Phase-field modeling of brittle fracture in materials with anisotropic surface energy and in thin sheets

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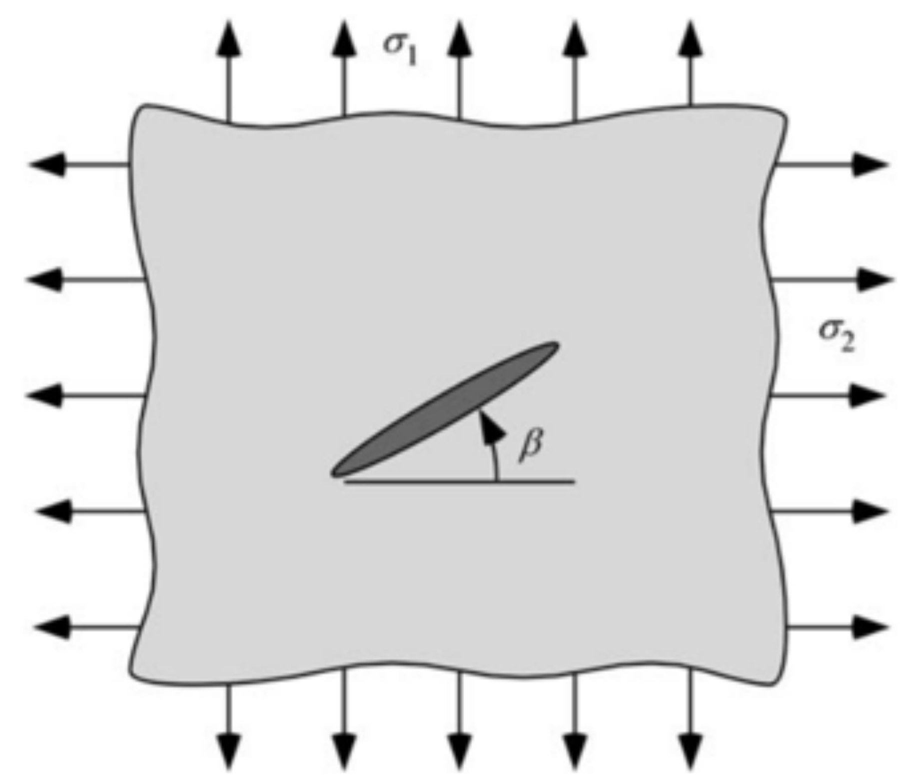
Motivation

Quasi-static crack propagation in brittle materials

If and when ? *Griffith's theory*

energy release rate reaches a critical value

$$G = G_c$$



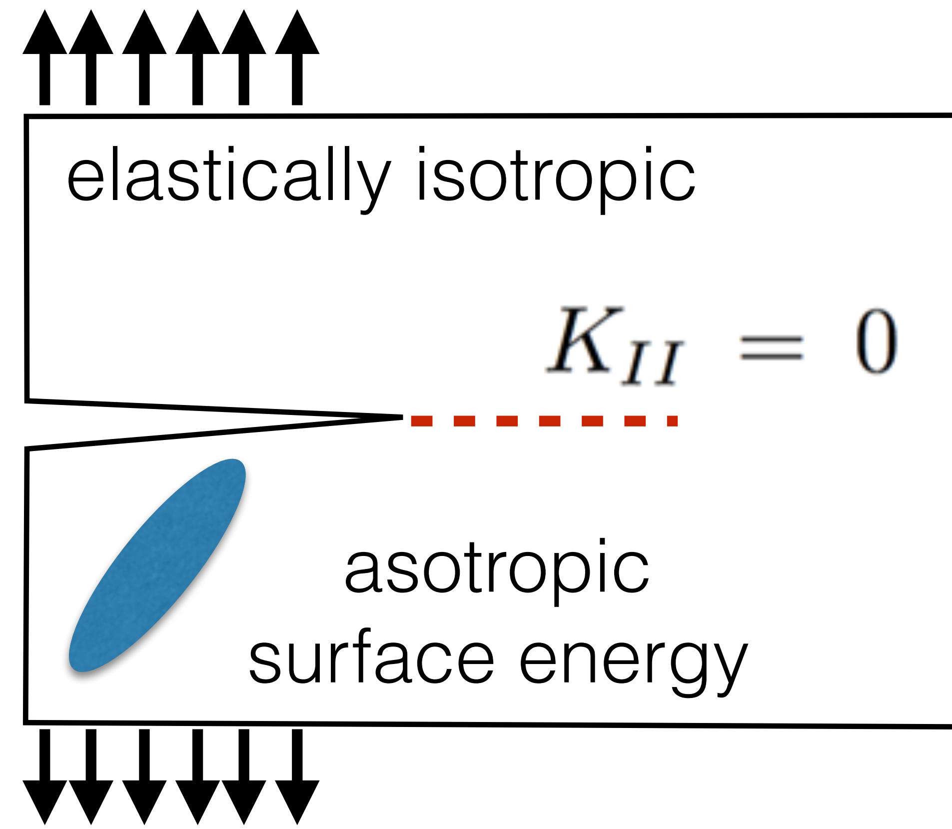
Which direction ?

- max hoop stress
- principle local symmetry
- max energy release rate (MERR)
- …

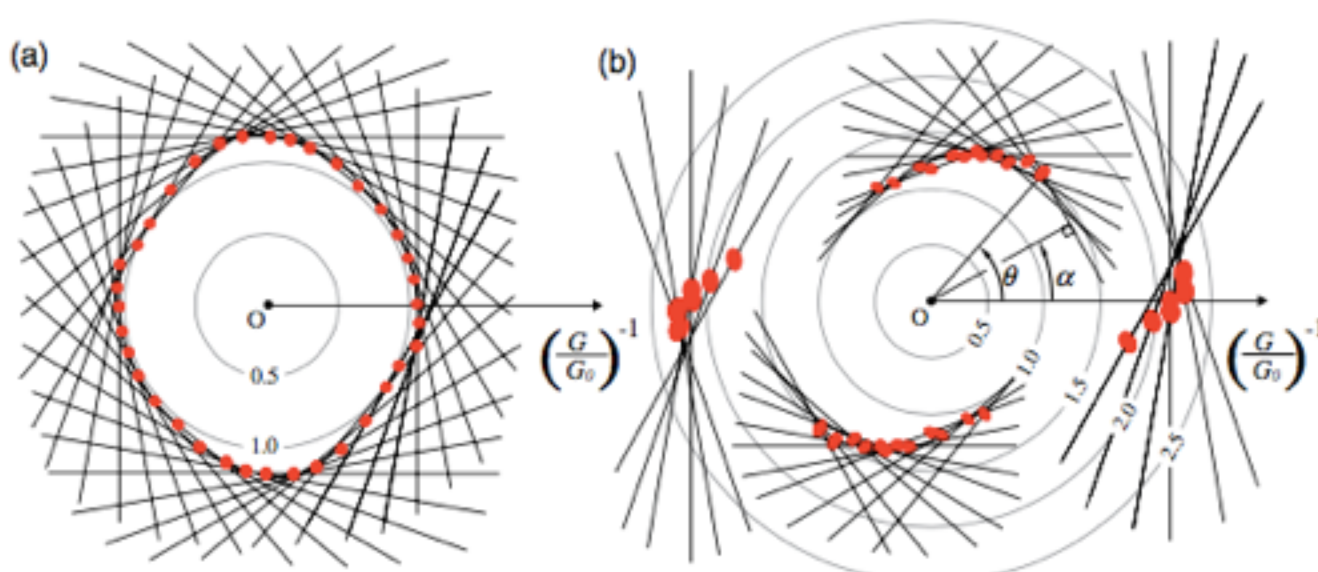
Motivation

As discussed by Alain and Benoit, brittle materials with anisotropic surface energy challenge our understanding of fracture.

Gurtin, Podio-Guidugli (98),
Hakim, Karma (05-09)
Chambolle, Francfort, Marigo (09),
...

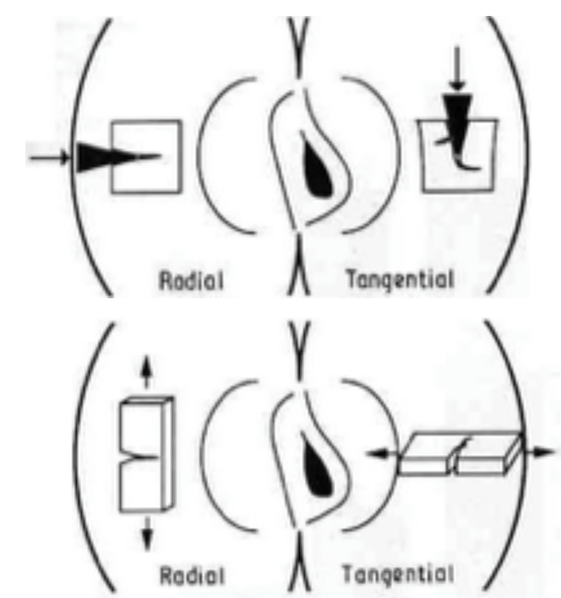


Many man-made and natural materials exhibit a strongly anisotropic surface energy.



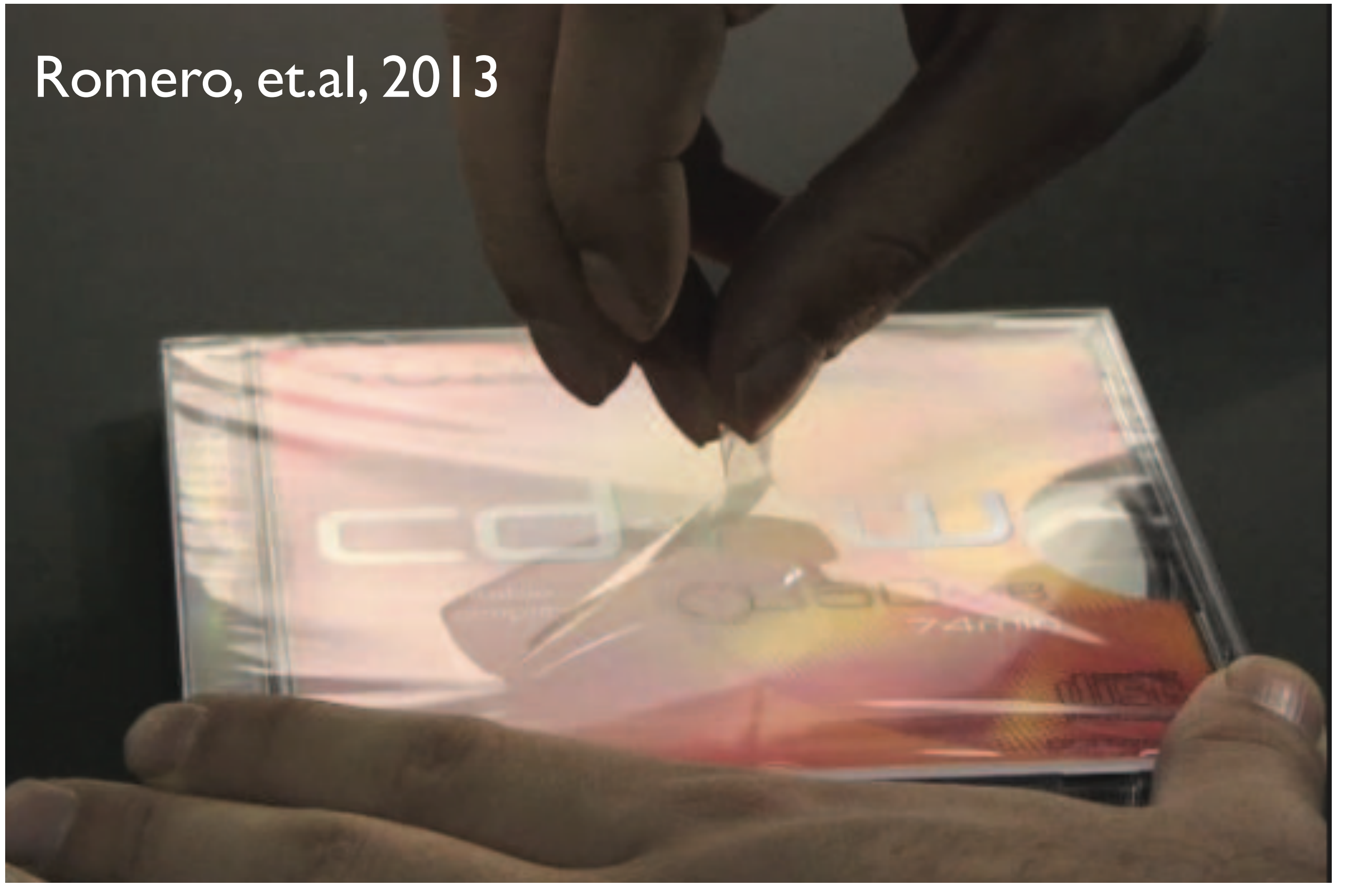
Takei et al (13)

apple flesh



Khan, et al, 1993

Motivation

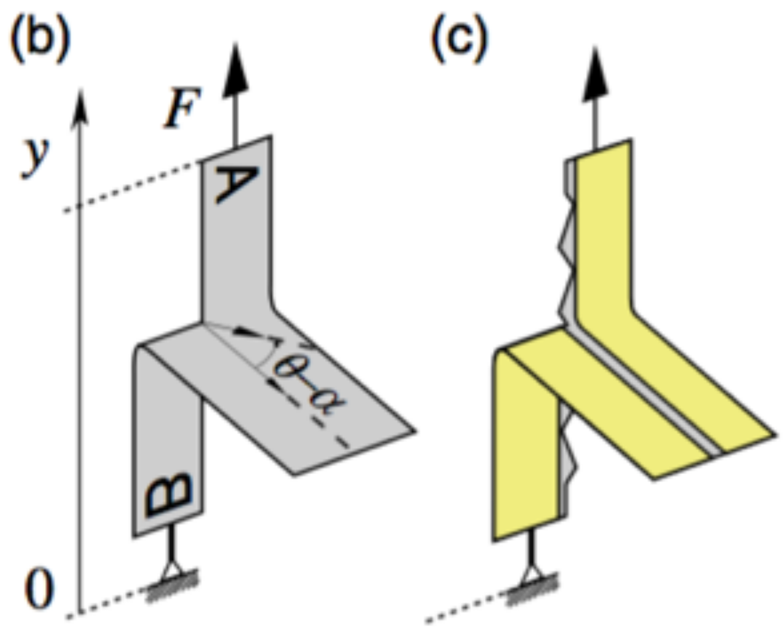


4 stress intensity factors (SIFs) (in-plane, bending, twisting)

Relation between SIFs and *G*? Path selection criterion?

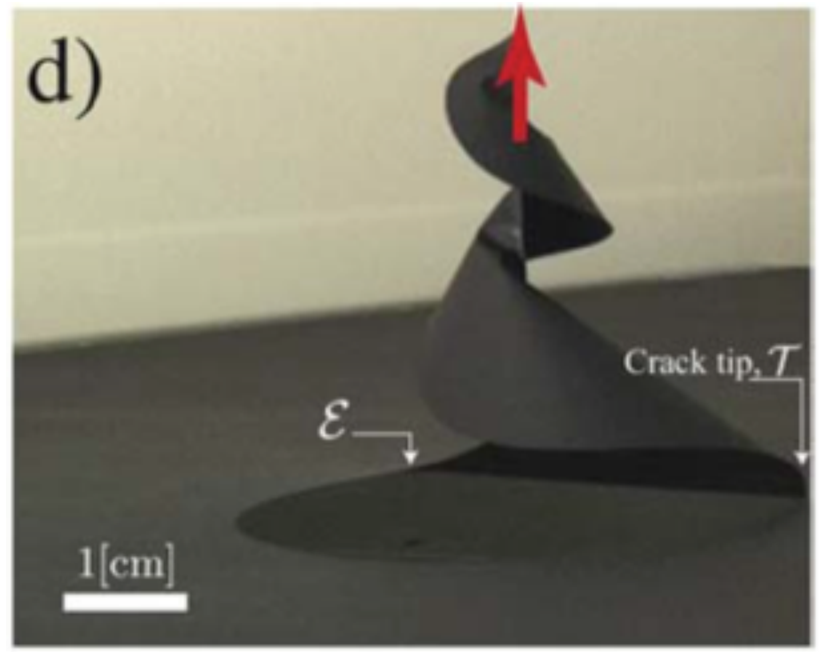
Large geometric nonlinearity

Motivation



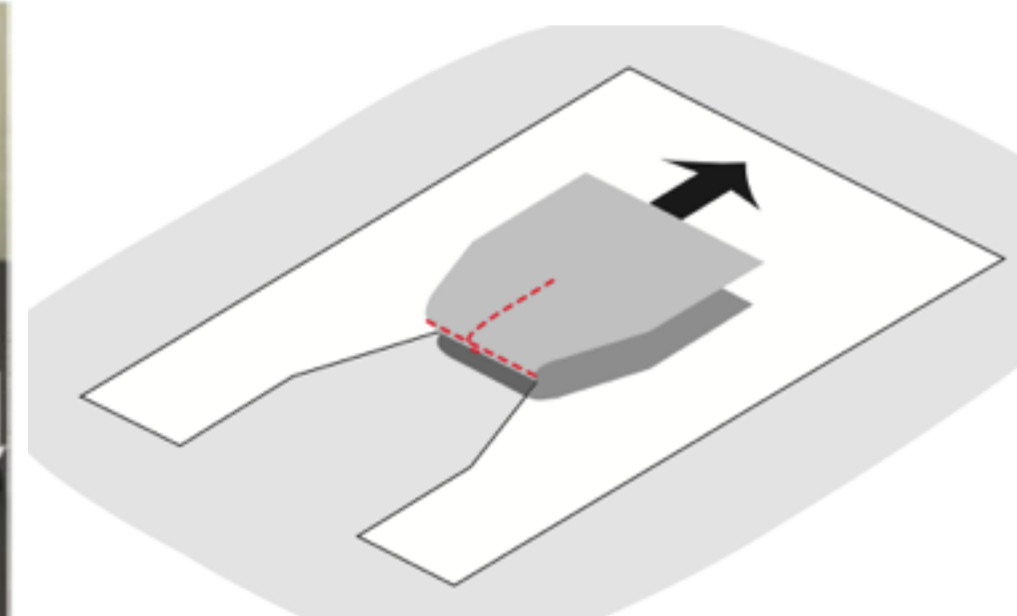
anisotropic films

Takei,et.al, *PRL*, 2013



non-adhesive films

Romero,et.al, *Soft matter*, 2013



tearing adhesive film

Hamm,et.al, *Nat Mater*,2008

A wealth of controlled experiments. In some regimes, crack path is well-described by minimal models based on <u>energetic arguments</u>.

Hypothesis: variational phase-field models of fracture may reproduce the observed phenomenology, and hence provide a general modeling framework.

Outline

1. **Phase-field modeling of fracture in materials with strongly anisotropic surface energy**

2. Phase-field modeling of fracture in brittle thin shells

3. Effect of shell geometry on crack propagation:

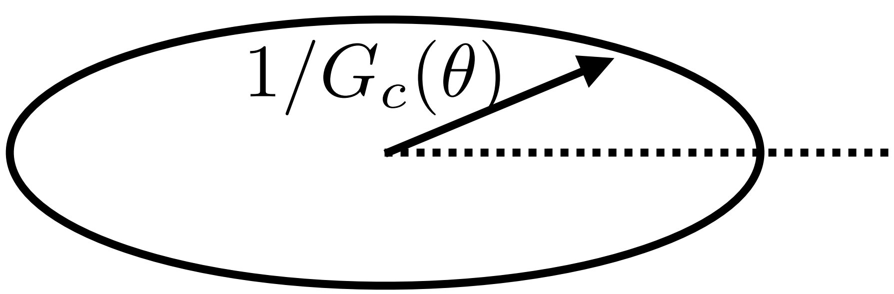
   G for a thin shell

Anisotropic surface energy

$$\Pi_{\rm tot}[\boldsymbol{u}, v] = \int_\Omega (v^2 + \eta_k) W(\boldsymbol{\varepsilon})\; d\Omega + \int_\Omega G_{\rm c} \left[\frac{(v-1)^2}{4\ell} + \ell |\nabla v|^2 \right]\; d\Omega,$$

Ambrosio-Tortorelli (90),
Bourdin, Francfort, Marigo (00)

isotropic fracture energy



Ellipse in inverse polar plot
two-fold anisotropy

$$\int_\Omega G_c \left[\frac{(v-1)^2}{4\ell} + \ell \nabla v^T \boldsymbol{A} \nabla v \right] d\Omega$$

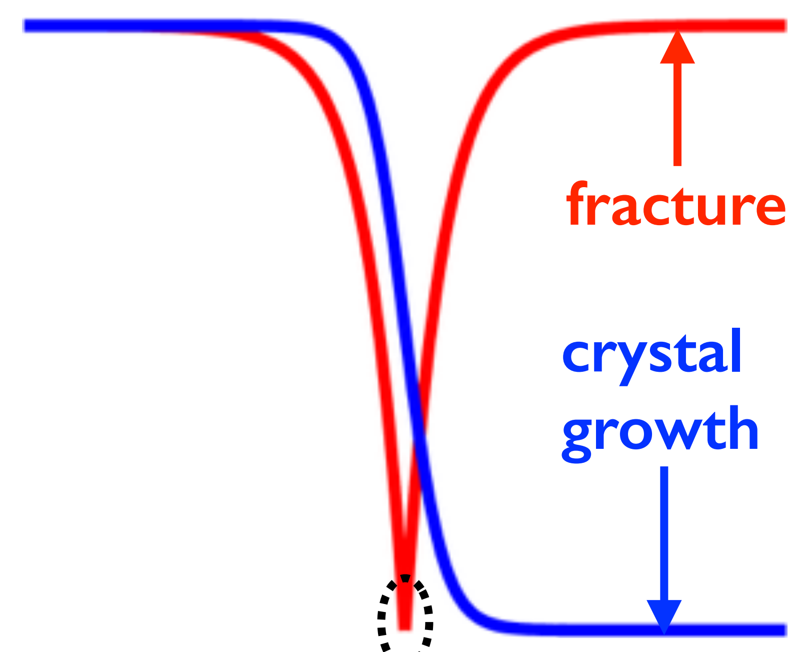
Hakim, Karma (05, 09)

anisotropic fracture energy

In phase-field modeling for crystal growth

$$G_c(\boldsymbol{n}) \;\; \text{with} \;\; \boldsymbol{n} = \frac{\nabla v}{|\nabla v|}$$

Kobayashi (93), Taylor, Cahn (98),
Torabi (09)



Anisotropic phase-field fracture model

Extended Cahn-Hilliard interface model

$$
f(v, \nabla v, \nabla^2 v) = f_0(v) + \boxed{\sum_{ij} \ell_{ij} \frac{\partial v}{\partial x_i} \frac{\partial v}{\partial x_j}} + \sum_{ijkl} \tilde{\alpha}_{ijkl} \frac{\partial v}{\partial x_i} \frac{\partial v}{\partial x_j} \frac{\partial v}{\partial x_k} \frac{\partial v}{\partial x_l}
$$

$$
+ \sum_{ijkl} \tilde{\beta}_{ijkl} \frac{\partial^2 v}{\partial x_i \partial x_j} \frac{\partial v}{\partial x_k} \frac{\partial v}{\partial x_l} + \boxed{\sum_{ijkl} \tilde{\gamma}_{ijkl} \frac{\partial^2 v}{\partial x_i \partial x_j} \frac{\partial^2 v}{\partial x_k \partial x_l}}.
$$

quadratic terms

Cahn and Hilliard (58)
Abinandanan and Haider (01)
Torabi, Lowengrub (12)

We focus on quadratic terms and cubic symmetry in 2D

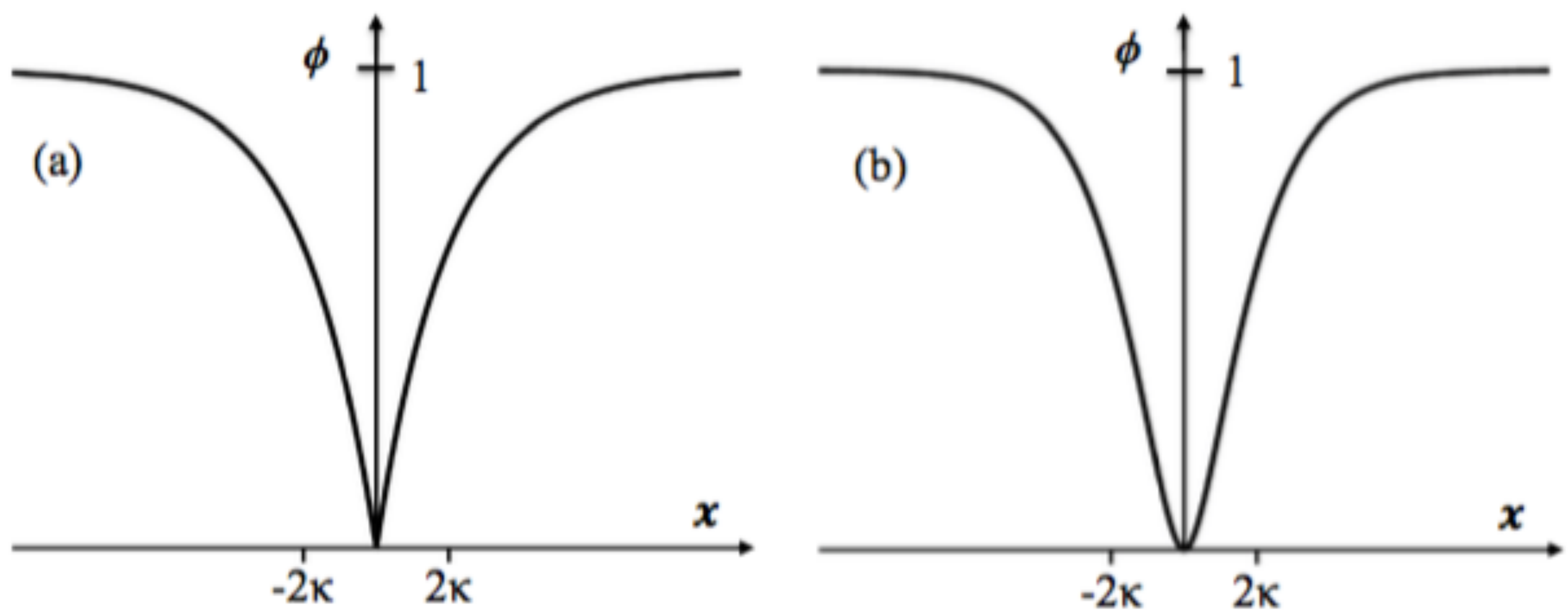
$\ell_{ij} = \ell \, \delta_{ij}$ $\qquad$ γ_{ijkl} has 3 independent coefs

Anisotropic phase-field fracture model

Fourth-order phase-field model with anisotropic surface energy

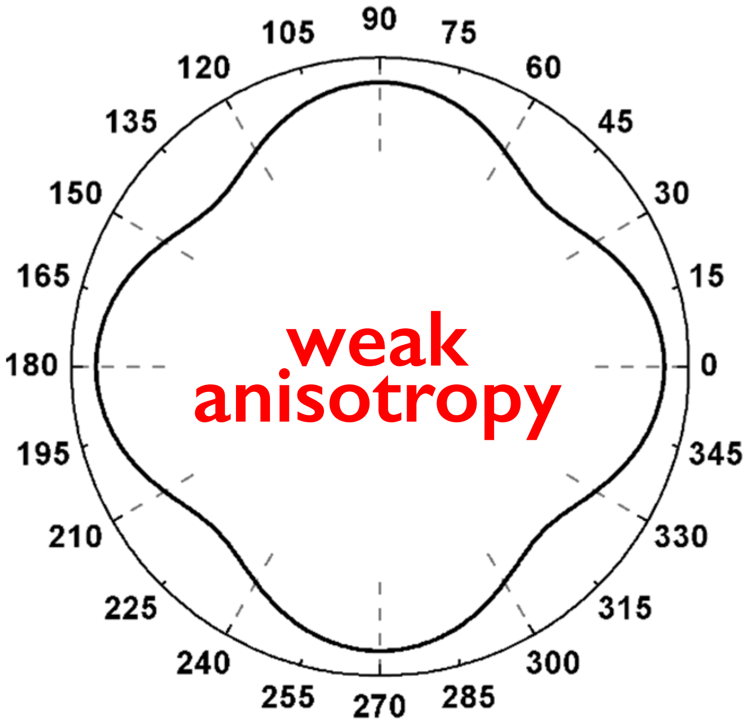
$$E[\boldsymbol{u}, v] = \int_\Omega (v^2 + \eta_k) W(\boldsymbol{\varepsilon})\, d\Omega + \boxed{\tilde{G}_c \int_\Omega f\left(v, \nabla v, \nabla^2 v\right) d\Omega}$$

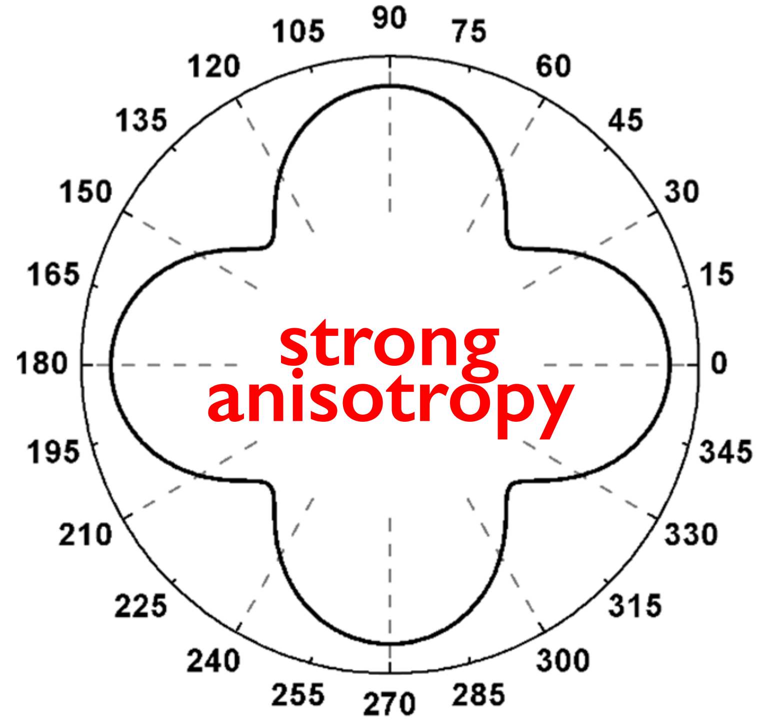
Bin Li, et.al, *IJNME*.2014



Fourth-order model by Borden et al (14) is a particular case.

Resulting anisotropic surface energy



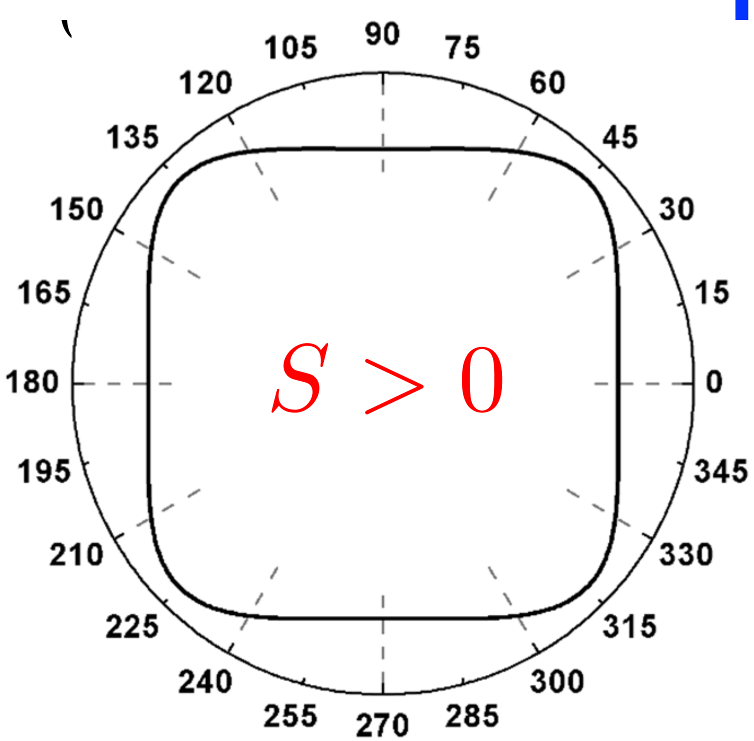


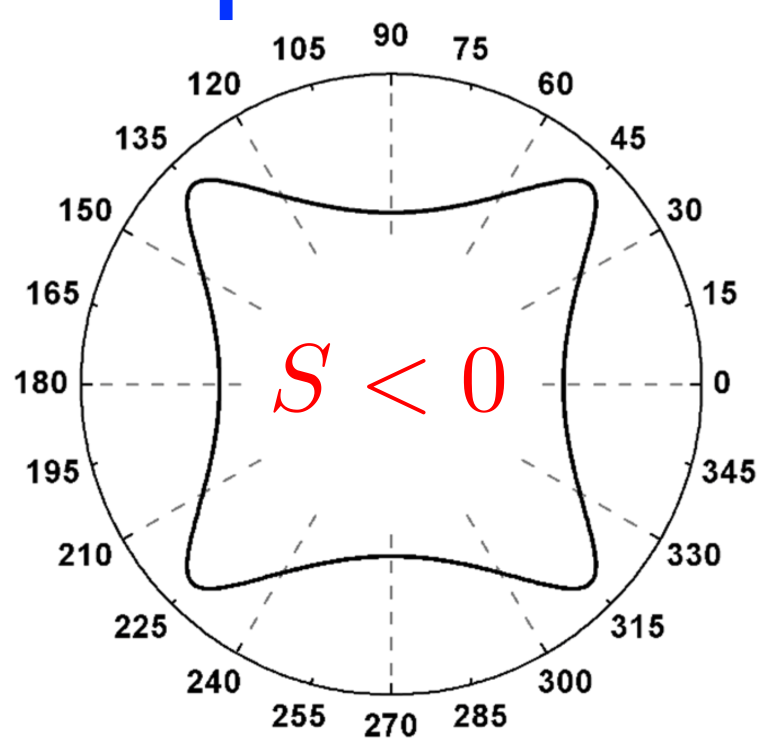
cubic symmetry

surface stiffness

$$S = G_c(\theta) + G_c''(\theta)$$

inverse polar plot





nonconvex surface energy

$$S < 0$$

convex surface energy

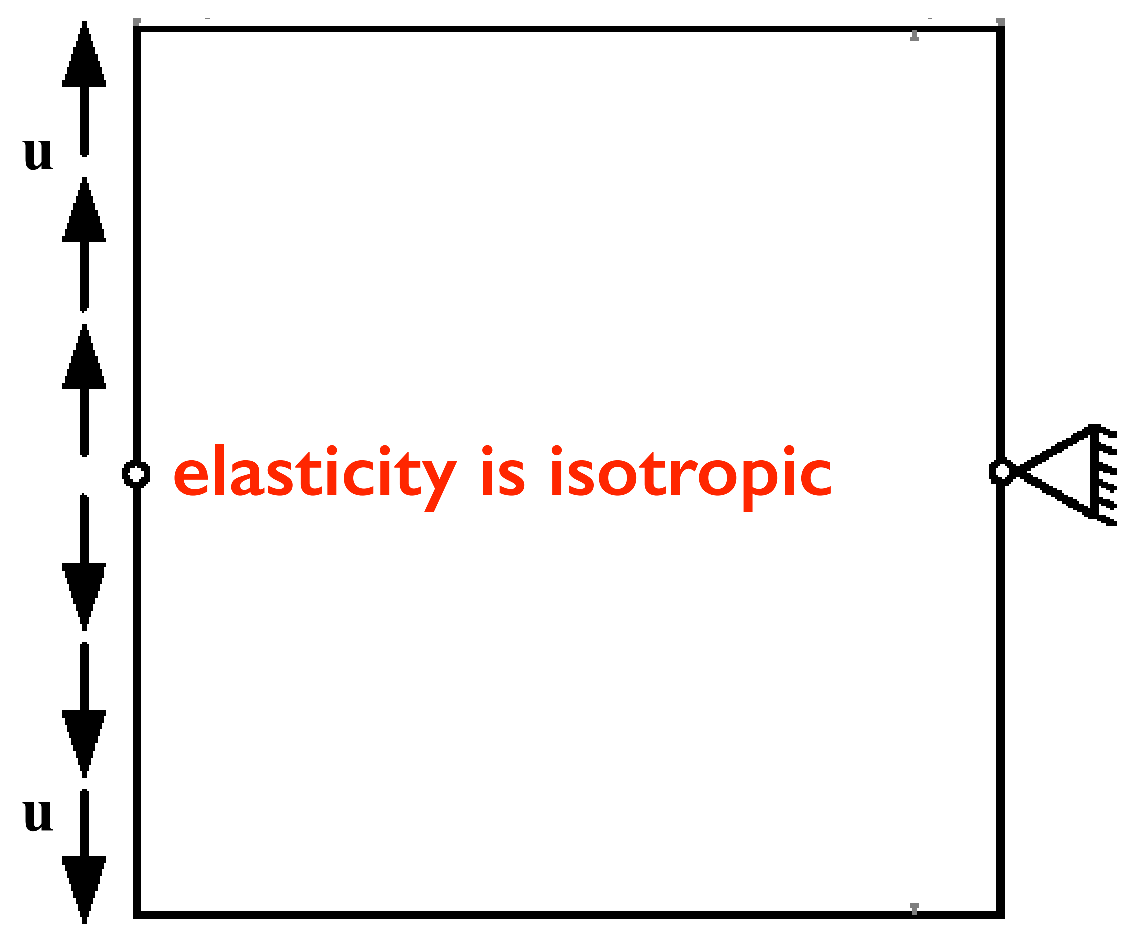
$$S > 0$$

Simulations

4th order PDE approximated with a Galerkin method based on smooth local maximum entropy (LME) meshfree basis functions.

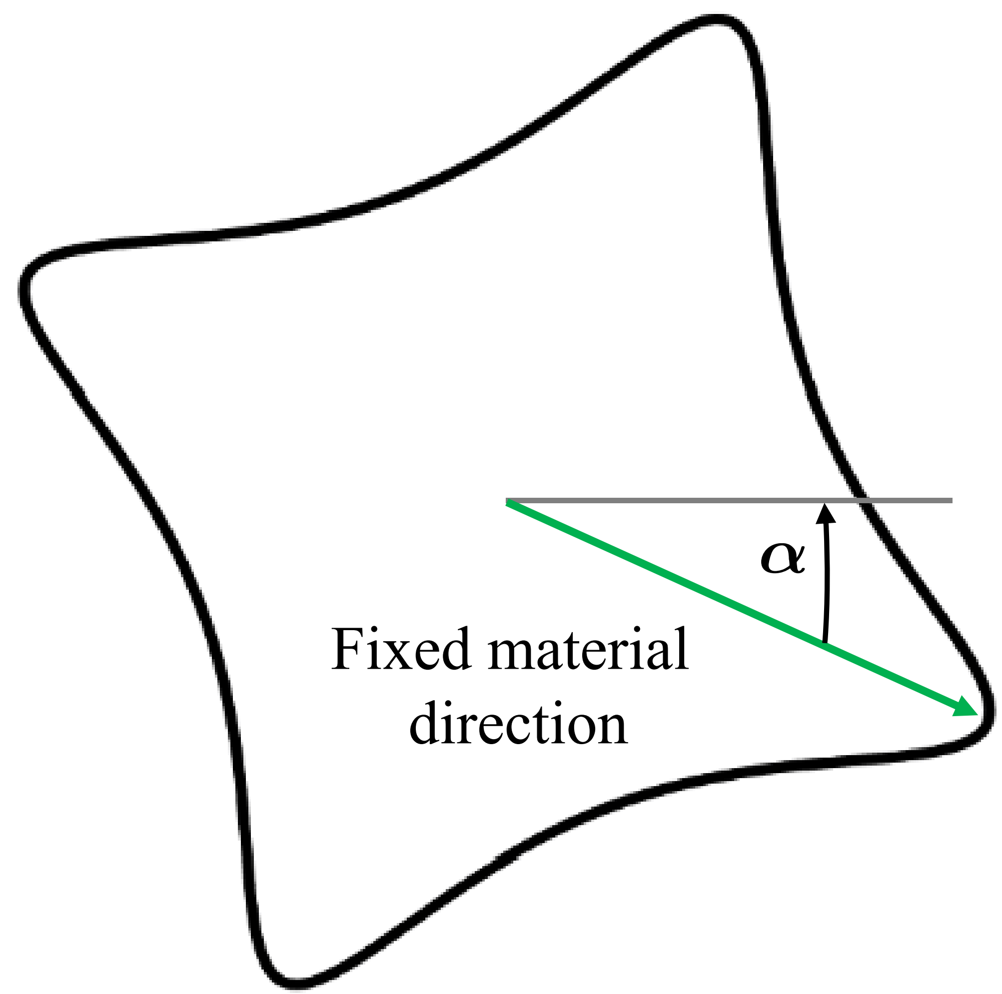
Arroyo, Ortiz, *IJNME*, 2006

Alternate minimization algorithm



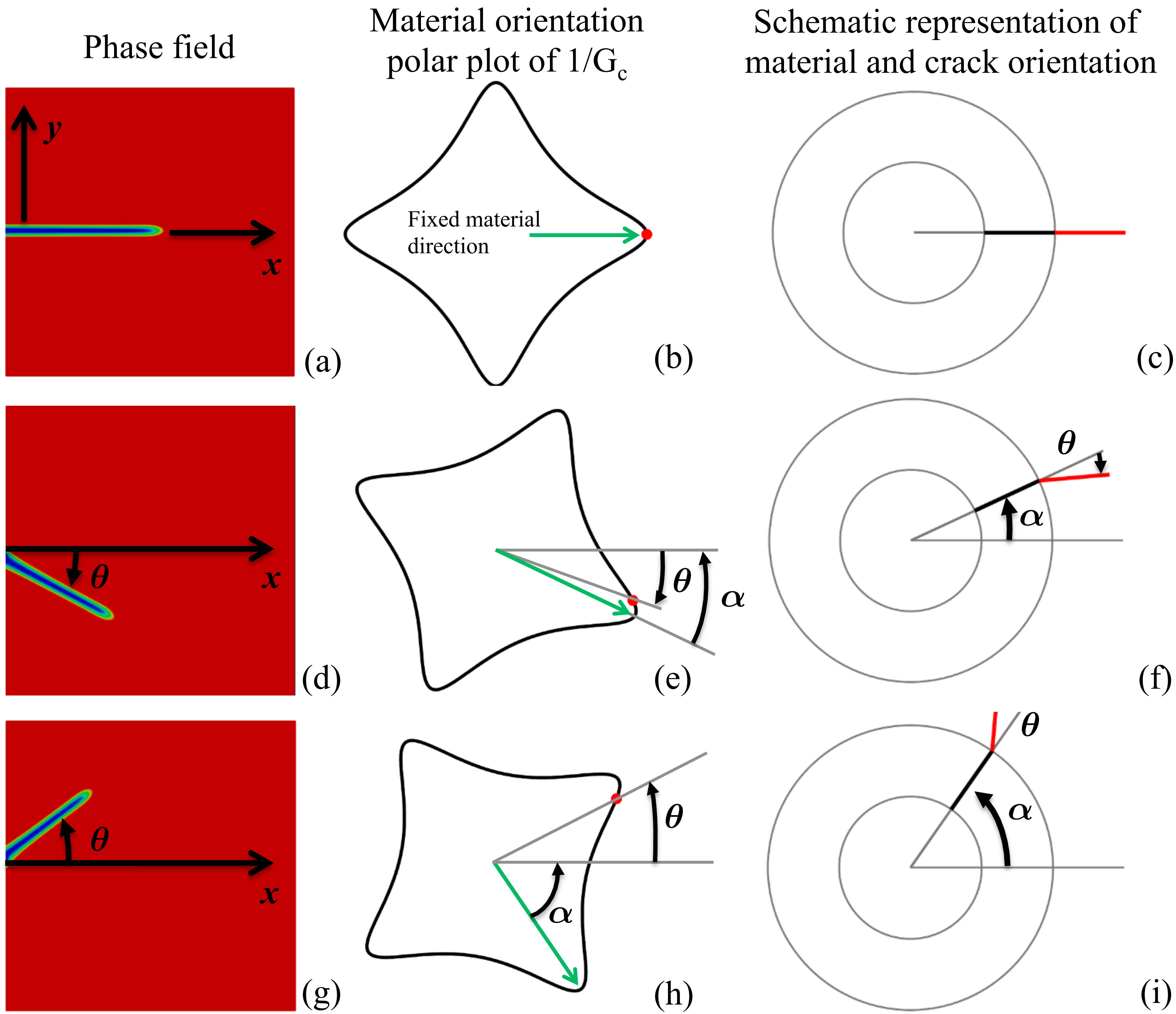
(a)

geometry and BCs

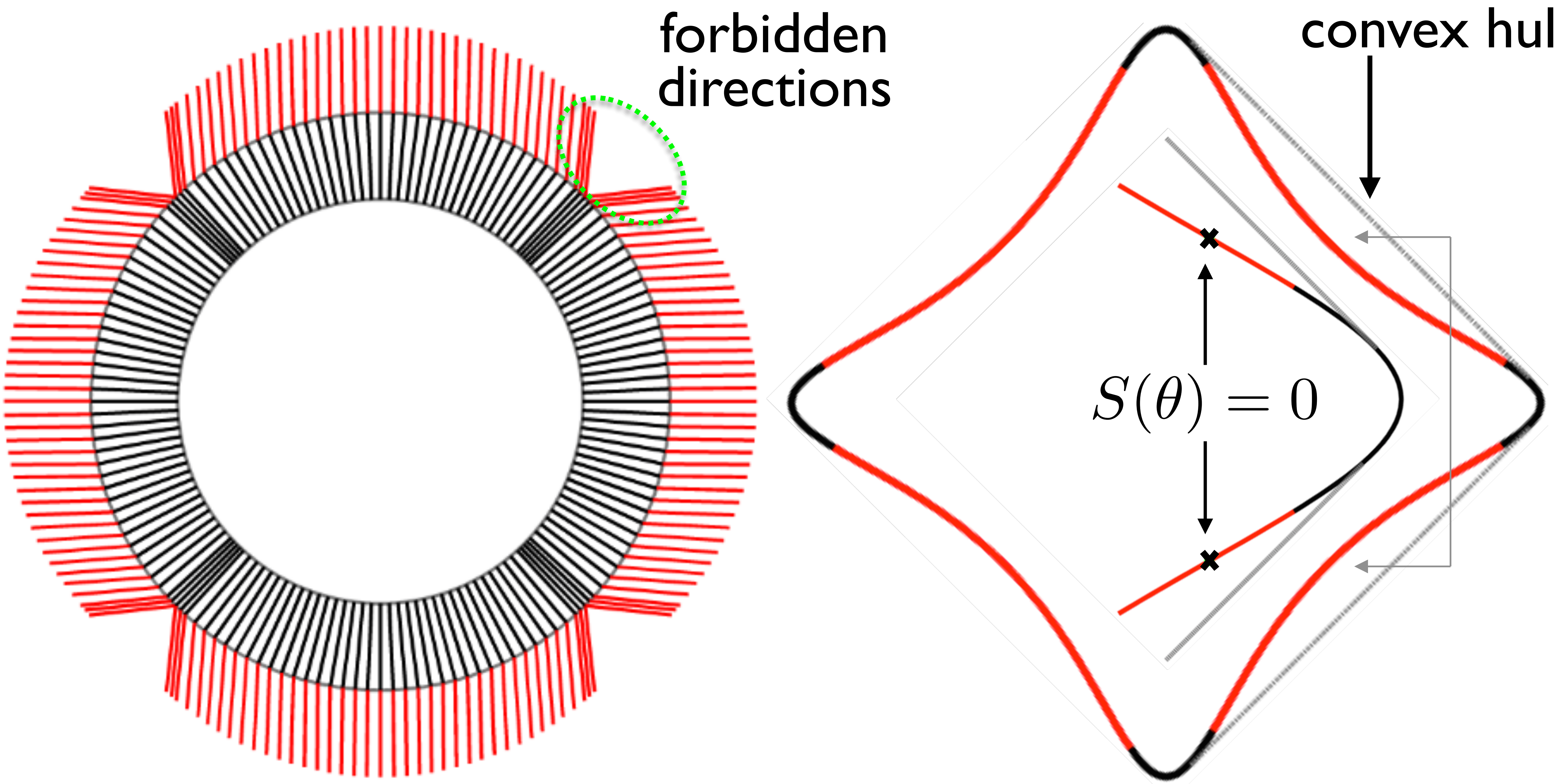


(b)

inverse polar plot of surface energy

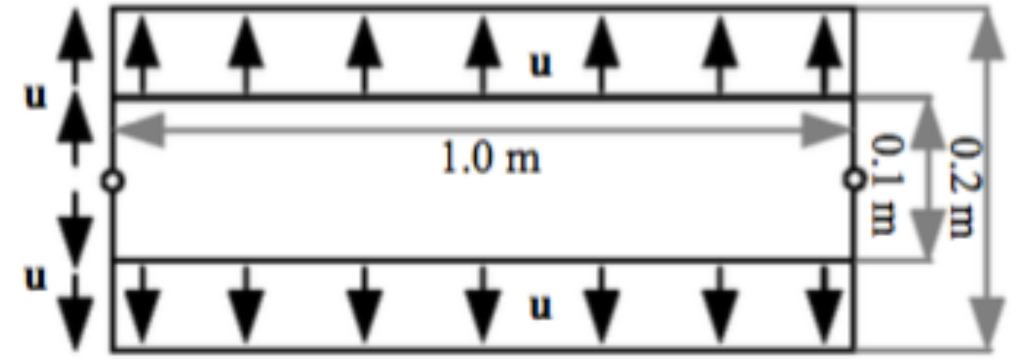

Phase field
Material orientation polar plot of 1/G$_c$
Schematic representation of material and crack orientation
y
x
(a)
Fixed material direction
(b)
(c)
θ
x
(d)
θ
α
(e)
θ
α
(f)
θ
x
(g)
θ
α
(h)
θ
α
(i)

Systematic dependence of crack propagation on material orientation



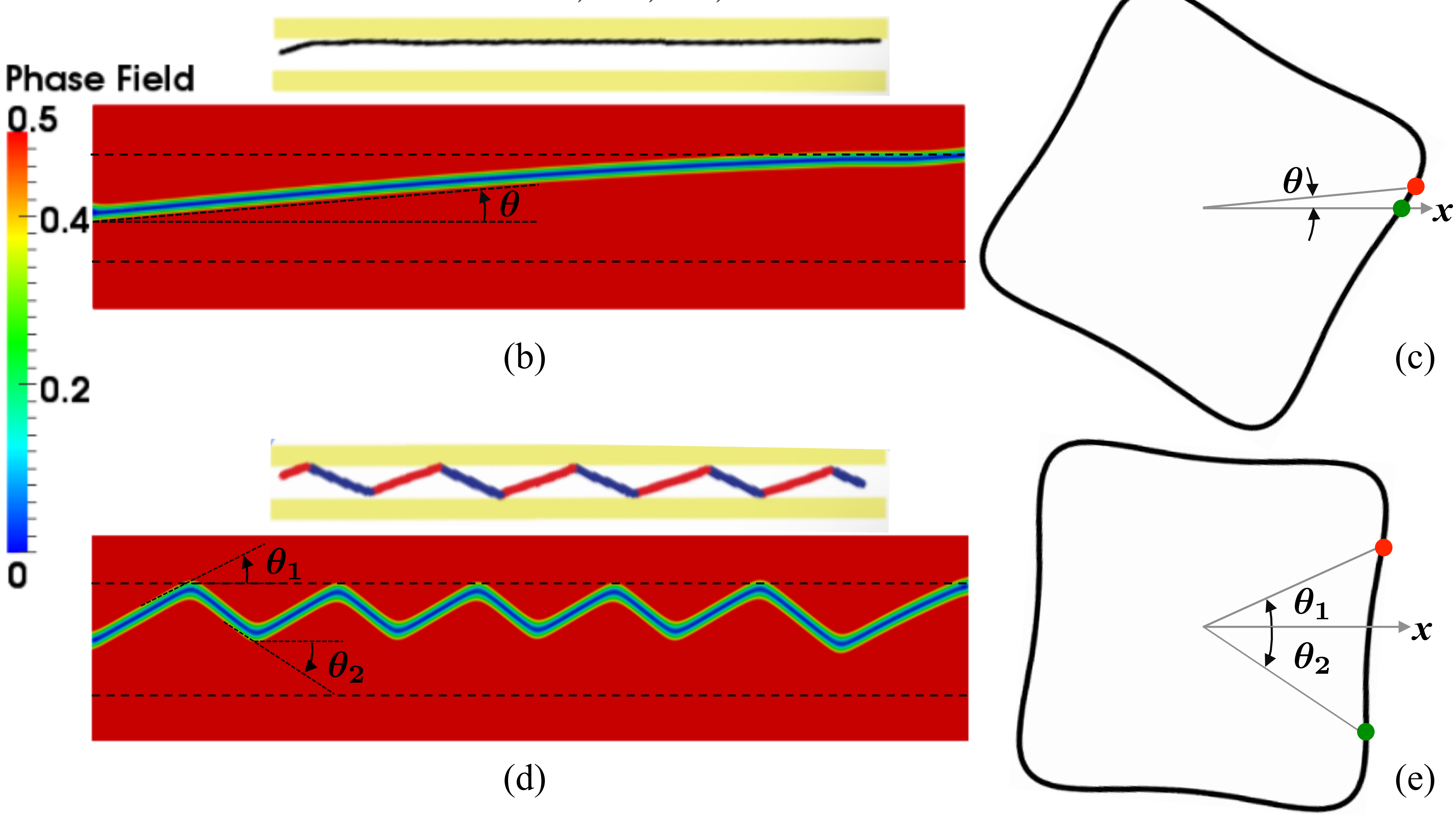
(a) (b)

Guided crack propagation

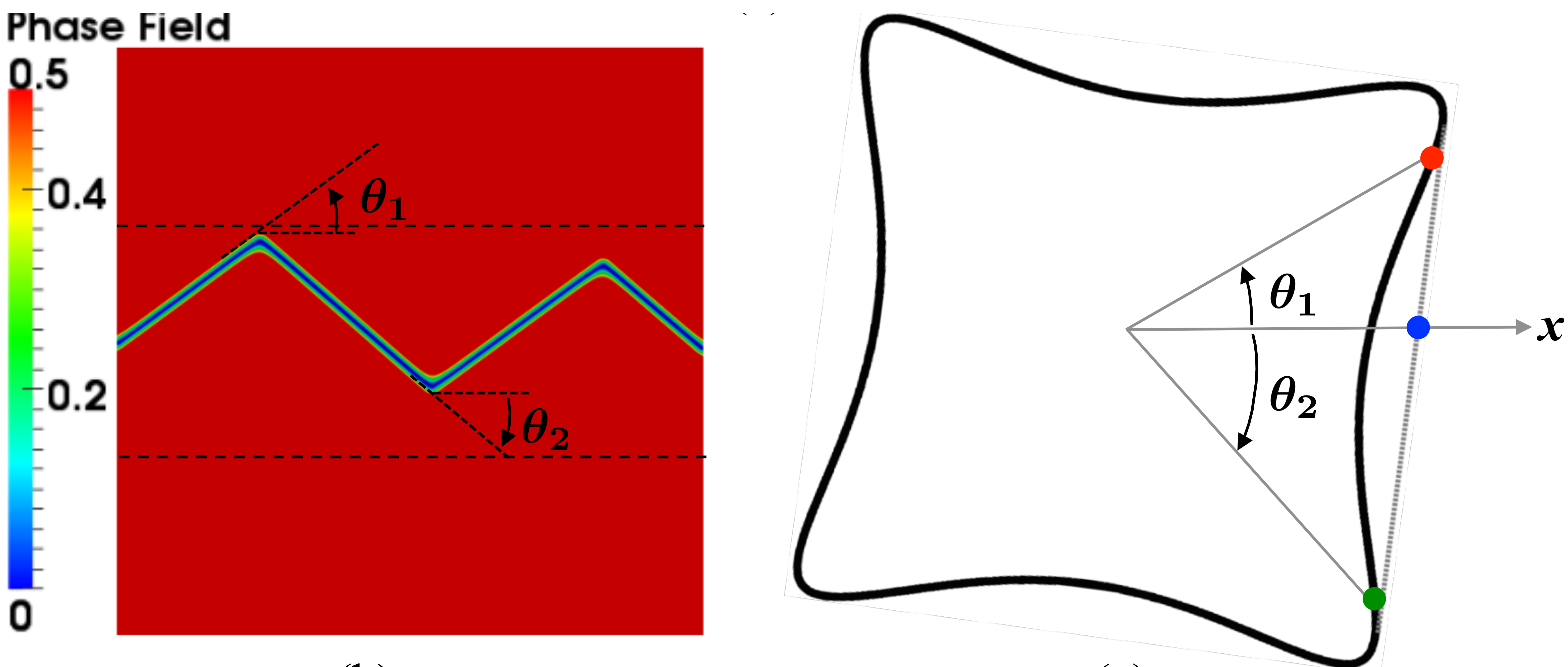


fully constrained displacement field at top and bottom bands

Takei,et.al, *PRL*, 2013



Guided crack propagation



(b) (c)

Average surface energy close to that of the blue point.

summary

1. Variational anisotropic phase-field formulation that can model the strongly anisotropic surface energy.
2. The numerical results exhibit the features of strongly anisotropic fracture.

many questions

1. What kind of angle dependence of $G(\theta)$ that can be described with the model, including all the 4th order tensors.
2. Understand the energetic penalty for crack kinking implicit in the phase-field model.
3. Model other symmetries, 3D…

Outline

1. Phase-field modeling of fracture in materials with strongly anisotropic surface energy

2. **Phase-field modeling of fracture in brittle thin shells**

3. Effect of shell geometry on crack propagation:

   G for a thin shell

phase-field model for (adhesive) thin sheets

$$\Pi[\boldsymbol{u}, v] = \boxed{\Pi_{\mathrm{ela}}[\boldsymbol{u}, v]} + \Pi_{\mathrm{adh}}[\boldsymbol{u}] + \boxed{\Pi_{\mathrm{fra}}[v]},$$

Elastic energy

$$\Pi_{\mathrm{ela}}[\boldsymbol{u}, v] = \int_{S_0} v^2 \boxed{W(\boldsymbol{\varepsilon}, \boldsymbol{\rho})}\, dS_0,$$

nonlinear Koiter thin shell

$\boldsymbol{\varepsilon}$ change of metric

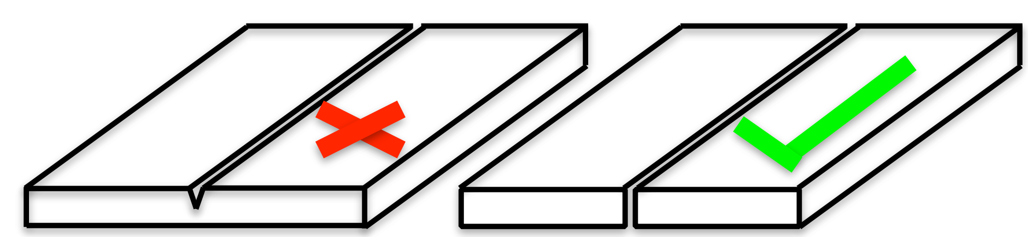
$\boldsymbol{\rho}$ change of curvature

Fracture energy approximation

$$\Pi_{\mathrm{fra}}[v] = \int_{S_0} G_{\mathrm{c}} \left[\frac{(v-1)^2}{4\ell} + \frac{\ell}{2} |\underline{\nabla_{\mathrm{s}} v}|^2 + \frac{\ell^3}{4} (\underline{\Delta_{\mathrm{s}} v})^2 \right] dS_0,$$

Borden, et.al, *CMAME*, 2014

gradient and Laplacian on surface



phase-field model for (adhesive) thin sheets

$$\Pi[\boldsymbol{u}, v] = \Pi_{\mathrm{ela}}[\boldsymbol{u}, v] + \boxed{\Pi_{\mathrm{adh}}[\boldsymbol{u}]} + \Pi_{\mathrm{fra}}[v],$$

Adhesion energy: cohesive zone model

$$\Pi_{\mathrm{adh}}[\boldsymbol{u}] = \int_{S_0} \Phi_{\mathrm{n}} \left[1 - \left(1 + \frac{\Delta_{\mathrm{n}}}{\delta_{\mathrm{n}}} \right) \exp\left(-\frac{\Delta_{\mathrm{n}}}{\delta_{\mathrm{n}}} - \frac{\Delta_{\mathrm{t}}^2}{\delta_{\mathrm{t}}^2} \right) \right] \, dS_0,$$

Δ_{n} and Δ_{t} are projected normal/tangential displacements

Xu, et.al, *JMPS*, 1994

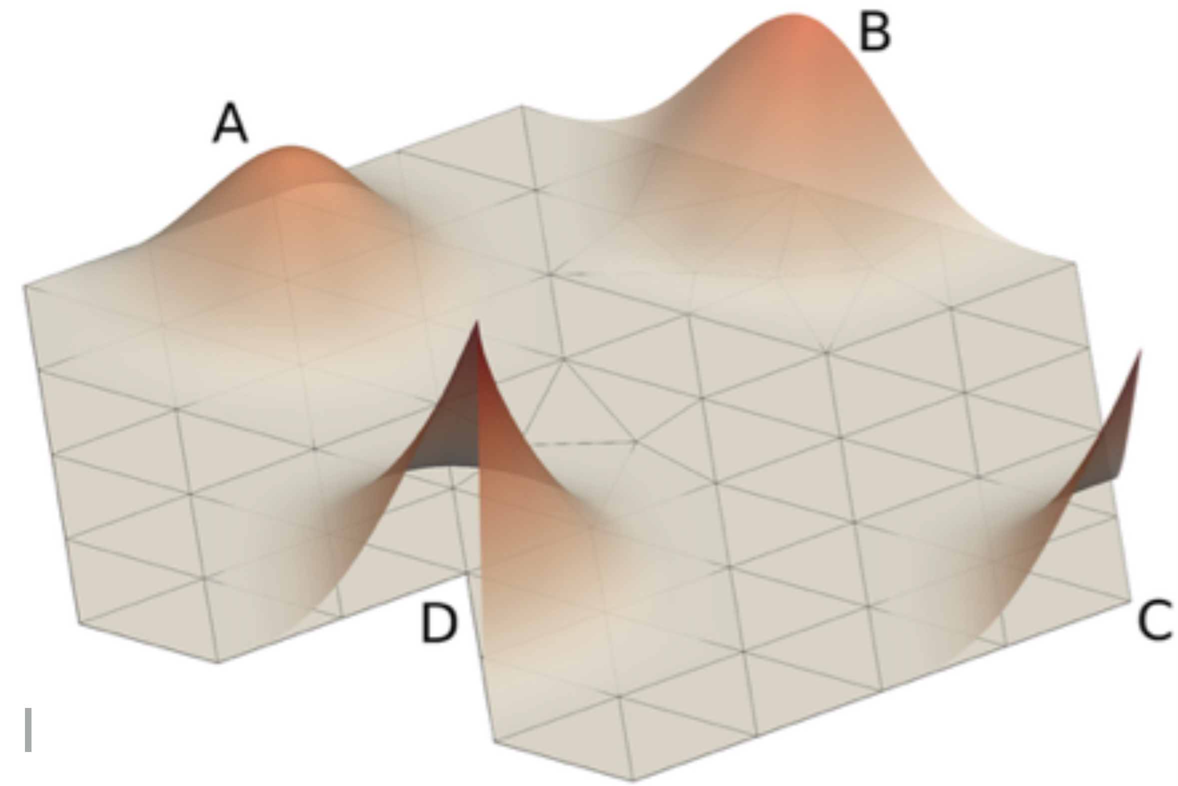
Model for fracture in thin adhesive shells:

$$\min_{\boldsymbol{u}, v} \Pi[\boldsymbol{u}, v] \quad \text{subject to} \quad \dot{v} \leq 0 \quad \text{(irreversibility)}$$

Numerical implementation

4th-order PDE (shell and phase-field), C^1 approximation is required

Subdivision surface finite elements



smooth approximation for $\boldsymbol{u}$ and v

Cirak,et.al, *IJNME*, 2000, 2011

Irreversibility $\dot{v} \leq 0$ is implemented by strain-history function

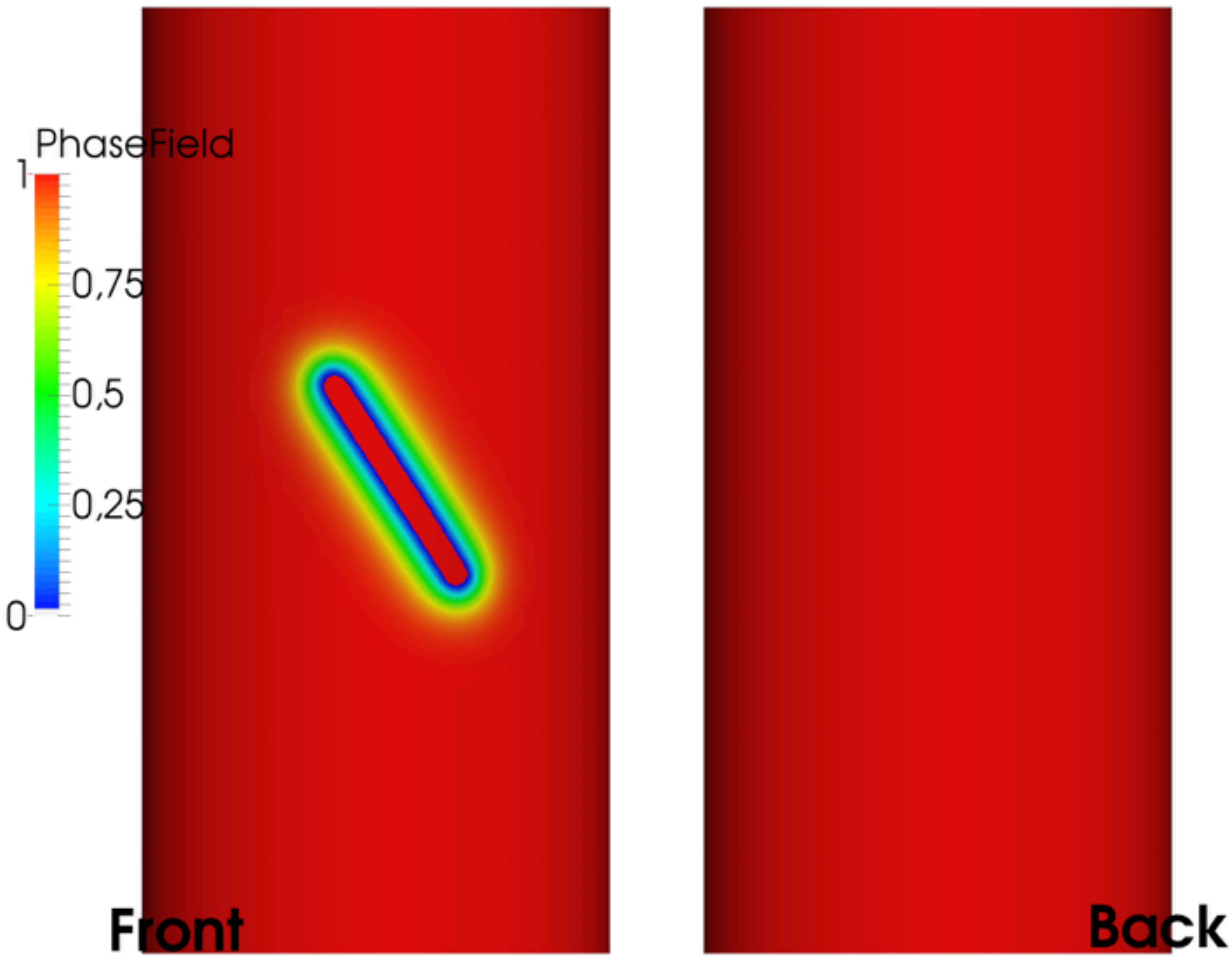
Miehe,et.al,*CMAME*,2010

Displacement of shell is solved by Newton's method.

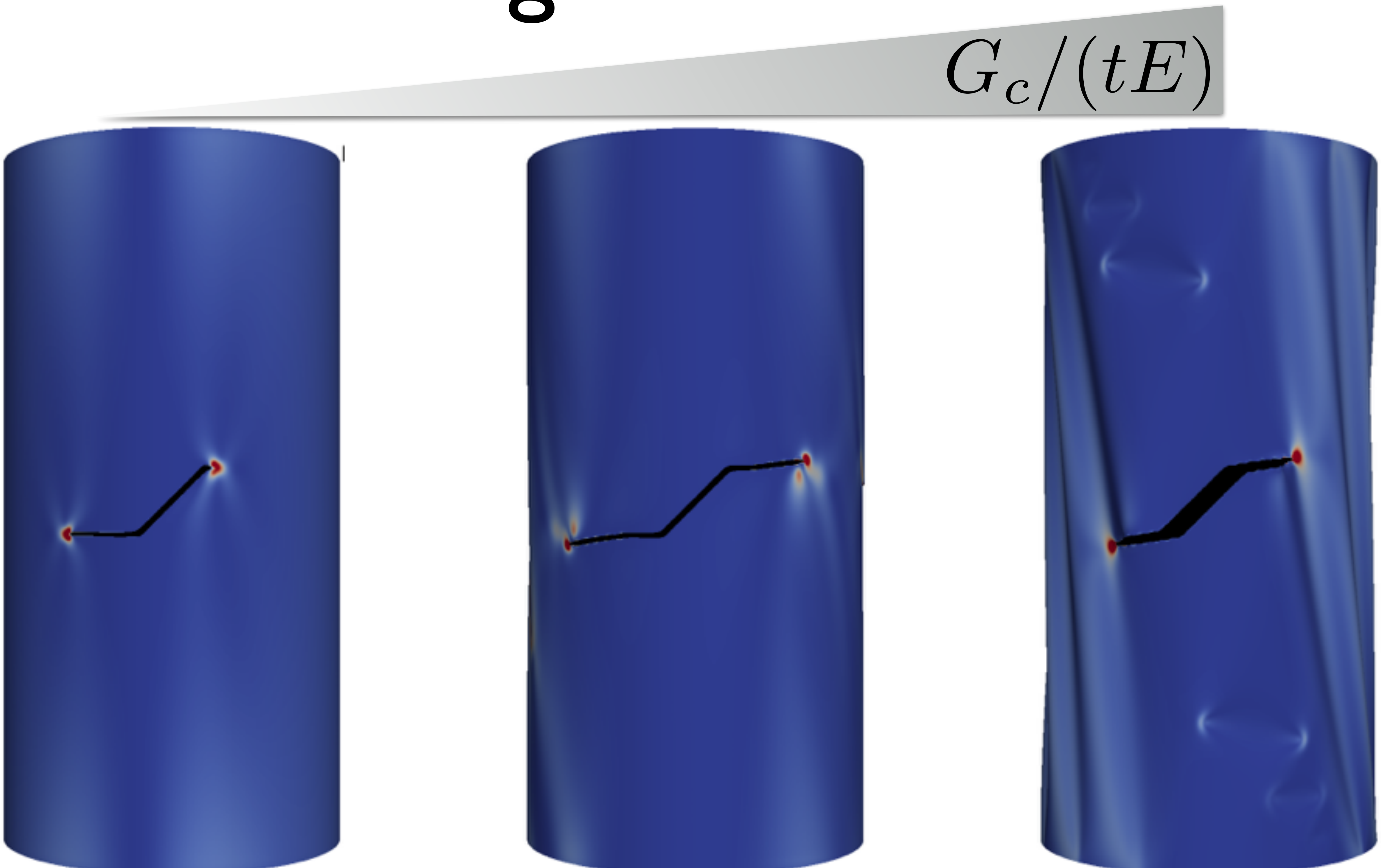
Alternate minimization algorithm.

Bourdin,*Interface Free Bound*,2007

buckling vs fracture



buckling vs fracture

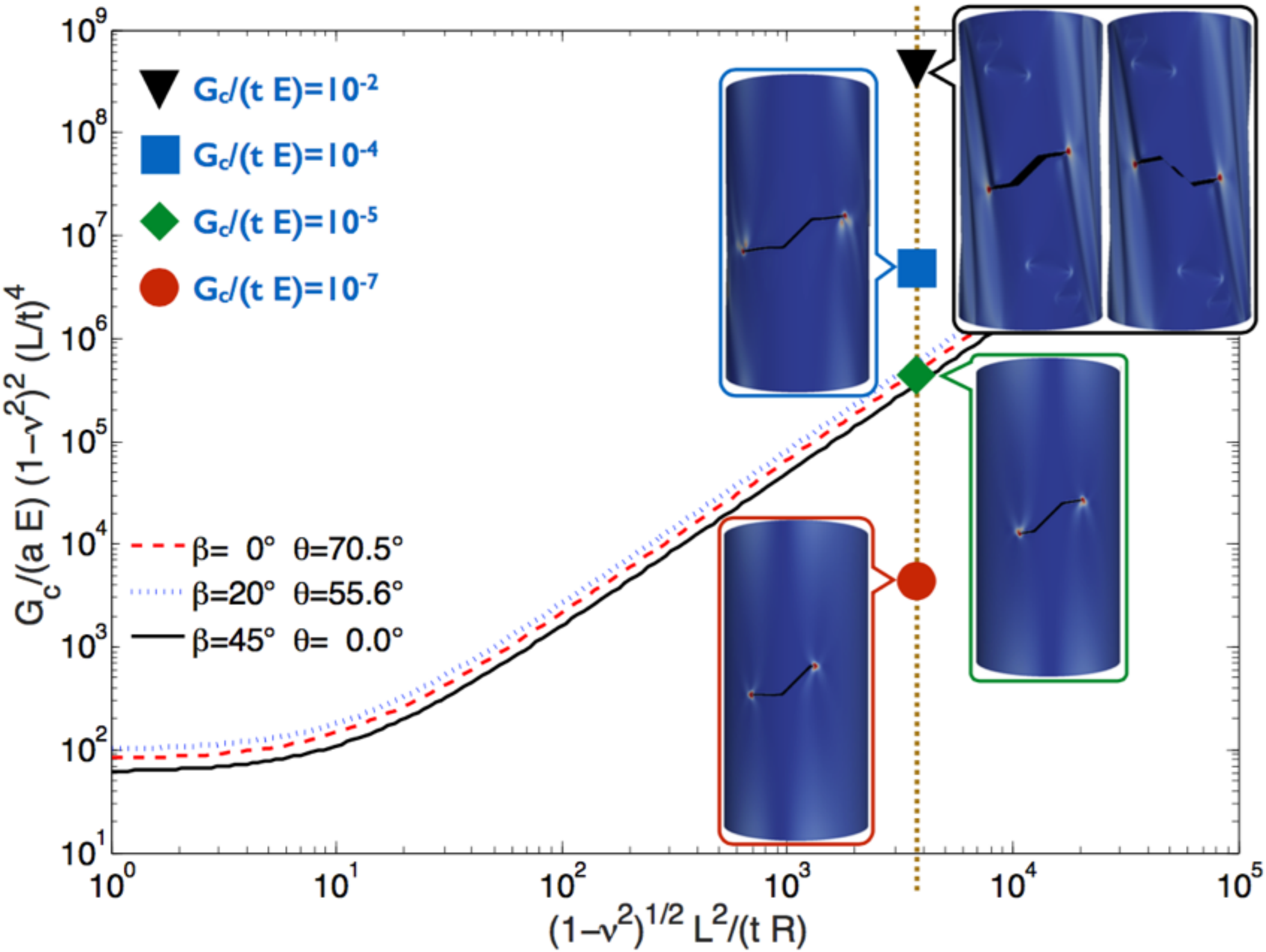


fracture without significant deformation

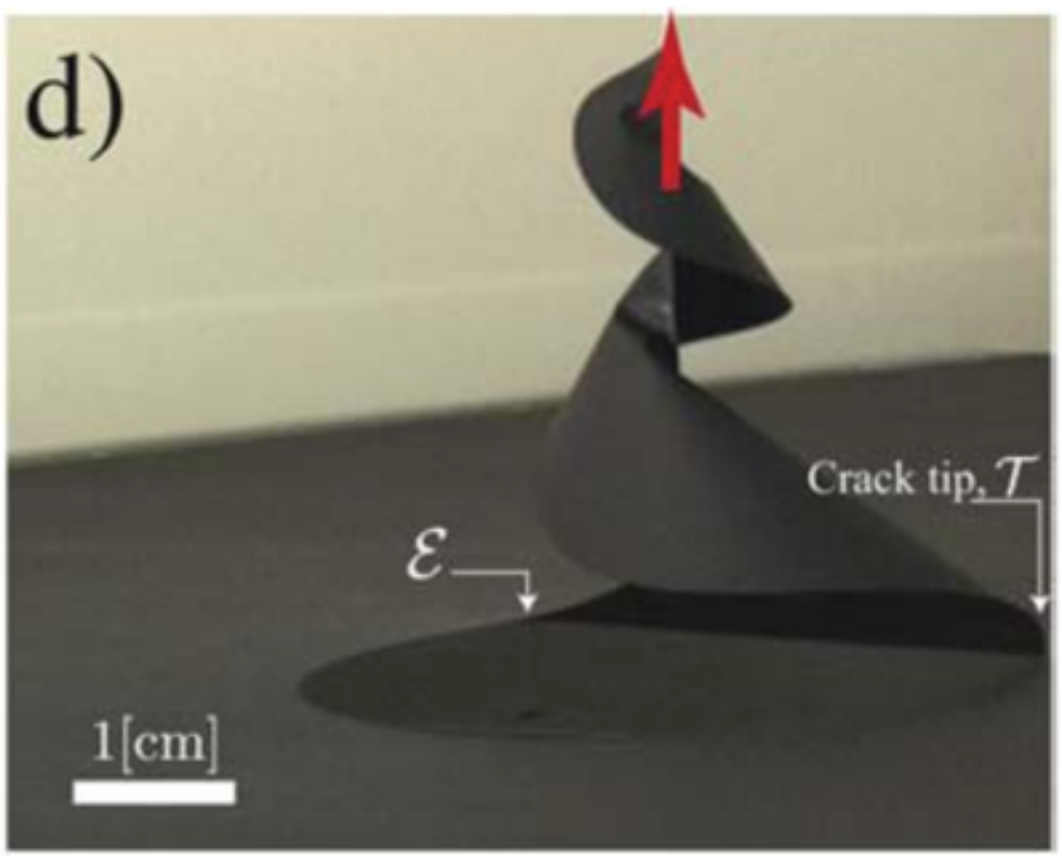
fracture with slight buckling

fracture and prominent buckling

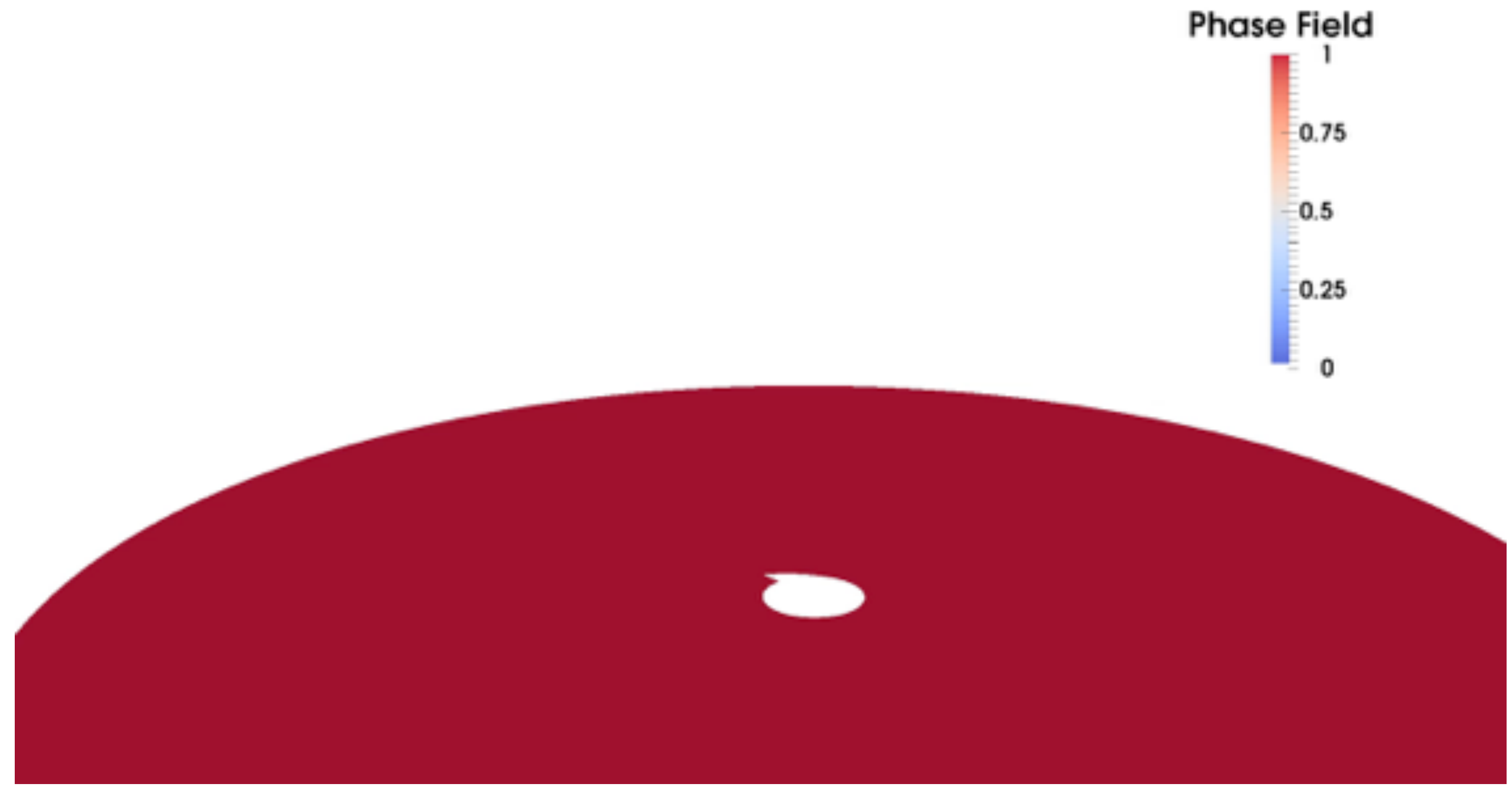
buckling vs fracture



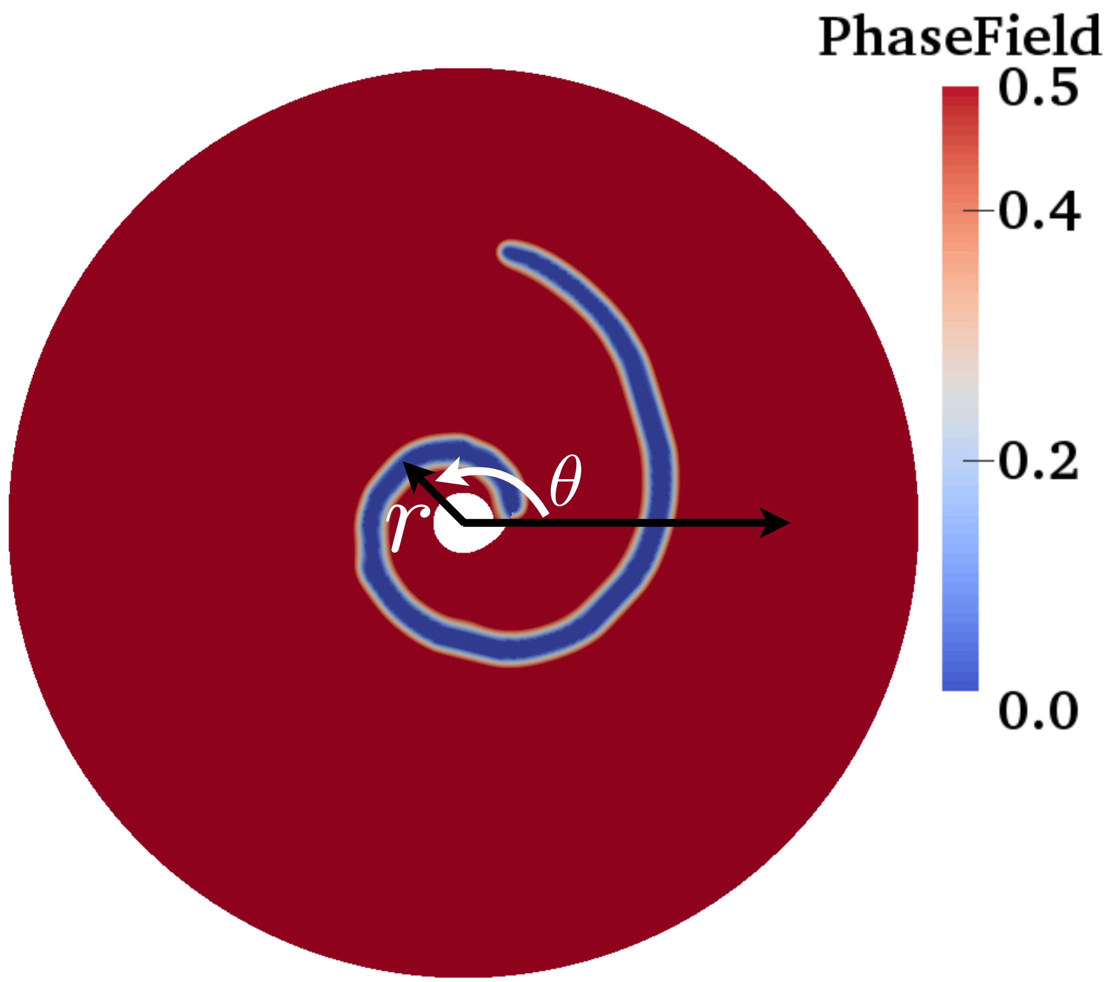
Spiraling tearing of thin sheets



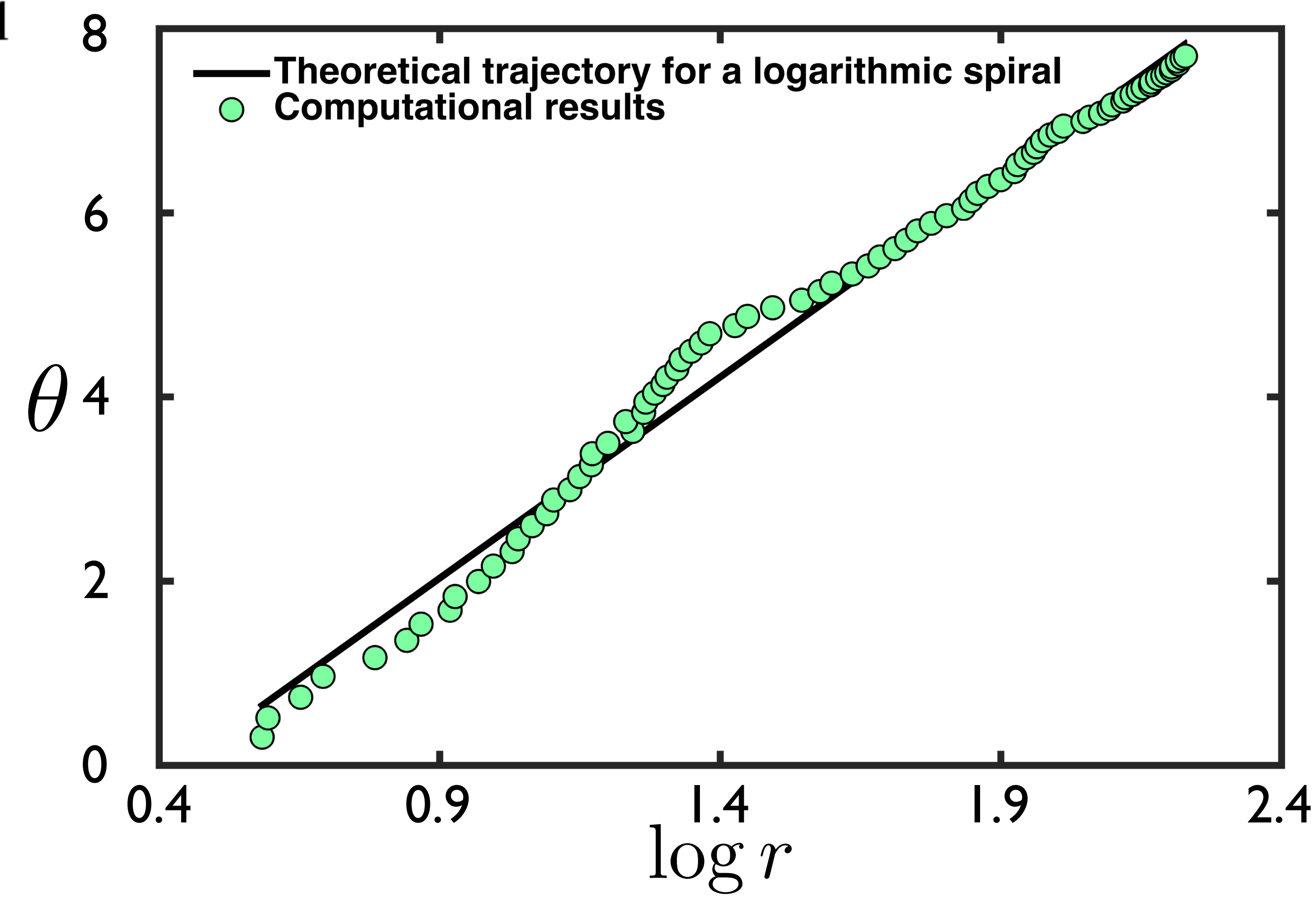
Romero, et.al, *Soft Matter*, 2013



Spiraling tearing of thin sheets

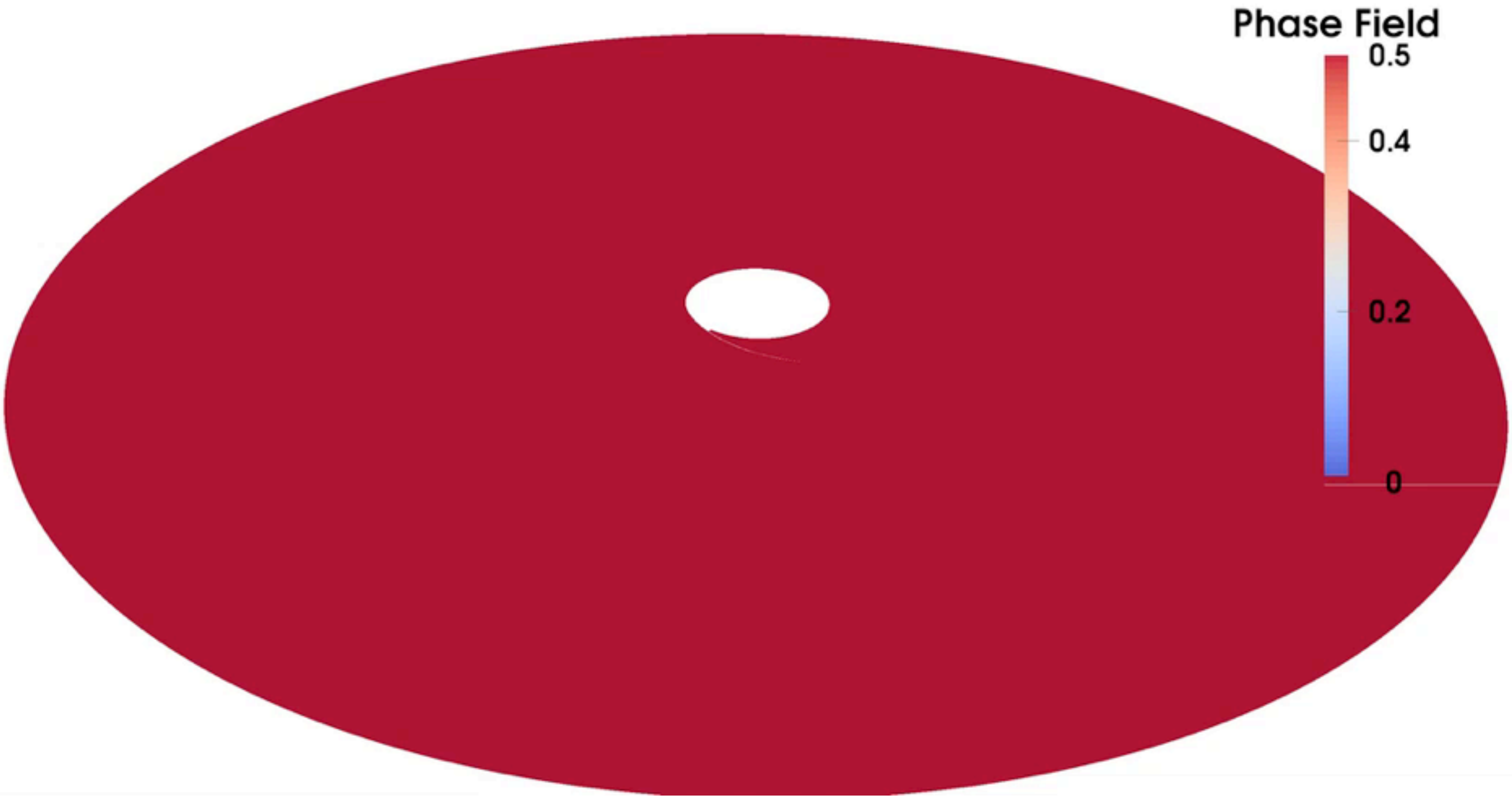


(a)

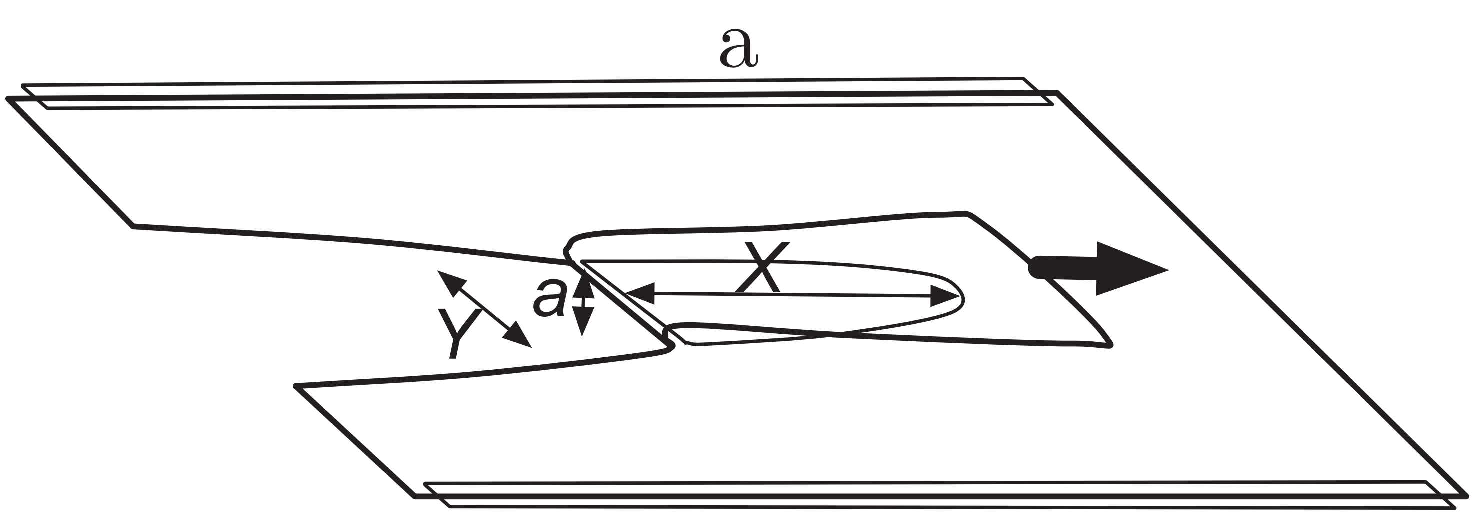


(b)

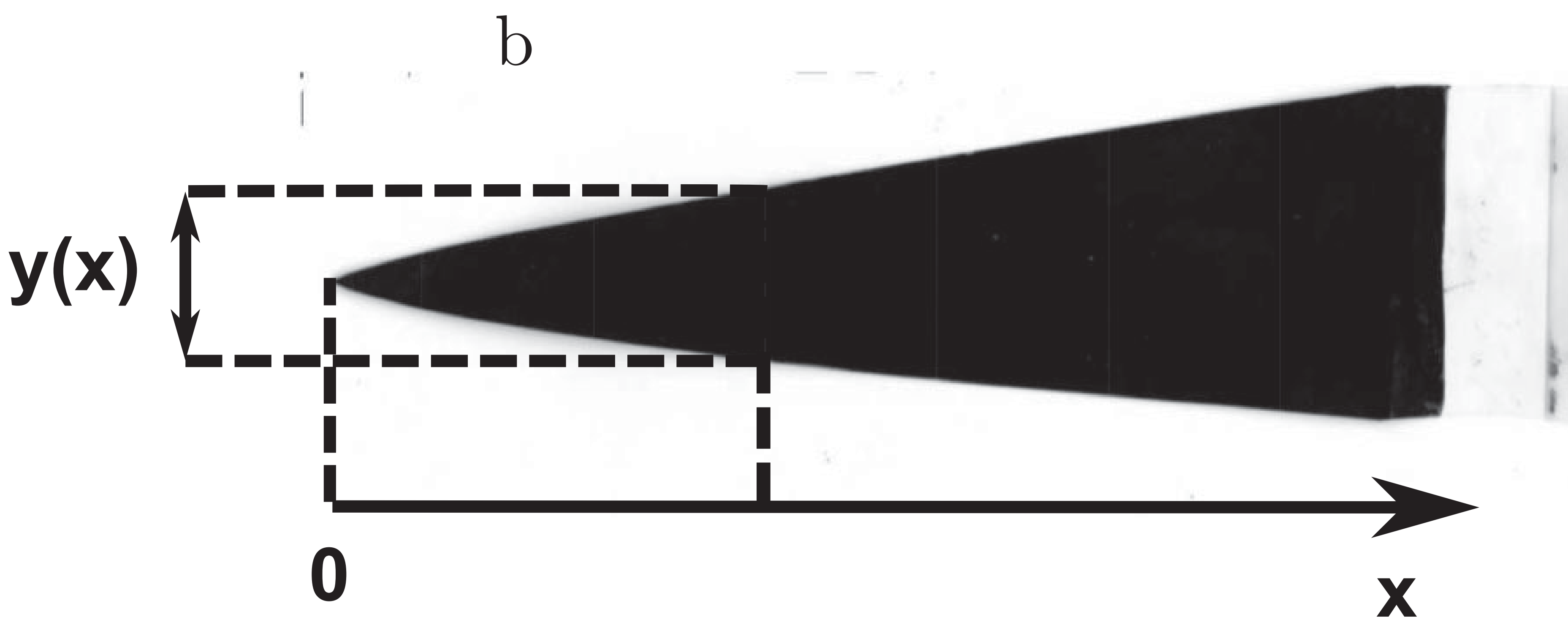
logarithmic spiral crack path


Phase Field
0.5
0.4
0.2
0

One-flap tearing of thin sheets



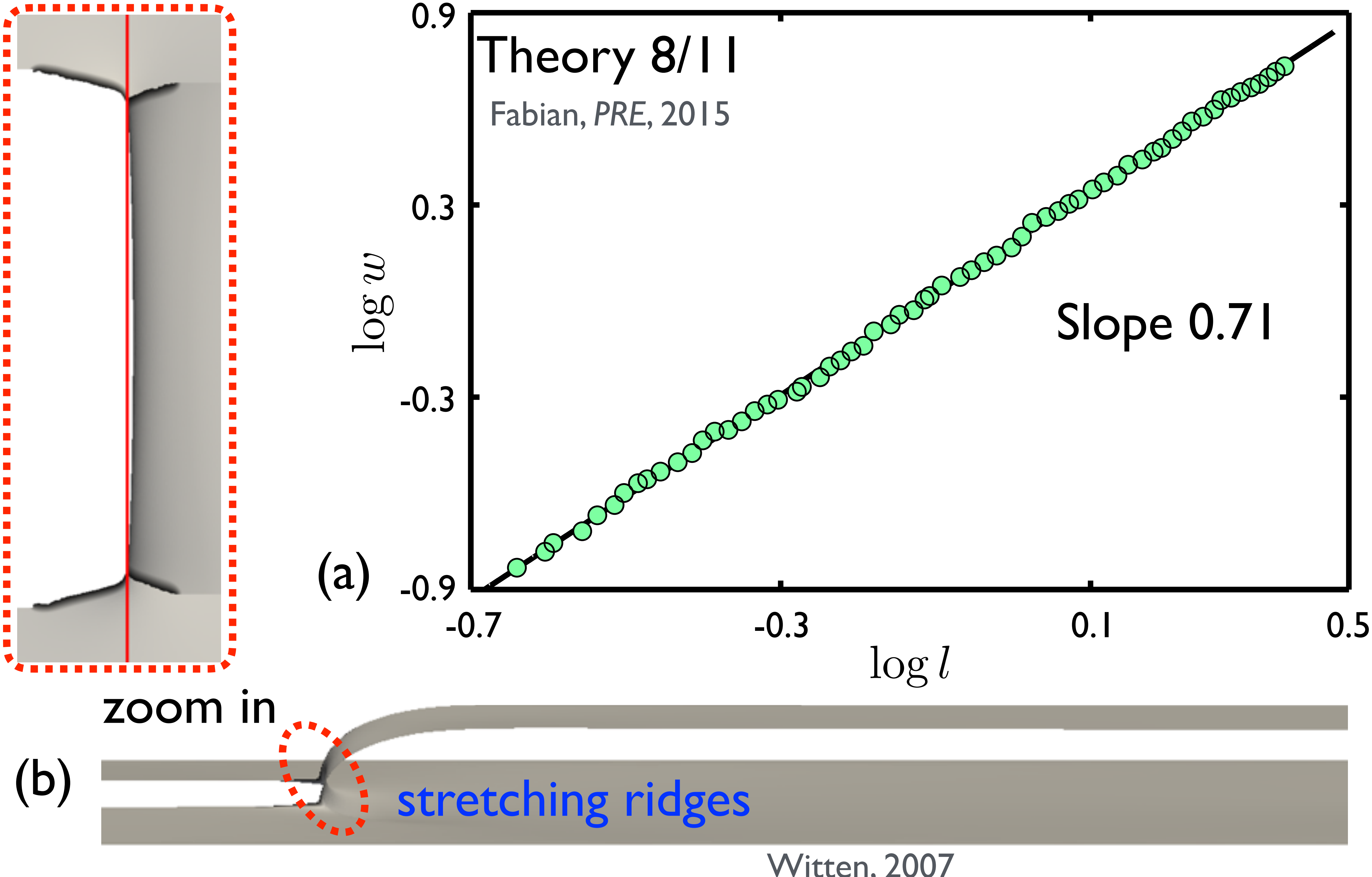
Bayart,et.al, *PRL*, 2011



$$Y \sim X^{(0.77 \pm 0.05)}$$

One-flap tearing of thin sheets

One-flap tearing of thin sheets

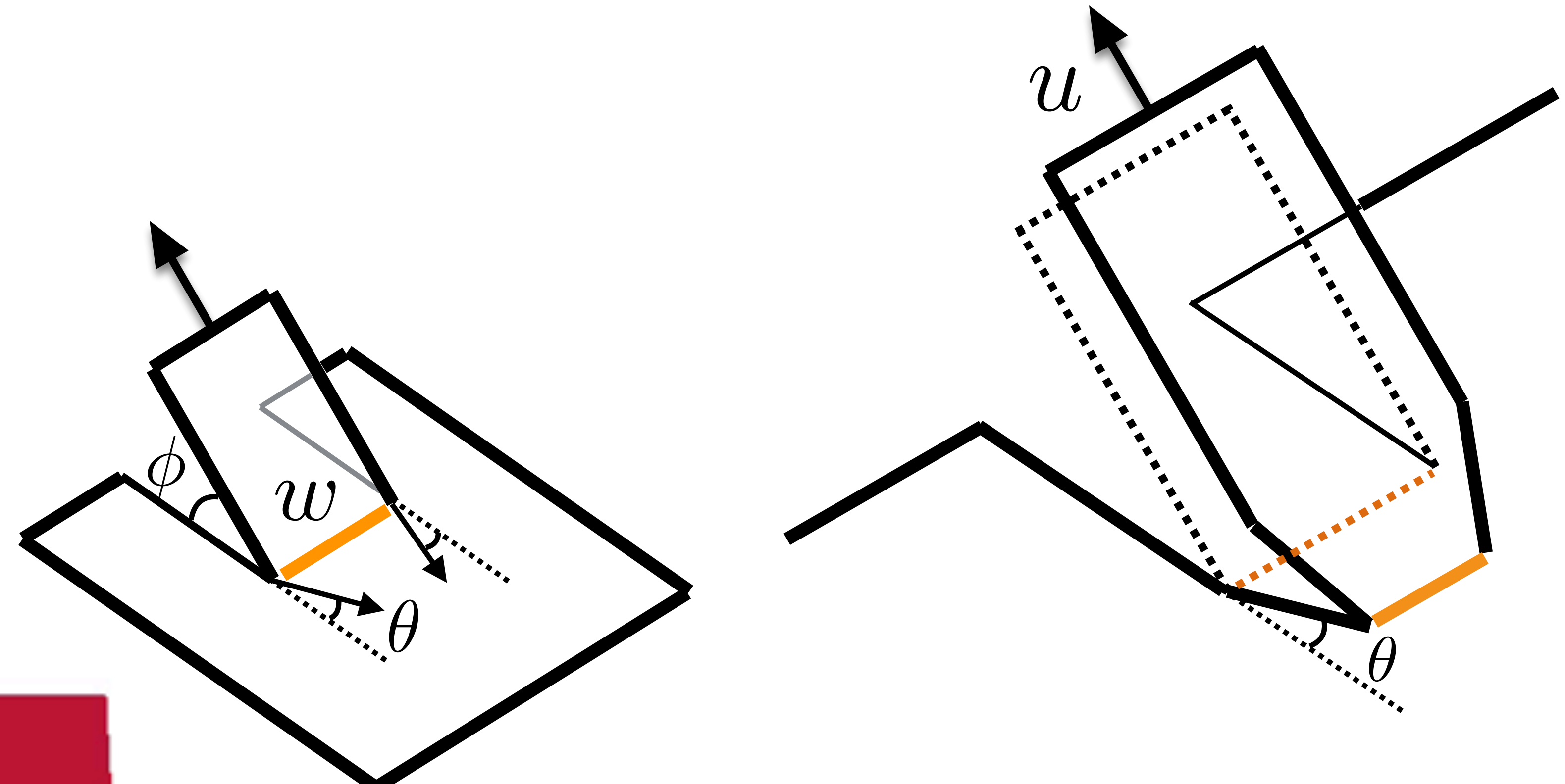


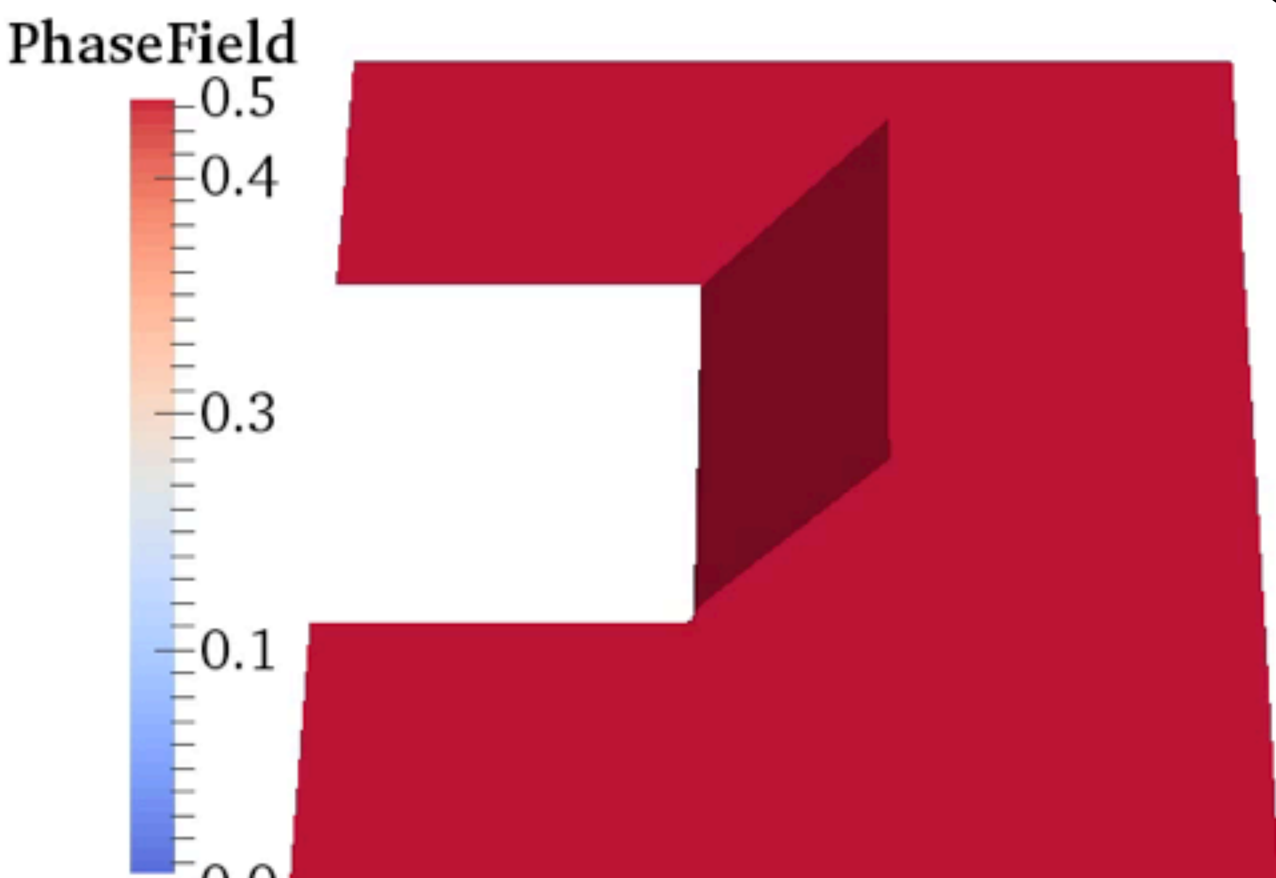
Tearing with Adhesion

Sheet adhered to flat substrate

strong adhesion

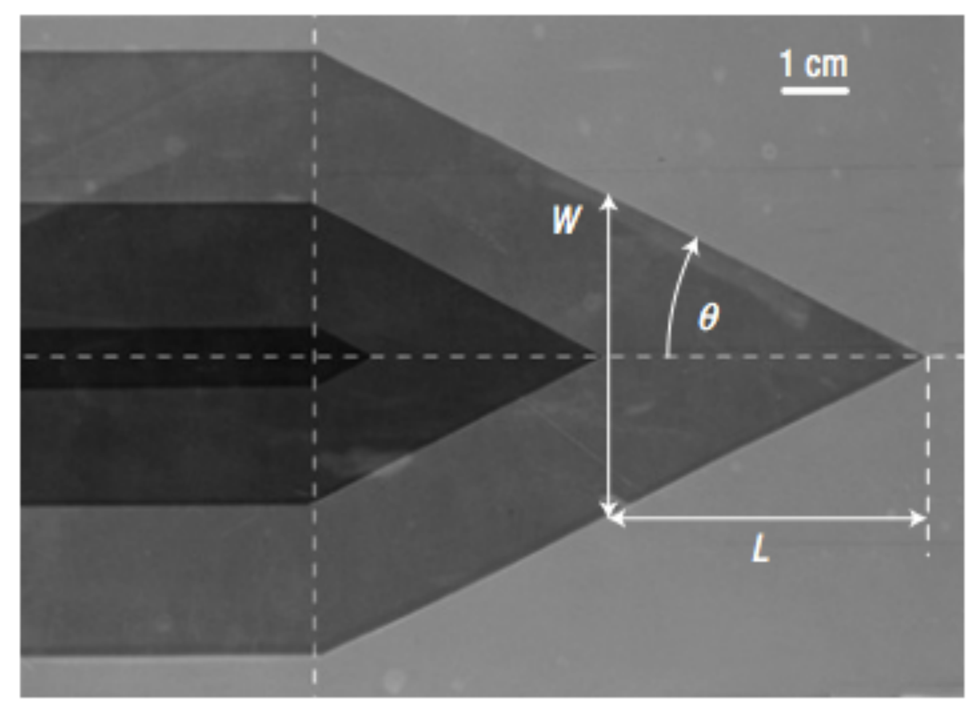
$$\Phi_n w \gg G_c t$$



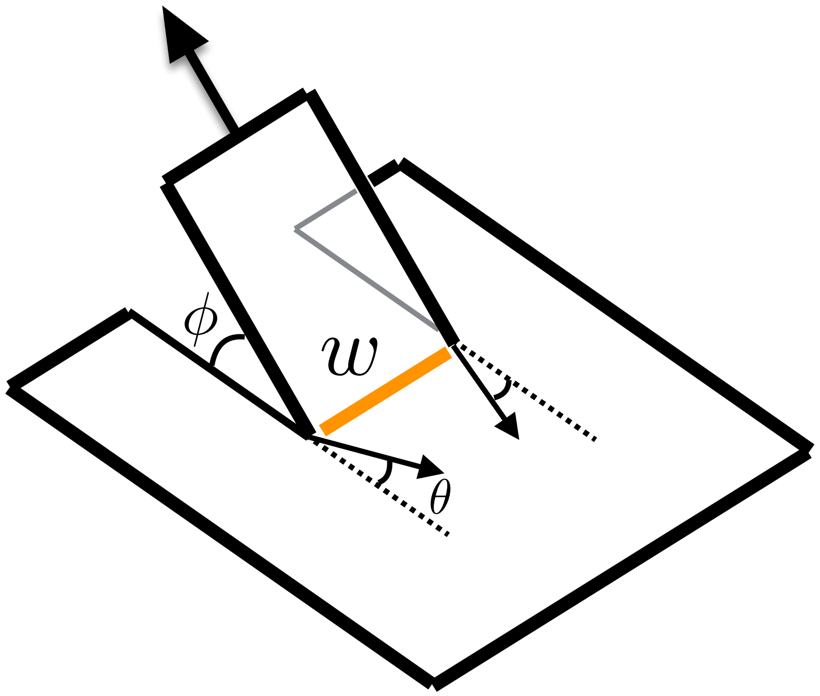


straight convergent cracks

Hamm,et.al *Nat Mater*, 2008



Sheet adhered to flat substrate



According to simple energetic model

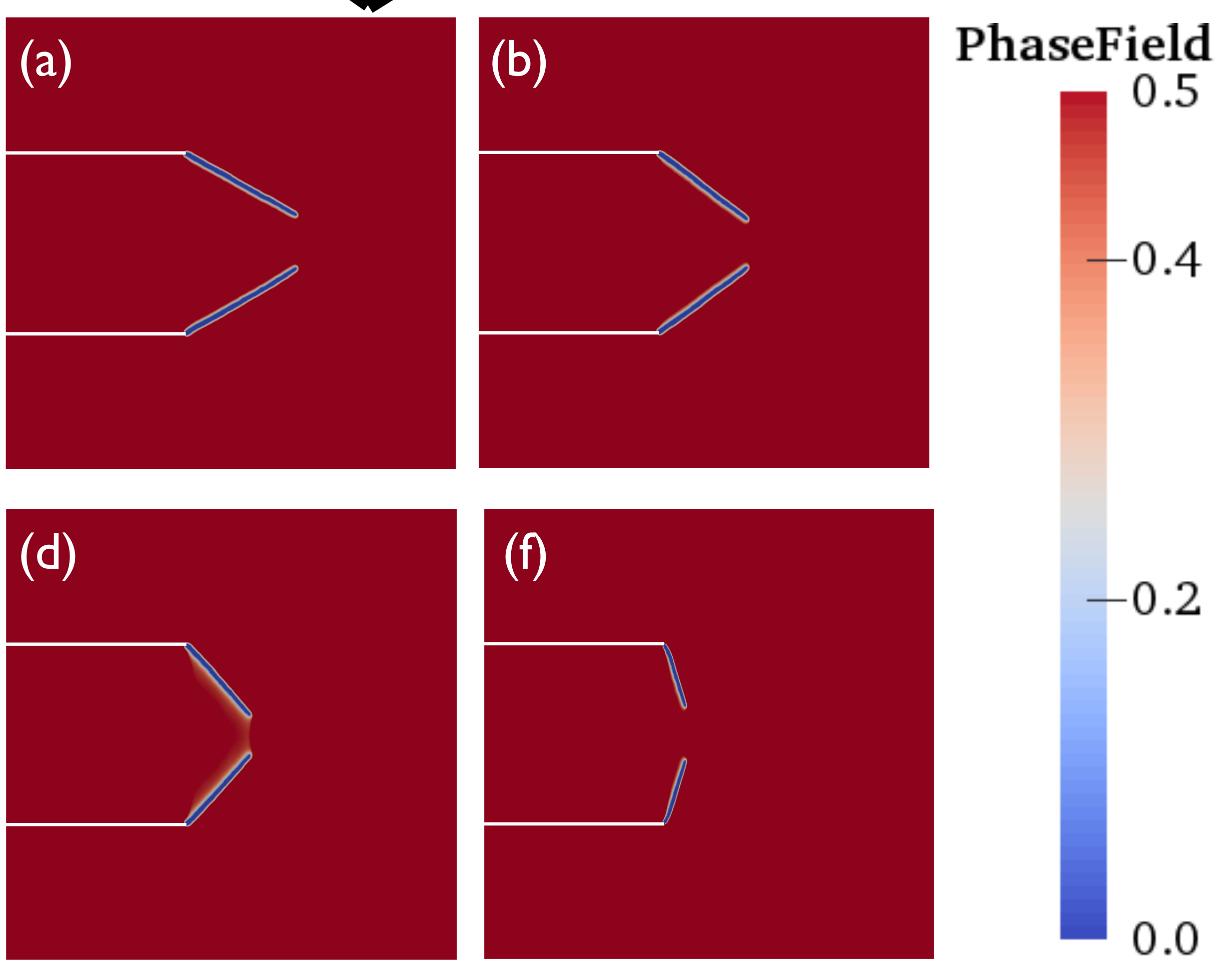
$$\sin(\theta) = \frac{\sqrt{2B\Phi_n}}{G_c t}\left[\frac{1-\cos(\phi/2)}{\sin(\phi/2)}\right]$$

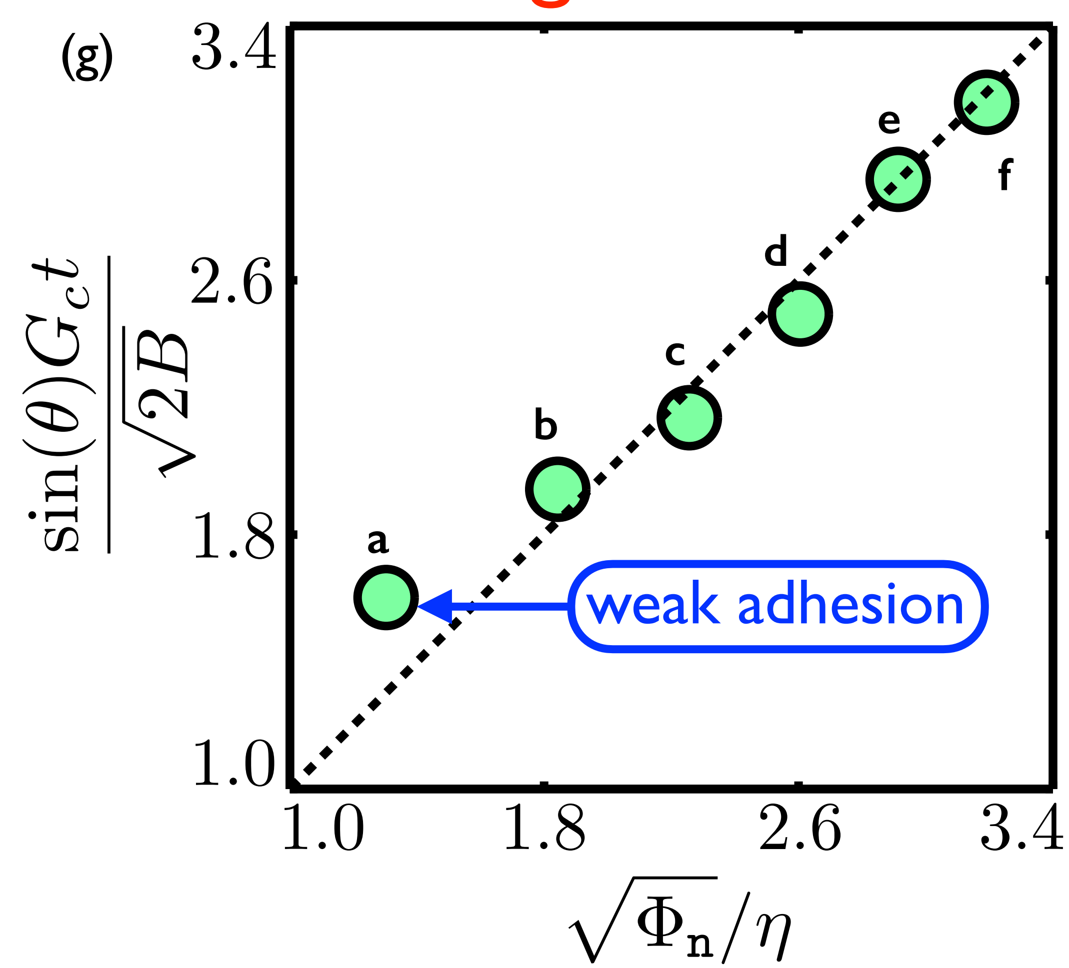
Hamm,et.al, *Nat Mater*, 2008, Roman, *IJF*, 2013

strong adhesion

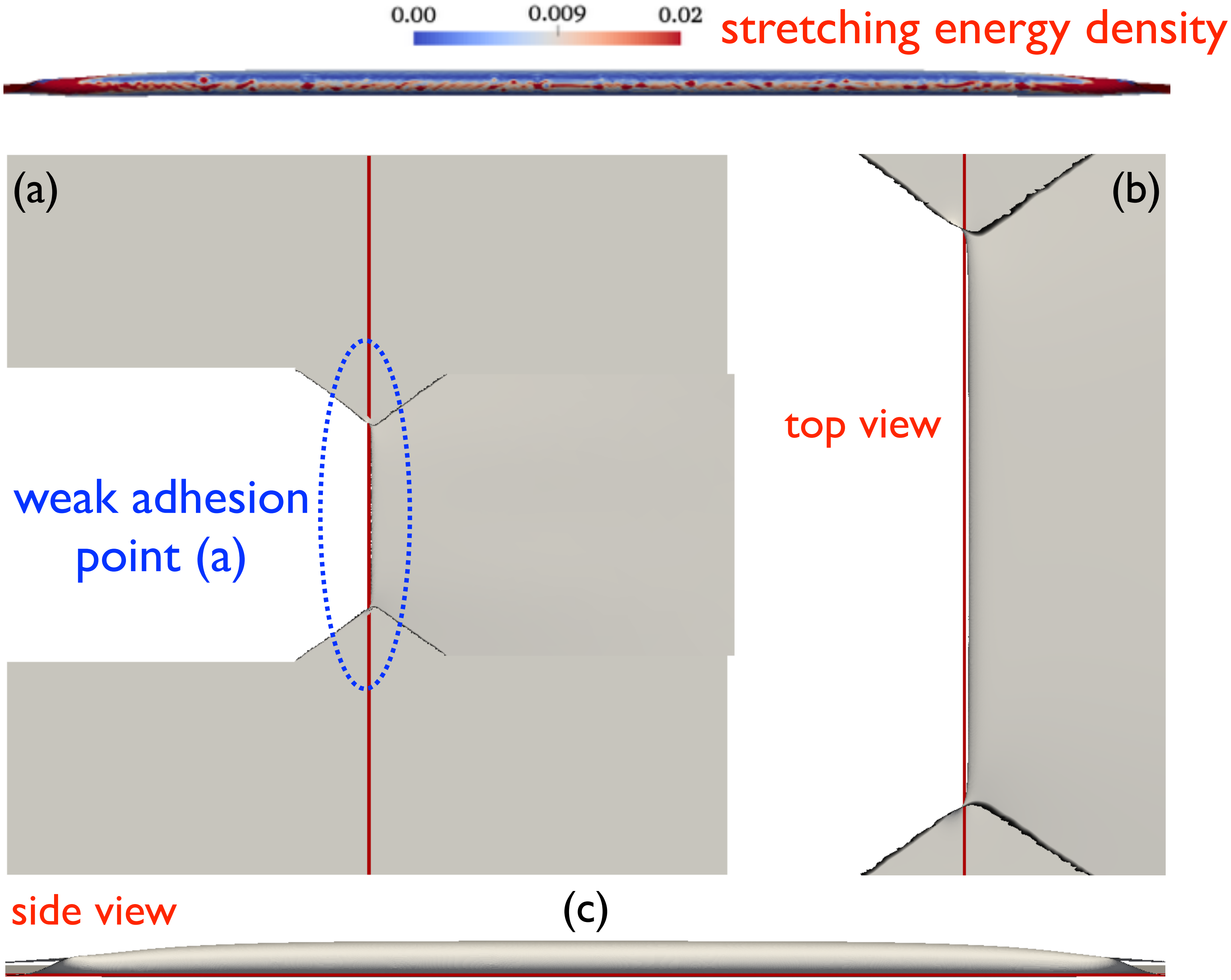
$$\Phi_n w \gg G_c t$$

change adhesion

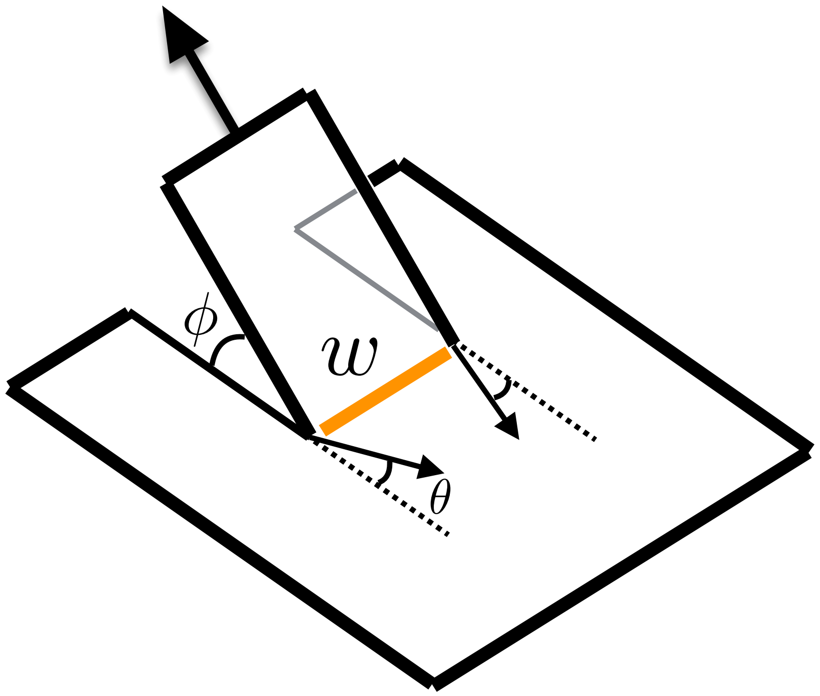




Sheet adhered to flat substrate



Sheet adhered to flat substrate

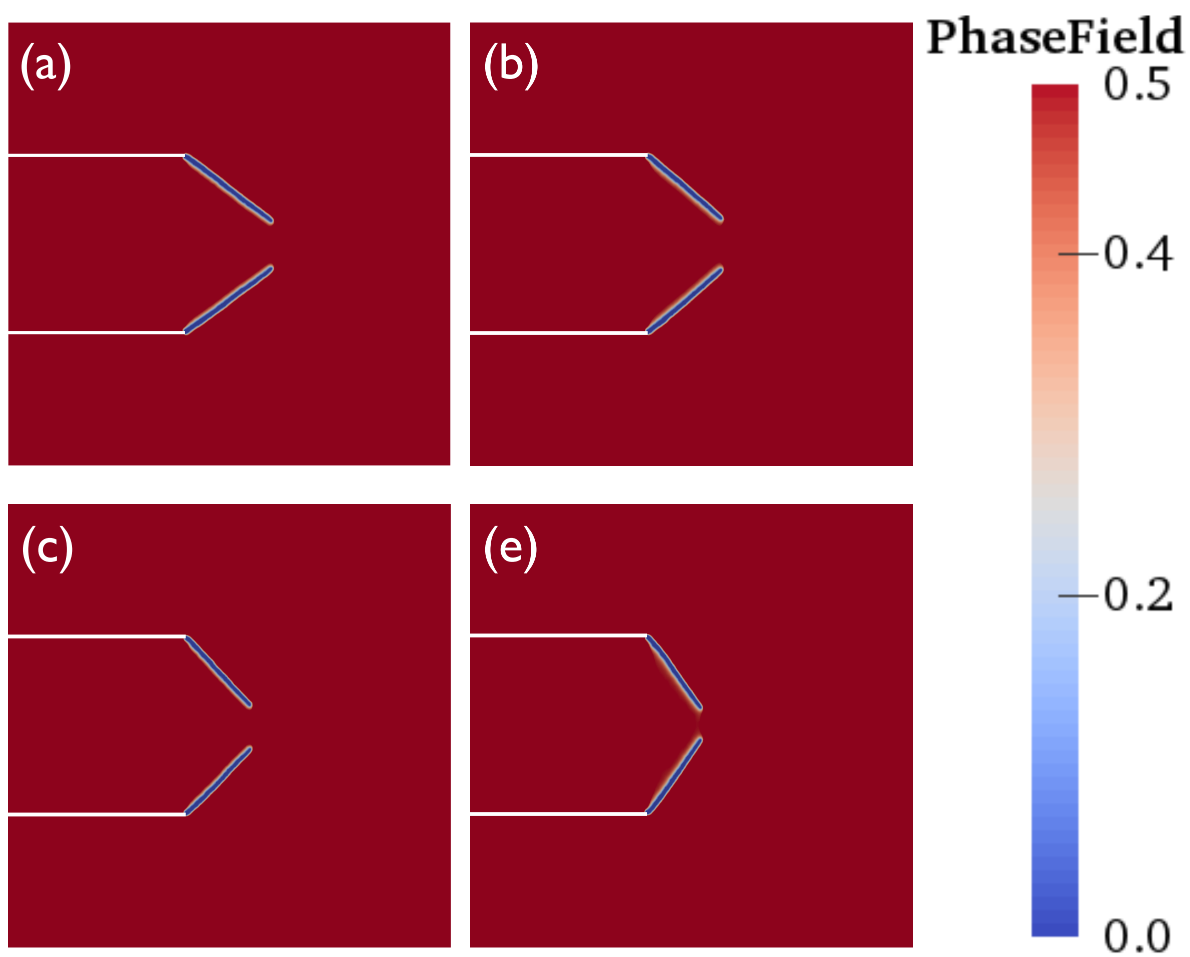


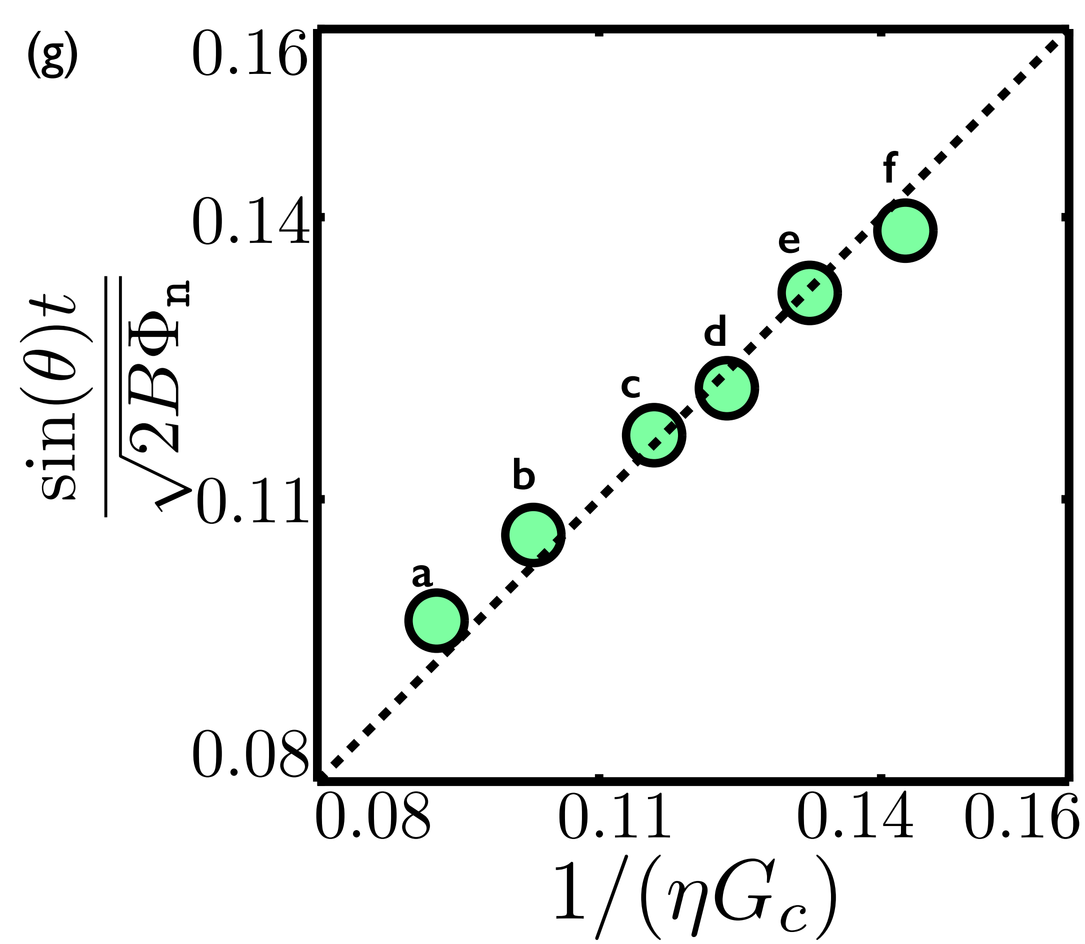
According to simple energetic model

$$\sin(\theta) = \frac{\sqrt{2B\Phi_n}}{G_c t}\left[\frac{1-\cos(\phi/2)}{\sin(\phi/2)}\right]$$

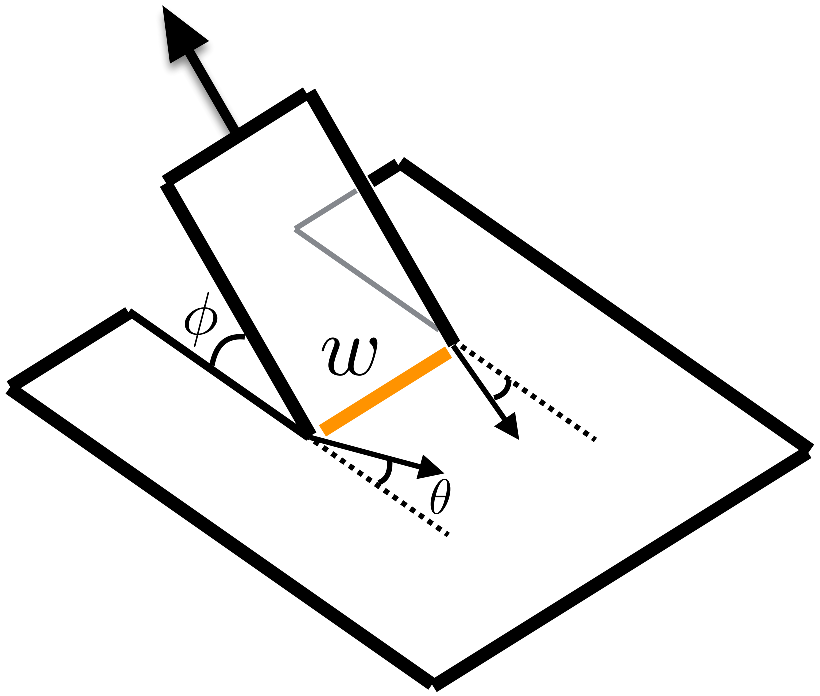
$$\Phi_n w \gg G_c t$$

change fracture energy





Sheet adhered to flat substrate

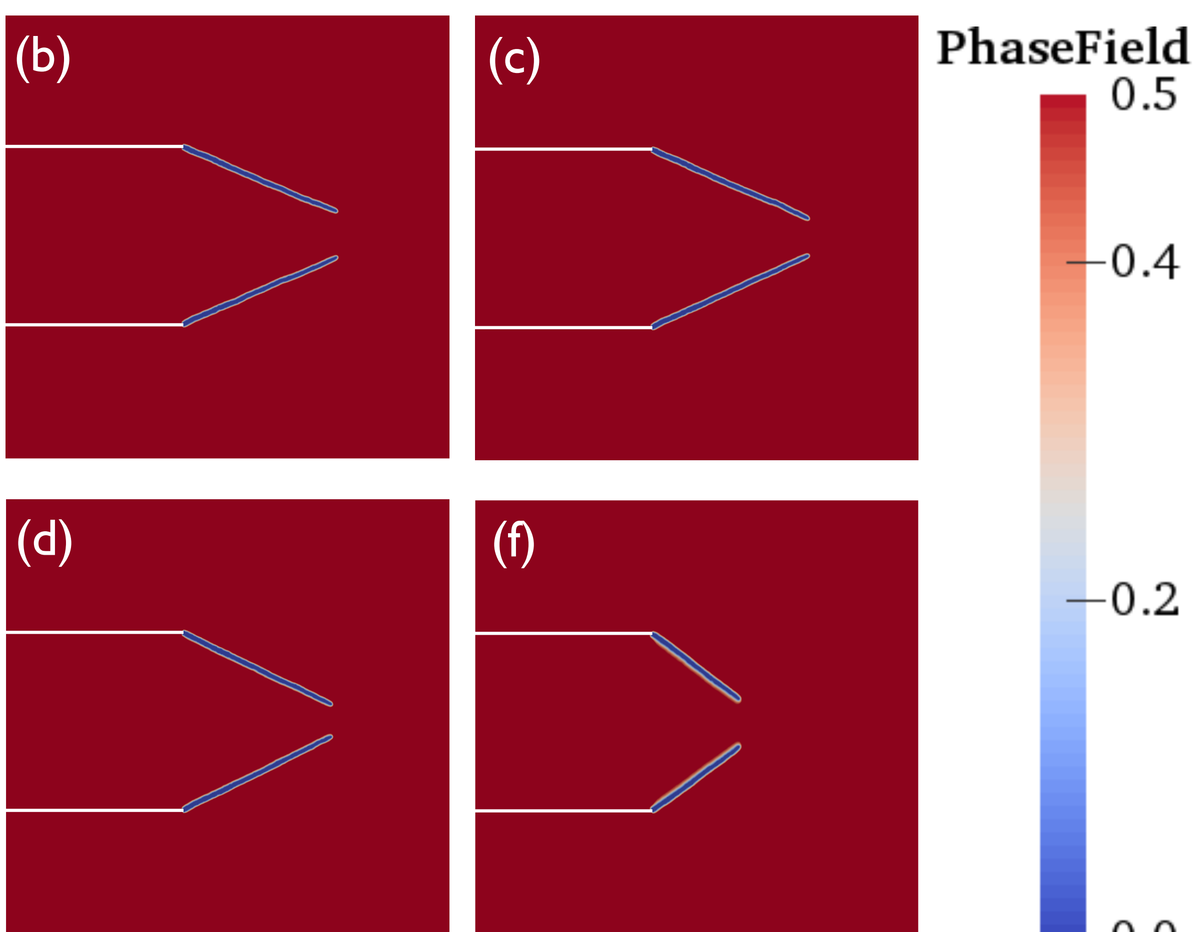


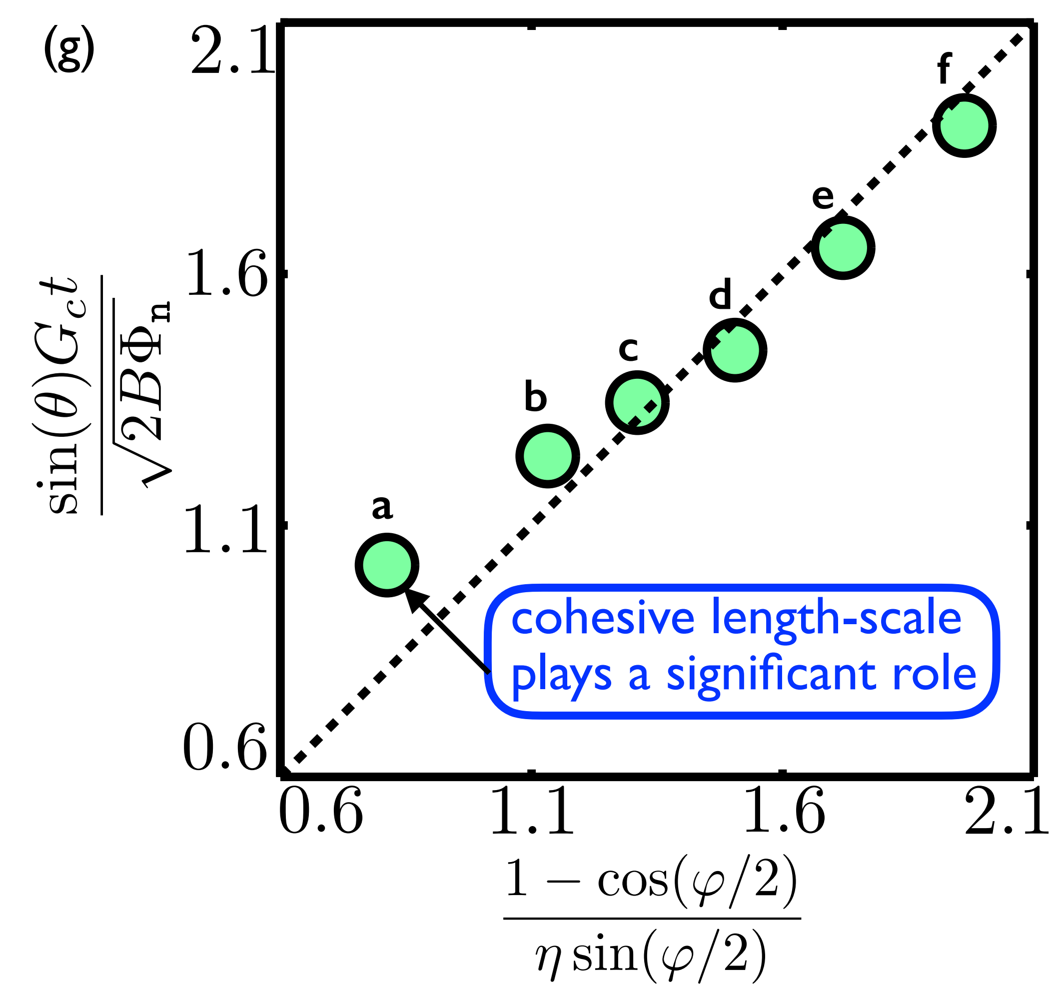
According to simple energetic model

$$\sin(\theta) = \frac{\sqrt{2B\Phi_n}}{G_c t}\left[\frac{1-\cos(\phi/2)}{\sin(\phi/2)}\right]$$

$$\Phi_n w \gg G_c t$$

change peeling angle



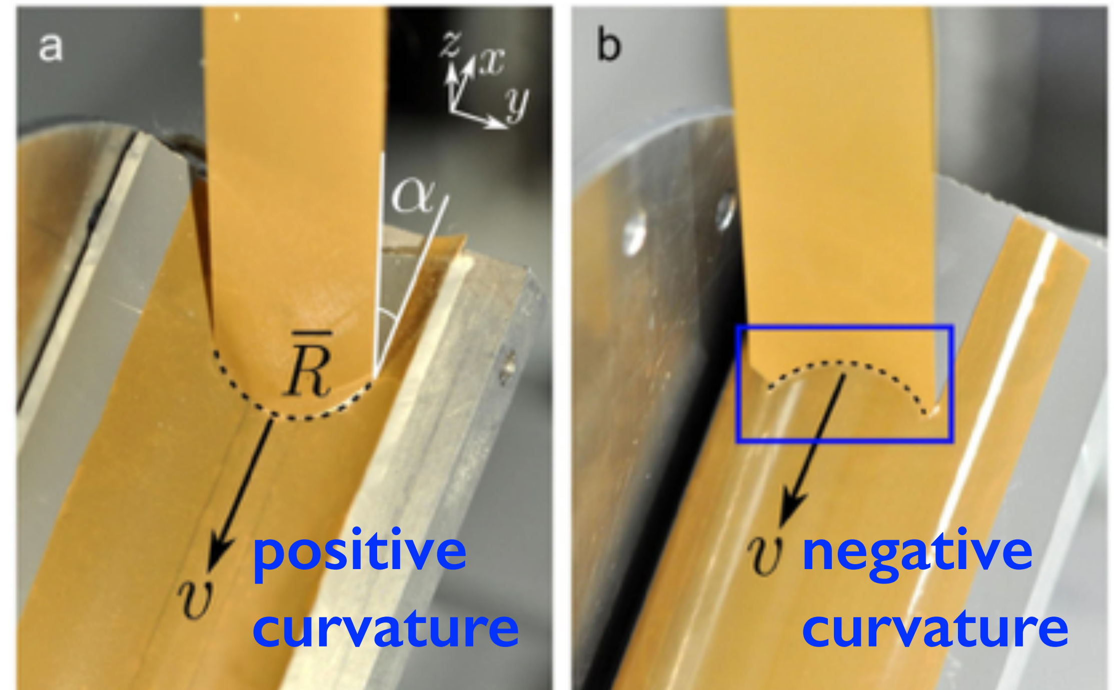


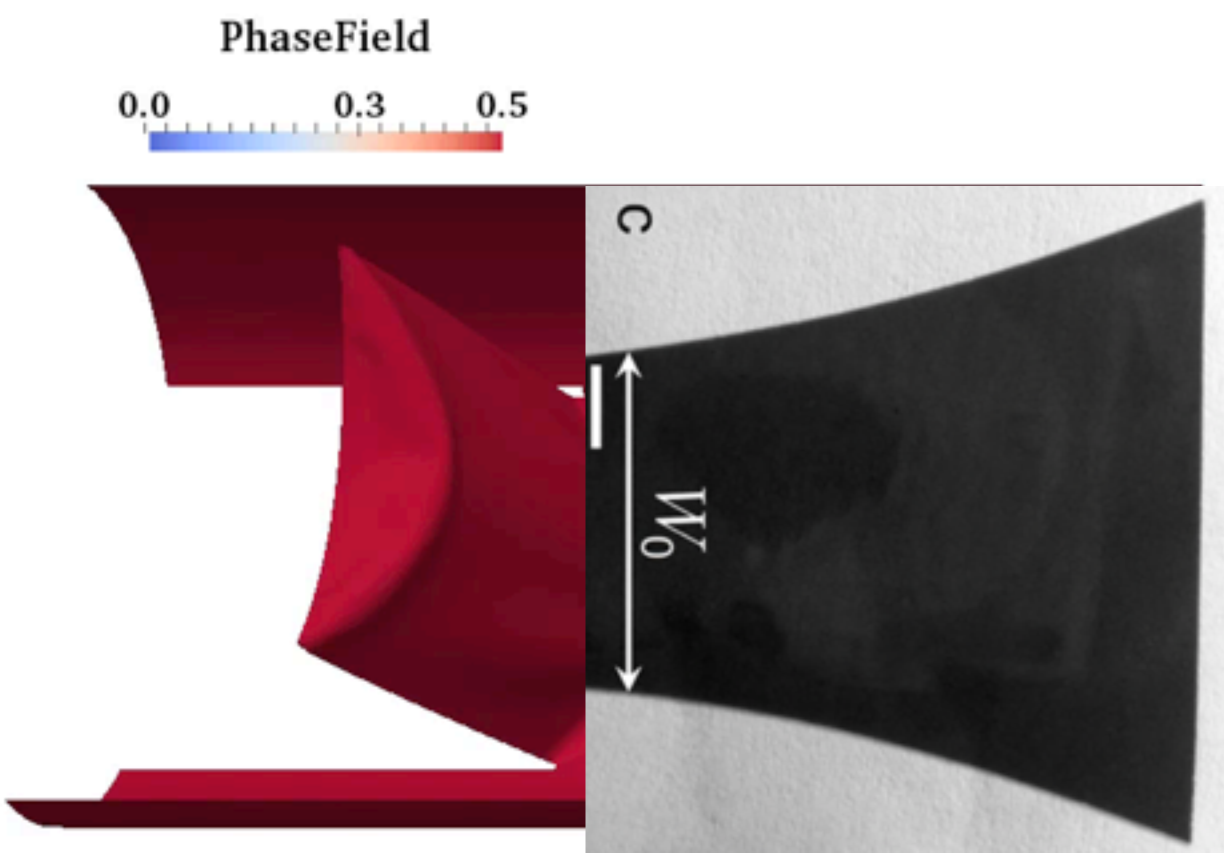
Sheet adhered on cylinder substrate

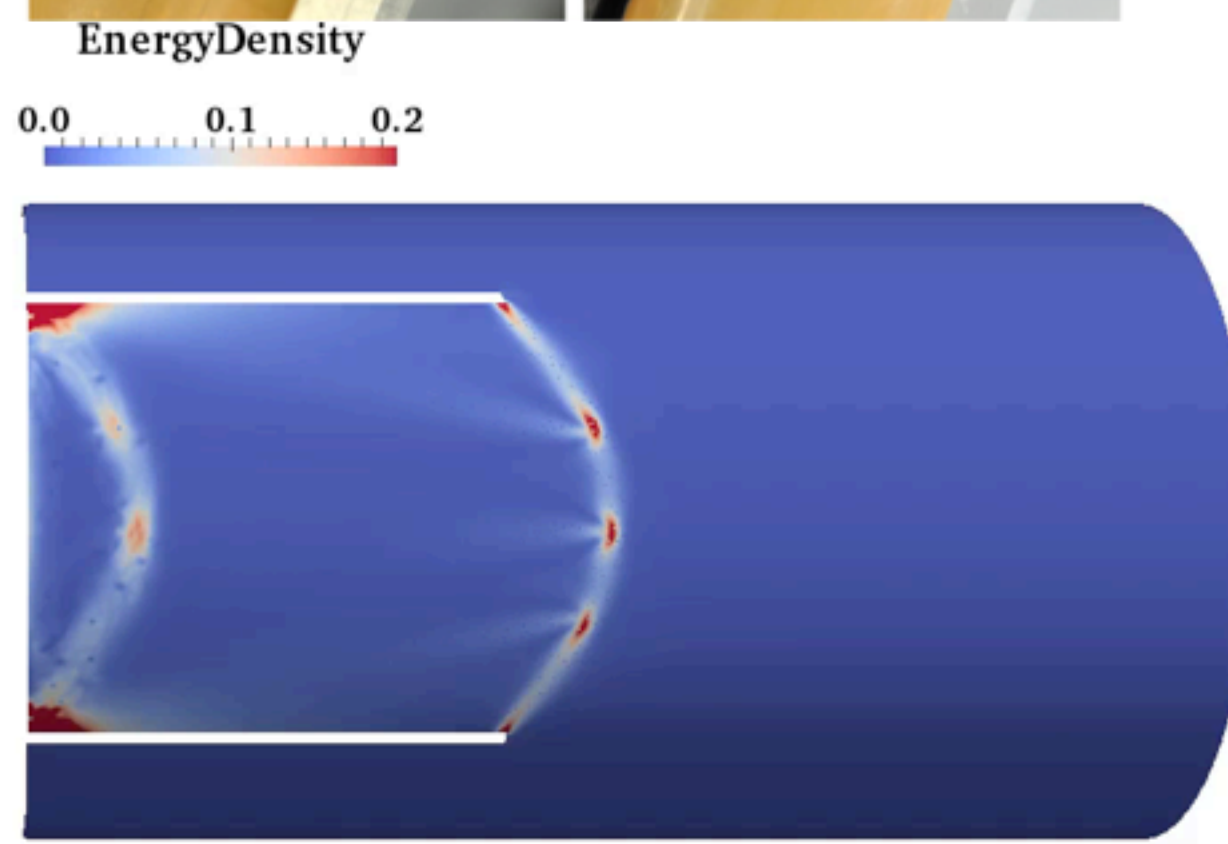
adhered on curved substrate

opening or closing tears
depending on sign of curvature

Kruglova,et.al, *PRL*, 2011





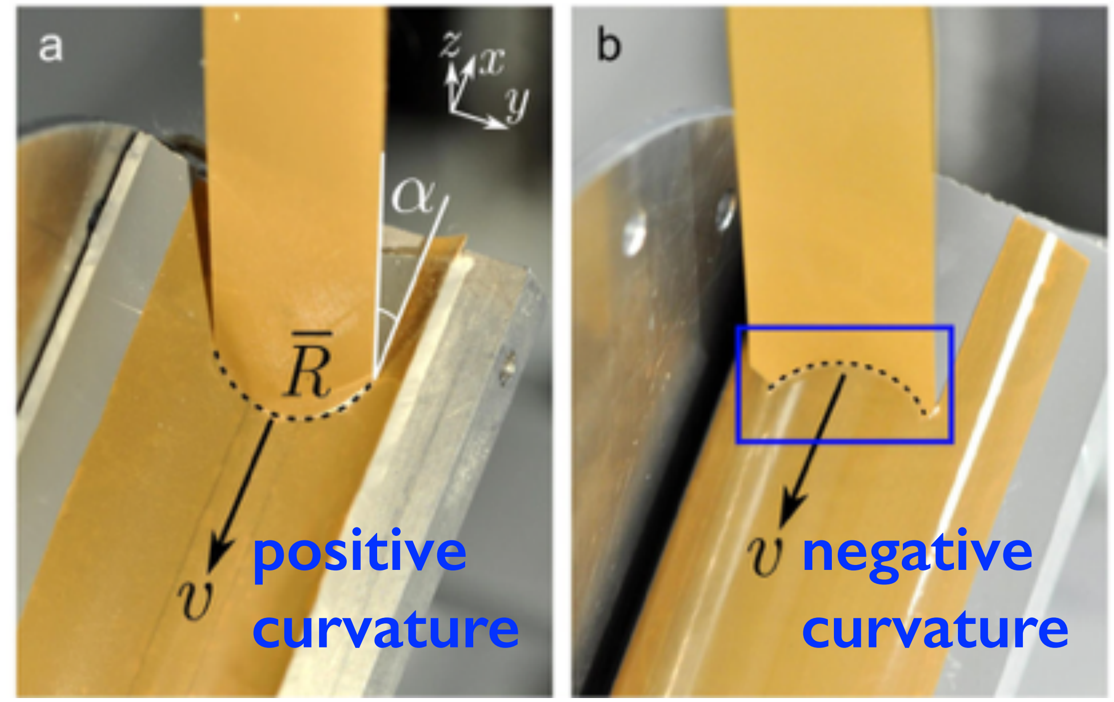


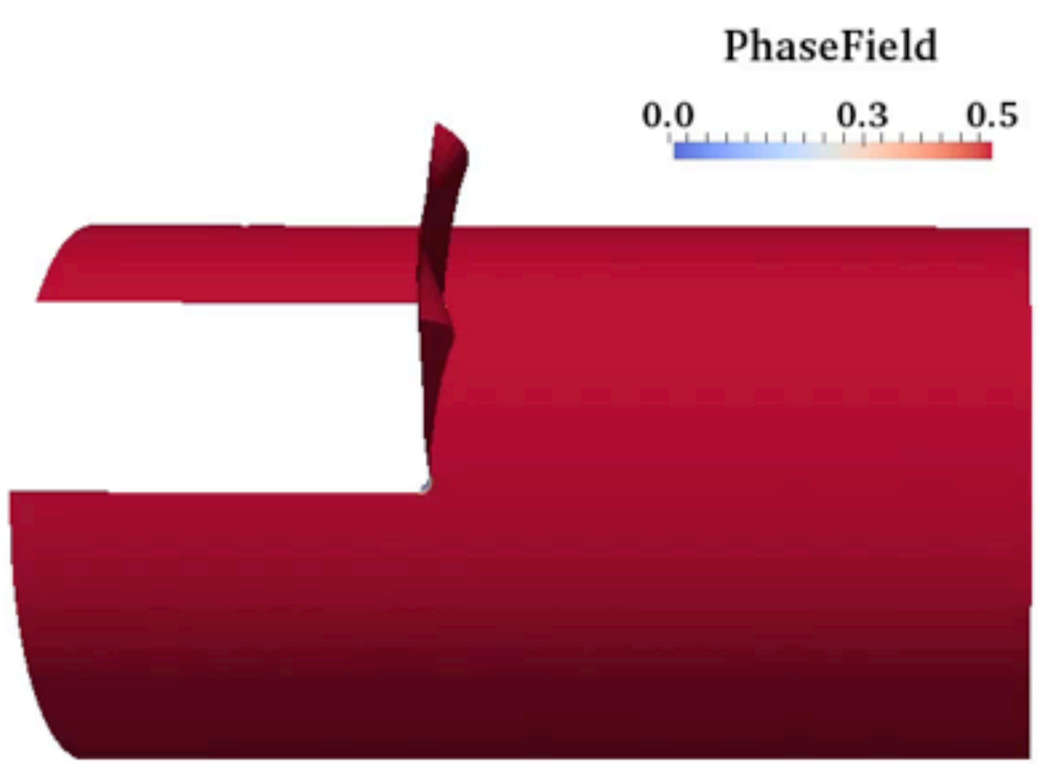
Sheet adhered on cylinder substrate

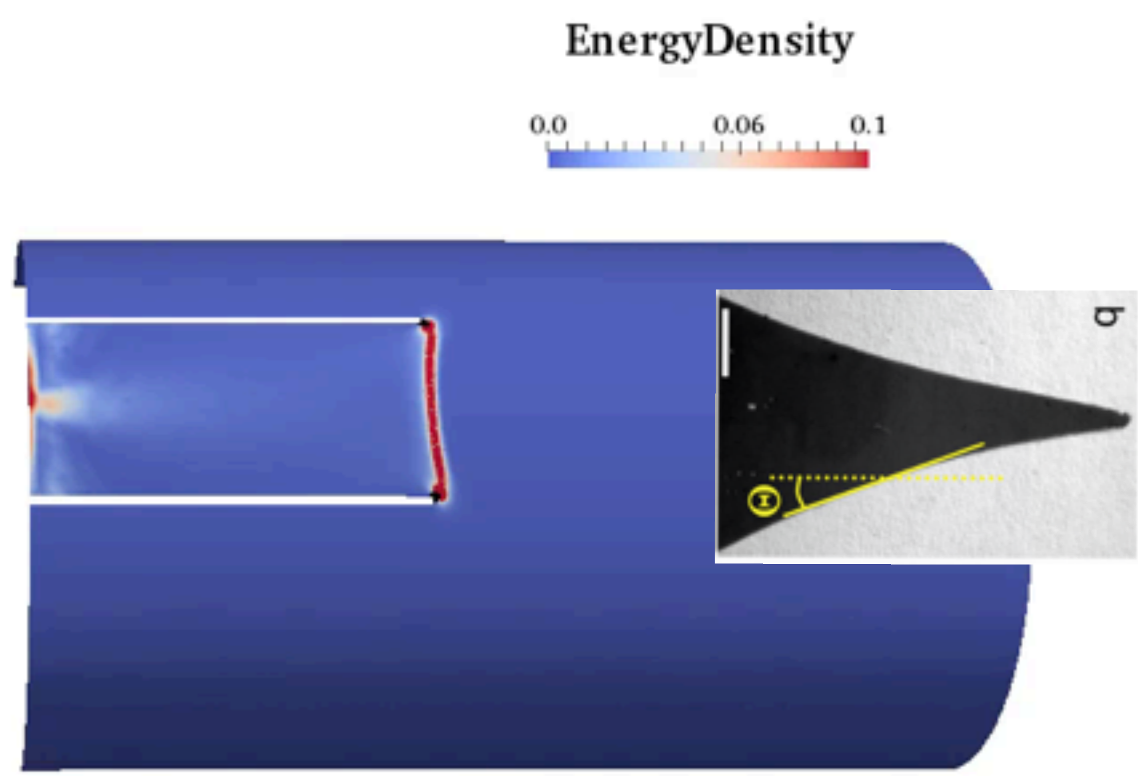
adhered on curved substrate

opening or closing tears depending on sign of curvature

Kruglova,et.al, *PRL*, 2011







Conclusions

1. Simple modeling and computational strategy for brittle fracture in thin elastic sheets accounting for geometric nonlinearity and adhesion.

2. Our simulations reproduce crack patterns observed in tearing experiments remarkably well.

3. Variational models of fracture naturally extend to thin shells. Good starting point to understand fracture in thin shells.

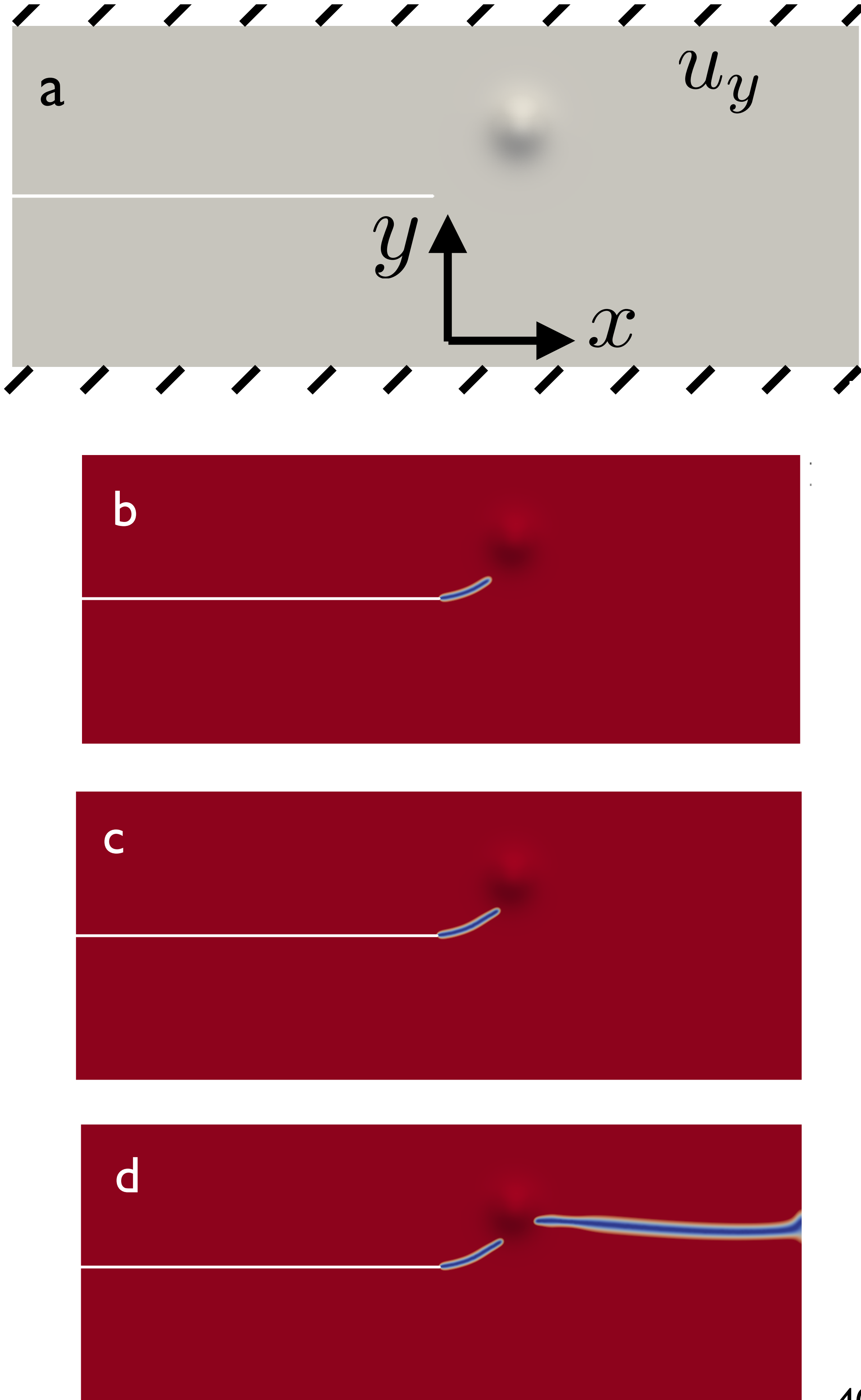
Outline

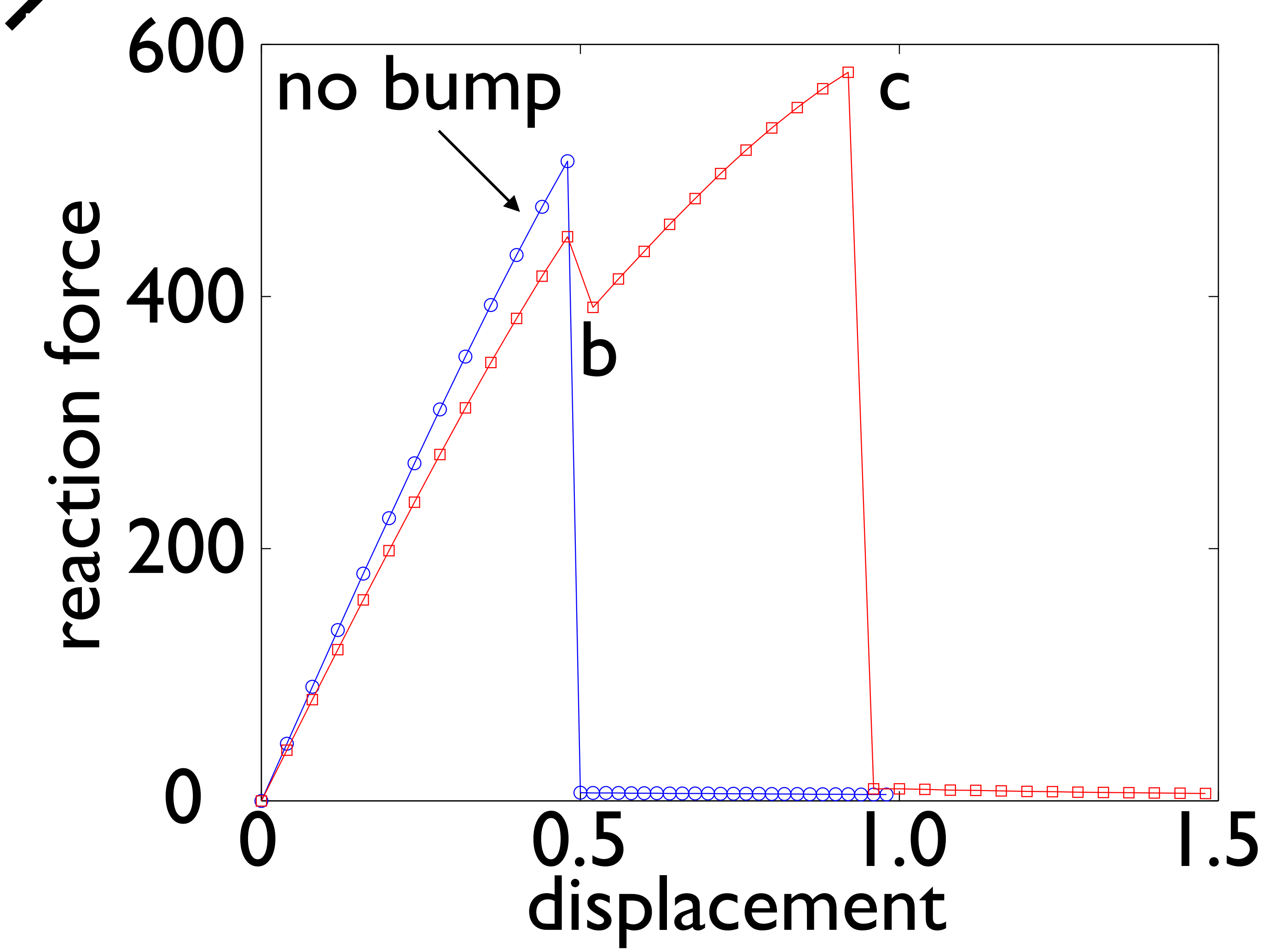
1. Phase-field modeling of fracture in materials with strongly anisotropic surface energy

2. Phase-field modeling of fracture in brittle thin shells

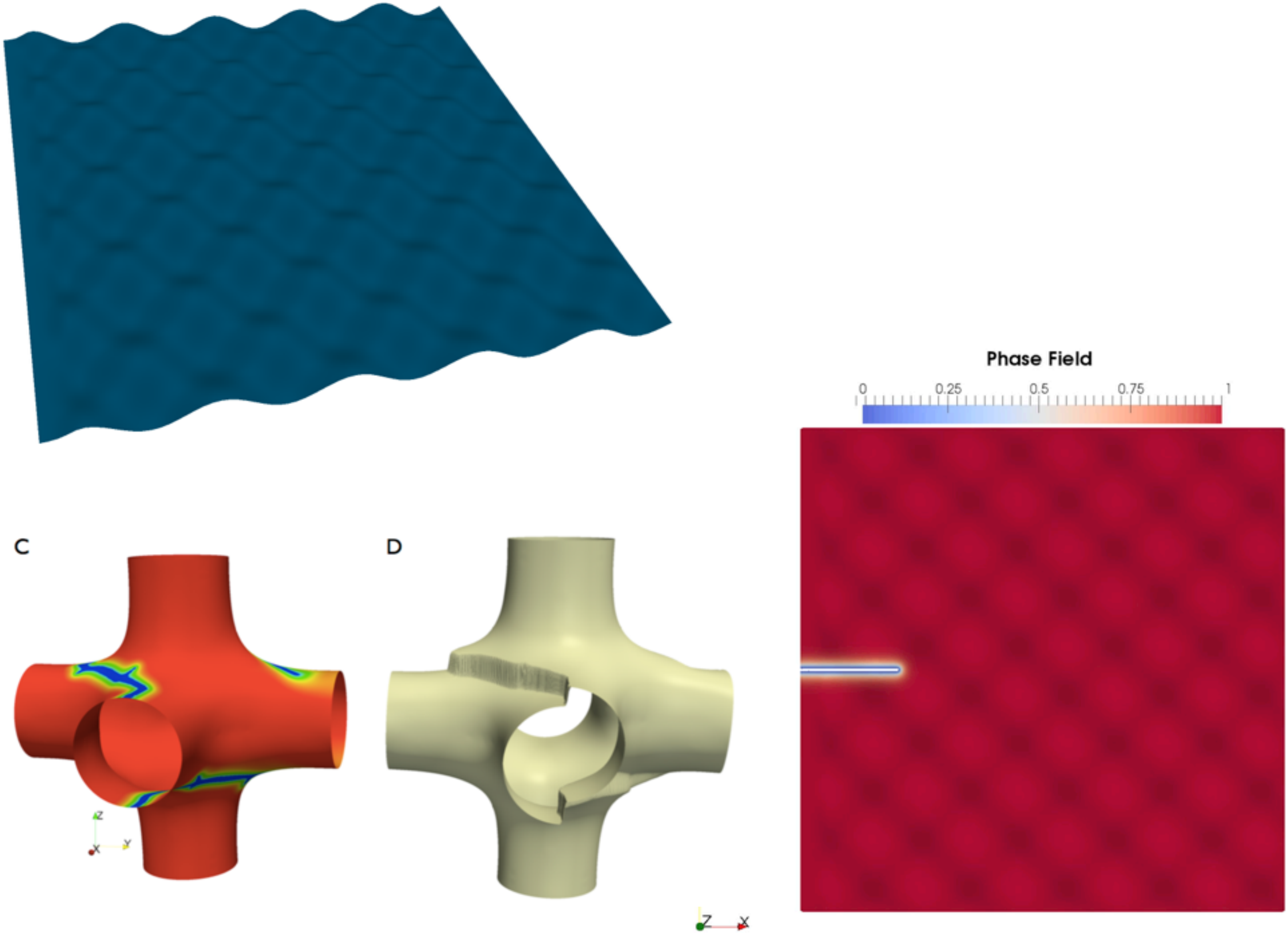
3. **Effect of shell geometry on crack propagation:**

   G **for a thin shell**



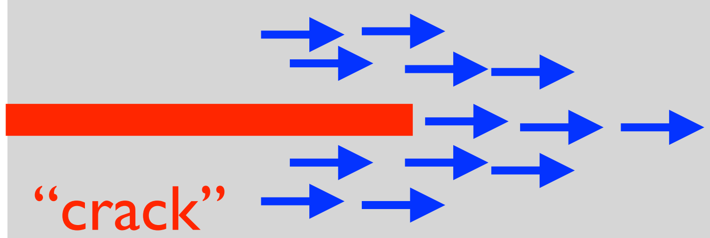


slightly more compliant
much tougher


Phase Field
0
0.25
0.5
0.75
1
C
D
Z
X
Y
Z
X

Calculation of G

$$\boldsymbol{V} = \left.\frac{d\Psi_\epsilon}{d\epsilon}\right|_{\epsilon=0}$$



material frame "X"

$$\Pi\,[\boldsymbol{u}] = \int_{\Omega_0} W\,(\boldsymbol{X}, \boldsymbol{u})\, d\Omega_0$$

heterogeneity

Consider a material rearrangement "moving" the crack

$$\Psi_\epsilon(X)$$
$$\Psi_0 = Id$$

$$\Pi_\epsilon[\boldsymbol{u}] = \int_{\Omega_0} W(\Psi_\epsilon^{-1}(X), \boldsymbol{u})\, d\Omega_0$$

$$G = -\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \Pi_\epsilon[\boldsymbol{u}_\epsilon]$$

$$= \int_{\Omega_0} \boldsymbol{J} \cdot \boldsymbol{V}\ d\Omega_0$$

$$\boxed{\boldsymbol{J} = \mathrm{div}\ \boldsymbol{B}}$$

Configurational force field

Eshelby tensor

Calculation of G for a shell

Intrinsic formulation for a geometrically linear Koiter shell

$$W\left(\boldsymbol{\varepsilon},\boldsymbol{\rho}\right) \qquad n^{\alpha\beta}=\frac{\partial W}{\partial \varepsilon_{\alpha\beta}}, \quad m^{\alpha\beta}=\frac{\partial W}{\partial \rho_{\alpha\beta}}$$

$$\varepsilon_{\alpha\beta}=\frac{1}{2}\left(u_{\alpha|\beta}+u_{\beta|\alpha}-2\,b_{\alpha\beta}w\right),$$

$$\rho_{\alpha\beta}=w_{|\alpha\beta}-c_{\alpha\beta}w+b^{\lambda}_{\alpha}u_{\lambda|\beta}+b^{\lambda}_{\beta}u_{\lambda|\alpha}+b^{\lambda}_{\alpha|\beta}u_{\lambda}$$

$$c_{\alpha\beta}=b^{\lambda}_{\alpha}b_{\lambda\beta}$$

$$\Pi[\boldsymbol{u},w]=\int_{\bar{\Omega}}\tilde{W}(\underline{\xi},\boldsymbol{b},\nabla\boldsymbol{b},\boldsymbol{u},\nabla\boldsymbol{u},w,\nabla^2 w)\sqrt{a}\,d\bar{\Omega}$$

heterogeneity

Calculation of G for a shell

material rearrangement "moving" the crack

$$\Pi_\epsilon[\boldsymbol{u}, w] = \int_{\bar{\Omega}} \tilde{W}(\Psi_\epsilon^{-1}(\xi), \boldsymbol{b}, \nabla \boldsymbol{b}, \boldsymbol{u}, \nabla \boldsymbol{u}, w, \nabla^2 w)\sqrt{a}\, d\bar{\Omega},$$

material rearrangement "moving" the crack and bumps

$$\int_{\bar{\Omega}} \tilde{W}(\Psi_\epsilon^{-1}(\xi), \boldsymbol{b}(\Psi_\epsilon^{-1}(\xi)), \nabla \boldsymbol{b}(\Psi_\epsilon^{-1}(\xi)), \boldsymbol{u}, \nabla \boldsymbol{u}, w, \nabla^2 w)\sqrt{a}\, d\bar{\Omega},$$

Calculation of G for a shell

$$
\begin{aligned}
G &= -\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \Pi_\epsilon[u_\epsilon, w_\epsilon] \\
&= -\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \int_{\bar{\Omega}} \tilde{W}(\Psi_\epsilon^{-1}(\xi), b, \nabla b, u_\epsilon, \nabla u_\epsilon, w_\epsilon, \nabla^2 w_\epsilon)\sqrt{a}\, d\bar{\Omega}.
\end{aligned}
$$

Configurational forces field

$$
J_\gamma = \boxed{M^{\beta}_{\gamma|\beta}} + \boxed{K}\hat{J}_\gamma + \boxed{\tilde{J}_\gamma}.
$$

divergence of Eshelby tensor

Gaussian curvature

non uniformity of curvature

Infinitesimal deformations but finite geometry

Calculation of G for a shell

Configurational forces field

$$J_\gamma = \boxed{M^{\beta}_{\gamma|\beta}} + \boxed{K}\hat{J}_\gamma + \boxed{\tilde{J}_\gamma}.$$

divergence of Eshelby tensor

Gaussian curvature

non uniformity of curvature

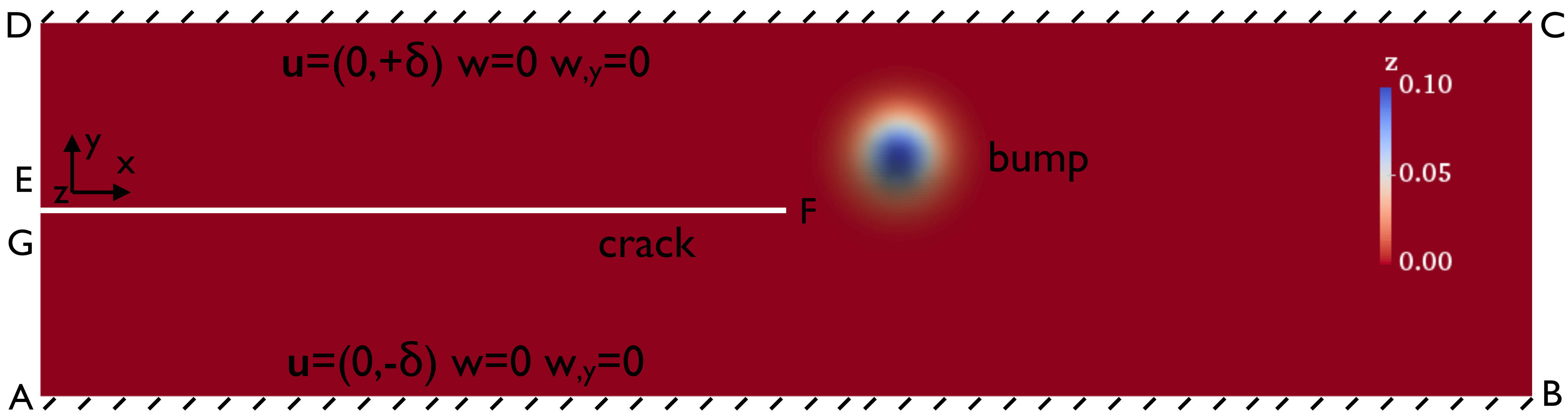
$$M^\beta_\gamma = \tilde{W}\delta^\beta_\gamma - l^{\alpha\beta}u_{\alpha|\gamma} - m^{\alpha\beta}w_{|\alpha\gamma} + m^{\alpha\beta}{}_{|\alpha}w_{|\gamma}$$

$$\hat{J}_\gamma = \mathrm{tr}\boldsymbol{l}\, u_\gamma - l_\gamma{}^\beta u_\beta + \mathrm{tr}\,\boldsymbol{m}\, w_{|\gamma} - m^\beta_\gamma w_{|\beta}$$

$$\tilde{J}_\gamma = \left(l^{\alpha\beta}w - 2m^{\alpha\mu}u^\beta{}_{|\mu}\right) b_{\alpha\beta|\gamma} - m^{\alpha\nu}u^\beta b_{\alpha\beta|\nu\gamma}$$

$$l^{\alpha\beta} = n^{\alpha\beta} + 2b^\alpha_\lambda m^{\lambda\beta}$$

Calculation of G for a shell



Gaussian curvature

$$G = \frac{1}{||\boldsymbol{a}_1||_{\text{tip}}} G_{\text{no bump}} + \boxed{G_K} + \boxed{G_{\boldsymbol{b}}}$$

non uniformity of curvature

$$\boxed{- \int_\Omega M^\beta_\gamma \, V^\gamma{}_{|\beta} \, d\Omega + \int_{EF \cup FG} m^{\alpha\beta} w_{|\gamma} V^\gamma{}_{|\alpha} \nu_\beta \, d\ell,}$$

"non-uniform" *V*

$\boldsymbol{V}$ velocity of the microstructure

Summary

1. Focusing on linear Koiter's thin shell theory, we have obtained expressions for the configurational force-field and for the energy release rate of a plate with a pre-crack and a finite shape disturbance.

2. We hope to get insight from these expressions, and possibly provide an understanding of how geometry affects crack propagation.