Multiscale assumptions

- Crack, Γ , propagates from the crack tip in a zig-zag direction towards the circumference. Path minimizes the total energy of the system, $\varepsilon(\Gamma)$:

$$\varepsilon(\Gamma) = \int_{\Gamma} 2\gamma ds \; - G(\bar{\alpha})$$

γ: Surface energy density

- Crack propagation is initiated when the total energy is negative.

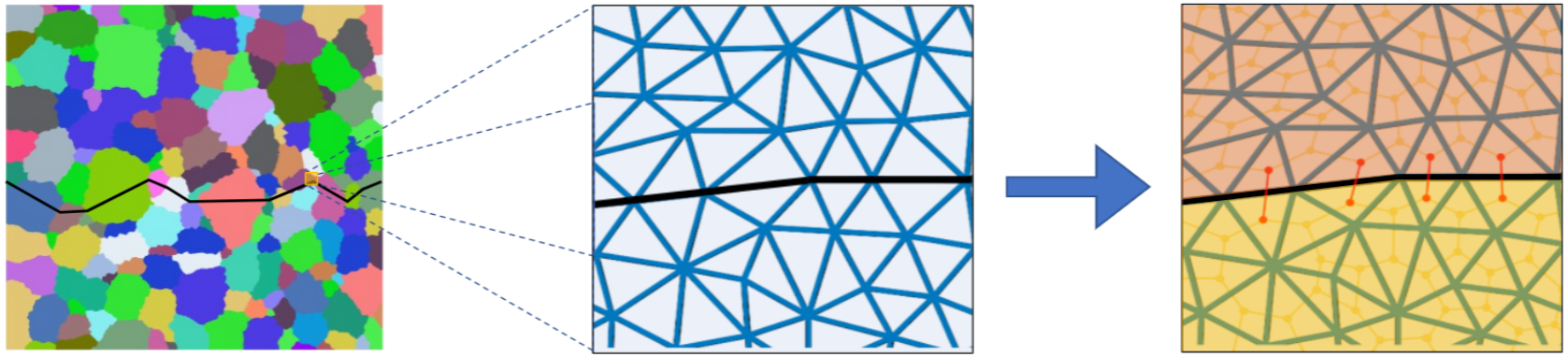


Tensile test, Mixed mode crack

Surface Energy is a microscopic object and energy release is a macroscopic object

Graph representation of Fracture

- Each element is treated as a vertex of graph
- A connection (Yellow) is drawn between two elements if they share an edge (Blue).



- Want to label elements above crack line as '$+1$' and below crack as '-1'.
- Surface energy of fracture encoded in the red edges of the Embedded graph.

Graph labeling problem: Pairwise formulation

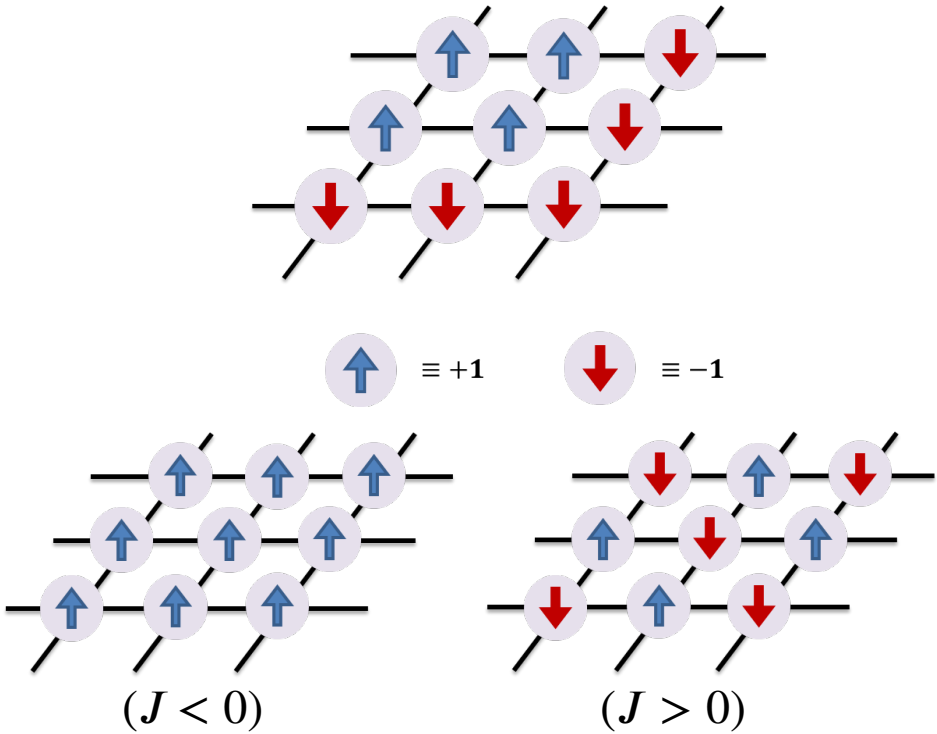
- Evolution of the state is determined by following energy

$$E(S) = \sum_{i}^{N} H_i S_i + \sum_{\langle ij \rangle} J_{ij} S_i S_j$$

S_i = spin (+1/-1) on i^{th} vertex

H_i = external field

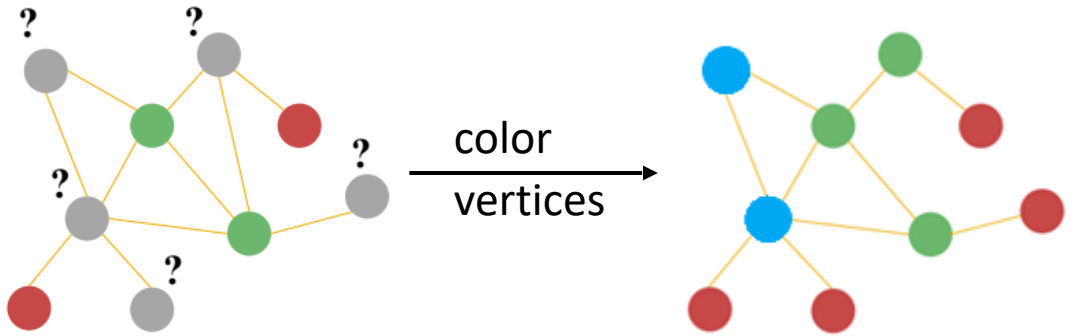
J_{ij} = interaction strength between different lattice points



Direct energy minimization

- First term enforces specific states at each node (Local behavior)
- Second term enforces relative spin of each neighbor (Non-local behavior)

Generalization to graph



Pairwise formulation for fracture problem

Want to label elements above crack line as '$+1$' and below crack as '-1' such that they minimize

$$\varepsilon(\Gamma) = \int_{\Gamma} 2\gamma ds \; - G(\bar{\alpha})$$

Modelling surface energy

A crack between element A and B means they have different labels

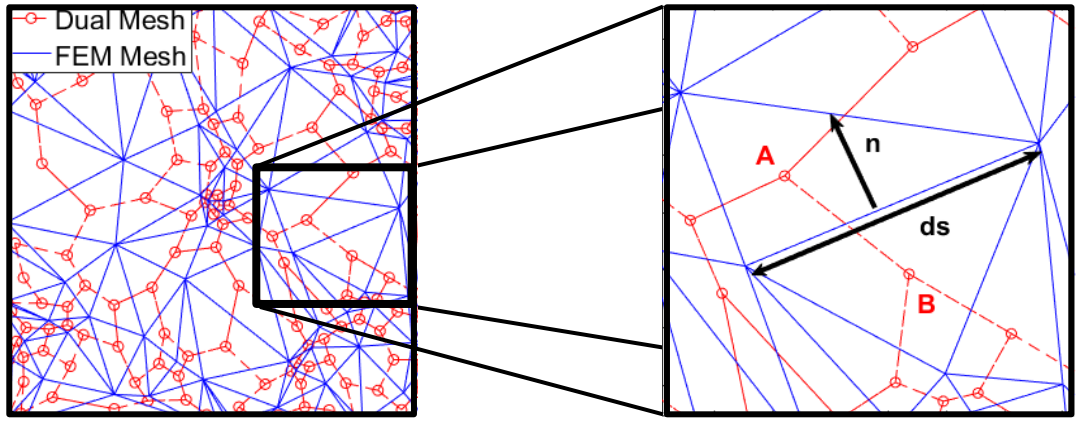
- Interaction term adds energy when A and B have different labels. Following function impose this condition:

$$1 - \delta_{s_A - s_B}$$

- Strength of the link $= 2\gamma\left(\vec{n}\right)\Delta s$

- Total surface energy is evaluated as

$$\sum_{\langle i,j \rangle} 2\gamma\left(\vec{n}\right)\Delta s\left(1 - \delta_{s_i - s_j}\right)$$



Pairwise formulation for fracture problem

Want to label elements above crack line as '$+1$' and below crack as '-1' such that they minimize

$$\varepsilon(\Gamma) = \int 2\gamma ds \; - G(\bar{\alpha})$$

Modelling energy release

Key idea: Find $g(x, l)$ such that

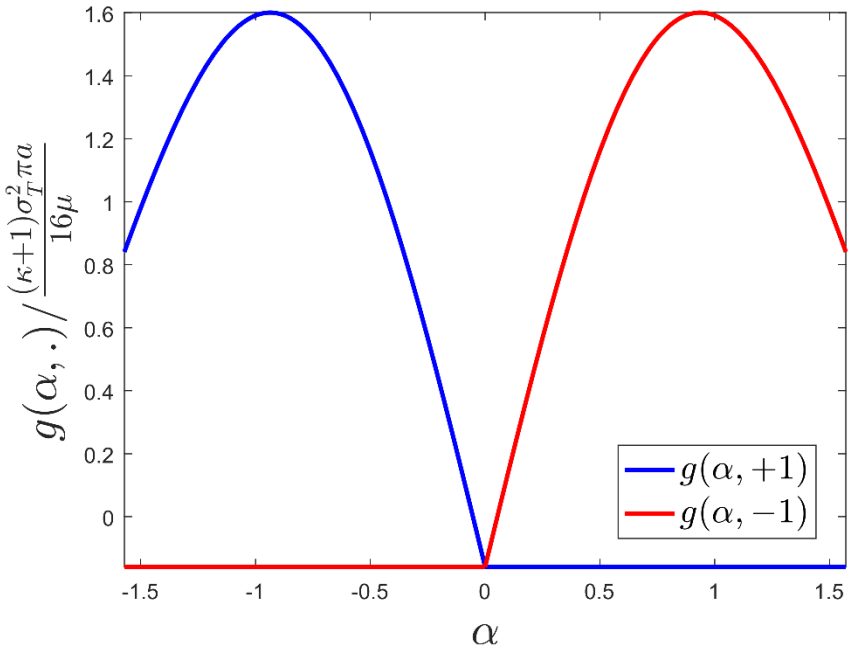
$$\lim_{A_i \to 0} \sum_{i \in \{1,\ldots,N_V\}} g(x_i, l_i) A_i = - G(\bar{\alpha})$$

x_i, l_i, A_i: Position, Label and Area of the i^{th}element

Can be done exactly if

- labeling is legitimate i.e. represents a single boundary
- G is a differentiable function

$$\varepsilon(\Gamma) \approx \sum_i g(x_i, l_i) A_i + \sum_{\langle i,j \rangle} 2\gamma\left(\vec{n}\right)\Delta s\left(1 - \delta_{s_i - s_j}\right)$$



Mode-1 fracture

$(\beta = 90^{\circ})$

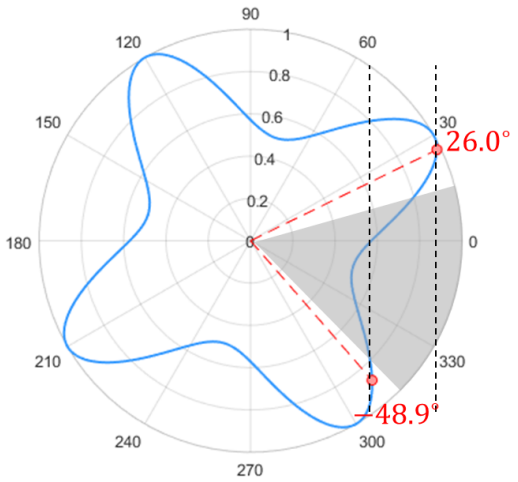
Method verification

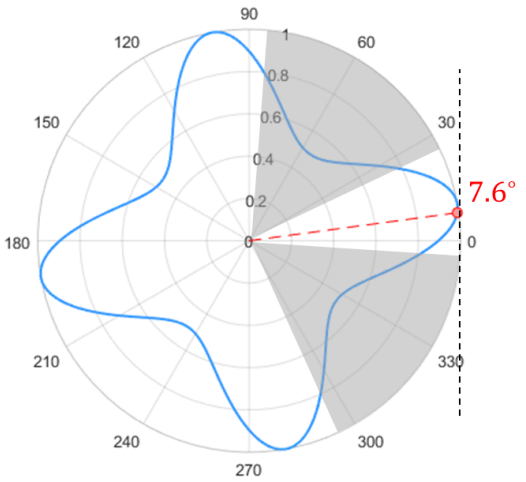
Quantitative tests:

- **Isotropic surface energy:**
  - Numerical prediction of average branched crack path angle, $\bar{\alpha}$, within 2° error of analytical and 4° error of experiments.
- **Anisotropic surface energy:**
  - For convex surface energy, $\bar{\alpha}$, within 4° error of analytical results.
  - For non-convex surface energy, fracture path shows smooth to rough transition in surface.

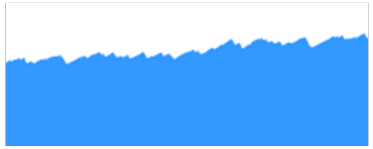
Qualitative tests:

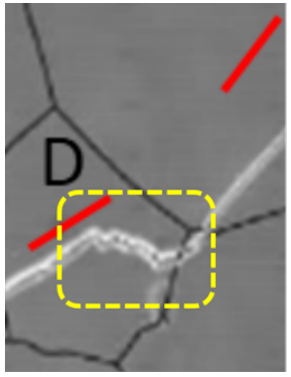
- **Effect of Grain Boundary**
  - Fracture path prefers grain boundaries with lower intergranular surface.
  - Crack path is affected before hitting the grain boundary.
  - This is a consequence of the global minimization of crack labeling problem.



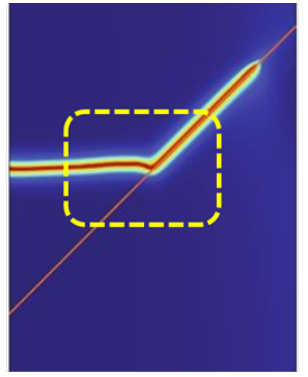


Forbidden regions for crack propagation

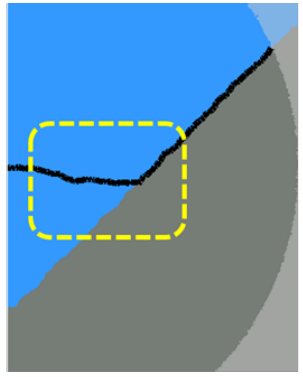




Experiment



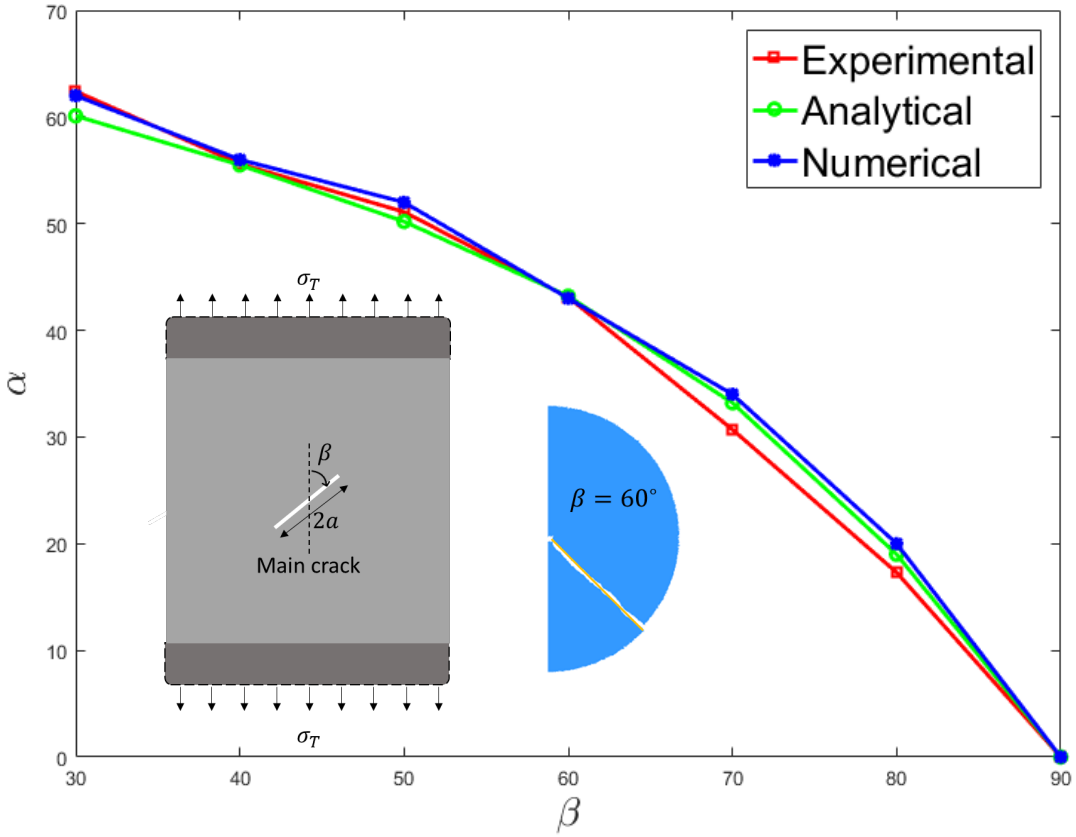
Phase field



Graph-based

Fracture in isotropic materials

- Estimating the macroscopic angle, $\bar{\alpha}_\Gamma$
- **Experiment***: plexiglass sheets with oblique cracks under tension.
- **Analytical**: Maximum energy release criteria
- Numerical prediction within 2° error from numerical and 4° error from experimental



* F. Erdogan and G. C. Sih. On the Crack Extension in Plates Under Plane Loading and Transverse Shear. *Journal of Basic Engineering*, 85(4):519–525, 12 1963

Mode-I failure with surface anisotropy

- Elastic properties are isotropic
- Surface energy

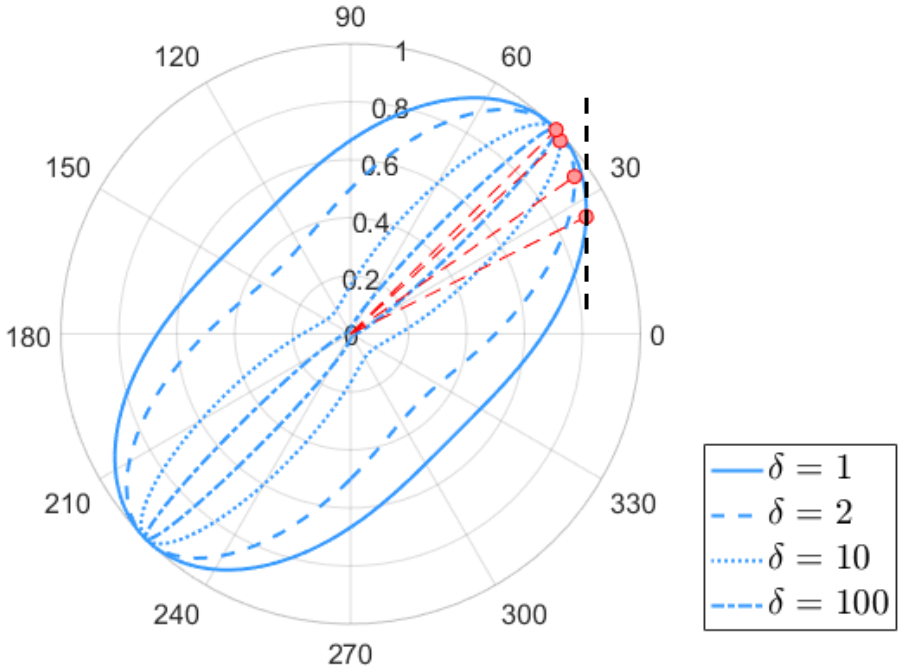
$$\gamma(\alpha) = \gamma_0(1 + \delta \sin^2(\alpha - \omega))$$

In absence of external load, preferred direction is $\alpha = \omega$.

<u>Wulff construction for Quasistatic brittle crack in Mode-I [1]:</u>

Step 1: Plot polar plot of γ^{-1} (Inverse of surface energy)

Step 2: Crack propagates along red line such that it intersects the blue line at a point with a vertical tangent.



Polar plot of Inverse surface energy

[1] Takei, Atsushi, et al. "Forbidden directions for the fracture of thin anisotropic sheets: an analogy with the wulff plot." *Physical review letters* 110.14 (2013): 144301.

Mode-I failure with surface anisotropy

- Elastic properties are isotropic
- Surface energy

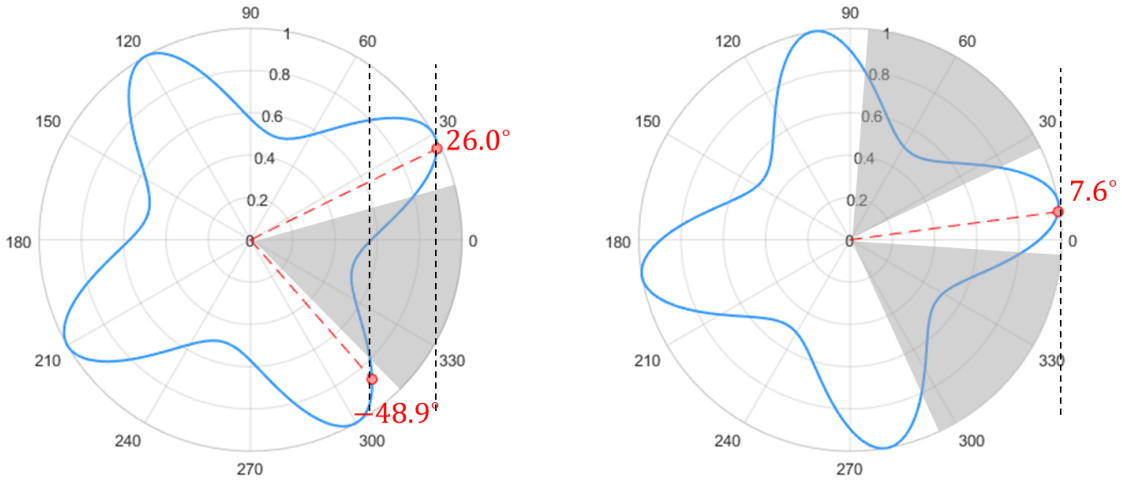
$$\gamma(\alpha) = \gamma_0(1 + \delta \sin^2 2(\alpha - \omega))$$

In absence of external load, bidirectional preference:

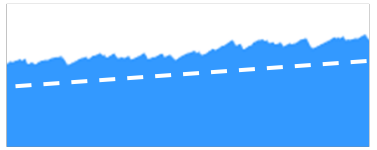
$$\alpha = \omega,\ \omega \pm 90^\circ$$

Wulff construction is still valid if intersection is convex

Cracks are not permitted in the non-convex regions



Forbidden regions for crack propagation



Effect: 1. Transition from one cleavage plane to another cannot be done smoothly due to forbidden regions

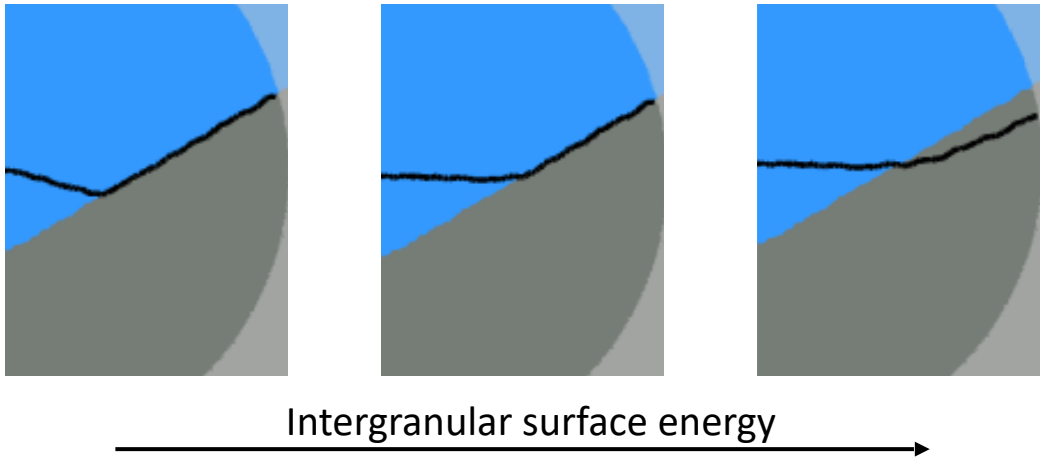
2. Switching between different preferred directions can reduce the macroscopic crack angle (white-dashed line)

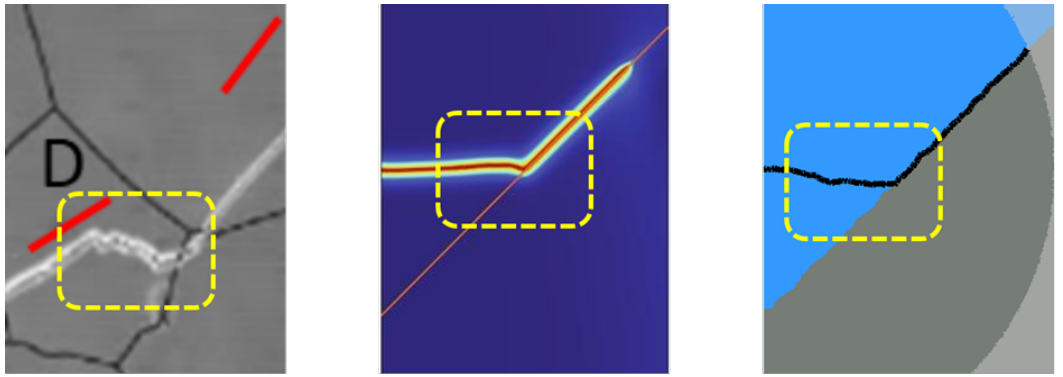
[1] Takei, Atsushi, et al. "Forbidden directions for the fracture of thin anisotropic sheets: an analogy with the wulff plot." *Physical review letters* 110.14 (2013): 144301.

Long range effects of grain boundary

Qualitative Results (Mode-I):

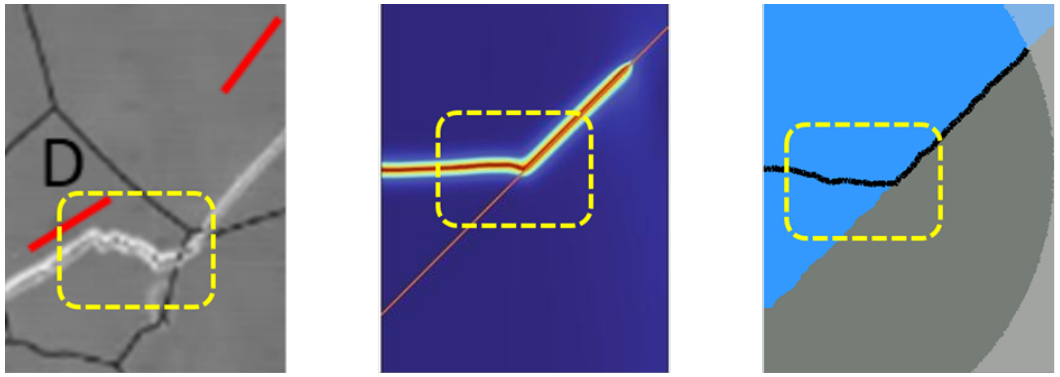
- As expected, fracture path prefers grain boundaries with lower intergranular surface.
- Crack path is affected before hitting the grain boundary.
- This is a consequence of the global minimization of crack labeling problem.
- Experimental results and Phase field methods reveal similar bending of crack before hitting the grain boundary. However, the length scale of this effect in Phase field is far smaller.





Validation: Effect of Grain Boundary

Experimental results and Phase field methods reveal similar bending of crack before hitting the grain boundary. However, the length scale of this effect in Phase field is far smaller



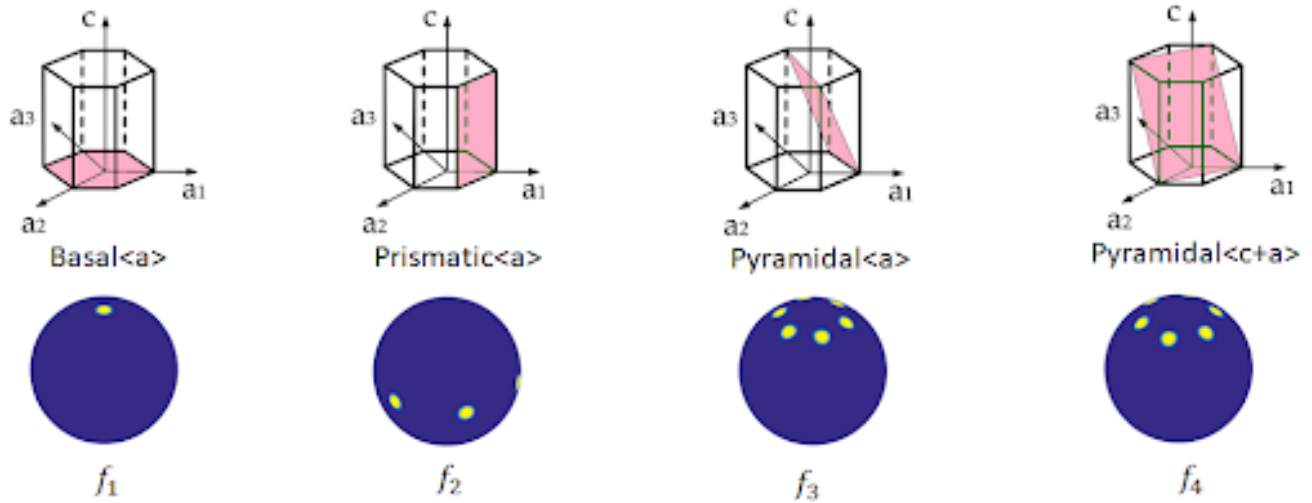
Experiment Phase field Graph-based

Modeling HCP materials

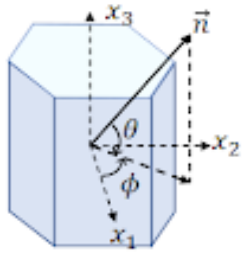
- HCP crystals is characterized by the symmetry group:

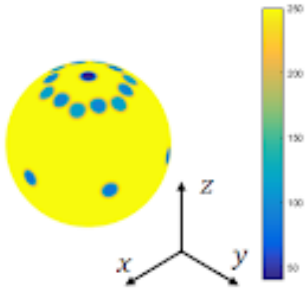
$\{R_z(\pi/3), R_x(\pi/2), -I\}$

- We introduce a 7-parameter model for surface energy:



$$\gamma = \gamma_0 + (\gamma_b - \gamma_0) f_1 + (\gamma_{pris} - \gamma_0) f_2 + (\gamma_{pyr<a>} - \gamma_0) f_3 + (\gamma_{pyr<c+a>} - \gamma_0) f_4$$

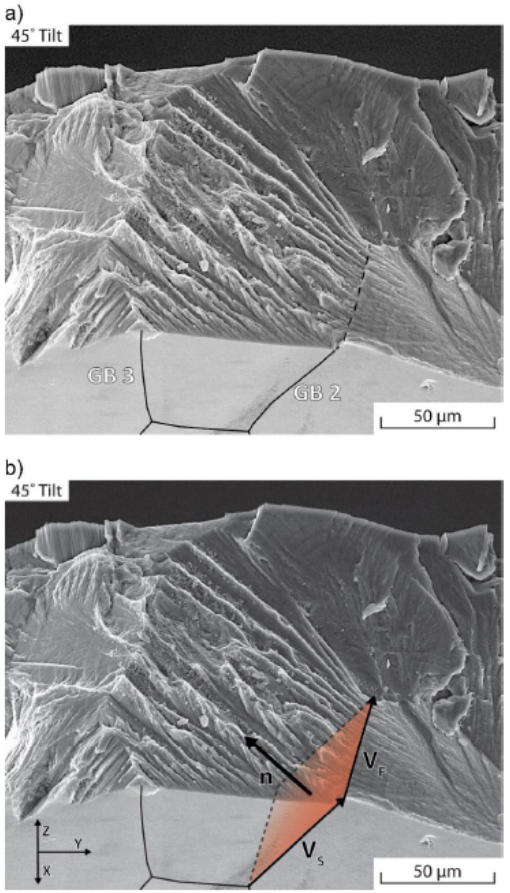




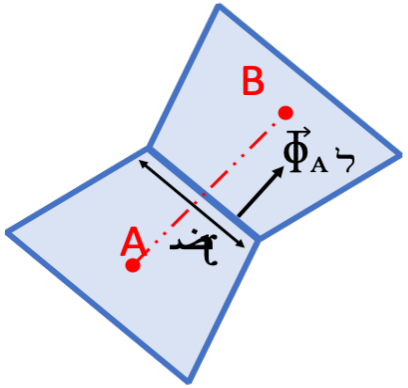
Representative Paper:

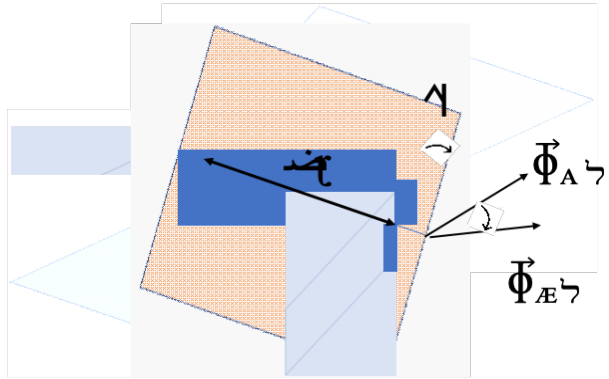
Srivastava S, Yaghoobi M, Adams J.F, Greeley D, Spear A.D, Allison J.E, Jones W and Sundararaghavan V(2020). "Fatigue crack growth in WE43 Mg alloy: thin foil fatigue experiment and graph-theoretic approach." Unpublished – Manuscript available on request

Thin foil experiments



- Crystalline fractured surfaces may exhibit an out-of-plane normal.
- Energy minimizing 3d normal can be pre-determined.





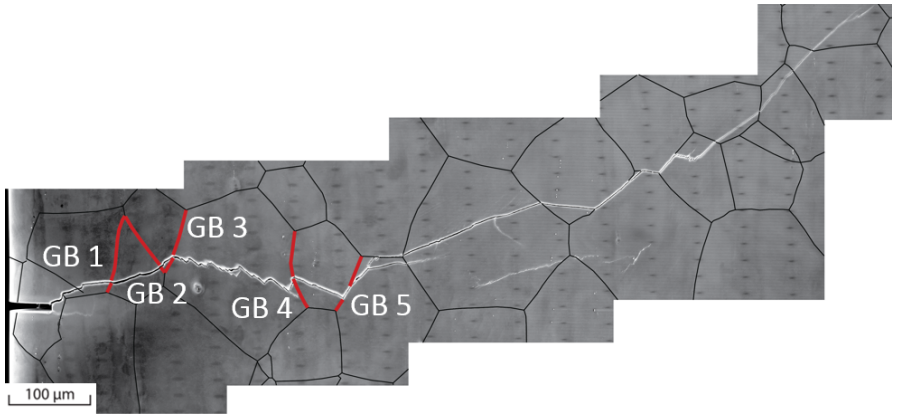
- Dihedral angle relates 2D and 3D cleaved surface

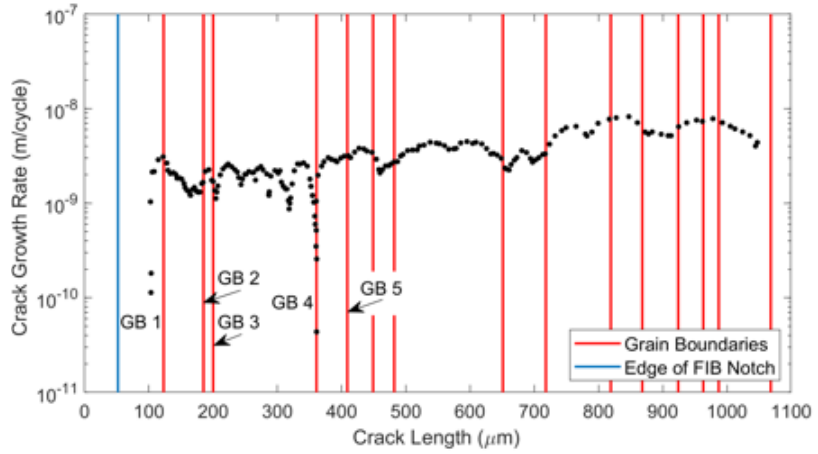
$$\vec{n}_{3D}(\psi) = [0,0,1]^T \sin\psi + \vec{n}_{2D}\cos\psi,$$

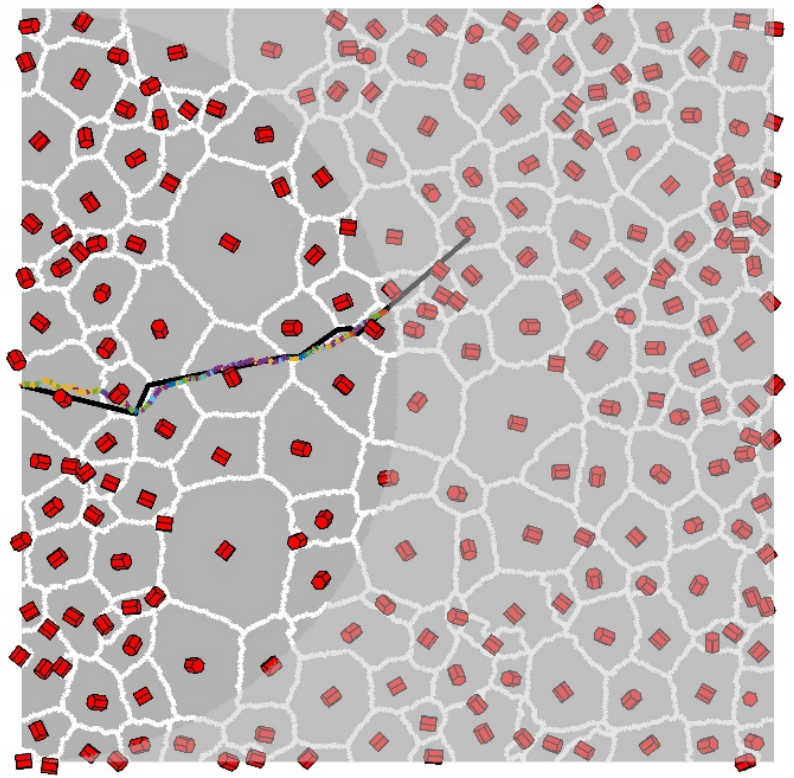
- Dihedral angle minimizes the net surface energy

$$\psi_D = argmin_{\psi\in(-\frac{\pi}{2},\frac{\pi}{2})}\gamma\left(\vec{n}_{3D}(\psi)\right)\sec\psi$$

Experimental comparisons: Foil 1



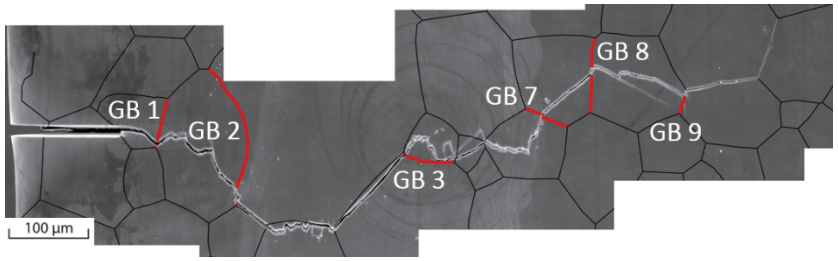


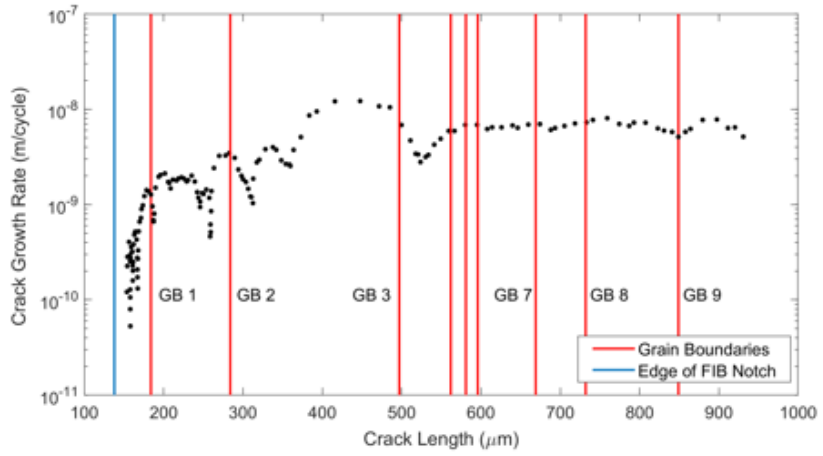


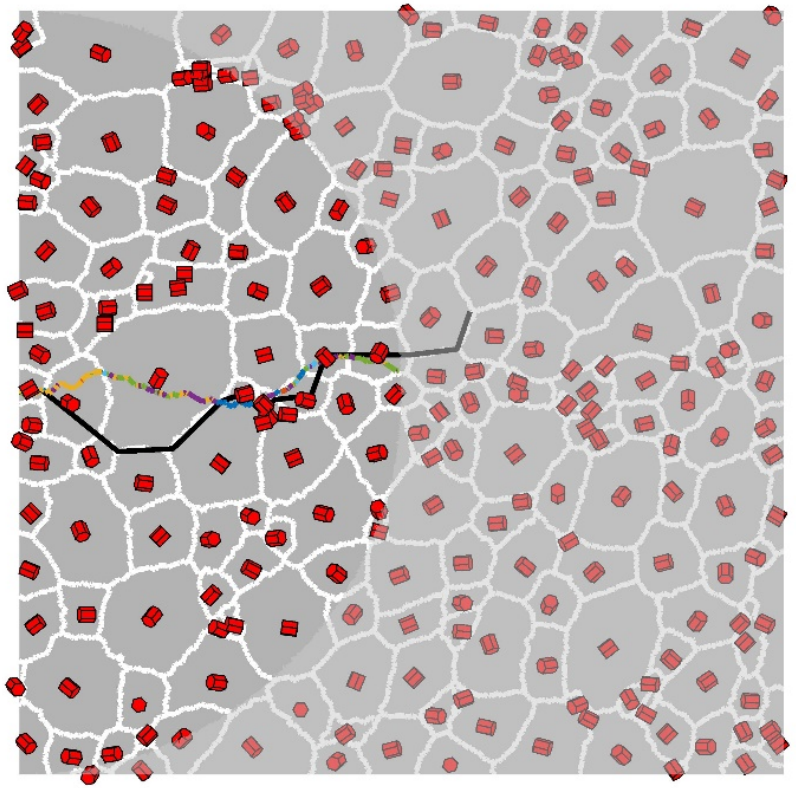
Fatigue cracks in alloys (Black line = Experiments)

Noncrystallographic
Intergranular
Basal
Prismatic
Pyramidal<a>
Pyramidal<c+a>

Experimental comparisons: Foil 2



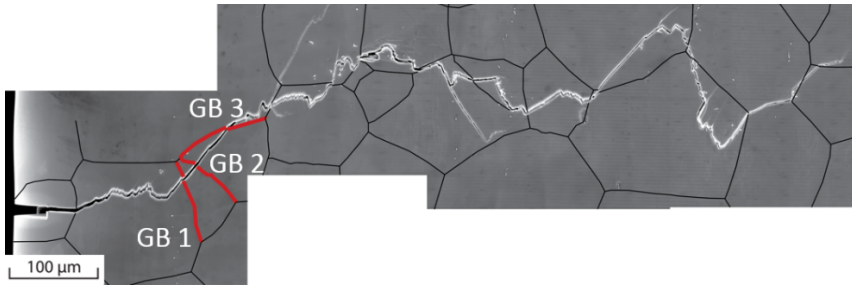


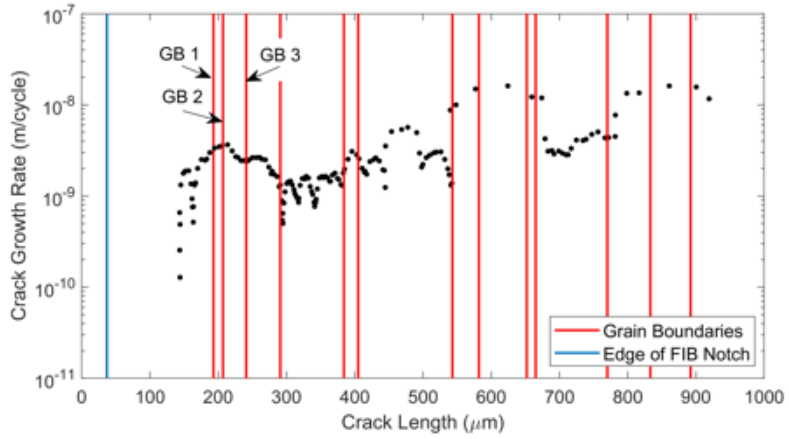


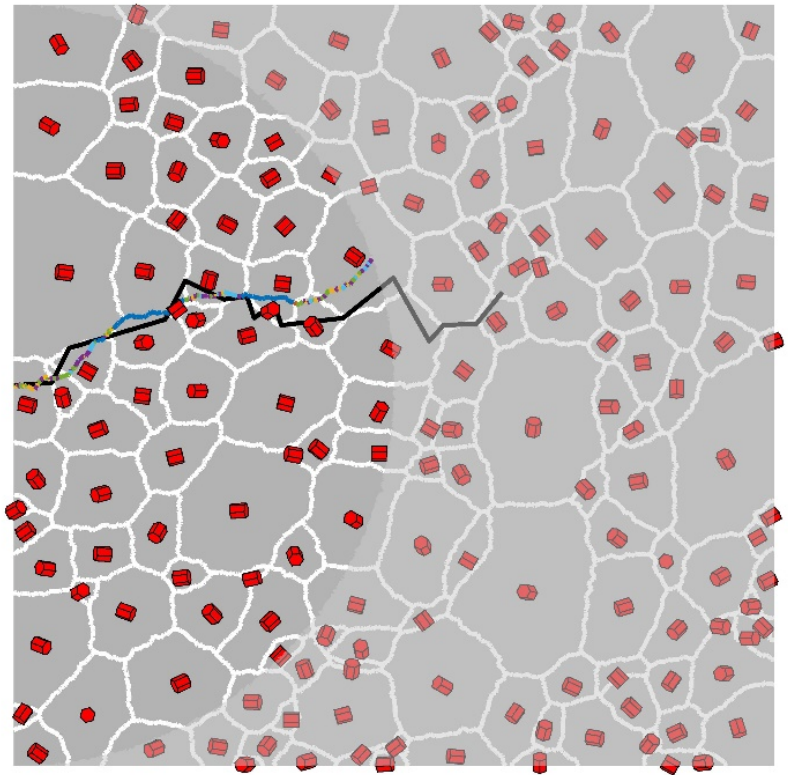
Fatigue cracks in alloys (Black line = Experiments)

Noncrystallographic
Intergranular
Basal
Prismatic
Pyramidal<a>
Pyramidal<c+a>

Experimental comparisons: Foil 3



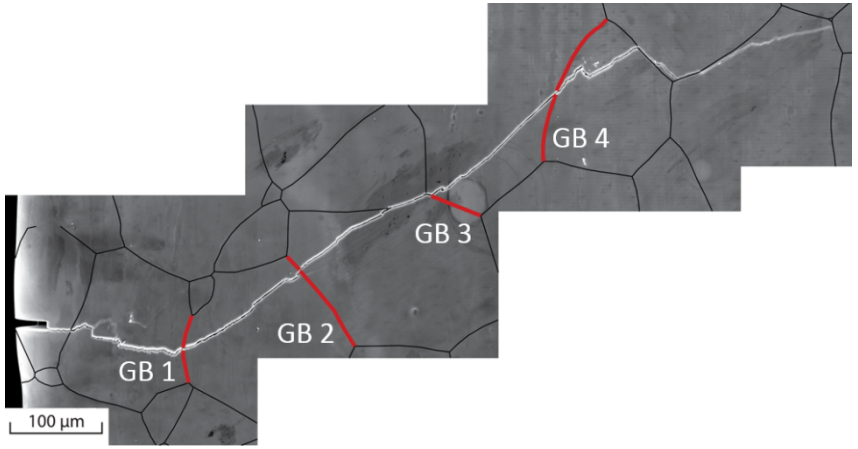


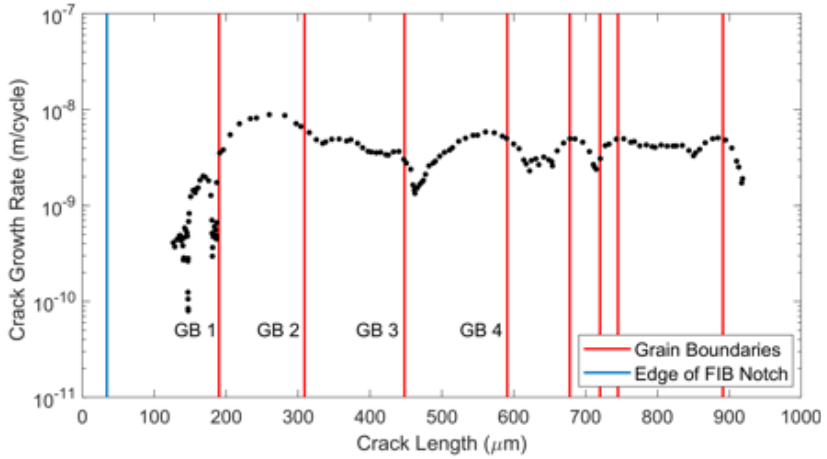


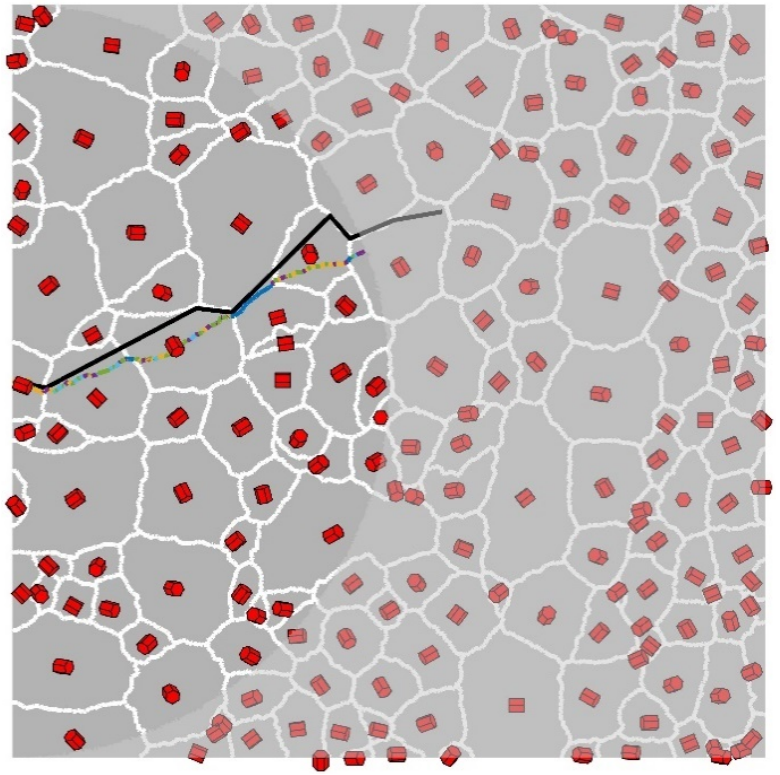
Fatigue cracks in alloys (Black line = Experiments)

Noncrystallographic
Intergranular
Basal
Prismatic
Pyramidal<a>
Pyramidal<c+a>

Experimental comparisons: Foil 4



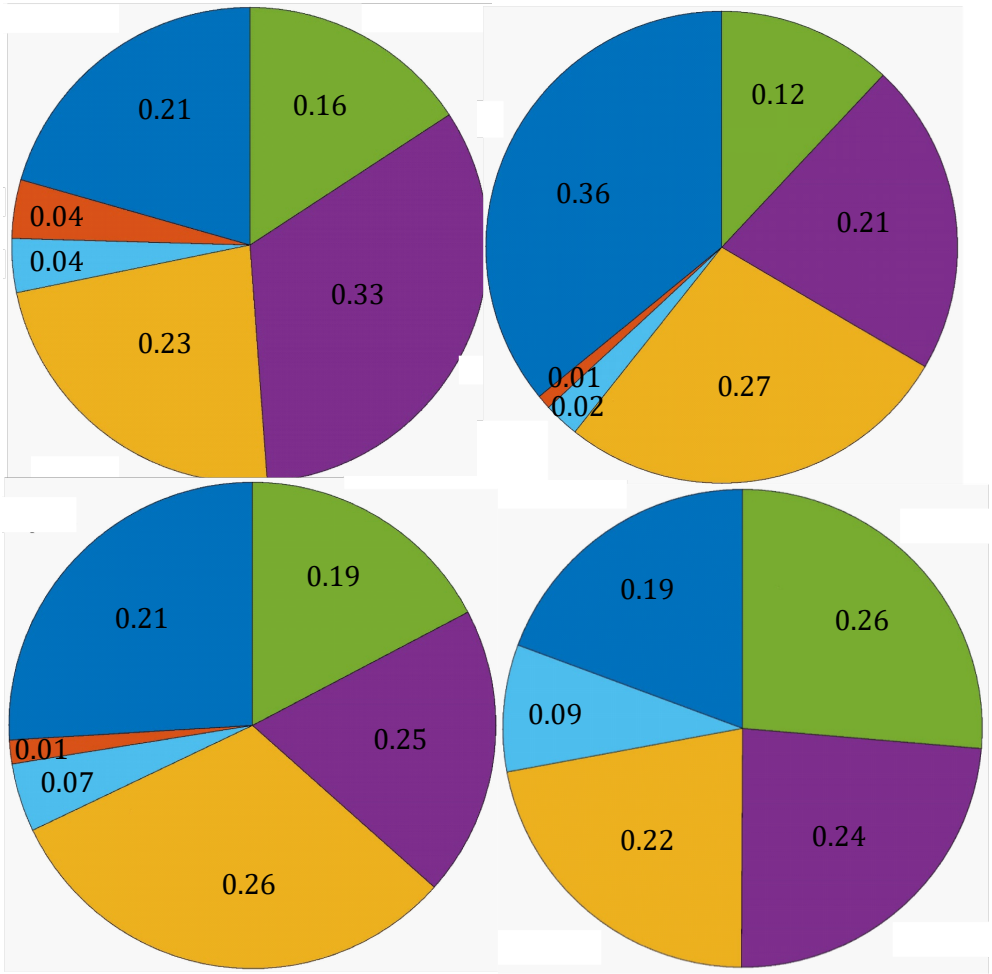


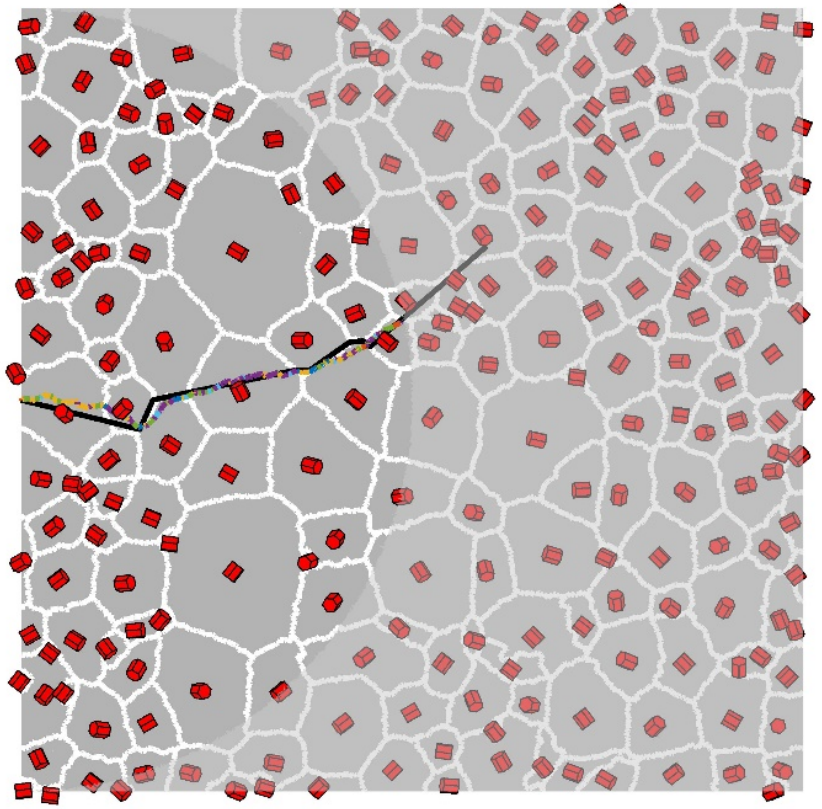


Fatigue cracks in alloys (Black line = Experiments)

Noncrystallographic
Intergranular
Basal
Prismatic
Pyramidal<a>
Pyramidal<c+a>

Learned statistics





Conclusion

- Developed a graph-labelling based approach to estimate microstructure crack path and tested it against analytical results.
- Experimental validation show promising results for WE43 alloy.

Computational complexity:

- The theoretical complexity for approximating Labeling (Rate-determining step) is $\mathrm{O}(N \log N)$.
- For practical mesh-sizes, estimating pairwise energy took most time (~ 1-2 mins on workstation).

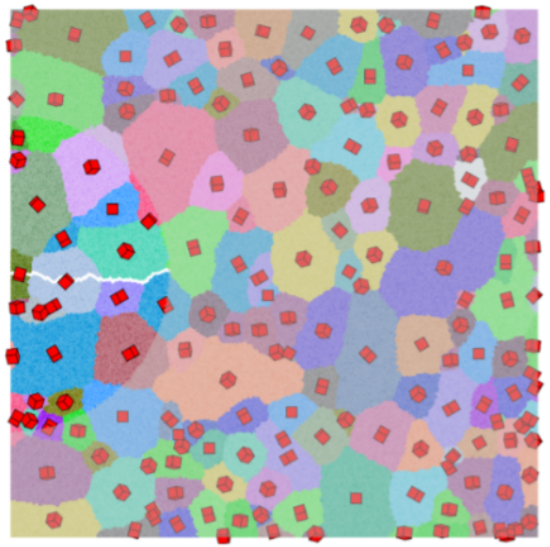
Theoretical extensions:

- This approach is also extended to study elastodynamic fracture (in the sense of *).
- Only the Graph-theoretic formulation for Minimum Energy (ME) criterion is presented but the approach can be extended to other fracture criteria such as Strain Energy (SE) criteria – useful for ductile fracture.

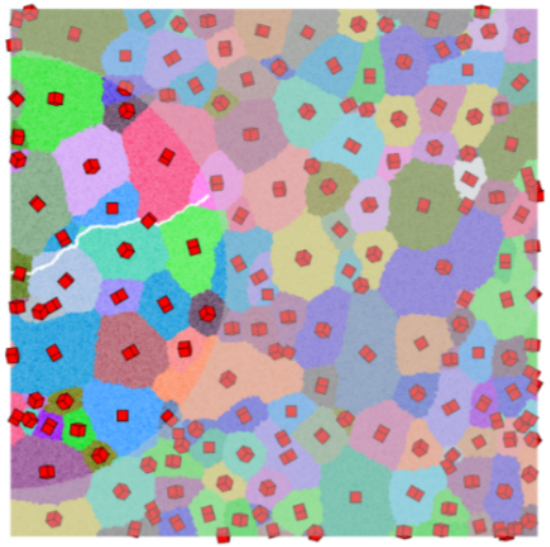
*L. B. Freund. *Energy concepts in dynamic fracture*, page 221–295. Cambridge Monographs on Mechanics. Cambridge University Press, 1990

Effect of radial step-size

- Small radius gives back homogeneous solution for the grain
- Large radius approaches macroscopic behavior



$\overline{r} = 0.3\times$ Image Size



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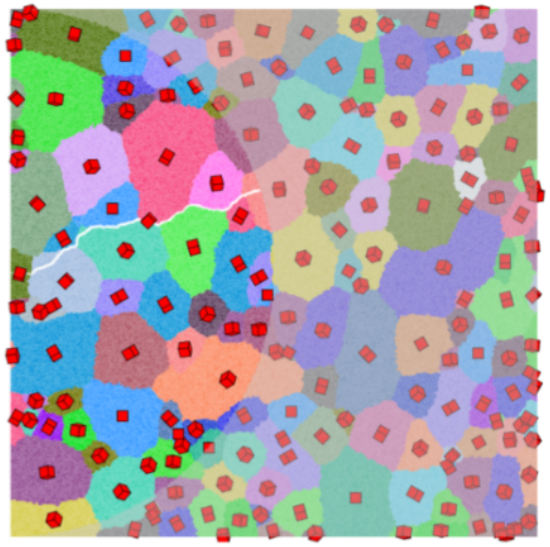


$\overline{r} = 0.5\times$ Image Size

Elastodynamic extension to Griffith's fracture

Assumption*: Constant velocity & no kinetic energy

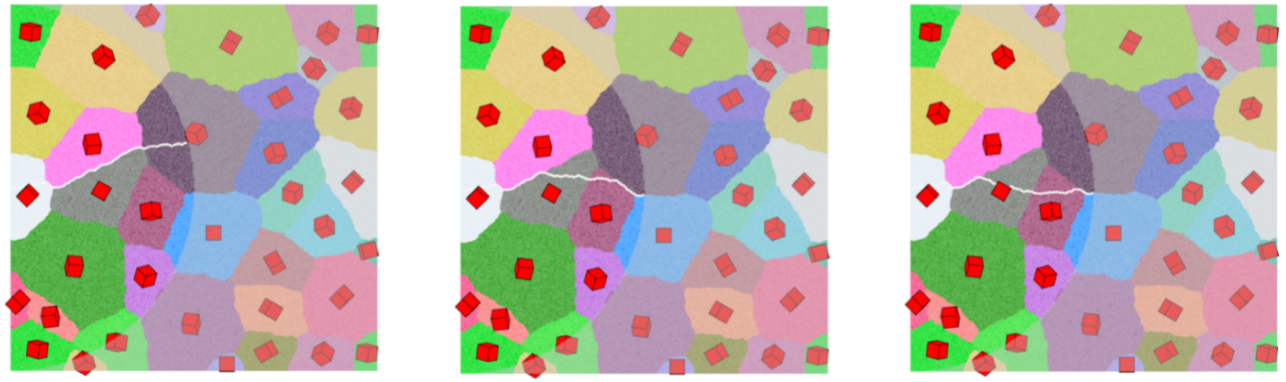
- Equilibrium crack in-plane strain mode - I failure with finite velocity (v) has an augmented energy release rate

$$\tilde{G}(v, \alpha) = A(v)G(\alpha)$$

- In the limiting case of quasistatic fracture, the solution can be recovered from the finite velocity case as

$$\lim_{v \to 0^+} A(v) = 1$$

- Similar results are available for Mode-II fracture



Application: 1. Relates load and velocity of the crack

2. Predicted crack path depends on the load

	Test - 1	Test - 2	Test - 3
$\frac{(\kappa+1)a\pi}{8\mu\gamma_0}\sigma_T^2$ (J/mm)	2.8	10.0	20.0
Microscopic surface energy (J)	1.36	1.41	1.43
Macroscopic energy release (J)	1.36	4.97	9.97
Total Energy (J)	0.00	−3.56	−8.54

*L. B. Freund. *Energy concepts in dynamic fracture*, page 221–295. Cambridge Monographs on Mechanics. Cambridge University Press, 1990

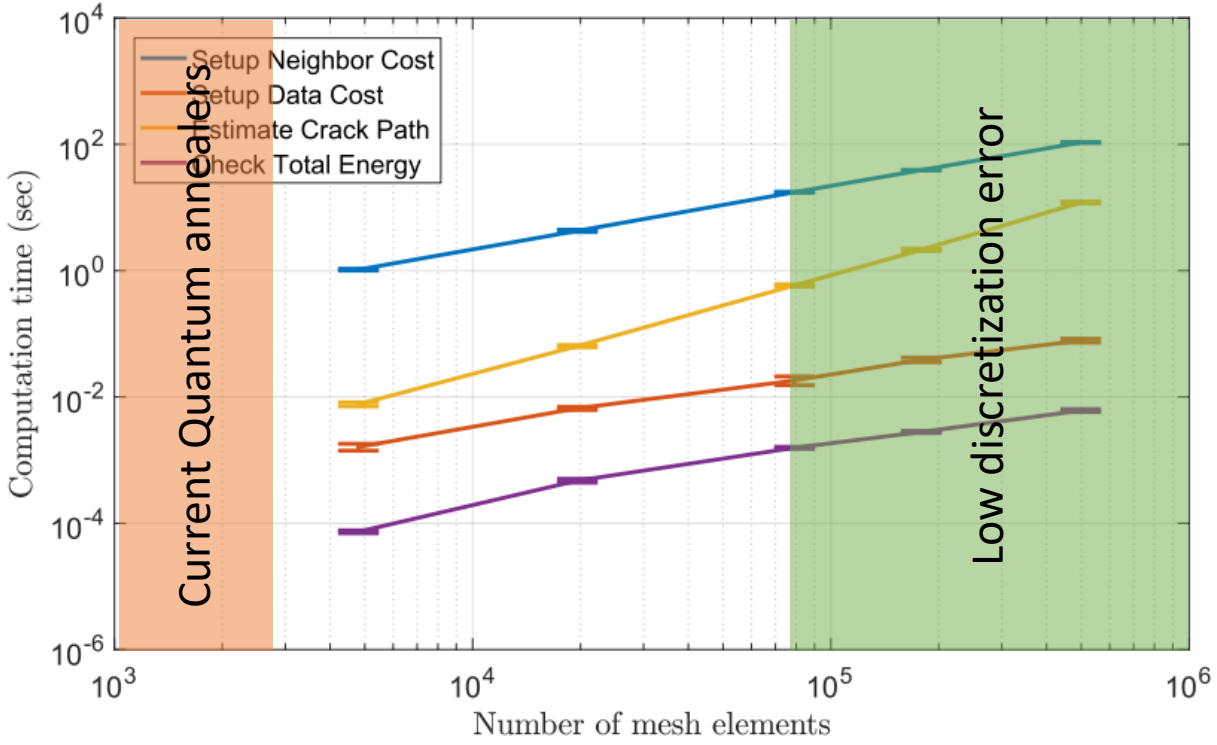
Computation on Quantum annealers

Classical cost:

- The theoretical complexity for approximating Labeling (Rate-determining step) is $\mathrm{O}(N \log N)$
- For practical mesh-sizes, estimating pairwise energy took most time (~ 1-2 mins on workstation)

Quantum Computation:

- Current annealers can't support the required computational size.
- If larger size annealers are made available in future, they can reduce complexity from $\mathrm{O}\left(N \log N\right)$ to $\mathrm{O}(N)$



Thank you