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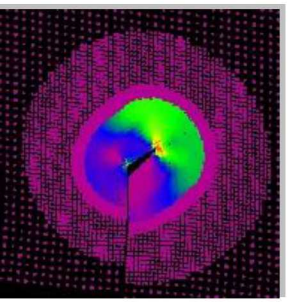

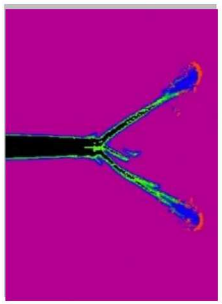

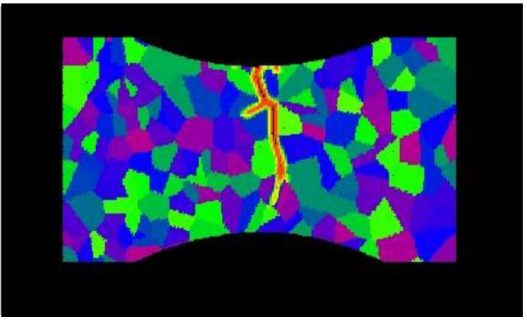

Peridynamic Modeling of Fatigue and Fracture

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Seminar at Los Alamos National Laboratory

November 5, 2019

Sandia National Laboratories

Exceptional service in the national interest

U.S. DEPARTMENT OF ENERGY

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Outline

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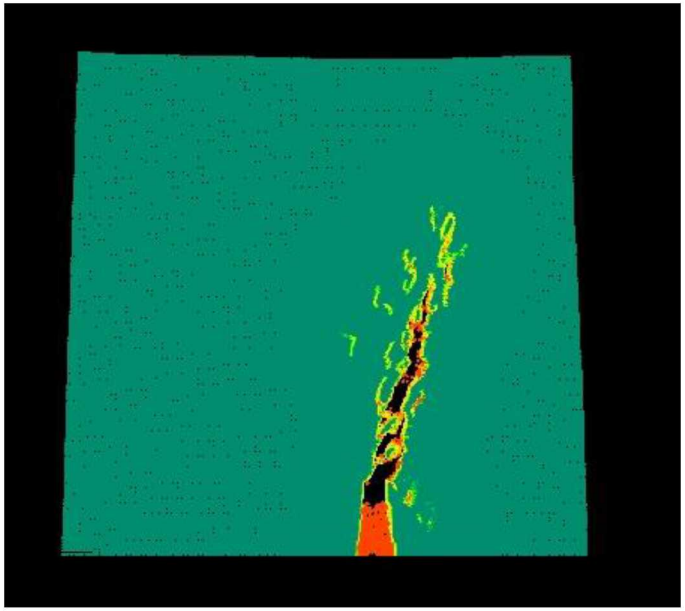
- Peridynamics background
- Dynamic fracture
  - Crack branching
  - Fragmentation
  - Spall
- Fatigue
  - Nucleation phase
  - Growth phase
  - Heterogeneity

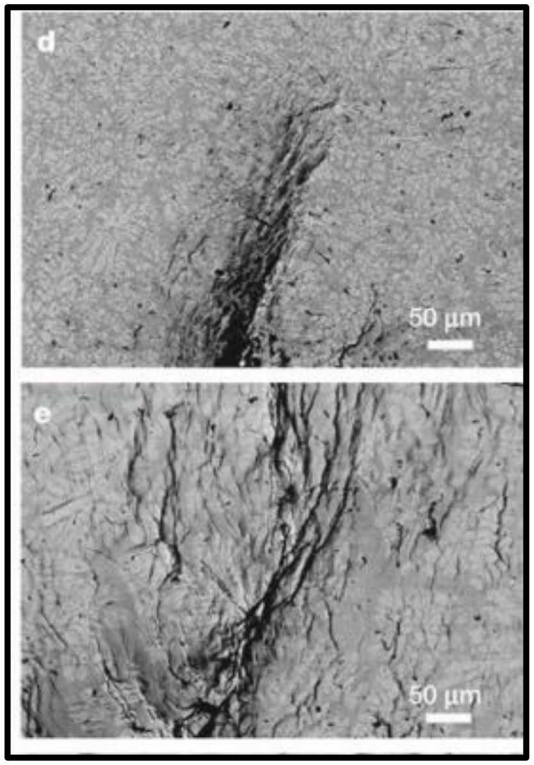
How does a crack nucleate and grow?

How does a continuous deformation become discontinuous?

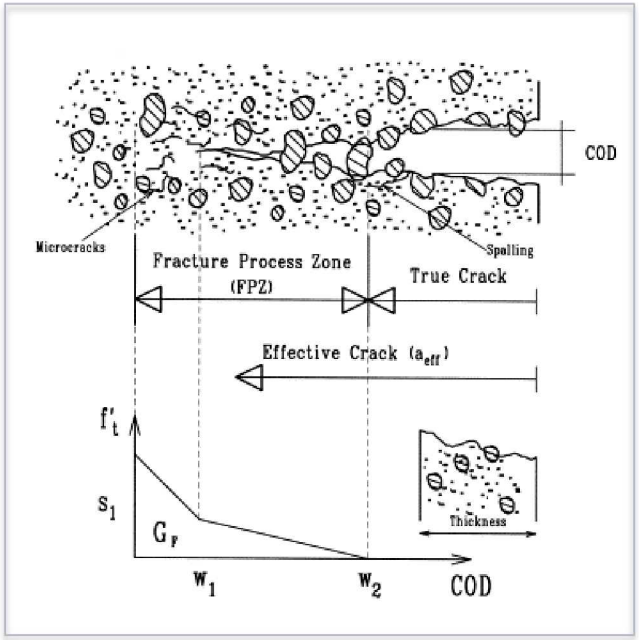
- To study this, we need a model that seamlessly transitions from one to the other within a consistent mathematical system.



Peridynamic simulation



Metallic glass crack tip*



Crack process zone idealization**

*Hofmann et al, Nature (2008)

**Abhimanew, https://commons.wikimedia.org/wiki/File:Fracture_Process_Zone.gif

Peridynamic answers to some simple questions

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- Why is fracture different from other kinds of deformation?
  - *It isn't.*
- Why are special modeling techniques needed for fracture?
  - *They aren't.*
- Why does nearly everybody think they are?
  - *Because nearly everybody uses partial differential equations (PDEs).*
    - What might work better?
      - *Integral equations.*

Typical damage progression in a notched composite panel
(photo courtesy Boeing)

Peridynamic* momentum balance

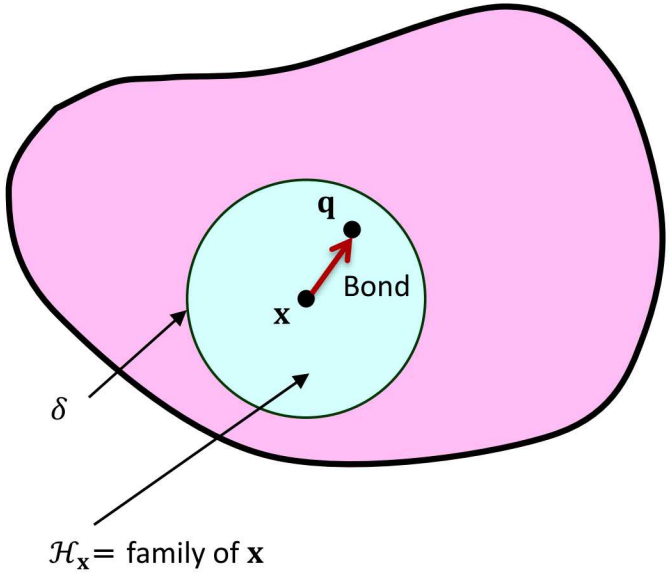
* Peri (near) + dyne (force)

- Any point $\mathbf{x}$ interacts directly with other points within a distance δ called the "horizon."
- The material within a distance δ of $\mathbf{x}$ is called the "family" of $\mathbf{x}$, $\mathcal{H}_{\mathbf{x}}$.

Peridynamic equilibrium equation

$$\int_{\mathcal{H}_{\mathbf{x}}} \mathbf{f}(\mathbf{q},\mathbf{x})\, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x}) = 0$$

$\mathbf{f}$ = bond force density (from the material model, which includes damage)



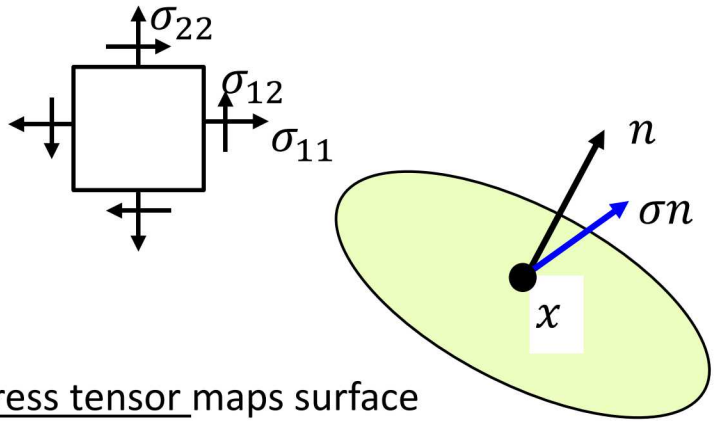
- If $\mathbf{f}$ satisfies $\mathbf{f}(\mathbf{x},\mathbf{q}) = -\mathbf{f}(\mathbf{q},\mathbf{x})$ for all $\mathbf{x},\mathbf{q}$ then linear momentum is conserved.

- SS, JMPS (2000)

The nature of internal forces

Standard theory

Stress tensor field
(assumes continuity of forces)



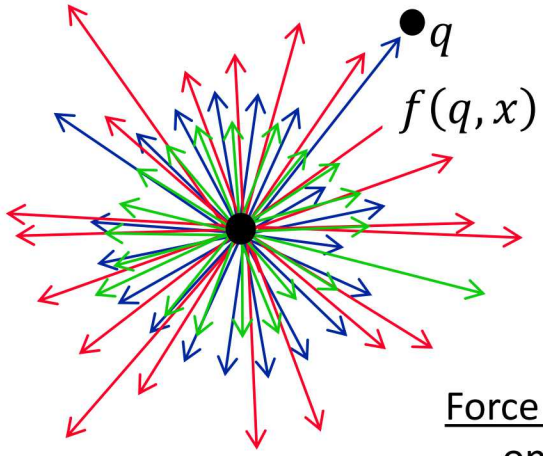
Stress tensor maps surface normal vectors onto surface forces

$$\rho\ddot{u}(x,t) = \nabla \cdot \sigma(x,t) + b(x,t)$$

Differentiation of surface forces

Peridynamics

Bond forces between neighboring points
(allowing discontinuity)



Force state maps bonds onto bond forces

$$\rho\ddot{u}(x,t) = \int_{H_x} f(q,x)dV_q + b(x,t)$$

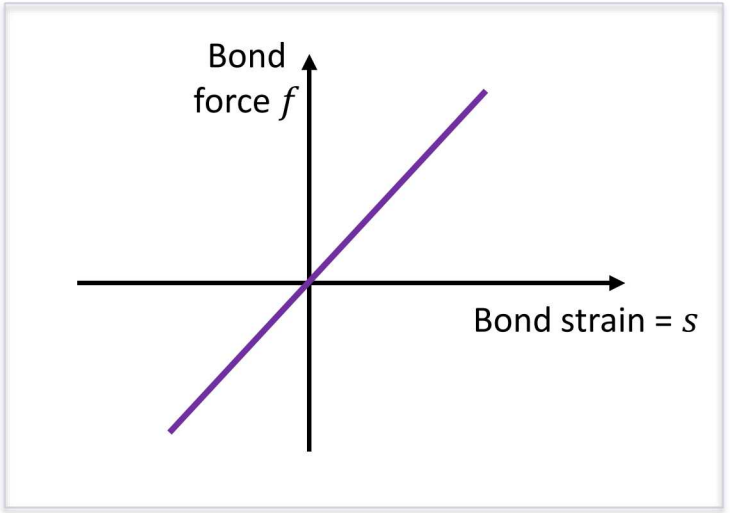
Summation over bond forces

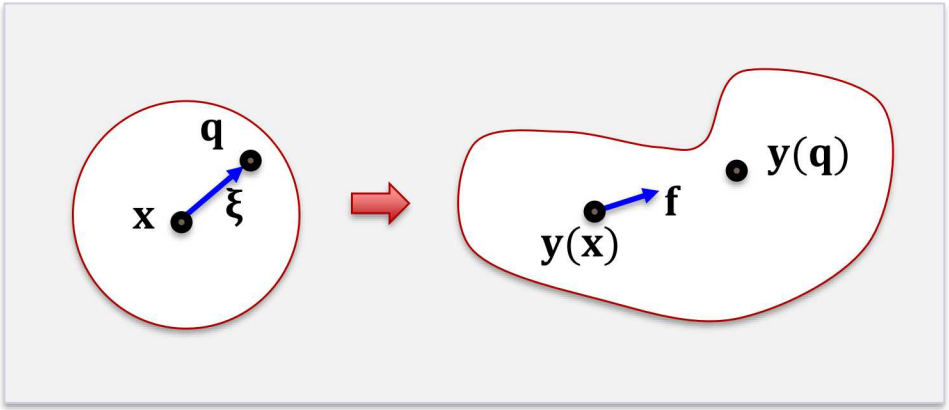
Simplest material model: Microelastic

- Each bond acts like a linear spring.

$$\mathbf{f} = cs\mathbf{M}$$

- s = bond strain = $\dfrac{|\mathbf{y}(\mathbf{q})-\mathbf{y}(\mathbf{x})|}{|\mathbf{q}-\mathbf{x}|} - 1.$
  - $\mathbf{M}$= deformed bond direction
  - $\boldsymbol{\xi}$= bond vector
  - $\mathbf{f}$= bond force density
  - c = spring constant
- Spring constant and horizon determine the wave speeds.
- Bond force is parallel to the deformed bond direction (ensures balance of angular momentum).





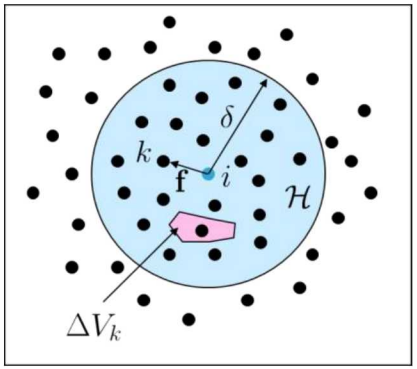
- SS, *JMPS* (2000)

Simple particle discretization

- Integral is replaced by a finite sum: resulting method is meshless and Lagrangian.

$$\rho\ddot{\mathbf{y}}(\mathbf{x},t) = \int_{\mathcal{H}} \mathbf{f}(\mathbf{x}',\mathbf{x},t)\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t) \longrightarrow \rho\ddot{\mathbf{y}}_i^n = \sum_{k\in\mathcal{H}} \mathbf{f}(\mathbf{x}_k,\mathbf{x}_i,t)\, \Delta V_k + \mathbf{b}_i^n$$

- Good:
  - Simple.
  - Linear and angular momentum conserved exactly.
    - Why: the discretized system is itself a peridynamic body.
- Bad:
  - If $\Delta x/\delta$ is held constant, fails to converge to PDEs as $\delta \to 0$.
  - Fails patch test for irregular grids.

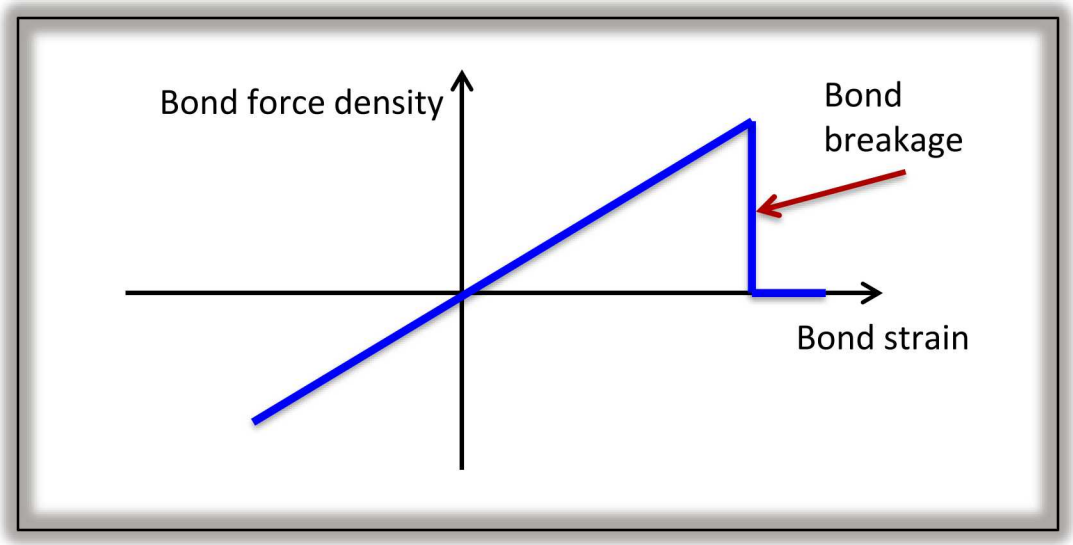


- Discontinuous Galerkin is another viable method (used in LS-DYNA).

- SS & Askari, *Computers and Structures* (2005)
- Bobaru, Yang, Alves, SS, Askari, & Xu, *IJNME* (2009)
- Chen & Gunzburger, *CMAME* (2011)
- Du, Tian, & Zhao, *SIAM J Numerical Analysis* (2013)
- Tian & Du, *SIAM J Numerical Analysis*. (2014)
- Ganzenmüller, Hiermaier, May, in *Meshfree methods for partial differential equations VII,* Springer (2015)
- Seleson & Littlewood, *Computers & Mathematics with Applications* (2016)
- Du, in *Handbook of peridynamic modeling* (2016)

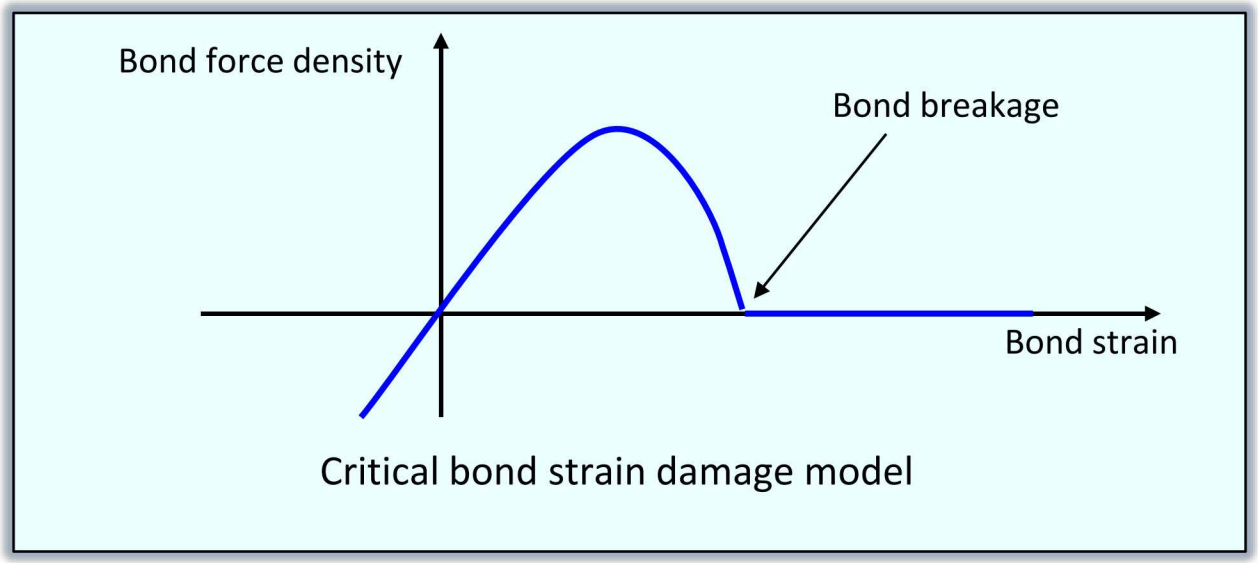
Bond based material models

- If each bond response is independent of the others, the resulting material model is called bond-based.
- The material model is then simply a graph of bond force density vs. bond strain.
- Damage can be modeled through bond breakage.
- Bond response is calibrated to:
  - Bulk elastic properties.
  - Critical energy release rate.



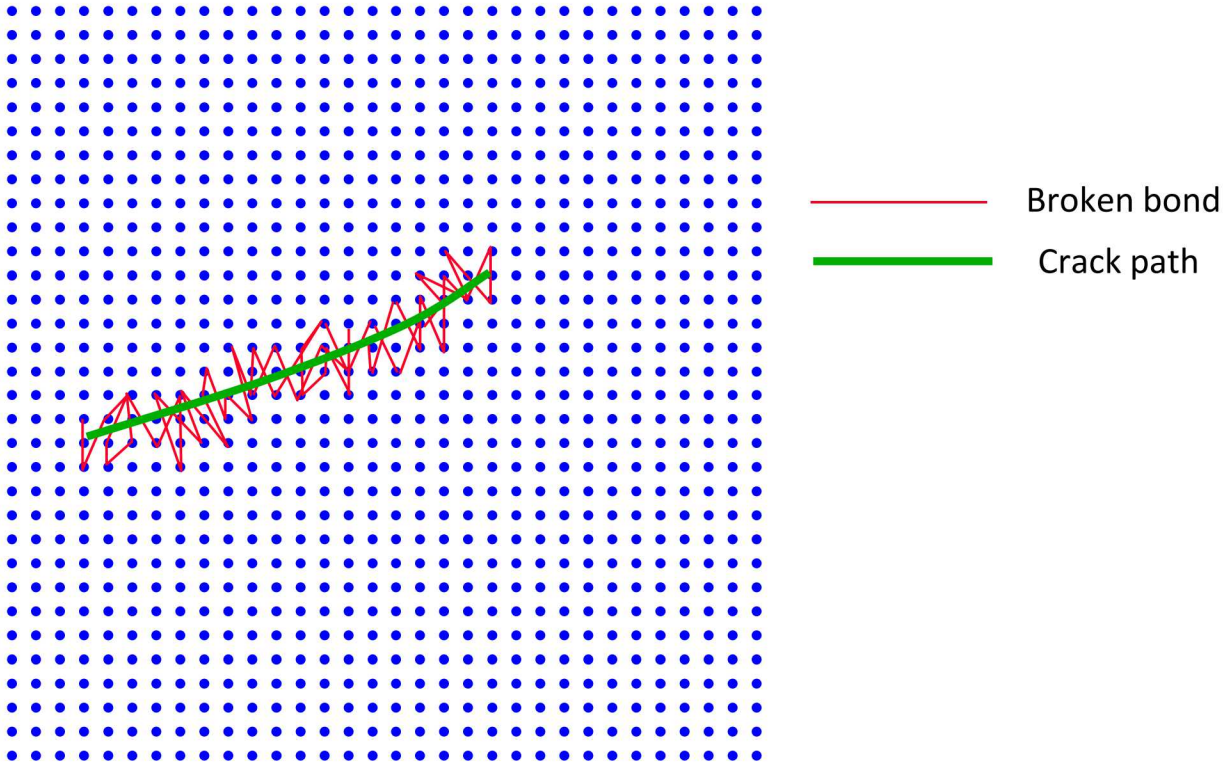
Damage due to bond breakage

- Recall: each bond carries a force.
- Damage is implemented at the bond level.
  - Bonds break irreversibly according to some criterion.
  - Broken bonds carry no force.
- Examples of criteria:
  - Critical bond strain (brittle).
  - Hashin failure criterion (composites).
  - Gurson (ductile metals).



Critical bond strain damage model

Autonomous crack growth

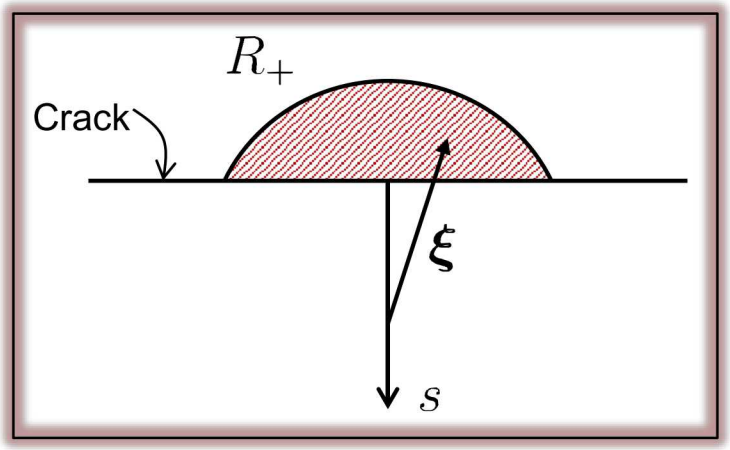


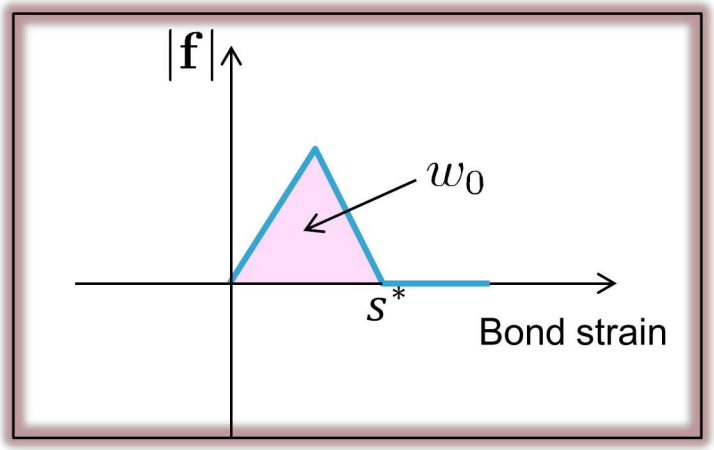
- When a bond breaks, its load is shifted to its neighbors, leading to progressive failure.

Critical bond strain:
Relation to critical energy release rate

If the work required to break the bond $\boldsymbol{\xi}$ is $w_0(\boldsymbol{\xi})$, then the energy release rate is found by summing this work per unit crack area (J. Foster):

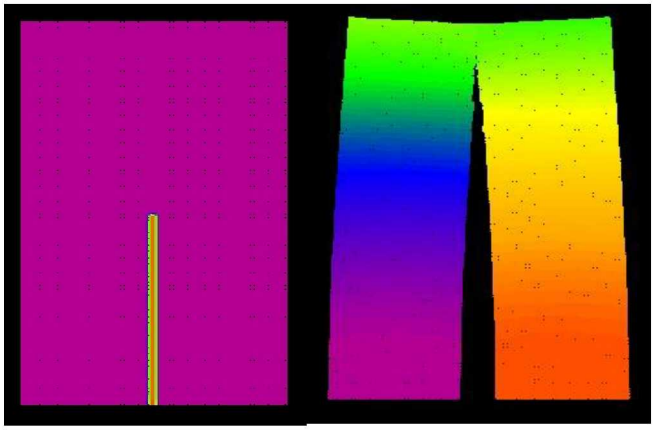
$$G = \int_0^{\delta} \int_{R_+} w_0(\boldsymbol{\xi})\, dV_{\boldsymbol{\xi}}\, ds$$

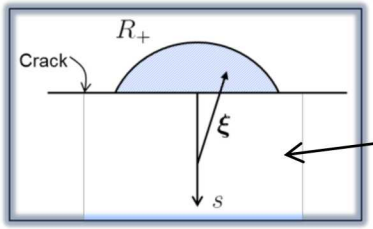




- Can then get the critical strain for bond breakage s^* in terms of G.
- Could also use the peridynamic J-integral as a bond breakage criterion.

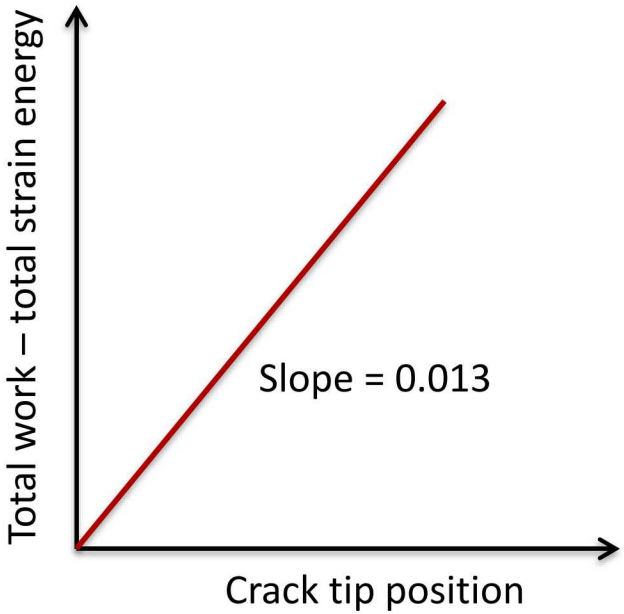
Constant bond failure strain reproduces the Griffith crack growth criterion





From bond properties, energy release rate should be

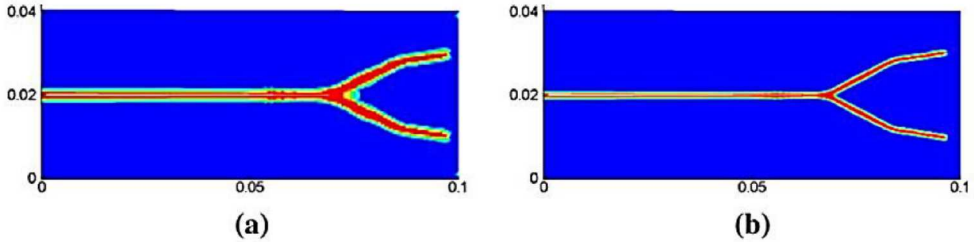
G = 0.013

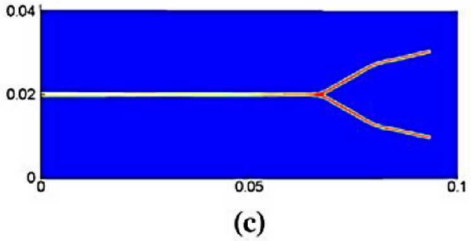


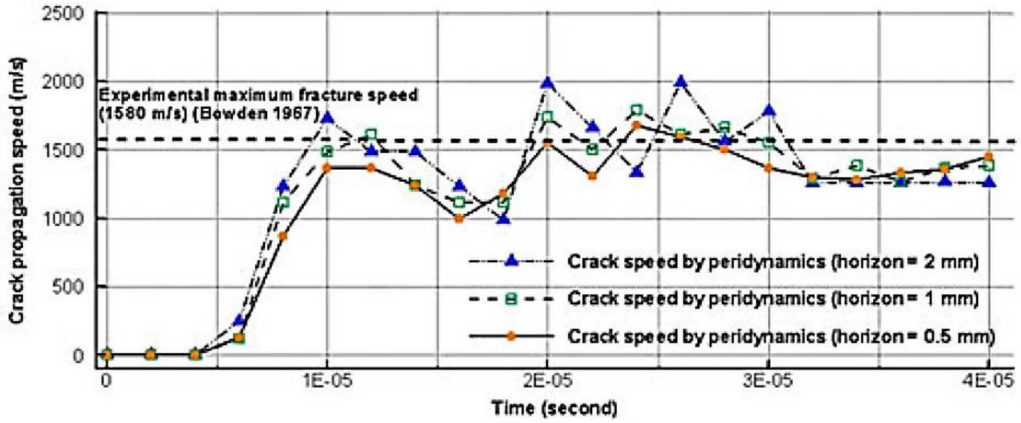
- This confirms that the energy consumed per unit crack growth area equals the expected value from bond breakage properties.

Brittle microelastic model reproduces measured dynamic crack velocity

- Fracture in soda-lime glass using 3 different grid spacings*.







- Ha & Bobaru, *Int J Fracture* (2010)
- *Agwai, Guven, & Madenci, *Int J Fracture* (2011)
- Ha & Bobaru, *Engin Fracture Mech* (2011)
- Dipasquale, Zaccariotto, & Galvanetto, *Int J Fracture* (2014)
- Bobaru & Zhang, *Int. J Fracture* (2015)
- Zhou, Wang, & Qian, *European J Mechanics-A/Solids*. (2016)

Fragmentation of an expanding cylinder driven by explosive

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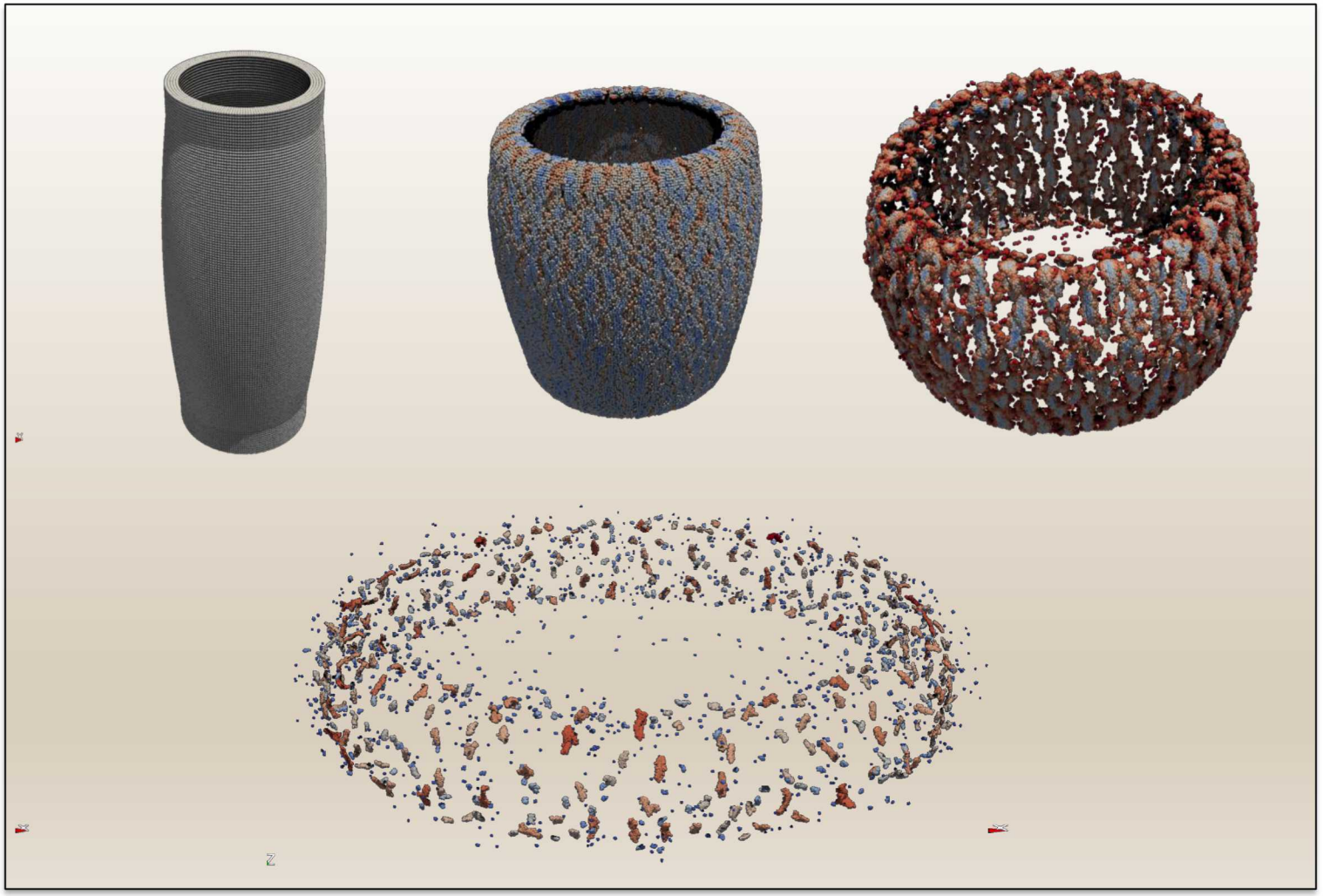
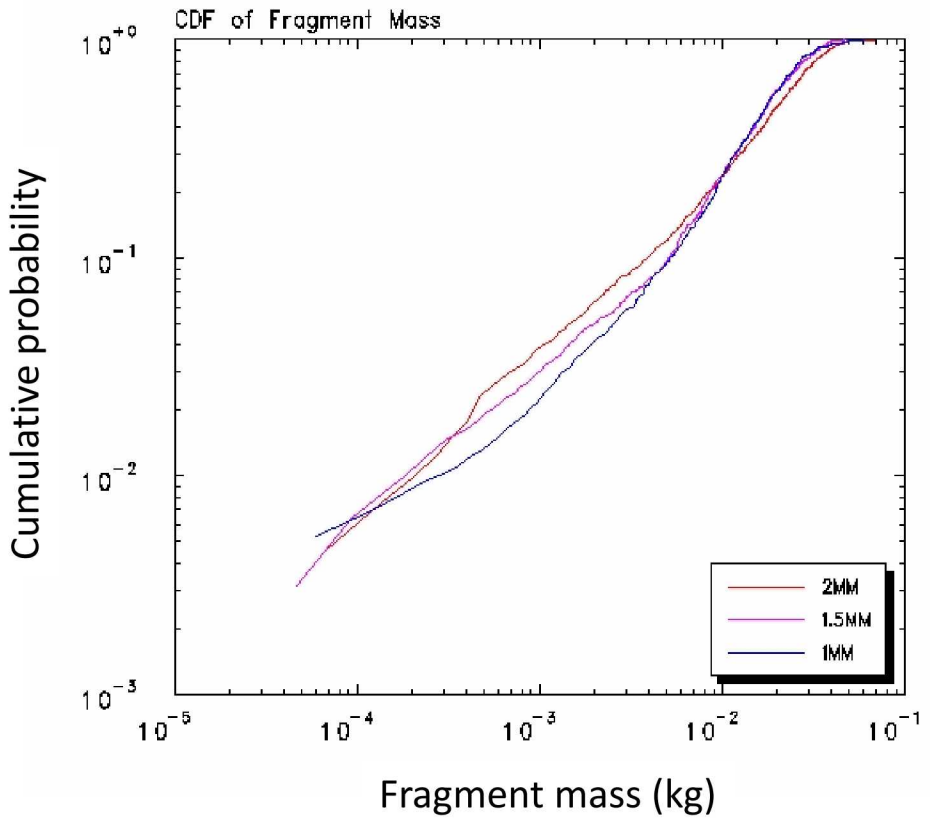
- Explosive is modeled by CTH, loads are applied to a peridynamic grid for the cylinder.



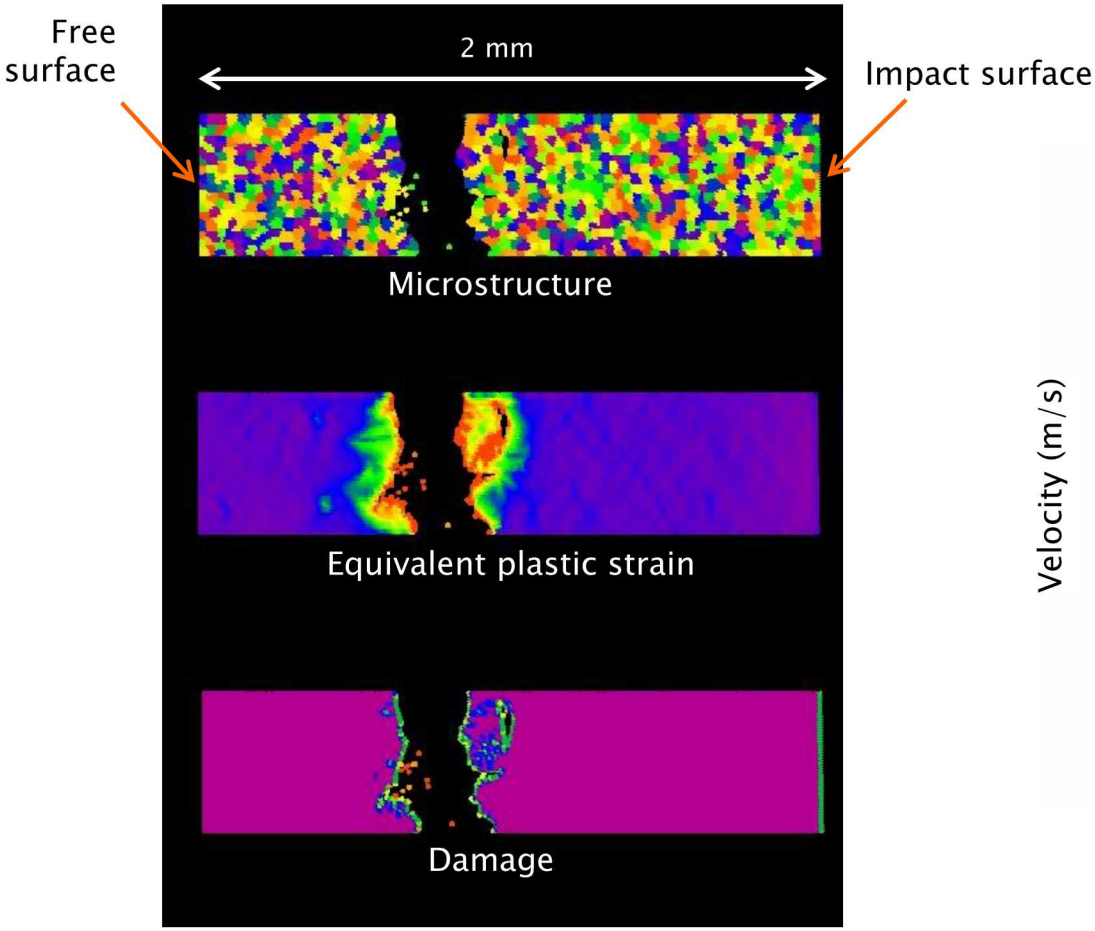
Fragmentation of an expanding cylinder: Convergence

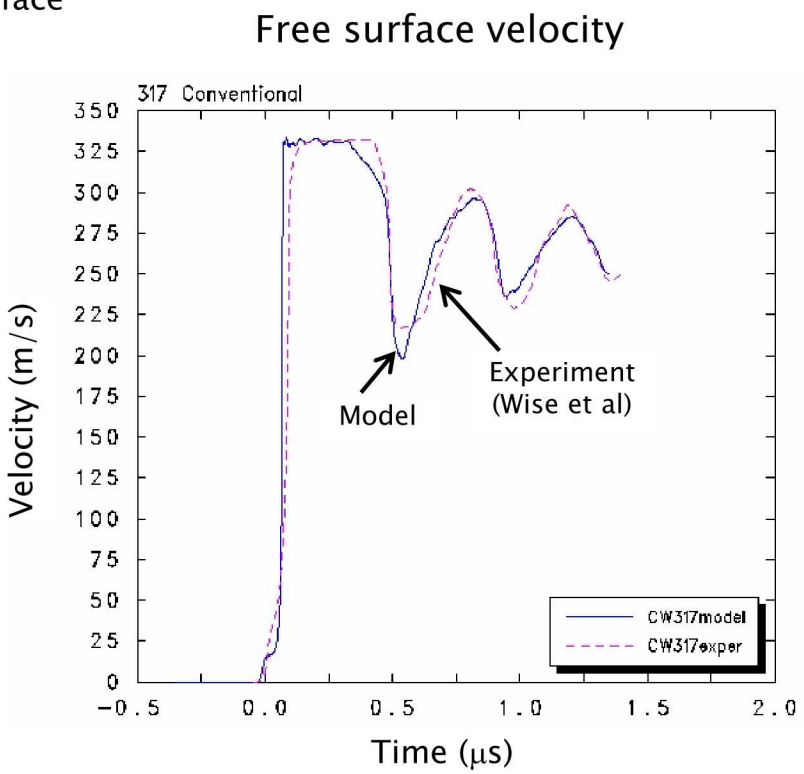
- Figure shows a CDF of fragment mass for three different grid spacings (1, 1.5, 2mm).
  - The 1 and 1.5mm curves are essentially identical for fragments larger than 5 grams.
  - This indicates the results are converging as the grid is refined.



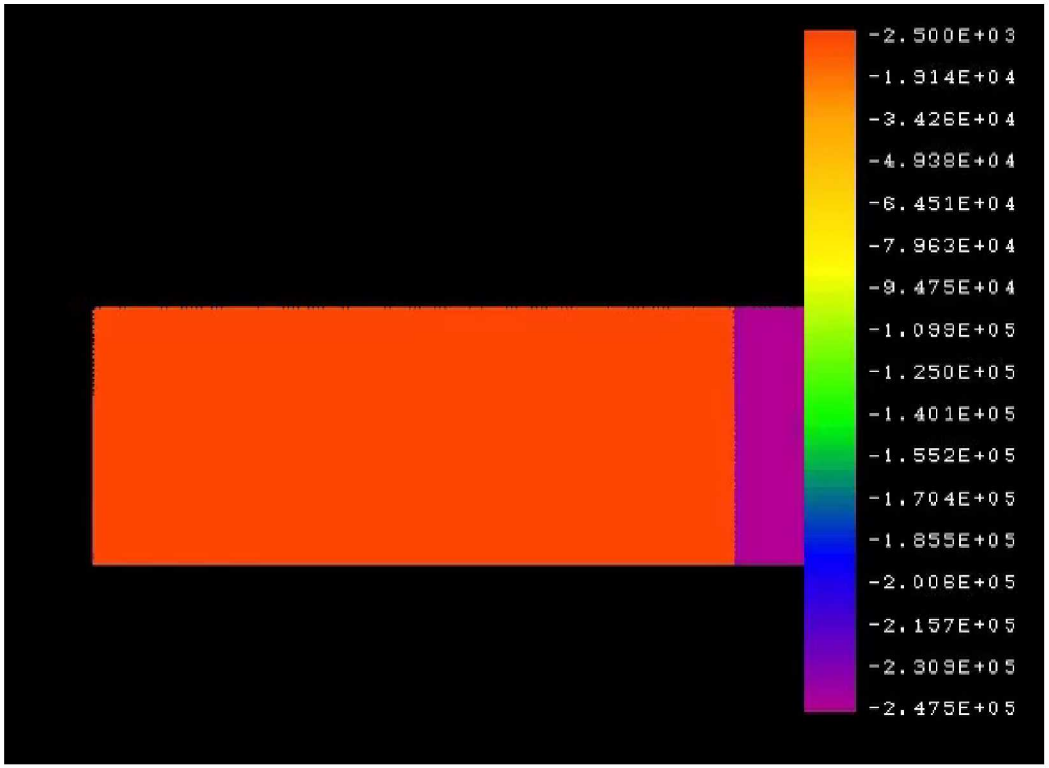
Spall: Microstructure affects the kinetics of fracture

- Peridynamic simulation of spall in steel (impact at 317m/s)

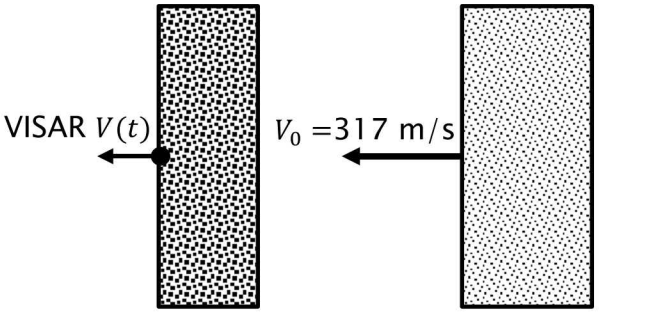




Spall video



Colors show velocity



Accumulation of damage: Hammering on a block

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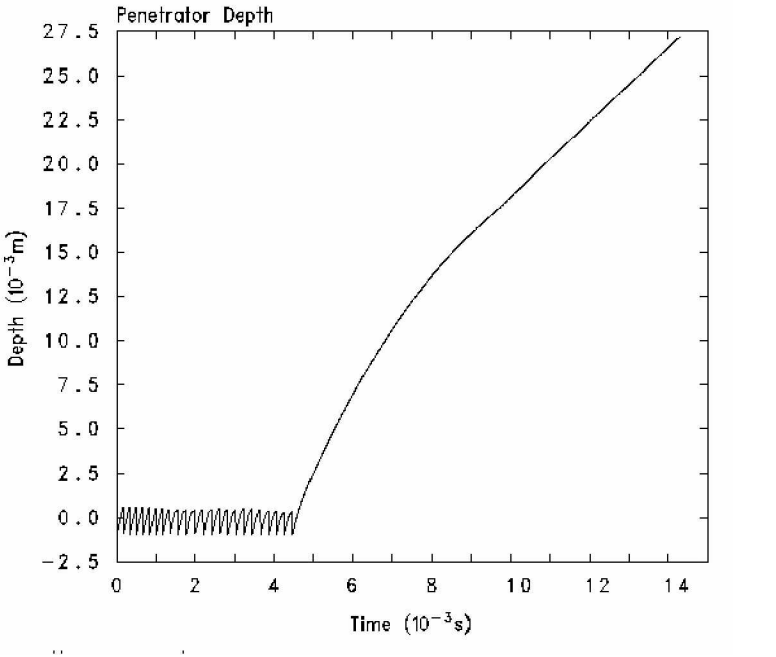
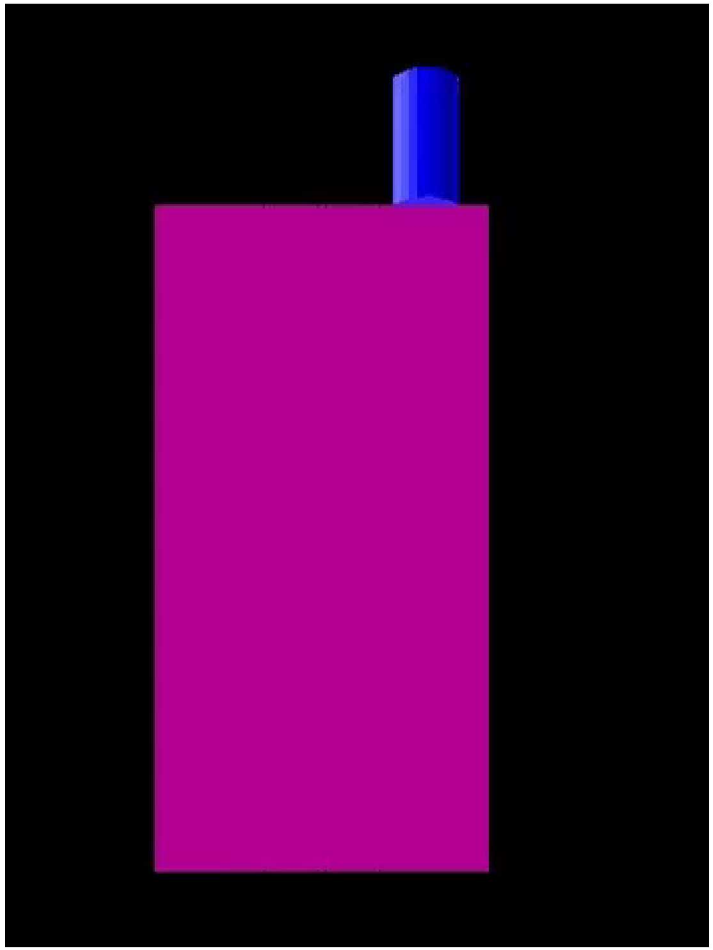


Penetration depth vs. time

Each peak is a strike.

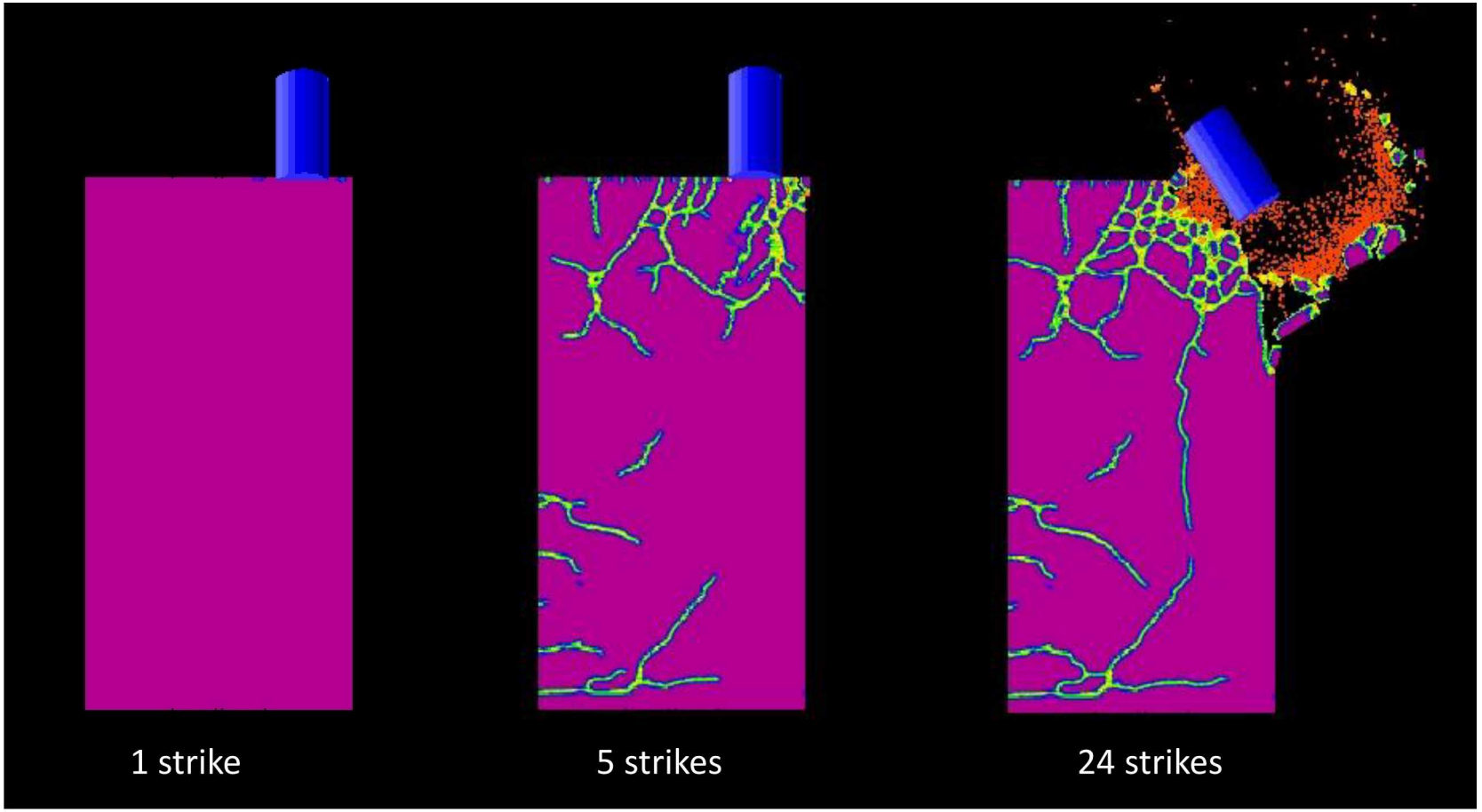
Break through at 24 strikes.

VIDEO



Colors show damage

Accumulation of damage: Hammering on a block



Colors show damage

Peridynamic vs. local equations

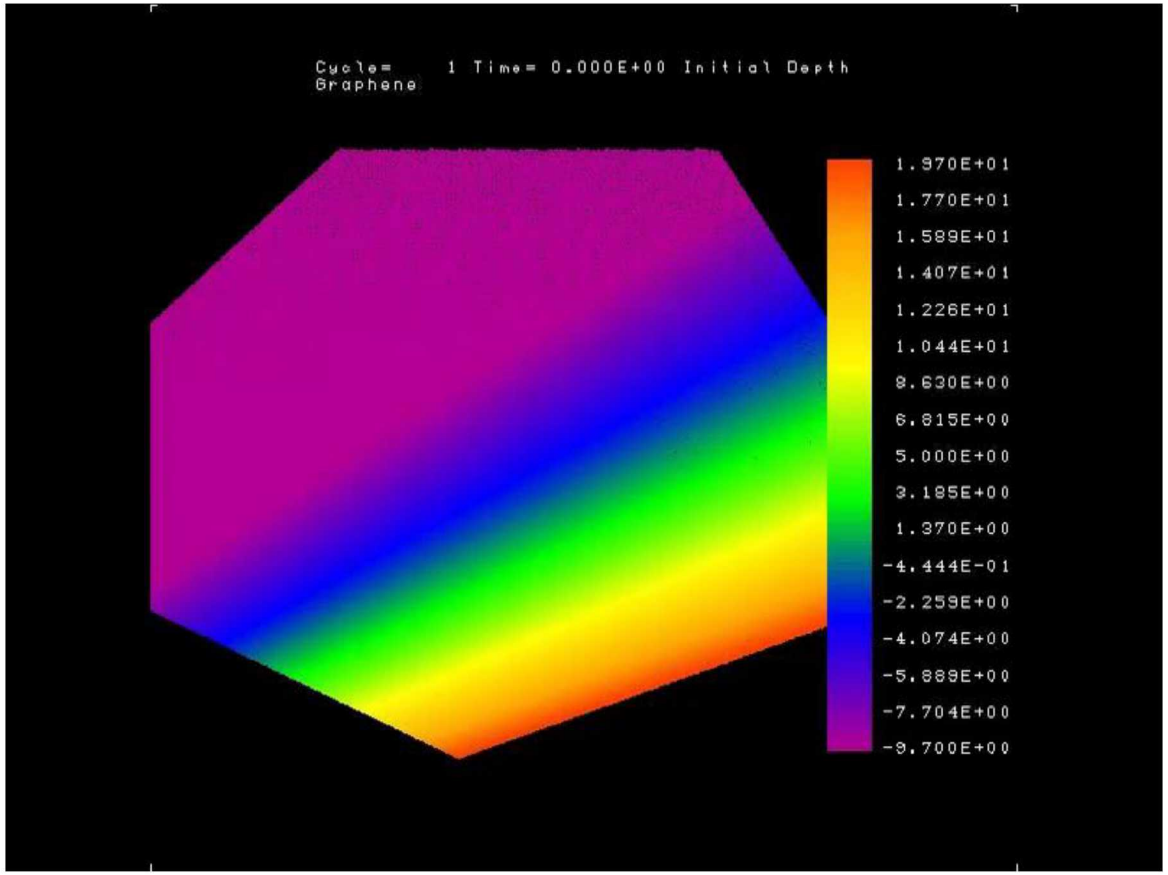
- The structures of the theories are similar, but peridynamics uses nonlocal operators.

Relation	*Peridynamic theory*	*Standard theory*
Kinematics	$\underline{\mathbf{Y}}\langle \mathbf{q}-\mathbf{x}\rangle = \mathbf{y}(\mathbf{q})-\mathbf{y}(\mathbf{x})$	$\mathbf{F}(\mathbf{x}) = \dfrac{\partial \mathbf{y}}{\partial \mathbf{x}}(\mathbf{x})$
Linear momentum balance	$\rho\ddot{\mathbf{y}}(\mathbf{x}) = \displaystyle\int_{\mathcal{H}} \Big(\mathbf{t}(\mathbf{q},\mathbf{x}) - \mathbf{t}(\mathbf{x},\mathbf{q})\Big)\, dV_{\mathbf{q}} + \mathbf{b}(\mathbf{x})$	$\rho\ddot{\mathbf{y}}(\mathbf{x}) = \nabla\cdot\boldsymbol{\sigma}(\mathbf{x}) + \mathbf{b}(\mathbf{x})$
Constitutive model	$\mathbf{t}(\mathbf{q},\mathbf{x}) = \underline{\mathbf{T}}\langle \mathbf{q}-\mathbf{x}\rangle, \qquad \underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}})$	$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(\mathbf{F})$
Angular momentum balance	$\displaystyle\int_{\mathcal{H}} \underline{\mathbf{Y}}\langle \mathbf{q}-\mathbf{x}\rangle \times \underline{\mathbf{T}}\langle \mathbf{q}-\mathbf{x}\rangle\, dV_{\mathbf{q}} = \mathbf{0}$	$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$
Elasticity	$\underline{\mathbf{T}} = W_{\underline{\mathbf{Y}}}$ (Fréchet derivative)	$\boldsymbol{\sigma} = W_{\mathbf{F}}$ (tensor gradient)
First law	$\dot{\varepsilon} = \underline{\mathbf{T}} \bullet \underline{\dot{\mathbf{Y}}} + q + r$	$\dot{\varepsilon} = \boldsymbol{\sigma}\cdot\dot{\mathbf{F}} + q + r$

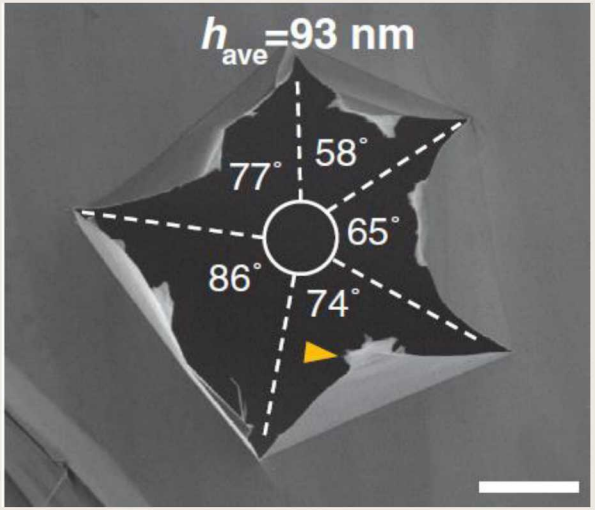
$$\underline{\mathbf{T}} \bullet \underline{\dot{\mathbf{Y}}} := \int_{\mathcal{H}} \underline{\mathbf{T}}\langle \boldsymbol{\xi}\rangle \cdot \underline{\dot{\mathbf{Y}}}\langle \boldsymbol{\xi}\rangle\, dV_{\boldsymbol{\xi}}$$

Microballistics: Perforation of a graphene laminate

- 600m/s 3.7μm sphere onto 50nm thick graphene laminate.



Video: Colors show initial position



Experiment
J-H Lee et al, Science (2014)

Ductile materials: Correspondence material models

- This is a type of state-based material model that uses a stress tensor as an intermediate quantity in computing bond forces.

$$\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle \rightarrow \mathbf{F} \rightarrow \boldsymbol{\sigma} \rightarrow \underline{\mathbf{T}}\langle\boldsymbol{\xi}\rangle$$

- This is the most convenient way to implement J_2 flow theory.
- Some overlap with SPH.

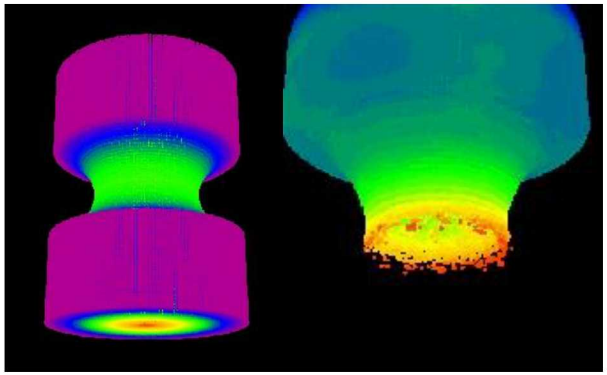
- SS, Epton, Weckner, Xu, & Askari, *J Elasticity* (2007)
- Warren, SS, Askari, Weckner, Epton, Xu, *Int J Solids & Structures* (2009)
- Tupek & Radovitzky, *JMPS* (2014)
- Bessa, Foster, Belytschko, & Liu, *Computational Mechanics* (2014)
- *SS, *CMAME* (2017)
- Du & Tian, *SIAM J Applied Math* (2018)
- Foster & Xu, *Int J Solids & Structures* (2018)
- Li, Hao, & Zhen, *CMAME* (2018)
- Nicely, Tang, & Qian, *CMAME* (2018)
- Chowdhury, P. Roy, D. Roy, & Reddy, *CMAME* (2019)
  - Ganzenmüller, Hiermaier, May, *Computers & Structures* (2015)

Ductile failure model implementation

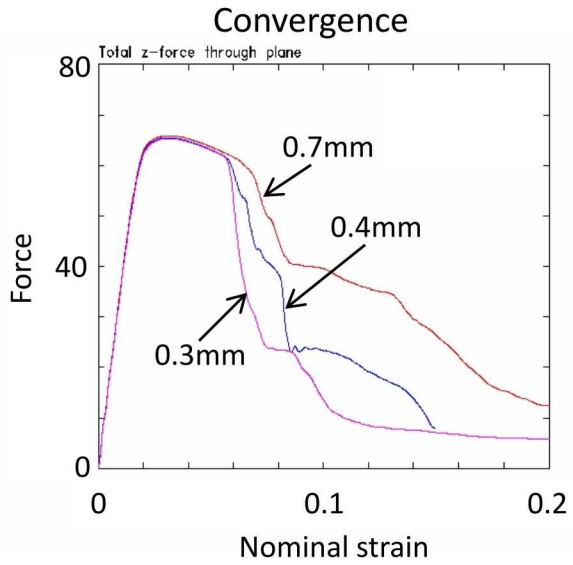
- It is essential to incorporate the effect of hydrostatic stress on ductile failure nucleation. How to map this effect onto bond breakage?
- One way: Wellman tearing parameter model.
- Start breaking bonds at **x** when

$$\int \left[\frac{2\sigma_1}{3(\sigma_1 - \bar{\sigma})}\right]^4 d\varepsilon^p = {\varepsilon^p}_f$$

where
σ_1 = maximum principal stress,
$\bar{\sigma}$= hydrostatic stress,
ε^p= equivalent plastic strain,
${\varepsilon^p}_f$ = failure strain in uniaxial tension.



Johnson-Cook plasticity with Wellman tearing model*



- G. W. Wellman, SAND2012-1343 (2012).

Fatigue: Cyclic strain in a bond

- For a given bond $\boldsymbol{\xi}$, the *bond elongation* is the change in bond length:

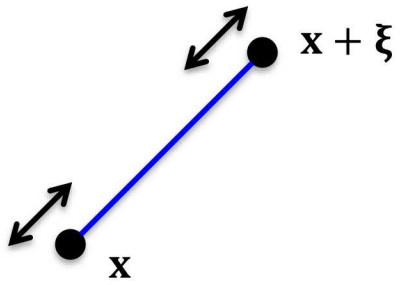
$$e = |\underline{\mathbf{Y}}\langle\boldsymbol{\xi}\rangle| - |\boldsymbol{\xi}| = |\mathbf{y}(\mathbf{x}+\boldsymbol{\xi}) - \mathbf{y}(\mathbf{x})|.$$

- The *bond strain* is the change in length over initial length:

$$s = \frac{e}{|\boldsymbol{\xi}|}.$$

- Let s^+ and s^- be the two extremes under cyclic loading of $\boldsymbol{\xi}$.
- The *cyclic bond strain* is defined by

$$\varepsilon = |s^+ - s^-|.$$

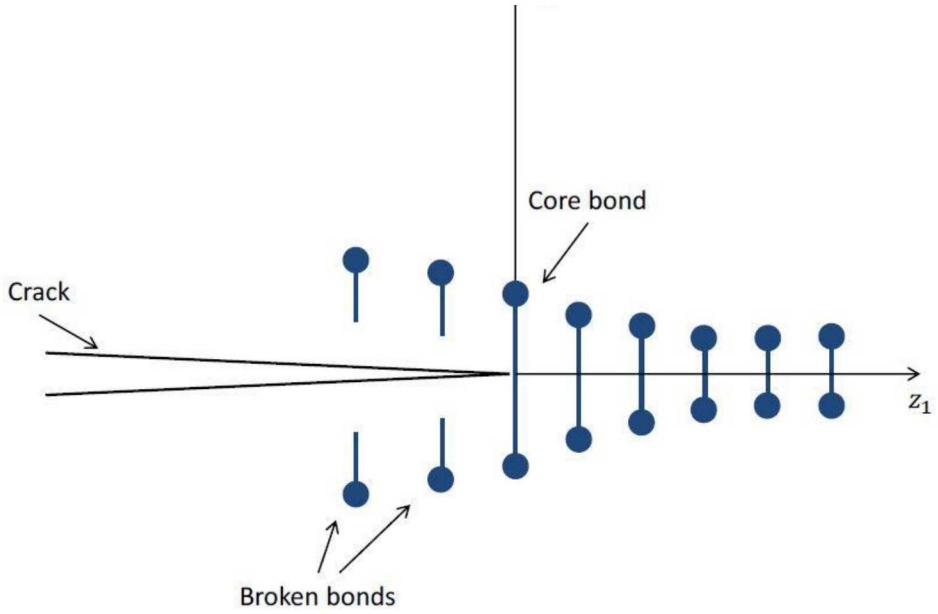


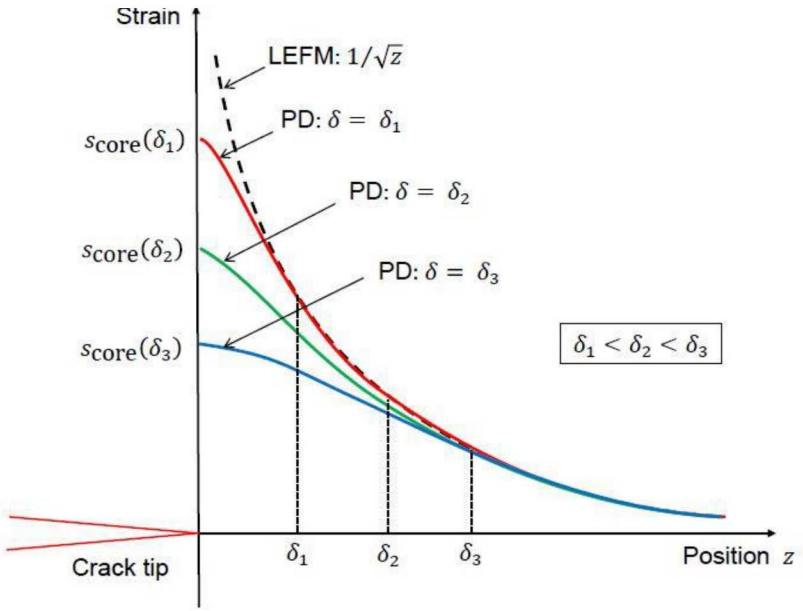
Structure of a crack tip field

- Let $\varepsilon_{\text{core}}(\delta)$ be the largest cyclic strain in any bond.
- Can show by a dimensional argument $\exists\ \hat{\varepsilon}_{\text{core}}$ such that

$$\varepsilon_{\text{core}}(\delta) = \hat{\varepsilon}_{\text{core}} \frac{\Delta K}{E\sqrt{\delta}}$$

where ΔK = cyclic stress intensity factor and E = modulus.





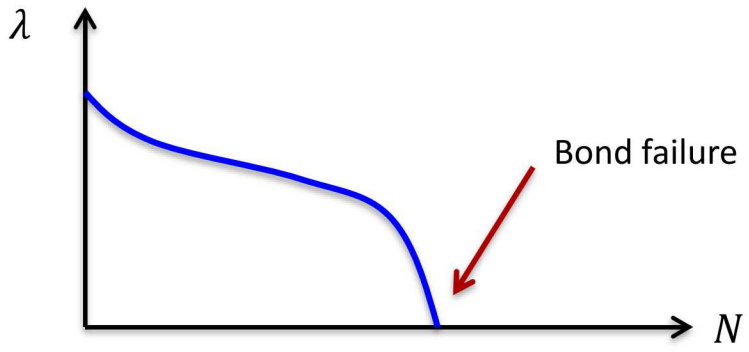
Remaining life of a bond

- Each bond in the body has a *remaining life* $\lambda(N)$ where N is the cycle number.
- The remaining life is monotonically decreasing over time.

$$\lambda(0) = 1, \qquad \dot{\lambda} \leq 0.$$

- The bond fails at the first cycle N when

$$\lambda(N) \leq 0.$$



Fatigue model

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- The fatigue model specifies how the remaining life of each bond depends on the loading.

$$\frac{d\lambda}{dN}(N) = -A\varepsilon^m$$

  where A and m are constants and ε is the cyclic bond strain.

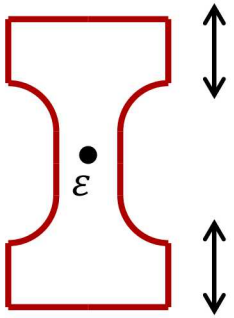
- The constants are calibrated separately for phases I and II (nucleation and growth).

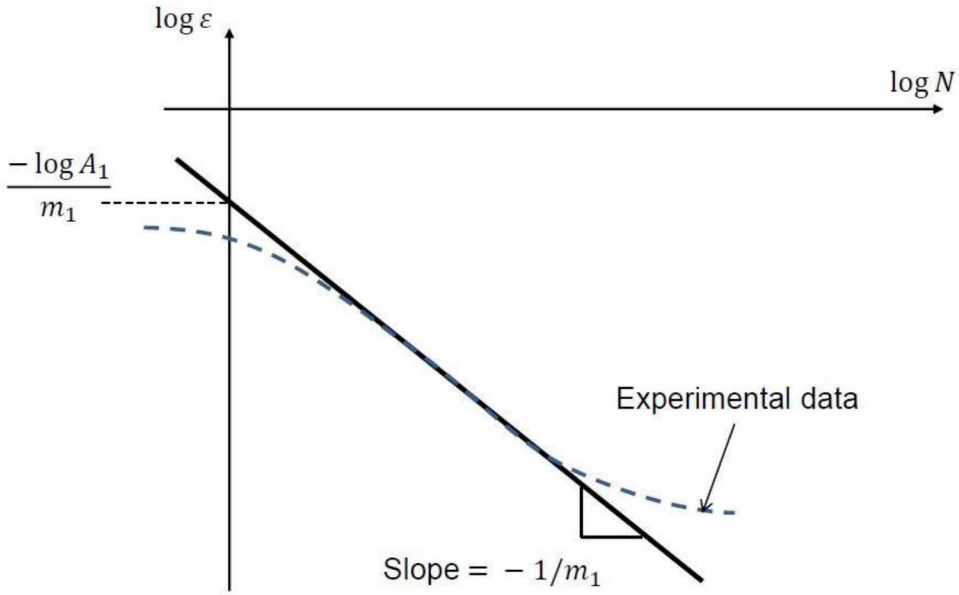
Phase I calibration from S-N data

- Run many cyclic loading tests at different values of ε (constant for each test).
- For each test, compute when damage starts:

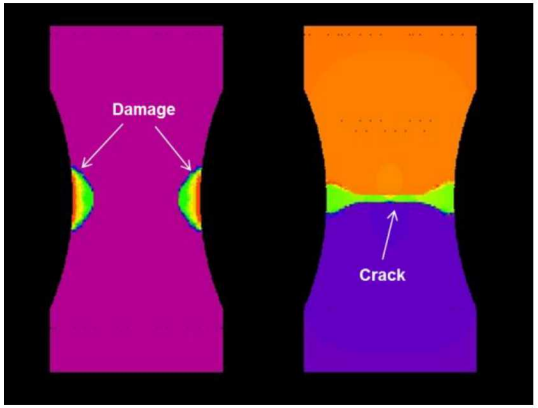
$$\frac{d\lambda}{dN}(N) = -A\varepsilon^m \qquad \Longrightarrow \qquad N = \frac{1}{A\varepsilon^m}.$$

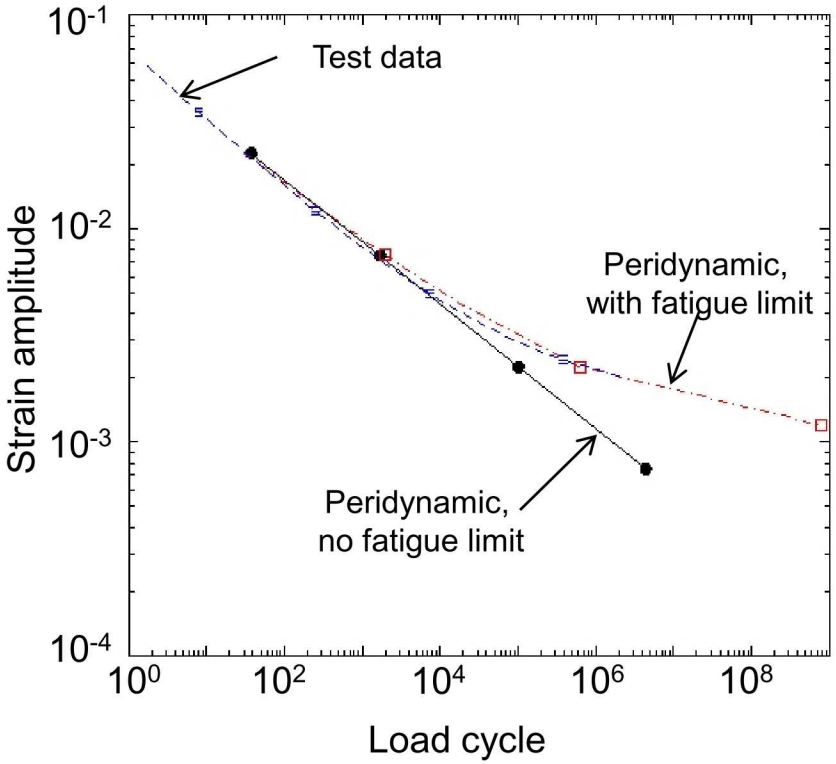
- Compare this to data on an ε-N plot, fit A and m.





Fatigue nucleation in aluminum alloy



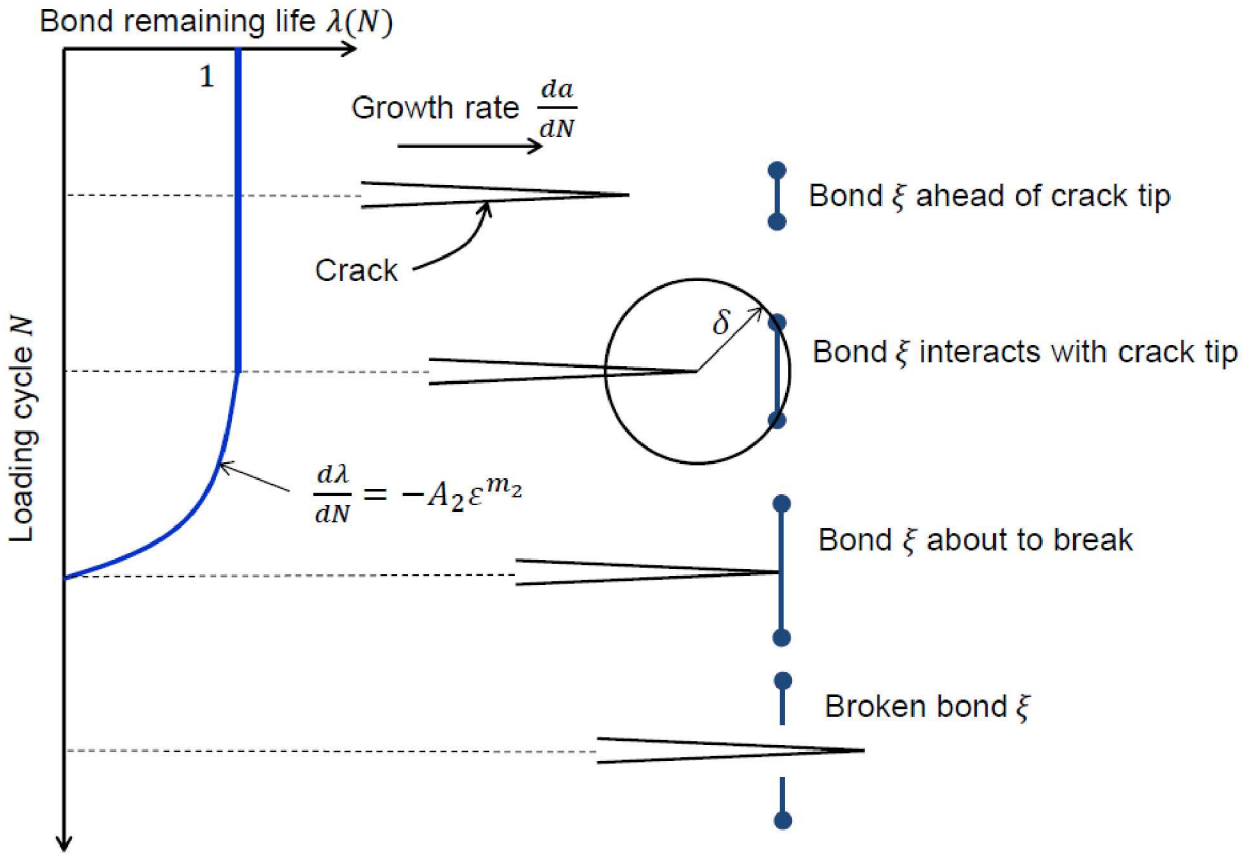


- Model with a fatigue limit:

$$\frac{d\lambda}{dN}(N) = -A\Big(\max(0, \varepsilon - \varepsilon_\infty)\Big)^m$$

Test data: T. Zhao and Y. Jiang. Fatigue of 7075-T651 aluminum alloy. International Journal of Fatigue, 30 (2008)834-849.

Growth: Bonds interact with the strain field near an approaching crack



Relate crack growth to remaining life

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- Evolution of remaining life:

$$\lambda(\delta) - \lambda(0) = \int_0^\delta \frac{d\lambda}{dz}\, dz = \int_0^\delta \frac{d\lambda}{dN}\frac{dN}{dz}\, dz.$$

- Recall

$$\frac{d\lambda}{dN} = -A\varepsilon^m.$$

- Denote by da/dN the crack growth rate.

$$1 - 0 = \frac{A}{da/dN}\int_0^\delta \varepsilon^m(z)\, dz$$

- Cyclic strain ahead of a crack:

$$\varepsilon(z) = \varepsilon_{\text{core}} f\left(\frac{z}{\delta}\right) = \frac{\Delta K}{E\sqrt{\delta}} f\left(\frac{z}{\delta}\right).$$

- Thus, for some c,

$$\frac{da}{dN} = cA\Delta K^m$$

Phase II calibration from Paris Law data

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- Now have
$$\frac{da}{dN} = cA\Delta K^m$$
where c and m are as yet unknown.
- Assume the Paris Law holds:
$$\frac{da}{dN} = C\Delta K^M$$
where C and M are constants that can be found from test data.
- Conclude
$$m = M.$$
- Need to do one computational simulation with an assumed value $C = 1$ to evaluate A.

Summary so far

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- Each bond has a remaining life $\lambda(N)$:

$$\lambda(0) = 1, \qquad \frac{d\lambda}{dN}(N) = -A\varepsilon^m, \qquad \lambda \leq 0 \text{ means failure.}$$

- In Phase I, use A and m from S-N data.
- In Phase II, use a different calibration from Paris law data.

Time mapping permits very large N

- We can avoid modeling each cycle explicitly.
- Define the *loading ratio* by

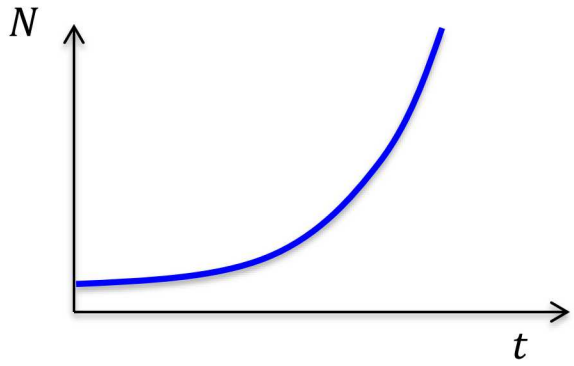
$$R = \frac{s^-}{s^+} \qquad \Longrightarrow \qquad \varepsilon = |s^+ - s^-| = |(1-R)s^+|.$$

- Map t to N:

$$N = e^{t/\tau}$$

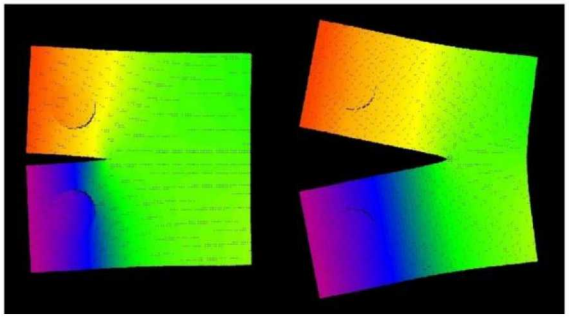
  where τ is a constant chosen according to convenience.

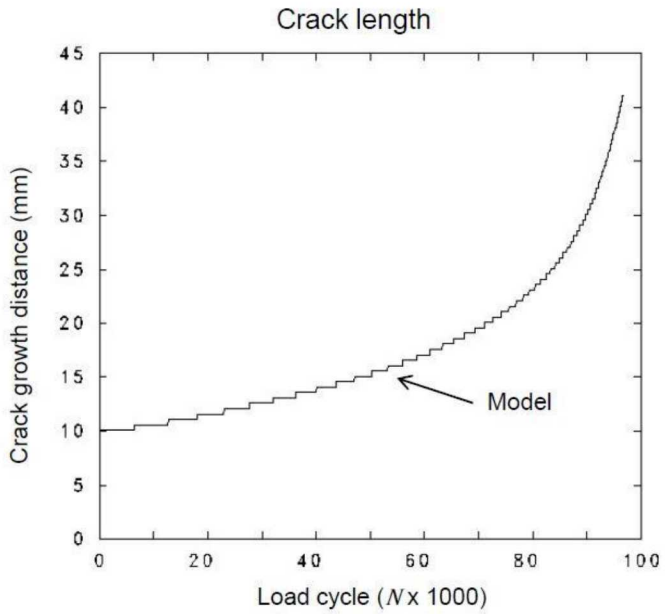
- Fatigue model in terms of t instead of N:

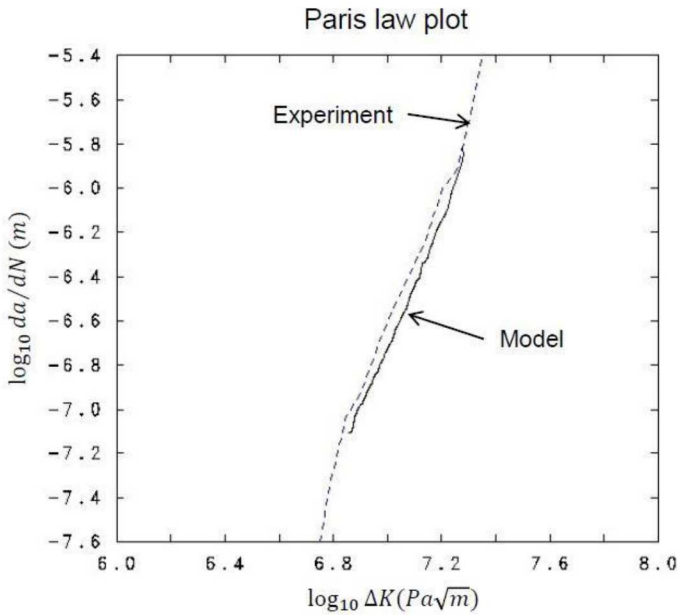


$$\frac{d\lambda}{dt} = \frac{d\lambda}{dN}\frac{dN}{dt} = \frac{-|1-R|AN}{\tau}|s^+|^m.$$

Fatigue crack growth in aluminum

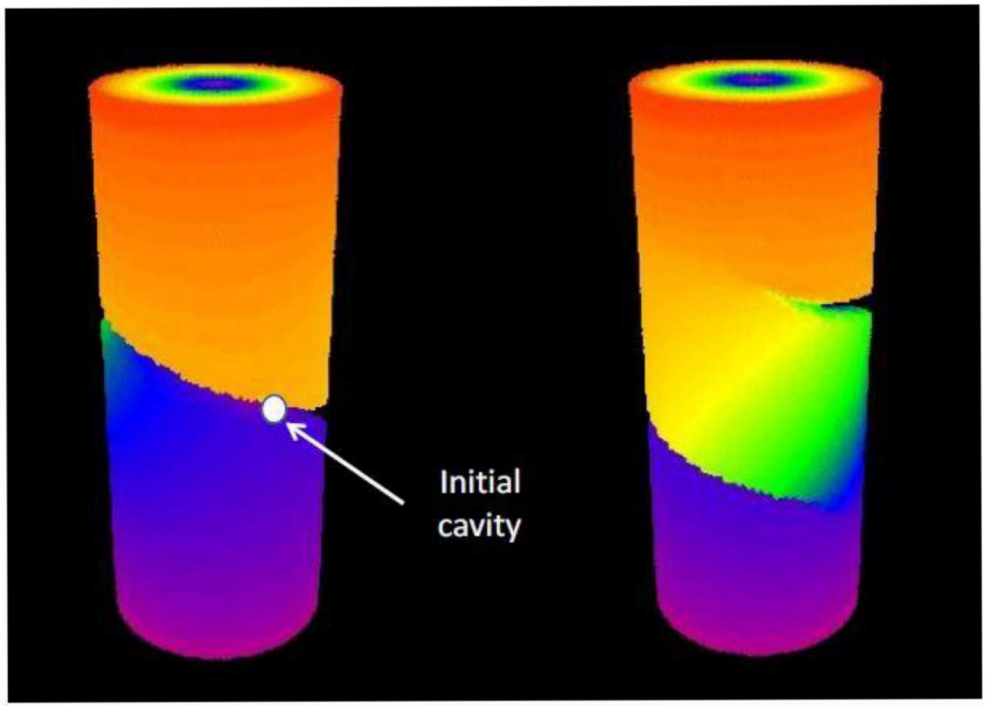






Test data: T. Zhao, J. Zhang, and Y. Jiang. A study of fatigue crack growth of 7075-T651 aluminum alloy. International Journal of Fatigue, 30 (2008) 1169-1180.

Spiral crack in a rod under torsion



Mesoscale:
Fatigue cracks at grain boundaries

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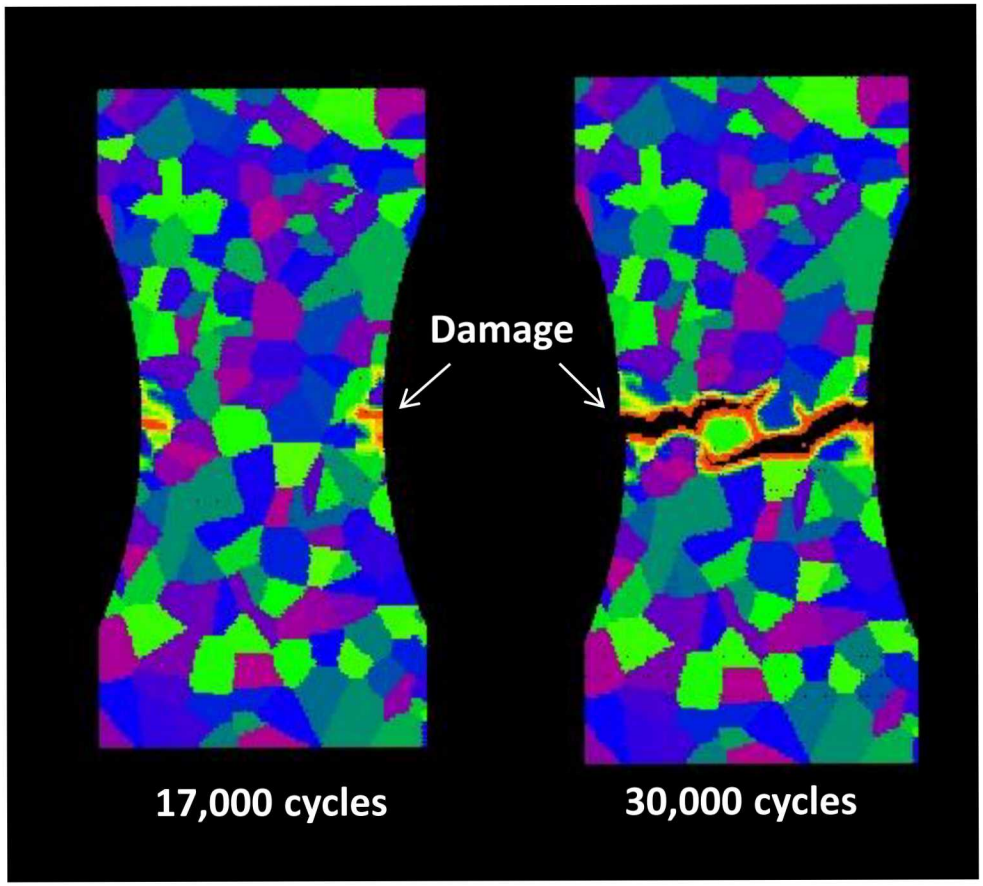
- Recall the peridynamic fatigue model: For a given bond,

$$\lambda(0) = 1, \qquad \frac{d\lambda}{dN} = -A\varepsilon^m$$

- Set:

$A = 5$ for bonds within a grain
$A = 50$ for bonds between grains

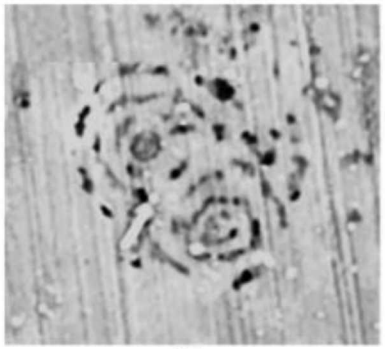


Fatigue crack growth between grains represented as Voronoi cells

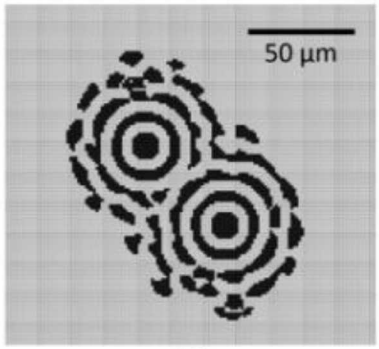
Corrosion

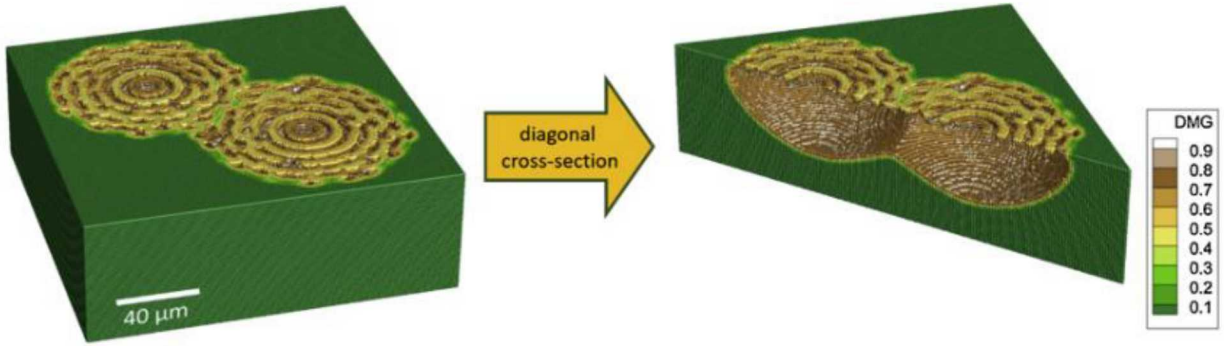
- Peridynamic simulation of corrosion pits and lacy covers*
  - Can use a peridynamic diffusion model for transport.

Experiment



Simulation





- Chen & Bobaru, JMPS (2015)
- Chen, Zhang, & Bobaru, J Electrochemical Society. (2016)
- De Meo, Diyaroglu, Zhu, E. Oterkus, & Siddiq, Int J Hydrogen Energy (2016)
- De Meo & E. Oterkus, Ocean Engineering. (2017)
- Li, Chen, Tan, & Bobaru, Materials Science and Engineering: A. (2018)
- *Jafarzadeh, Chen, Zhao, & Bobaru, Corrosion Science (2019)

Discussion

- Method treats continuous and discontinuous deformations according to the same equations.
  - Cracks nucleate according to the local conditions
  - Autonomous crack growth
- Fatigue model uses cyclic bond strain instead of actual bond strain.
  - Actual loading cycles are not computed.