郭永怀力学进展讲座, 中国科学院力学所,
April 17, 2020

A century of fracture mechanics: from Griffith theory to machine learning based modelling

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A*Star, Singapore

Acknowledgments
Bo Ni, Xing Liu (Brown University), Zhigong Song (IHPC, Singapore)

中科院力学国际分学会论坛

The 1st International Conference on Mechanics for Global Challenges

4 - 9 July 2021, Singapore (www.icmgc.org)

*Sponsored by CSTAM, NTU, NUS, A*STAR*
Co-organized with
The Materials Research Society of Singapore (MRS-S) in conjunction with the 11th International Conference on Materials for Advanced Technologies (ICMAT 2021)

Topics:

Mechanics for energy applications
Biomechanics and Mechanobiology
Mechanics for flexible electronics and health applications
Mechanics for soft and metamaterials
Mechanics of bio-inspired and biomimetic systems
Mechanics of low-dimensional materials
Mechanics for space exploration
Mechanics for manufacturing and robotics
Mechanics for food and plant sciences
Mechanics of structural materials
Mechanics of multifunctional materials and structures
Applications of machine learning in mechanics

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Outline

1. **Griffith and related theories in fracture mechanics**
    1. Introduction
    2. Griffith theory of fracture
    3. Other landmark theories in fracture mechanics

2. **Application of machine learning in fracture mechanics**
    1. Motivation
    2. ML-based solutions to fracture problems
    3. ML–assisted topographical design of thin structures
    4. ML-based atomic potential for fracture simulations
    5. Physics-informed NN for inverse fracture problems

3. **Summary and outlook**

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Alan Arnold Griffith (1893-1963)

First paper in fracture mechanics (1920)

VI. *The Phenomena of Rupture and Flow in Solids.*

By A. A. Griffith, *M. Eng.* (*of the Royal Aircraft Establishment*).

Communicated by G. I. Taylor, *F.R.S.*

Received February 11,—Read February 26, 1920.

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https://www.researchgate.net/figure/a-Alan-A-Griffith-b-reproduction-of-the-essential-statement-from-Griffiths-paper_fig4_260975561

A. A. Griffith, Philosophical transactions of the royal society of London. Series A, 221, 163 (1921).

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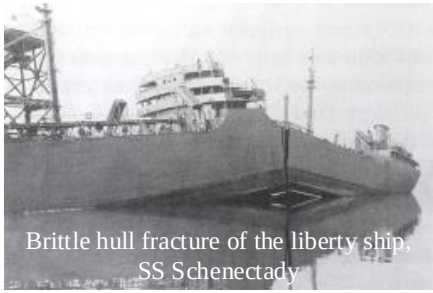
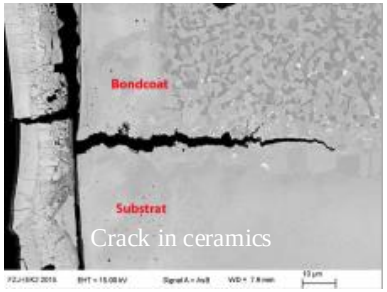
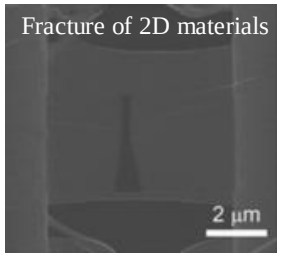
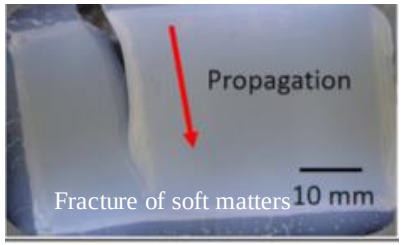
Fracture problems are everywhere!

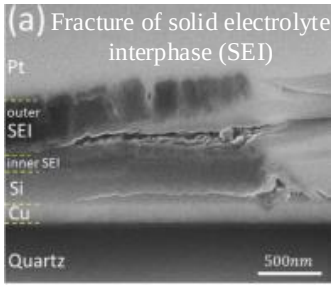
A. Catastrophic failures of structures and materials









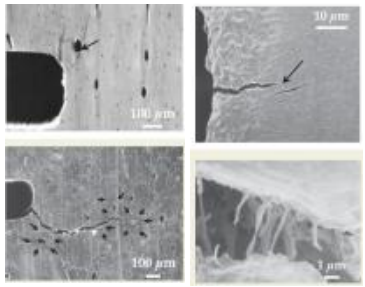


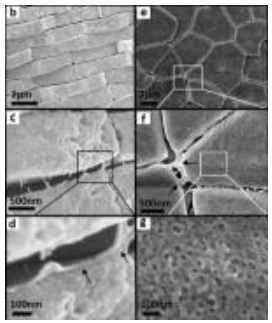
Wikipedia, Advanced Materials 29.2 (2017): 1604201., Gels 4.2 (2018): 53., Nano Energy 68 (2020): 104257.

B. Biomaterials

Bone

Abalone shell: Nacre

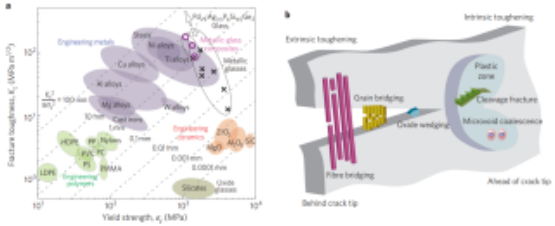




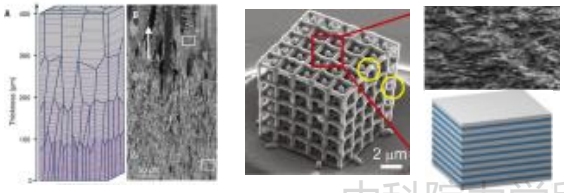
Ritchie RO, et al. Plasticity and toughness in bone., Song et al, Acta Mechanica Sinica 34.1 (2018): 143-150.

C. Materials design

Conflicts of strength v.s. toughness



Gradient nanomaterials, metamaterial and bio-mimic composites



Ritchie RO. Nature materials. 2011 Nov;10(11):817-22., Cheng, et al, Science 362.6414 (2018): eaau1925., Zhang, Gao, et al, PNAS 116.14 (2019): 6665-6672., Du, et al. Nature communications 10.1 (2019): 1-8.

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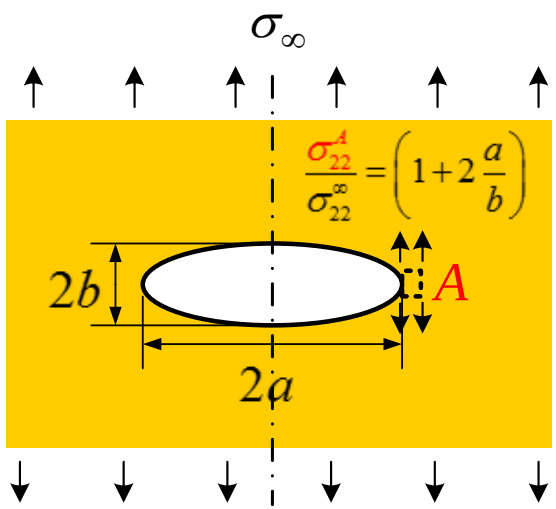
So, let's appreciate Griffith's theory

Inglis' stress solution



- Linear elastic solution for an ellipsoidal hole,

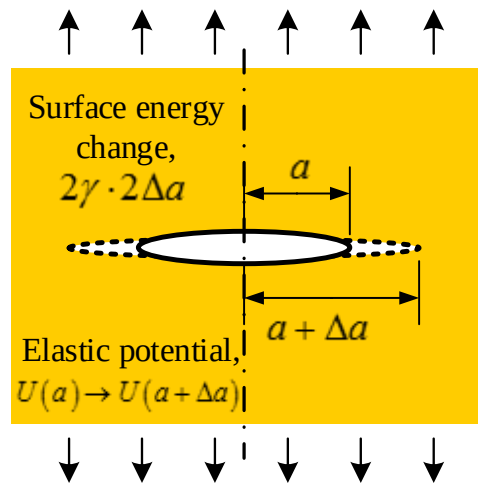
$$\sigma_{\max} = \sigma_\infty \left(1 + 2\frac{a}{b}\right)$$

- For a crack-shape limit,

$$\sigma_{\max} \to \infty \text{ as } b \to 0$$

- **Paradox**: Crack would propagate under ***arbitrarily small loading*** under the maximal stress/strain criterion.

Griffith's energy-based fracture criterion



Elastic energy

$$U = U_0 - \frac{(\sigma_\infty)^2}{E}\pi a^2$$

Surface energy

$$2\gamma \cdot 2a$$

- Total energy:

$$\Gamma = U + 4\gamma a$$

- 2nd law of thermodynamics ($\delta\Gamma \le 0$)

$$\partial\Gamma / \partial(2a) = 0 \longrightarrow \text{Griffith criterion} \quad G = G_c$$

Energy release rate: $G = -\frac{\partial U}{\partial(2a)} = \frac{1}{E}(\sigma_\infty)^2 \pi a$ -- *Driving force*

Surface energy: $G_c = 2\gamma$ -- *Material resistance*

A. A. Griffith, Philosophical transactions of the royal society of London. Series A, 221, 163 (1921).
C. E. Inglis, Trans Inst Naval Archit 55, 219, (1913)

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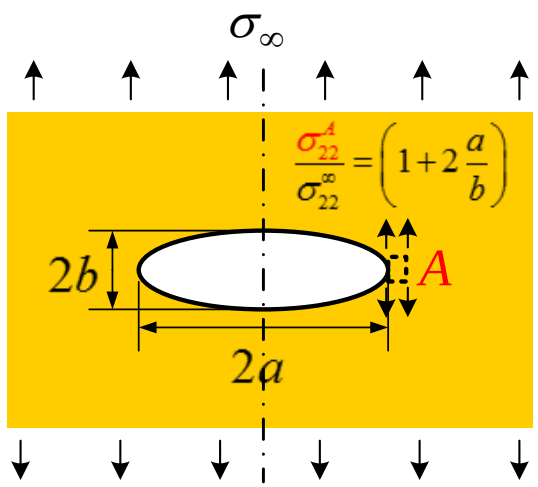
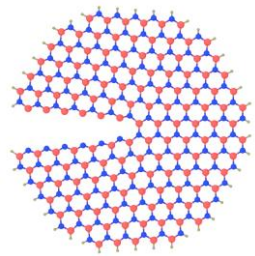
Unify Inglis and Griffith views!



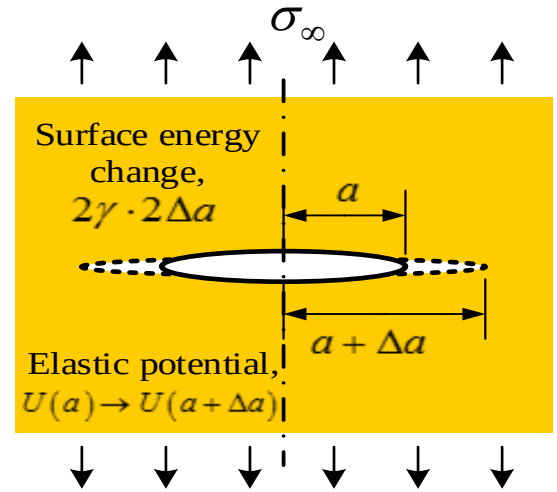


Atomic view of crack tip

Theoretical strength σ_{th}

Crack tip curvature ρ

Atomic radius a_0



Rewrite Inglis solution as:

$$\sigma_{\max} = \sigma_\infty \left(1 + 2\frac{a}{b}\right) \approx 2\sigma_\infty \sqrt{a/\rho} = \sigma_{th}$$

$$\sigma_\infty \sqrt{a} = \frac{1}{2}\sigma_{th}\sqrt{\rho} \longrightarrow \sigma_{th} = \sqrt{\frac{2\gamma E}{(\pi/4)\rho}}$$

Griffith criterion:

$$G = \frac{1}{E}(\sigma_\infty)^2 \pi a = 2\gamma$$

$$\sigma_\infty \sqrt{a} = \sqrt{\frac{2\gamma E}{\pi}} \longrightarrow \sigma_{th} = \sqrt{\frac{2\gamma E}{(\pi/4)\rho}}$$

Polanyi's (1921) interpretation

Elastic energy/atom $\xrightarrow{\textit{fracture}}$ surface energy/atom

$$a_0^3 \frac{(\sigma_{th})^2}{2E} = \gamma a_0^2 \longrightarrow \sigma_{th} = \sqrt{\frac{2\gamma E}{a_0}}$$

A. A. Griffith, Philosophical transactions of the royal society of London. Series A, 221, 163 (1921).
C. E. Inglis, Trans Inst Naval Archit 55, 219 (1913)
V. M. Polanyi, Z. Phys.7, 323-327 (1921)

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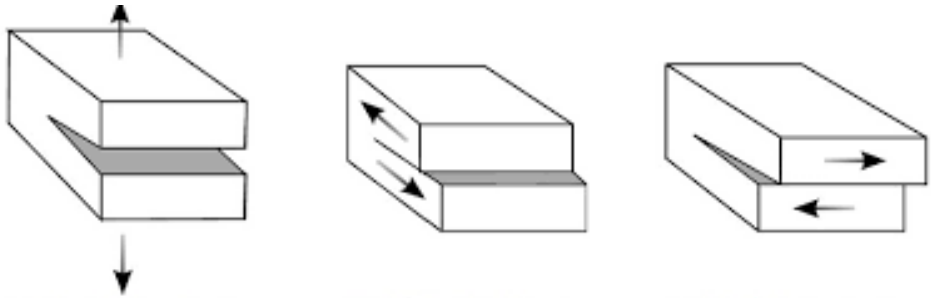
G.R. Irwin

Irwin's stress intensity factor & K-field

(key local concept for the study of multiple cracks and 3D cracks)



(a) Mode 1 (peeling) (b) Mode 2 (sliding) (c) Mode 3 (tearing)

The stress field near a crack tip has a ***universal*** asymptotic form (K-field):

$$\sigma_{ij}(r,\theta) = \frac{K}{\sqrt{2\pi r}}\hat{\sigma}_{ij}(\theta) \quad as \quad r \to 0$$

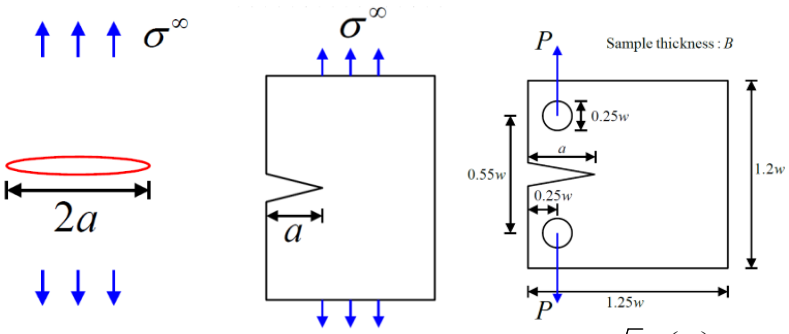
$$G = \begin{cases} \dfrac{1}{E}K^2 & for\ \ plane\ stress \\ \dfrac{(1-\nu^2)}{E}K^2 & for\ \ plane\ strain \end{cases}$$

Griffith criterion: $G = G_c$

Irwin criterion: $K = K_{Ic}$

K_{Ic} : fracture toughness

Stress intensity factor handbooks



$K_I = \sigma^\infty\sqrt{\pi a}$ $\quad K_I = 1.12\sigma^\infty\sqrt{\pi a}$ $\quad K_I = \dfrac{P\sqrt{a}}{Bw}f\left(\dfrac{a}{w}\right)$

$$f\left(\frac{a}{w}\right) = 29.6 - 185.5\left(\frac{a}{w}\right) + 655.7\left(\frac{a}{w}\right)^2 - 1017\left(\frac{a}{w}\right)^3 + 639\left(\frac{a}{w}\right)^4$$

G. R. Irwin, Trans. ASME, Ser. E, J. Appl. Mech. 24, 361 (1957)
G. R. Irwin, in Elasticity and Plasticity / Elastizität und Plastizität, edited by S. Flügge (Springer Berlin Heidelberg, Berlin, Heidelberg, 1958), pp. 551.

Tada, Hiroshi, et al. The stress analysis of cracks handbook. Vol. 130. New York: ASME press, 2000.

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J.R. Rice

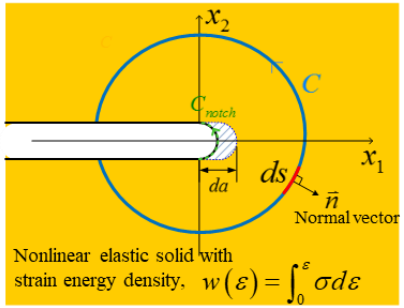
Rice's J-integral and HRR field

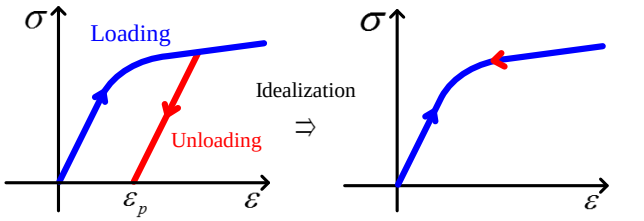
(enabled practical applications of fracture mechanics to most engineering materials)

J.W. Hutchinson

- Griffith's G extended to arbitrarily nonlinear solids by a path-independent integral

$$J = \int_C \left(w n_1 - \sigma_{kj} n_j \frac{\partial u_k}{\partial x_1} \right) ds = G$$





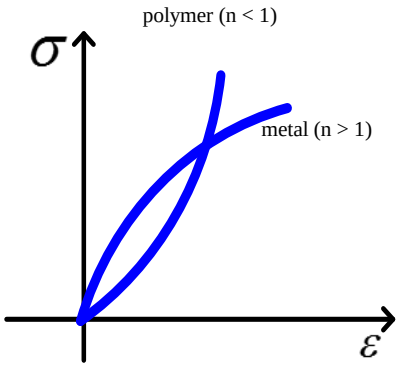
Elastic-plastic deformation

Nonlinear elastic deformation

J. R. Rice, Journal of applied mechanics 35, 379 (1968).

- Irwin's K-field extended to J-field (HRR)

$$\frac{\varepsilon}{\varepsilon_Y} = \frac{\sigma}{\sigma_Y} + \alpha \left(\frac{\sigma}{\sigma_Y} \right)^n$$



$$\begin{cases} \dfrac{\sigma_{ij}}{\sigma_Y} = \left(\dfrac{J}{\alpha \varepsilon_Y \sigma_Y I_n} \dfrac{1}{r} \right)^{\frac{1}{n+1}} \tilde{\sigma}_{ij}(\theta) \\ u_i = \alpha \varepsilon_Y r \left(\dfrac{J}{\alpha \varepsilon_Y \sigma_Y I_n r} \right)^{\frac{n}{n+1}} \tilde{u}_i(\theta) \end{cases}$$

J. Hutchinson, JMPS 16, 13 (1968).
J. Rice and G. F. Rosengren, JMPS 16, 1 (1968).

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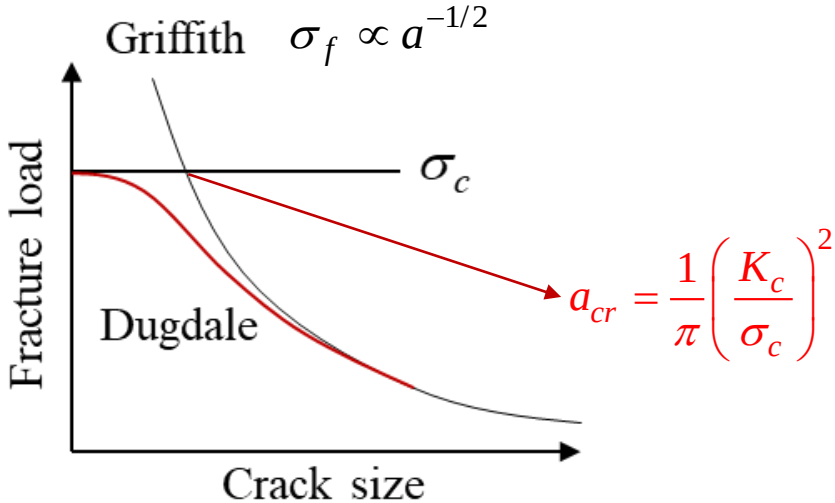
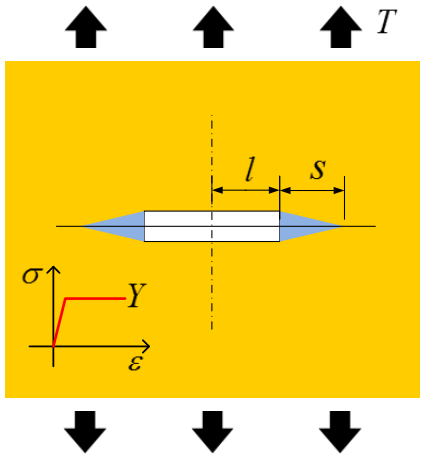
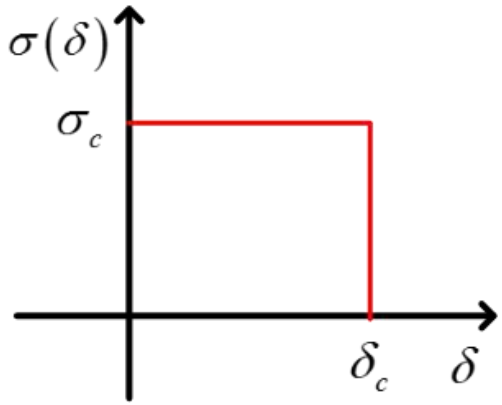
Barenblatt-Dugdale cohesive model of fracture

(concept of small-scale-yielding; also useful for fracture simulations)





Traction-separation law:



Relation to Griffith

$$G = J = \int_0^{\delta_{tip}} \sigma(\delta)\, d\delta = \sigma_c \delta_{tip}$$

$$G_c = \int_0^{\delta_c} \sigma(\delta)\, d\delta = \sigma_c \delta_c$$

$$G = G_c \quad \Rightarrow \quad \delta_{tip} = \delta_c$$

CTOD criterion

D. S. Dugdale, JMPS 8, 100 (1960).
G. I. Barenblatt, in Advances in applied mechanics (Elsevier, 1962), pp. 55.
A. A. Wells, in Proceedings of the crack propagation symposium 1961

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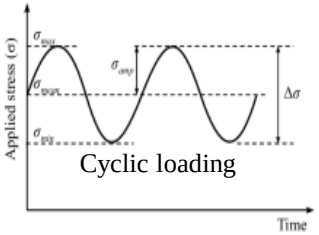
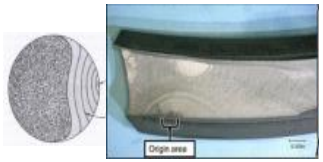
P.C. Paris

Paris' law of fatigue crack growth

(fatigue fracture accounts for >90% failure in engineering materials)



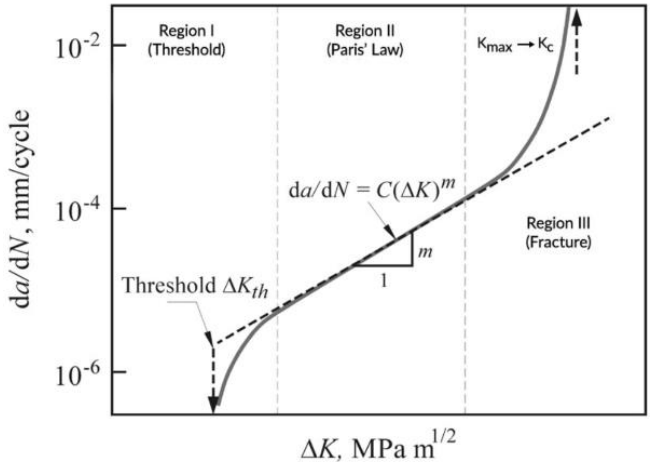
Cyclic loading



Fatigue crack surface

Accident due to fatigue crack of the engine blade

http://newsinflight.com/2018/05/04/fatigue-crack-on-southwest-cfm56-7b-failed-engine-blade-ntsb/



Paris' law

$$\frac{da}{dN} = C\left(\Delta K\right)^m$$

P. Paris, M. Gomez, and W. Anderson, University of Washington 13 (1961).
P. Paris, 1962. Ph.D. Dissertation, Lehigh University.

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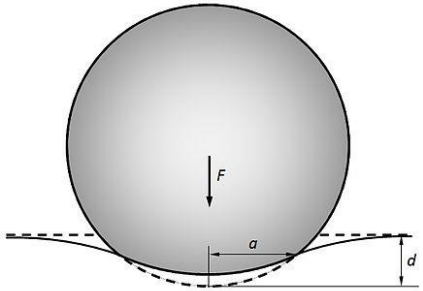
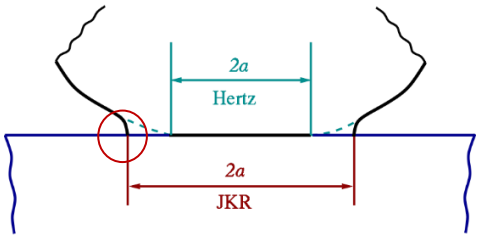
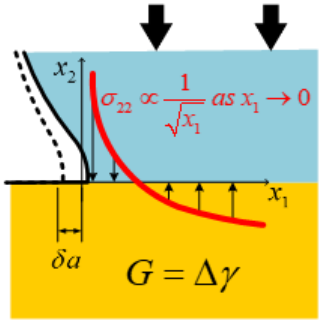
Analogy between adhesion and fracture







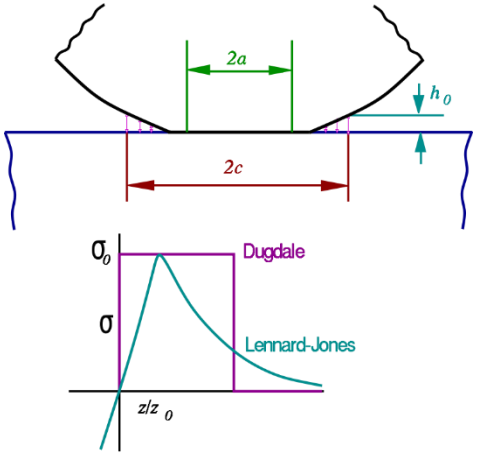
JKR model: Griffith's theory extended to adhesive contact

$$p(r) = p_0\left(1-\frac{r^2}{a^2}\right)^{1/2} + p_0^{'}\left(1-\frac{r^2}{a^2}\right)^{-1/2}, \quad F_c = -3\Delta\gamma\pi R, \quad \Delta\gamma = \gamma_1 + \gamma_2 - \gamma_{12}$$

Maugis model: Dugdale model extended to adhesive contact

$$p(r) = p^H(r) + p^D(r)$$

$$p^D(r) = \begin{cases} -\dfrac{\sigma_0}{\pi}\cos^{-1}\left[\dfrac{2a^2}{c^2-r^2}-1\right] & r < a \\ -\sigma_0 & a \le r \le c \end{cases}$$



K. L. Johnson, K. Kendall, and A. Roberts, Proceedings of the royal society of London. A. 324, 301 (1971).
D. Maugis, Journal of colloid and interface science 150, 243 (1992).
https://en.wikipedia.org/wiki/Contact_mechanics

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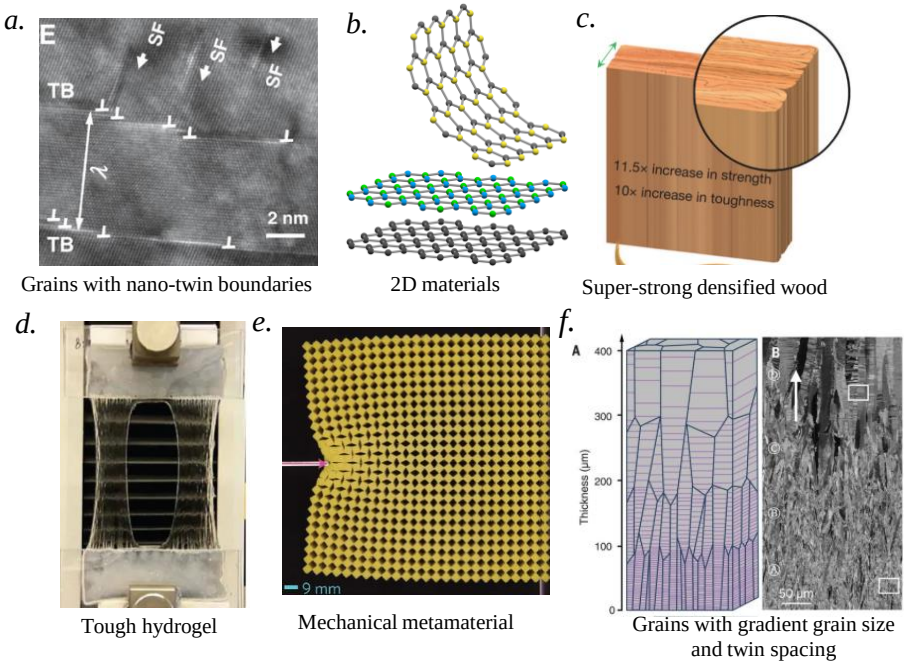
Current research in fracture mechanics and applications

Never-ending innovations in new materials



Grains with nano-twin boundaries

2D materials

Super-strong densified wood

Tough hydrogel

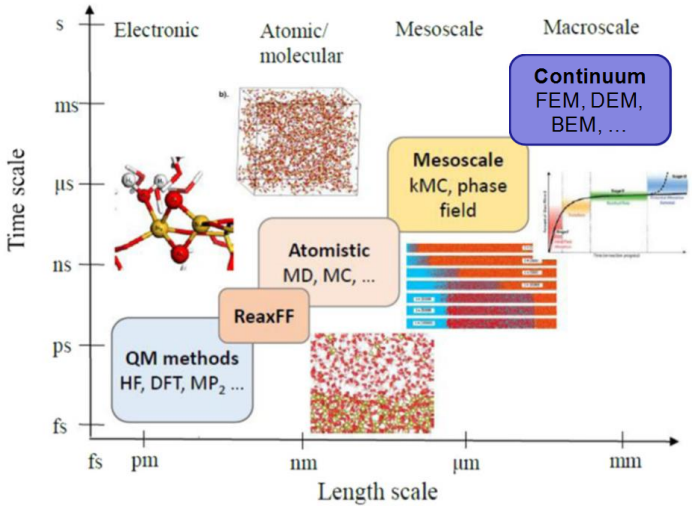
Mechanical metamaterial

Grains with gradient grain size and twin spacing

Lu et al, science 324.5925 (2009): 349-352., Song, Jianwei, et al. Nature 554.7691 (2018): 224-228., Sun, Jeong-Yun, et al. Nature 489.7414 (2012): 133-136., Coulais, Corentin, et al. Nature Physics 14.1 (2018): 40-44., Cheng, et al, Science 362.6414 (2018): eaau1925.

- Nanostructured materials
- Low dimensional materials
- Bio- or bio-mimetic materials
- Soft materials
- Meta-materials
- Gradient materials
- ……

Multiscale modeling



- Toughening mechanisms/strategies
- Controlled fracture
- Fracture patterns/device fabrication
- Interfacial fracture
- Switchable/super adhesion
- Fragmentation
- ……

Du, Jincheng, et al., npj Materials Degradation 1.1 (2017): 1-12.
Agrawal, Ankit, and Alok Choudhary. Apl Materials 4.5 (2016): 053208.

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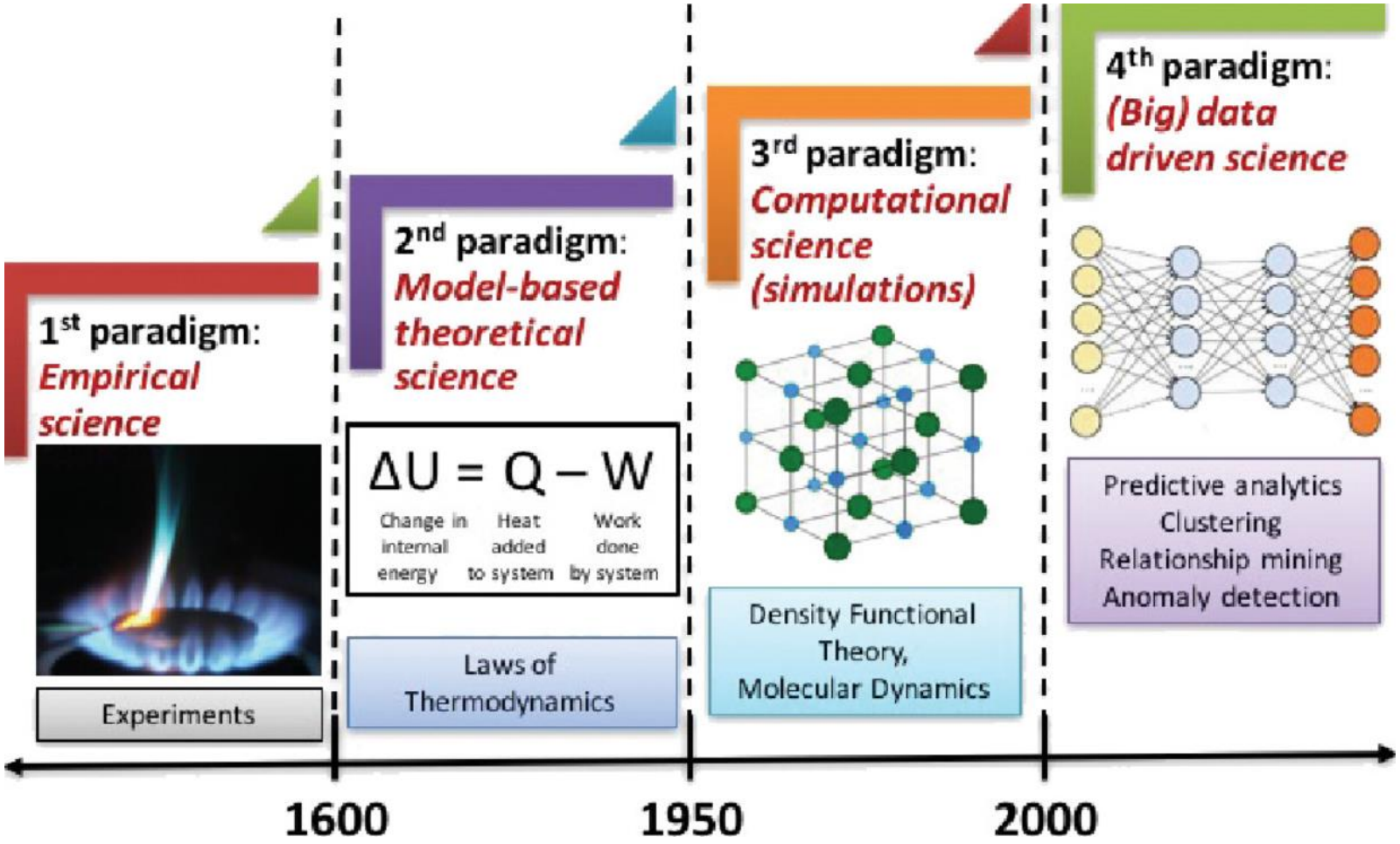
New paradigm through big data & machine learning



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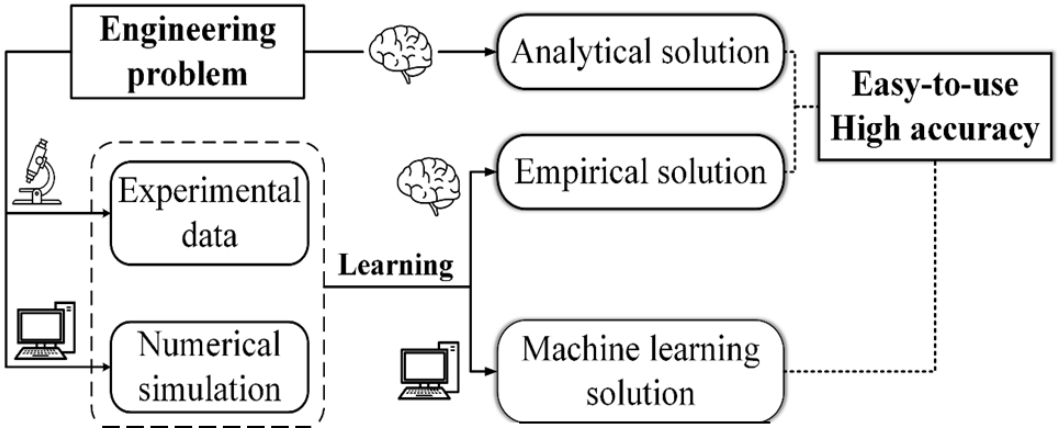
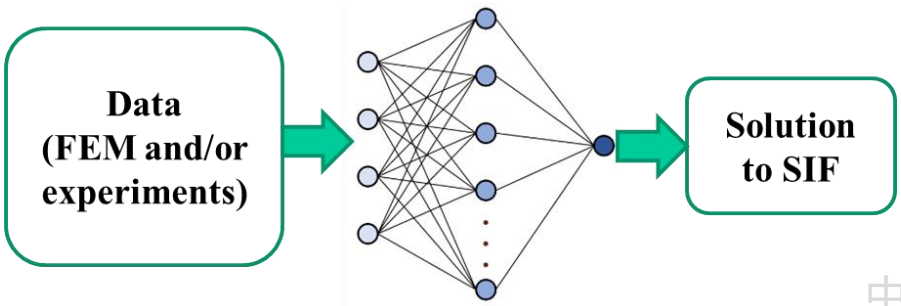
Du, Jincheng, et al., npj Materials Degradation 1.1 (2017): 1-12.
Agrawal, Ankit, and Alok Choudhary. Apl Materials 4.5 (2016): 053208.

ML-based solutions to fracture problems



- **<u>Rapid and accurate</u>** evaluation of SIF is required in experimental measurement of fracture toughness of materials.
- Analytical/empirical solutions exist only for relatively simple geometries, while increasingly c**omplex geometries** are being used for small scale testing due to the practical use of FIB instrument.
- Computational methods (e.g., FEM) are not always readily accessible to experimentalists.



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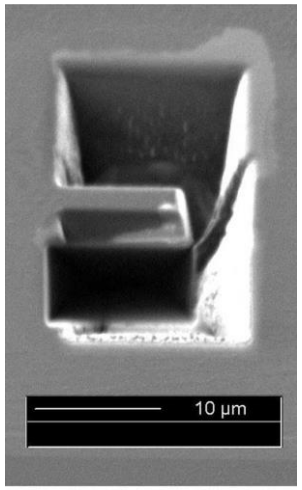
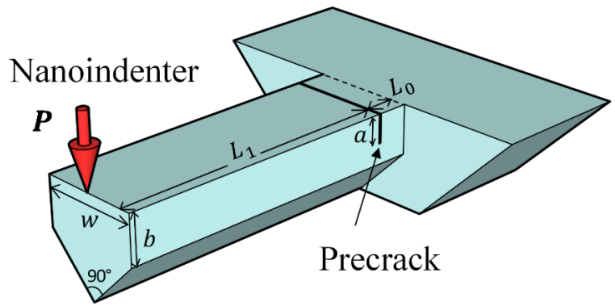
A microscale fracture sample



Fracture toughness measurement



$$K_I = \Gamma(P, w, b, a, L_0, L_1)$$

Empirical solution:

$$K_{Ic} = \sigma_c \sqrt{\pi a}\, F\left(\frac{a}{b}\right)$$

$$\sigma = \frac{PLy}{I}$$

$$y = \frac{\frac{b^2 w}{2} + \frac{w^2}{4}\left(b + \frac{w}{6}\right)}{bw + \frac{w^2}{4}}, \quad F(a/b) = 1.85 - 3.38\left(\frac{a}{b}\right) + 13.24\left(\frac{a}{b}\right)^2 - 23.26\left(\frac{a}{b}\right)^3 + 16.8\left(\frac{a}{b}\right)^4,$$

$$I = \frac{wb^3}{12} + \left(y - \frac{b}{2}\right)^2 bw + \frac{w^4}{288} + \left[\frac{w}{6} + (b - y)\right]^2 \frac{w^2}{4}$$

D. Di Maio, S.G. Roberts, J. Mater. Res. 20 (2005) 299–30232 (2017) 1211.

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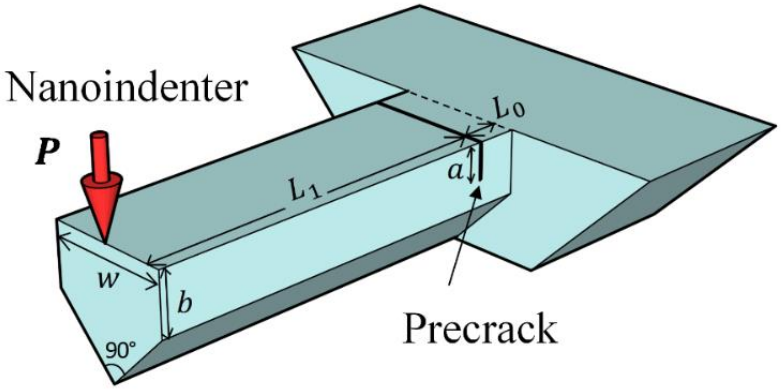
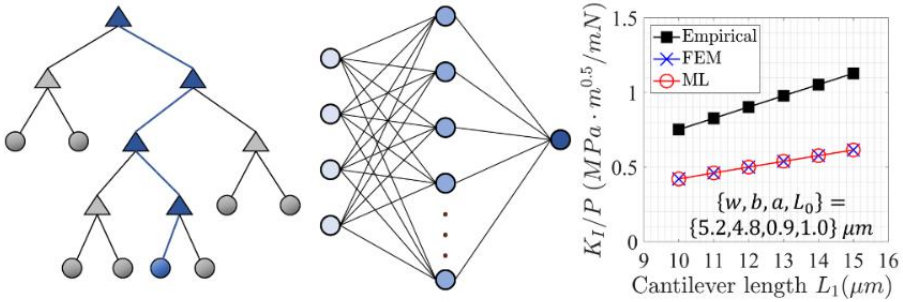
ML-based solution

Fracture toughness measurement



$$K_I = \Gamma(P, w, b, a, L_0, L_1)$$

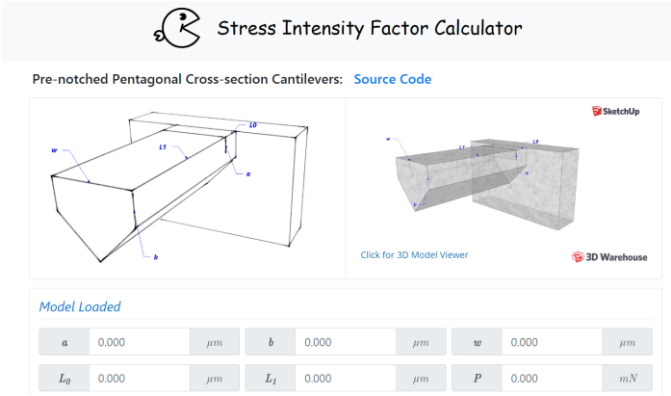
Machine learning solutions Γ



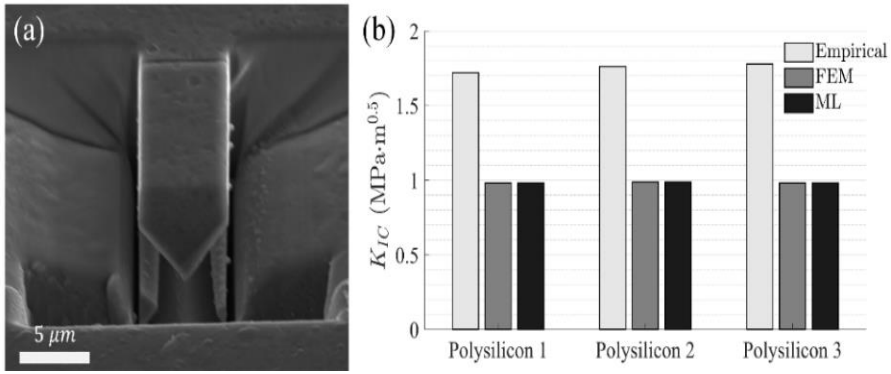
Regression trees Neural networks Accuracy

Web-based applications

Easy-to-use
High accuracy



https://hint1412.github.io/XLiu.github.io/SIF



(X. Liu, C.A. Athanasiou, N.P. Padture, B.W. Sheldon, H. Gao, Acta Mater., Vol. 19, pp. 105-112, 2020)

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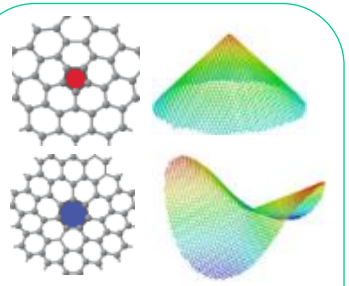
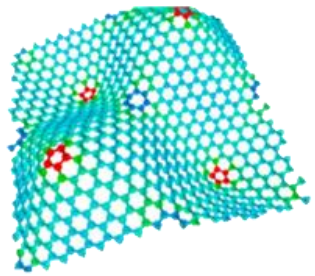
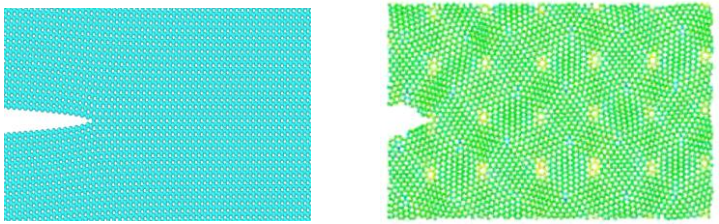
Topological toughening in 2D materials



Engineering **topological defect** distribution

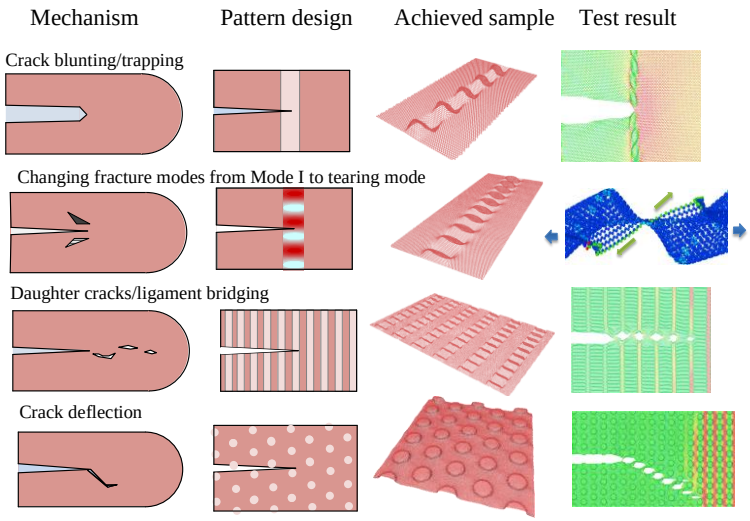


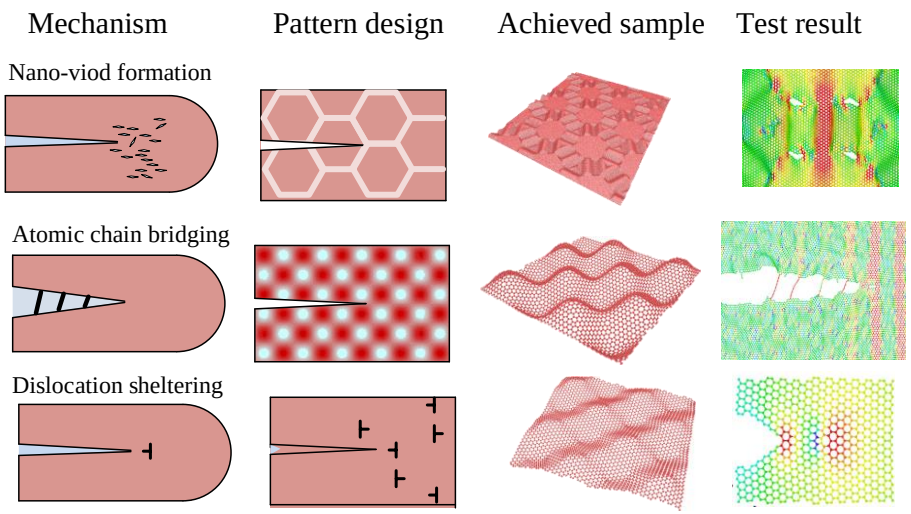
Achieve designed out-of-plane configuration



Activate novel **toughening mechanisms**: daughter crack initiation and atomic-scale bridging

Topology induced toughening mechanisms





Zhang, et al. EML 1 (2014): 3-8.
Ni, et al. "Topological design of graphene." Handbook of Graphene, Volume 2: Physics, Chemistry, and Biology (2019): 1.

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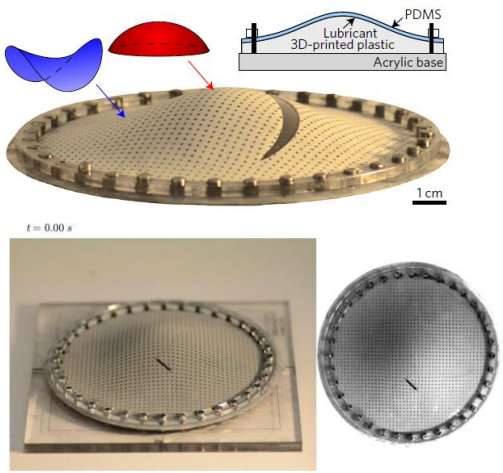
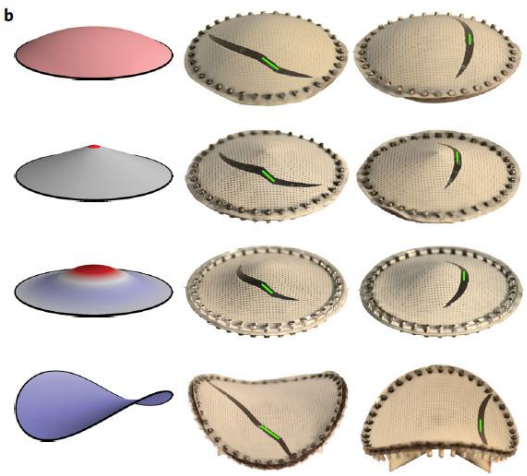
Topographical toughening in thin structures

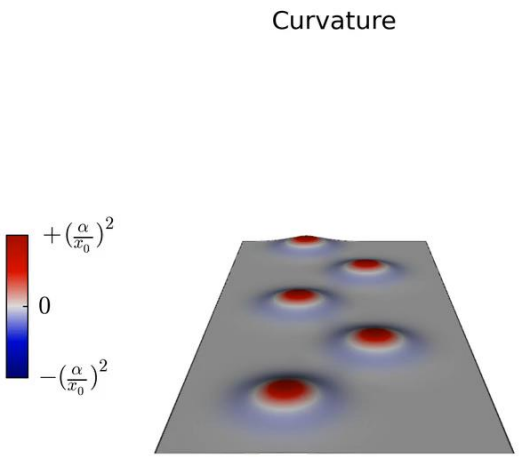
Draping a flat sheet onto a curved surface



Crack kinks due to curvature induced stress

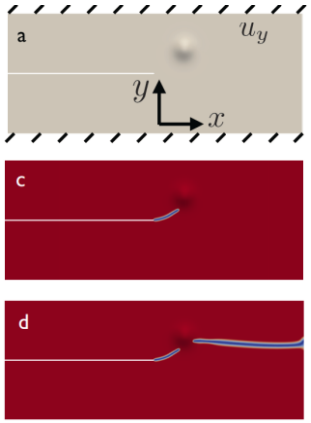


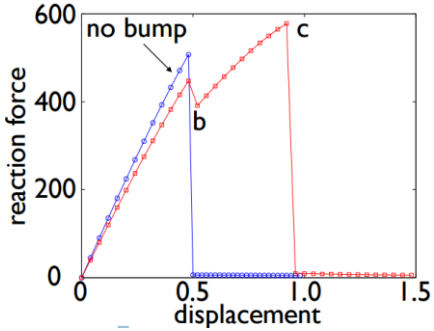
Phase field modeling of tuning crack paths with curvature landscape



Mitchell et al. Nature Materials (2016)

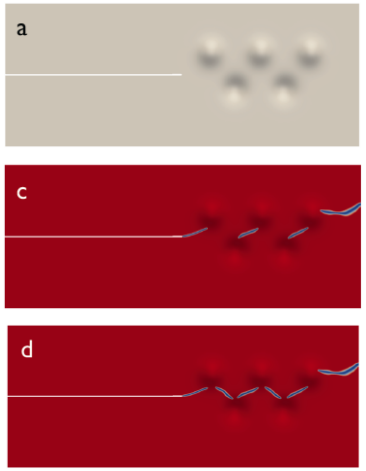
Phase filed modeling of interaction between an edge crack and a bump in a thin sheet



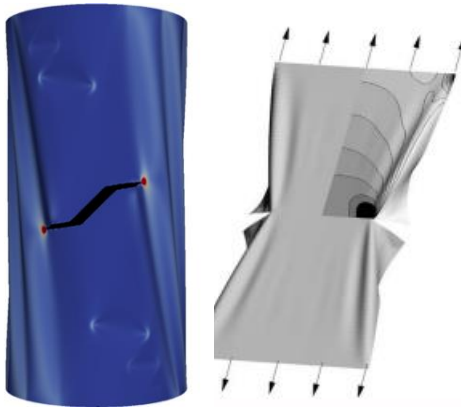


Marino Arroyo group, 2016.
Bin Li, PhD thesis, 2016

Tuning crack path with initial curvature



Buckling vs Fracture



Zavattieri, Pablo D. JAM 73.6 (2006): 948-958.

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Physics-informed neural networks (PINN)

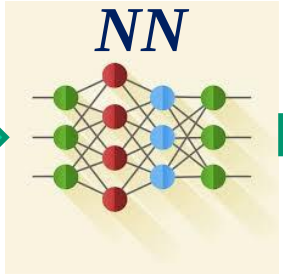
G. Karniadakis

Traditional Mechanics

PDE → → **Prediction**

Validation by experiments

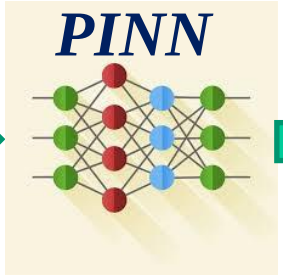
Machine Learning

Data → 

→ **Prediction**

Training by minimizing a loss function

PINN

PDE + Data (experiment & simulation) → 

→ **Prediction**

Training by minimizing a combined loss function

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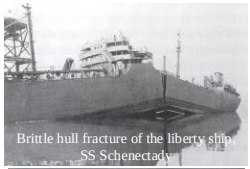
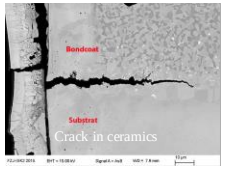
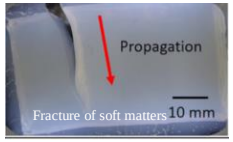
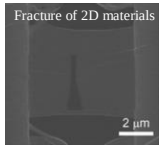
Raissi, Perdikaris, Karniadakis, J. Comp. Phys. 378, 686-707, arXiv:1711.10561; arXiv:1711.10566

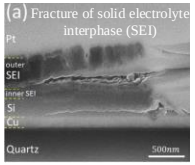
Summary and outlook











Fracture Mechanics

Fundamentals
Energy release rate
SIF & K-field
Fracture toughness
J-integral & HRR field
Paris law
Cohesive models
Adhesion & fracture
…..

New tools
ML solutions for SIFs
PINN for inverse fracture problems
ML-assisted topographical design
ML-based atomic potential for fracture simulations
…..

New applications
Nano materials
Low-D materials
Soft materials
Bio- or bio-mimic materials
Meta-materials
Gradient materials
…..

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Thank you!

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