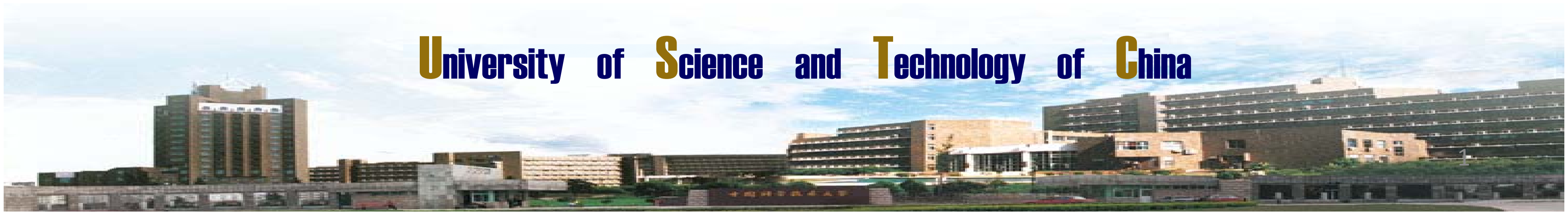
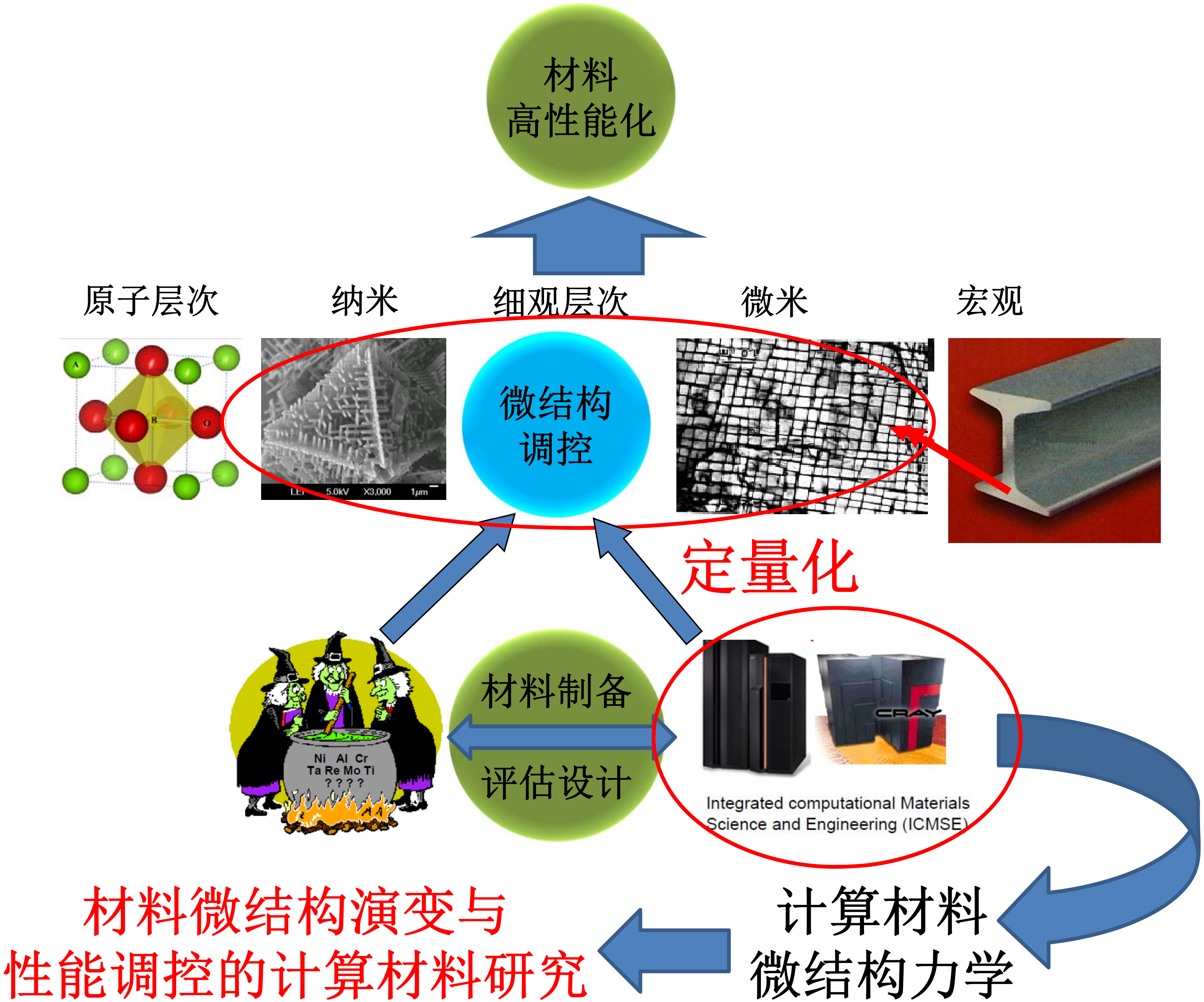
薄膜材料细观结构演化的相变力学分析

倪勇

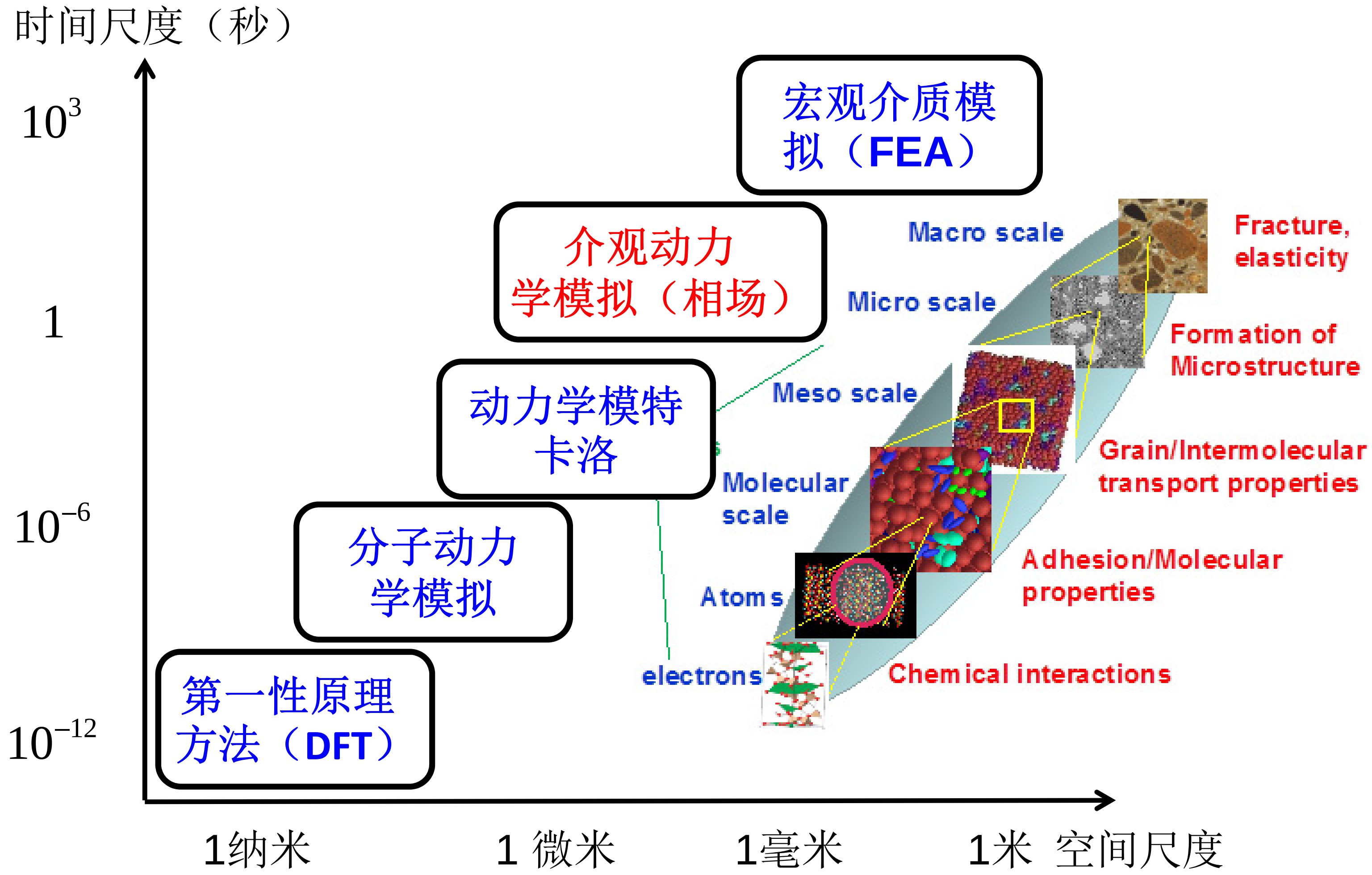
中国科学技术大学近代力学系，
材料力学行为与设计中科院重点实验室





材料
高性能化
原子层次
纳米
细观层次
微米
宏观
5.0kV X3,000 1μm
微结构
调控
定量化
Ni Al Cr
Ta Re Mo Ti
? ? ? ?
材料制备
评估设计
CRAY
Integrated computational Materials
Science and Engineering (ICMSE)
计算材料
微结构力学
材料微结构演变与
性能调控的计算材料研究

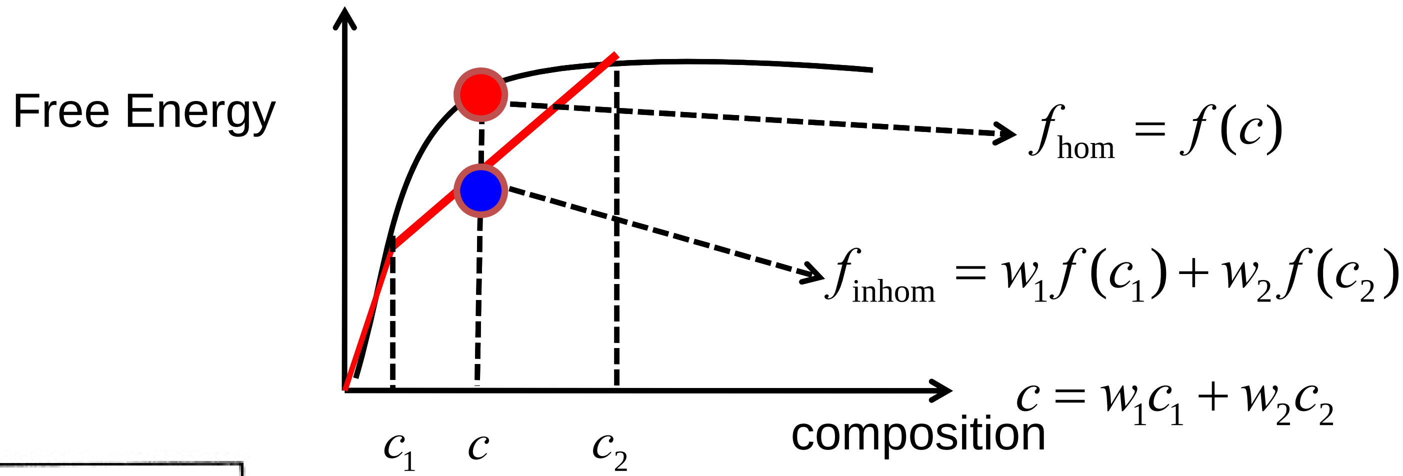
多尺度材料模拟

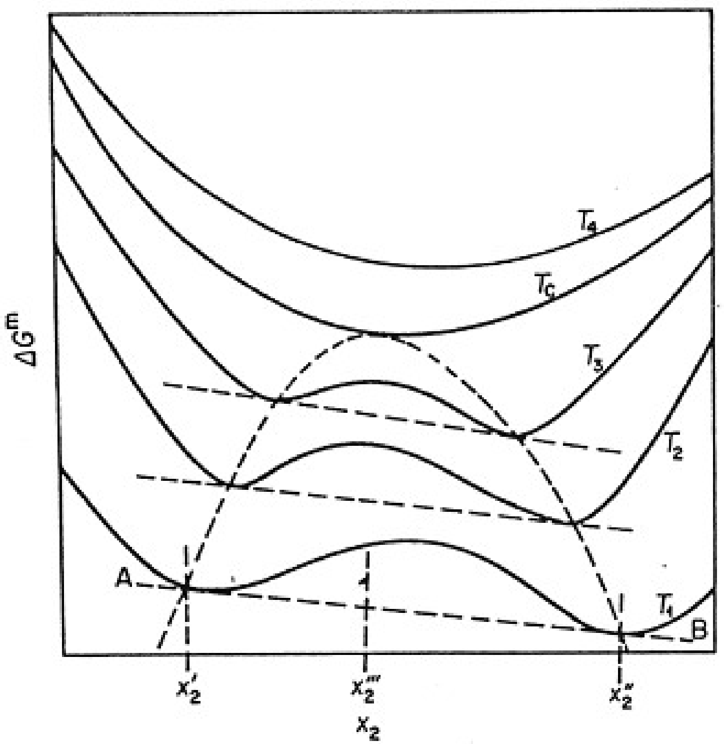


时间尺度（秒）
10^3
1
10^-6
10^-12
宏观介质模拟（FEA）
介观动力学模拟（相场）
动力学模特卡洛
分子动力学模拟
第一性原理方法（DFT）
Macro scale
Micro scale
Meso scale
Molecular scale
Atoms
electrons
Fracture, elasticity
Formation of Microstructure
Grain/Intermolecular transport properties
Adhesion/Molecular properties
Chemical interactions
1纳米
1 微米
1毫米
1米
空间尺度

相变简介

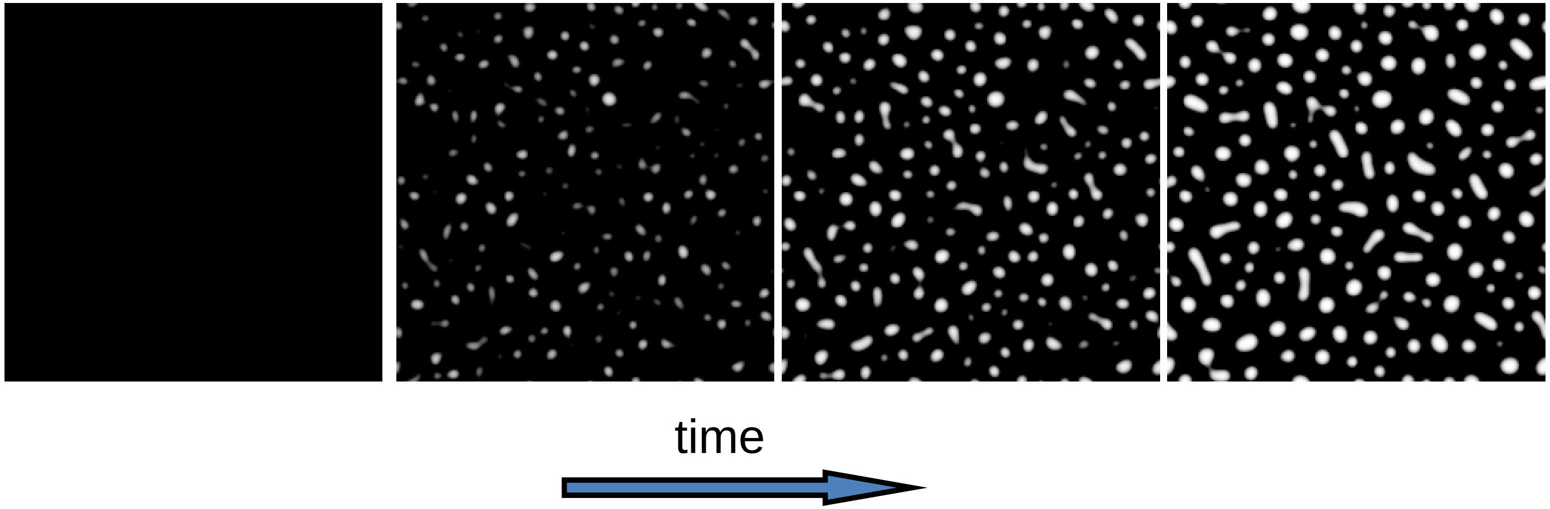
Instability of a supersaturated solid solution

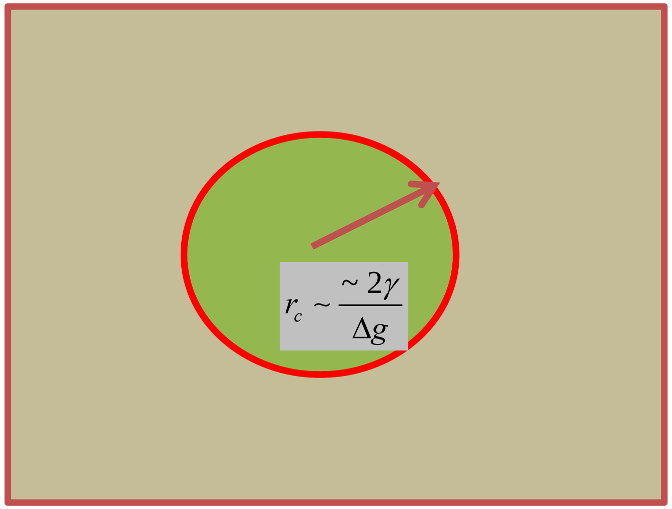


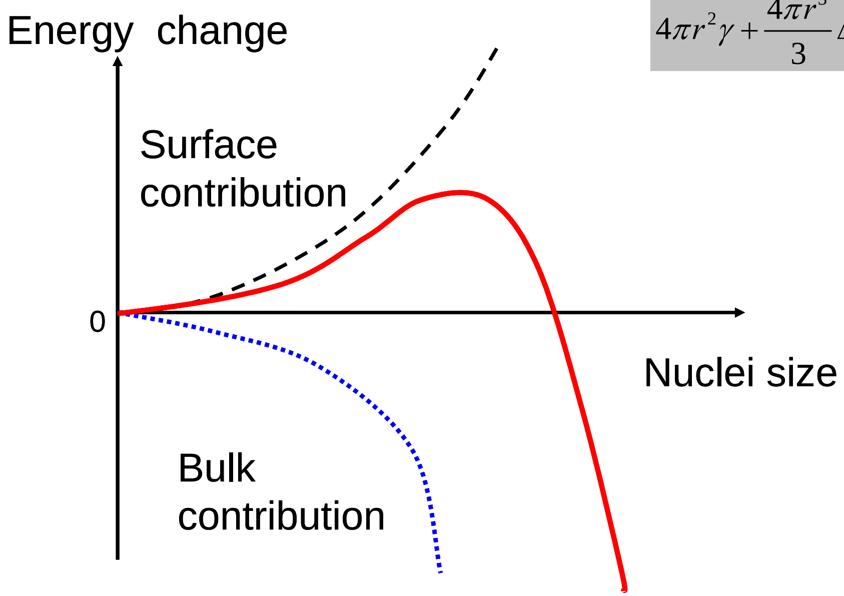


自由能曲线变凸时 $f_{\mathrm{inhom}} < f_{\mathrm{hom}}$

Microstructures produced by conventional nucleation

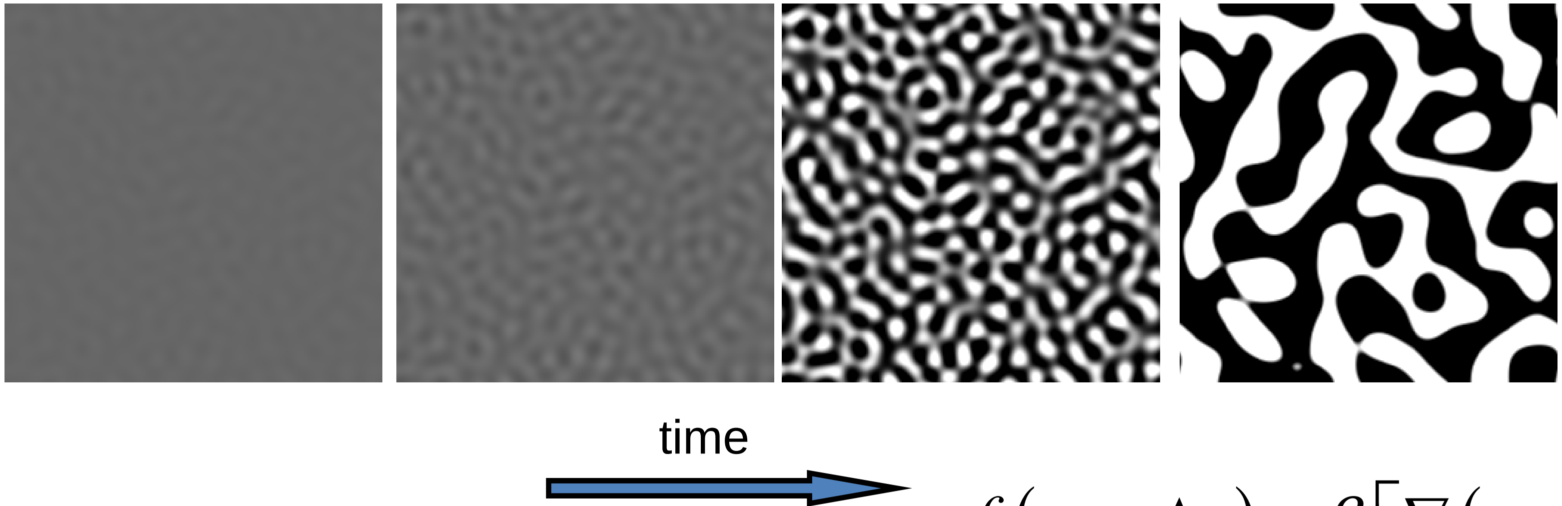


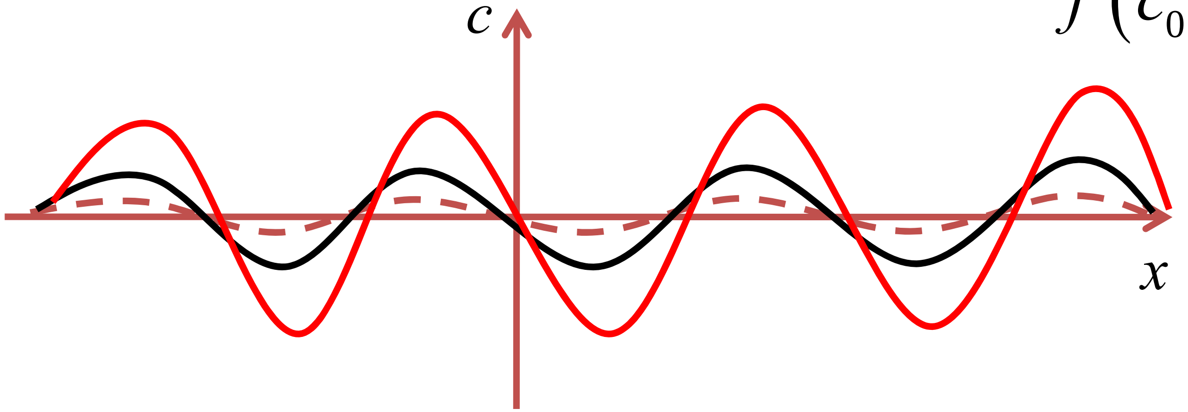




$$4\pi r^2 \gamma + \frac{4\pi r^3}{3} \Delta G \leq 0$$

Microstructures produced by spinodal decomposition



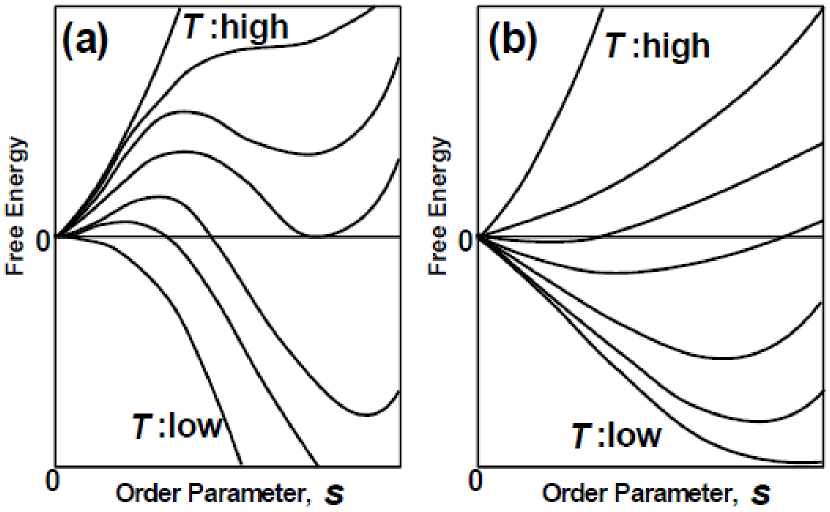


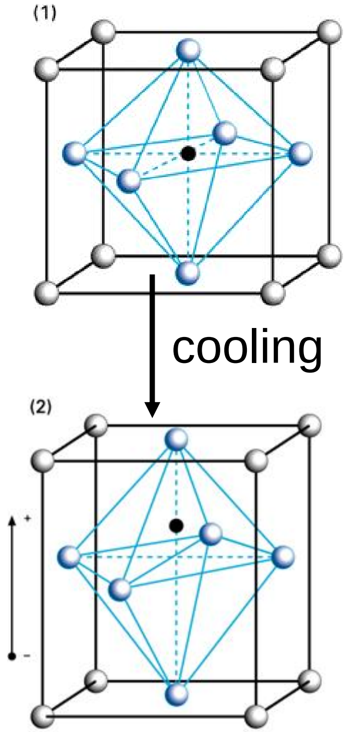
$$f\left(c_0+\Delta c\right)+\beta\left[\nabla\left(c_0+\Delta c\right)\right]^2$$

$$\Delta c=\delta\sin\frac{2\pi}{\lambda}x$$

$$\lambda_c\sim 2\pi\sqrt{-\beta\,/\,\frac{\partial^2 f}{\partial c_0^2}}$$

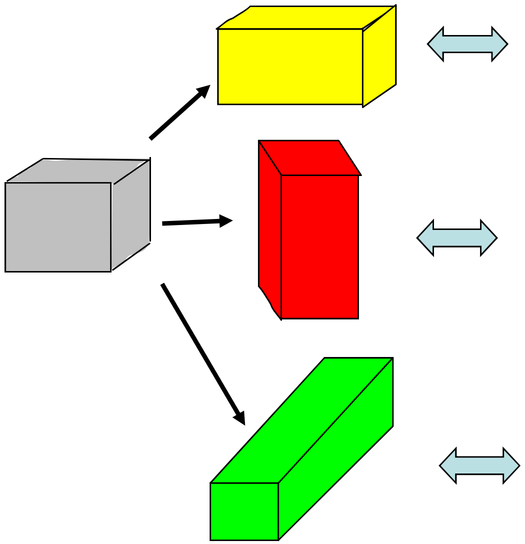
Displacive transformation





corresponding transformation strain

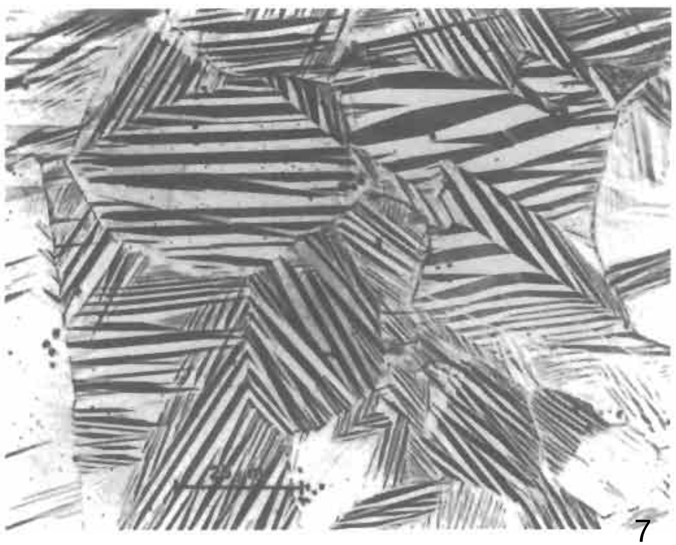
$$\varepsilon_{ij}^{o}(\mathbf{r}) = \sum_{p=1}^{3} \varepsilon_{ij}^{oo}(p)\eta_p(\mathbf{r},t)$$



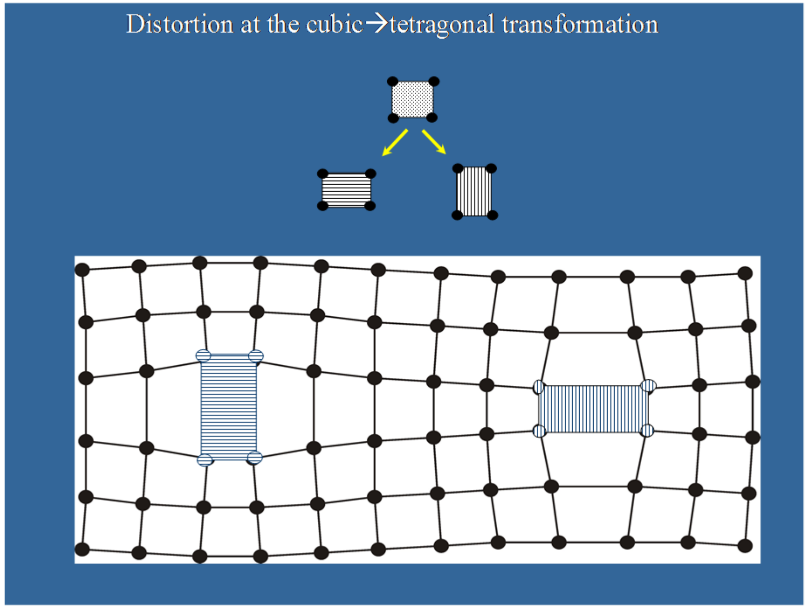
$$\begin{pmatrix} \varepsilon_c & 0 & 0 \\ 0 & \varepsilon_a & 0 \\ 0 & 0 & \varepsilon_a \end{pmatrix}$$

$$\begin{pmatrix} \varepsilon_a & 0 & 0 \\ 0 & \varepsilon_a & 0 \\ 0 & 0 & \varepsilon_c \end{pmatrix}$$

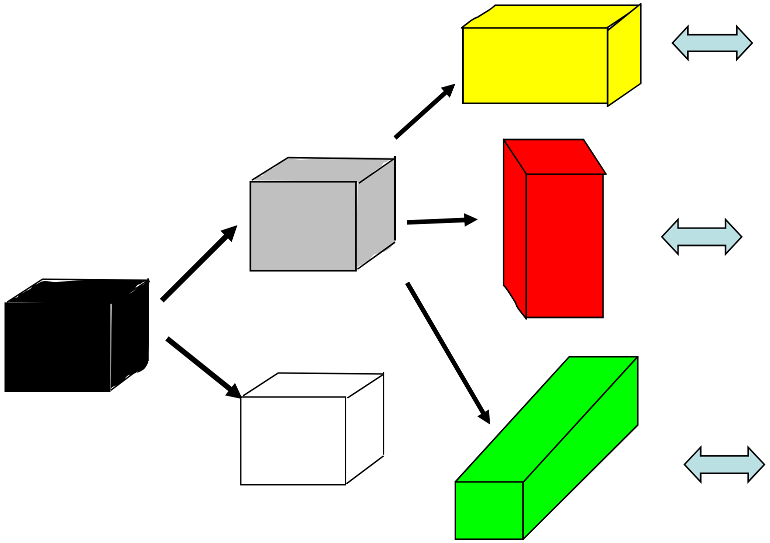
$$\begin{pmatrix} \varepsilon_a & 0 & 0 \\ 0 & \varepsilon_c & 0 \\ 0 & 0 & \varepsilon_a \end{pmatrix}$$



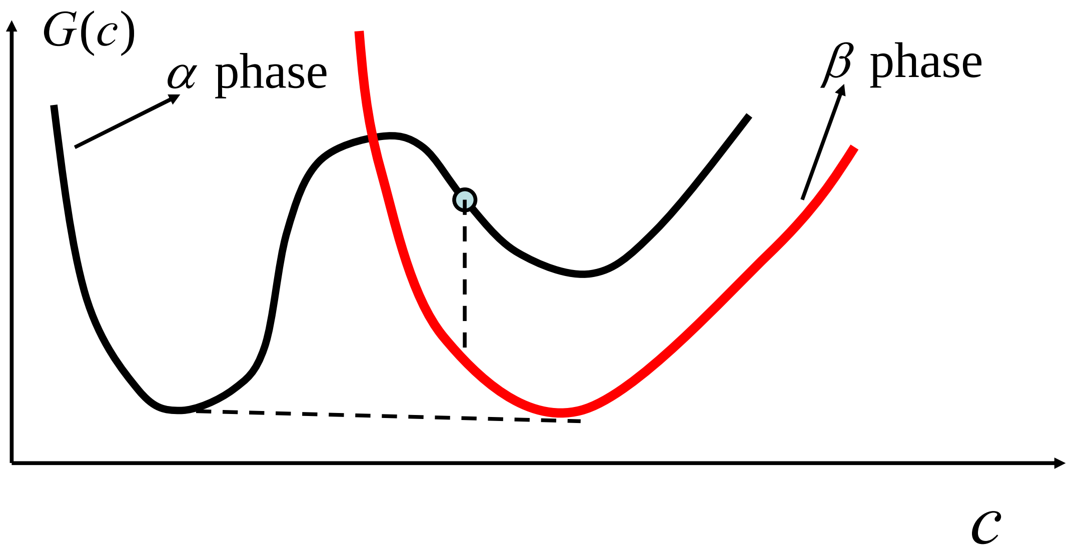
Coupled-diffusive-displacive phase transformation



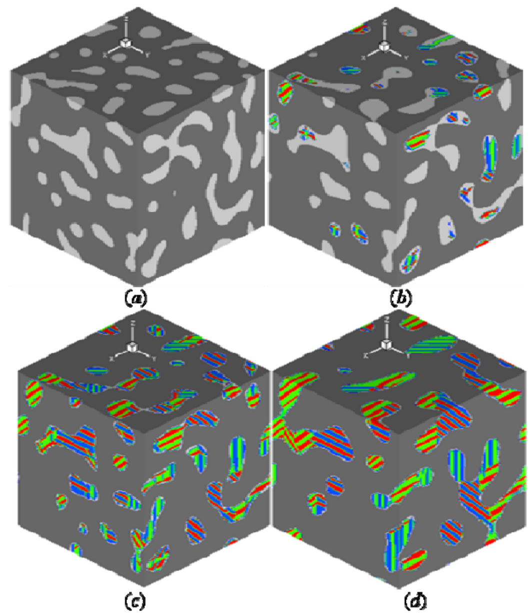
corresponding transformation strain



$$\begin{pmatrix} \varepsilon_c & 0 & 0 \\ 0 & \varepsilon_a & 0 \\ 0 & 0 & \varepsilon_a \end{pmatrix} \quad \begin{pmatrix} \varepsilon_a & 0 & 0 \\ 0 & \varepsilon_a & 0 \\ 0 & 0 & \varepsilon_c \end{pmatrix} \quad \begin{pmatrix} \varepsilon_a & 0 & 0 \\ 0 & \varepsilon_c & 0 \\ 0 & 0 & \varepsilon_a \end{pmatrix}$$

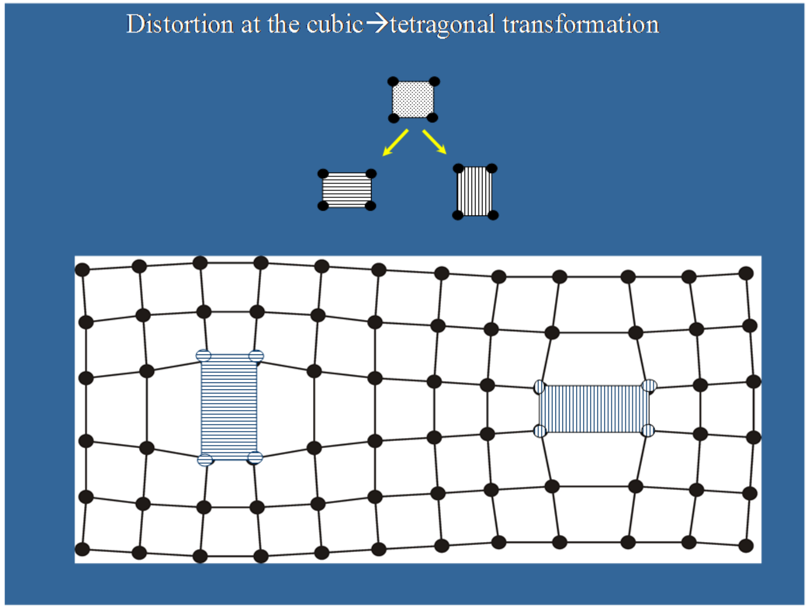


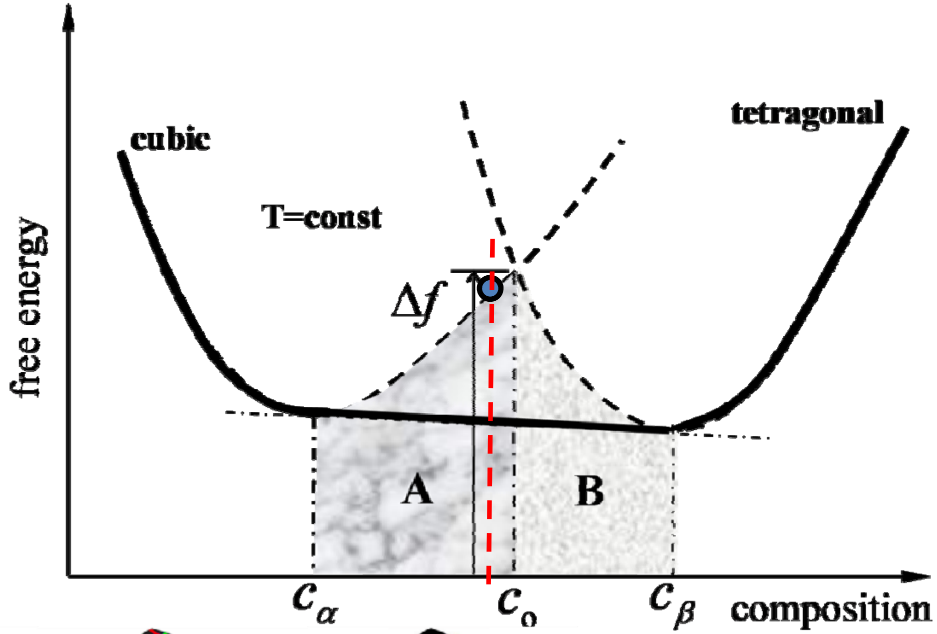
A schematic free energy curve vs composition

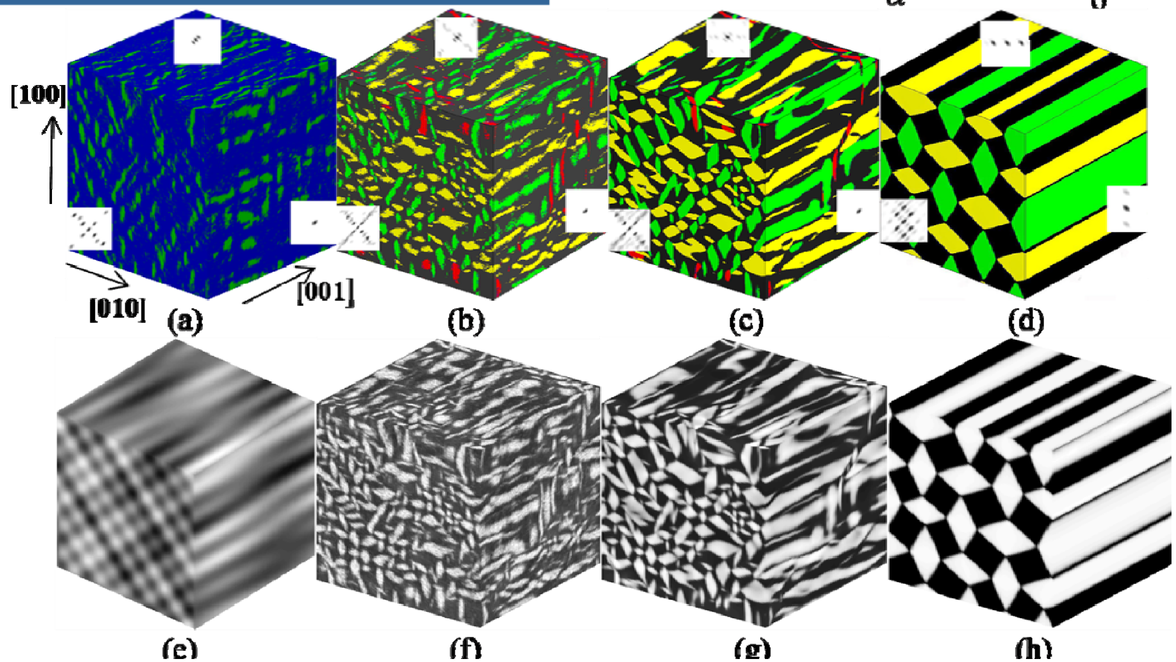


Pseudospinodal decomposition

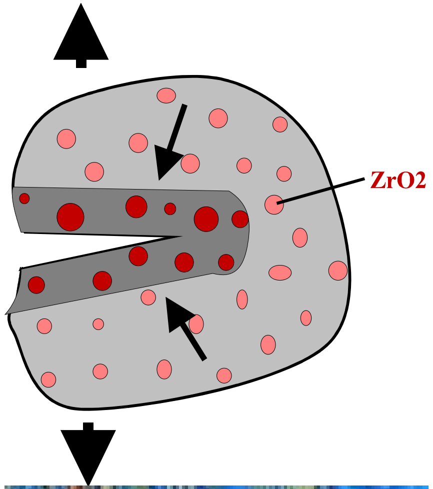
*

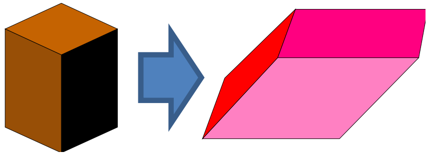




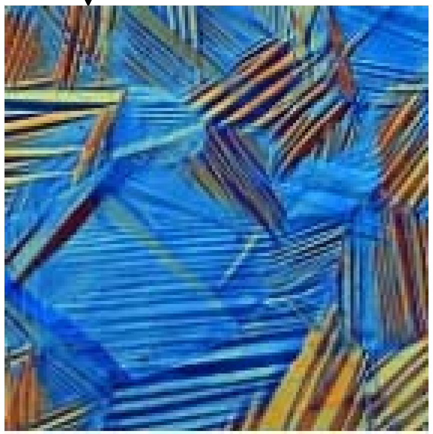


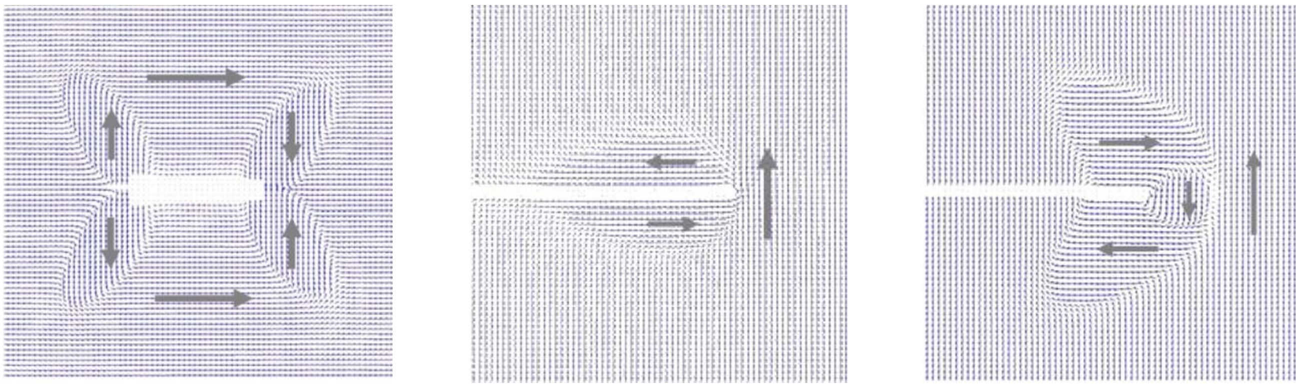
相变力学





裂尖二氧化锆相变增韧
（Budiansky et al,1983）



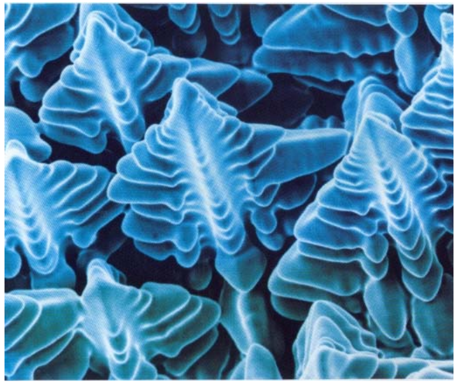


马氏体相变

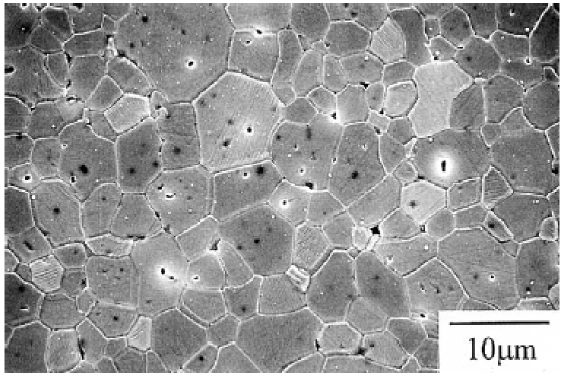
铁电体断裂力学

相变力学与微结构演化

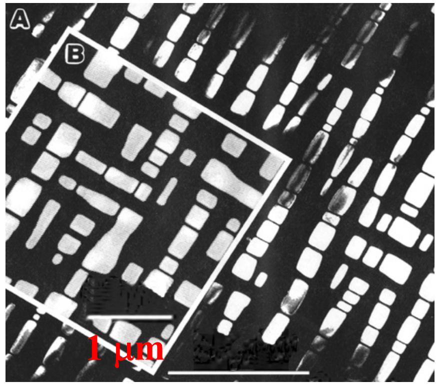
Microstructural evolution: instability→growth→pattern formation



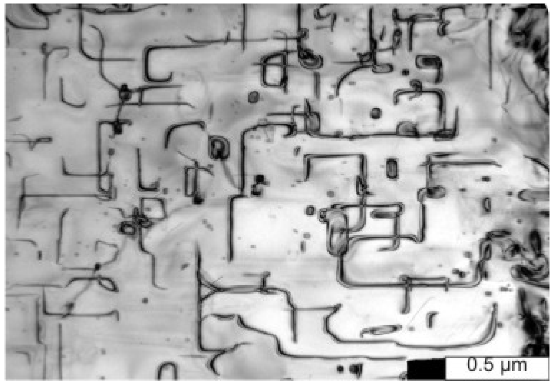
Solidification



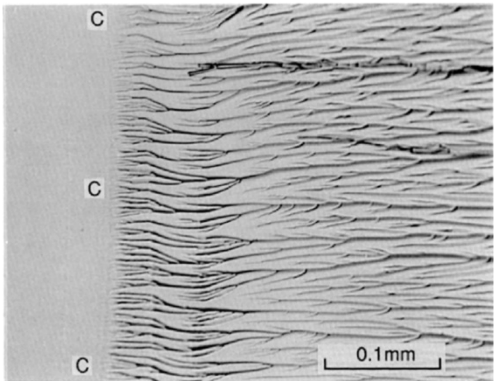
Grain growth



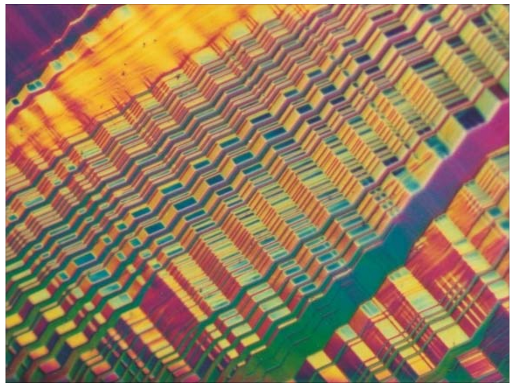
Precipitation



Dislocation network



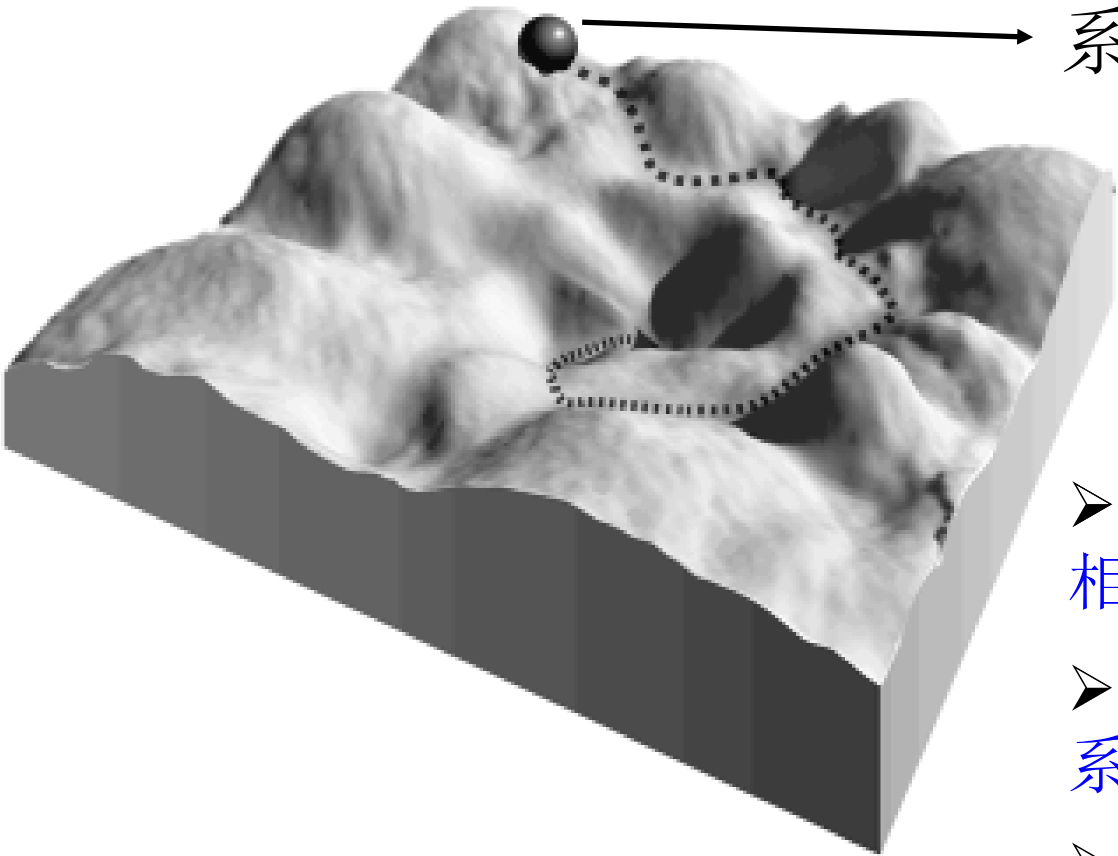
Crack pattern



Ferro domain

From the google images

相场方法的基本原理



系统在构形空间中演化

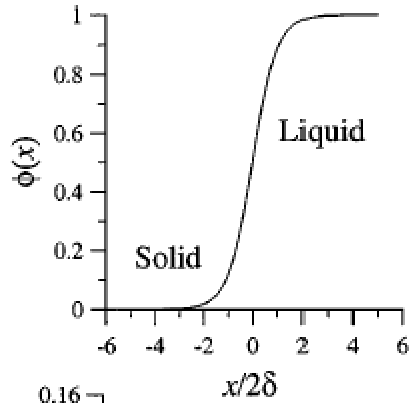
- 系统描述:
  相场变量选择，扩散界面
- 系统演化:
  系统不可逆熵产生大于0
- 热力学: 多重热力学力做功
- 动力学: 多重热力学流耗散

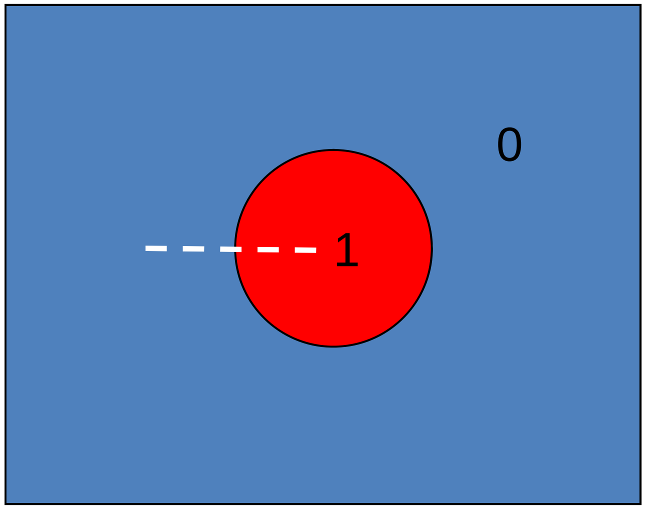
相场方法的基本原理

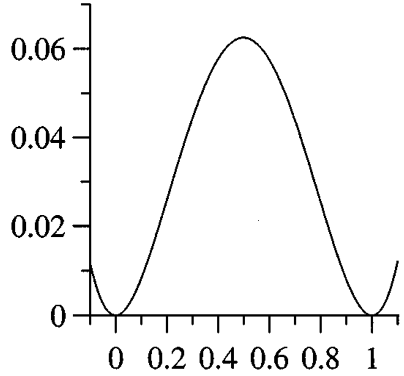
➢ 系统描述:

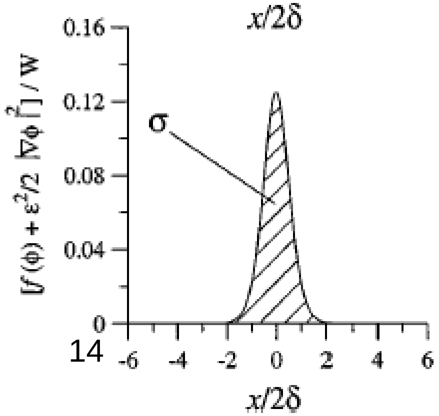
相场变量选择，扩散界面

•对于非均匀的连续体系，需要采取扩散-界面进行描述，即利用各种守恒和非守恒场变量（如：浓度、结构、取向、长程有序等）的空间梯度描述各相之间的扩散-界面。

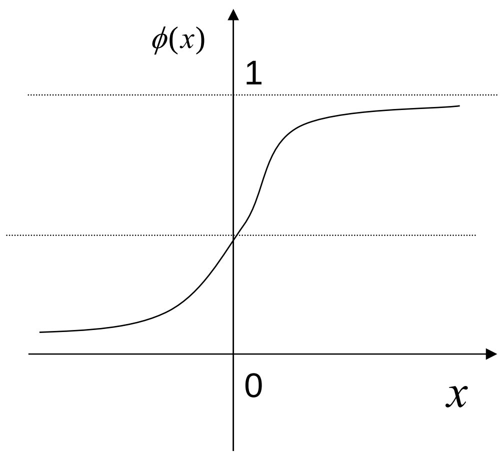








$$F = \int [f(\phi) + \frac{\varepsilon^2}{2}(\nabla \phi)^2] dV$$



相场热力学与动力学方程

$$F\left(c,\eta,\varepsilon,\nabla c,\nabla\eta\right)$$

守恒序参量：遵循C-H方程
非守恒序参量：遵循C-A方程

$$\frac{\partial c(\mathbf{r},t)}{\partial t}=\nabla(M\nabla\frac{\delta F}{\delta c(\mathbf{r},t)})+\zeta^{c}(\mathbf{r},t)$$

多个序参量：多物理场耦合

$$\frac{\partial \eta_p(\mathbf{r},t)}{\partial t}=-L\frac{\delta F}{\delta \eta_p(\mathbf{r},t)}+\zeta_p^{\eta}(\mathbf{r},t)$$

非平衡热力学：
不可逆熵产生大于0

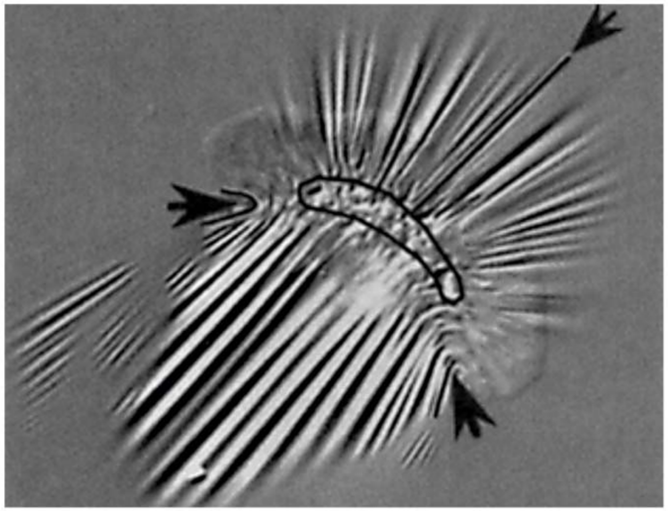
动力学：输运，界面反应 …

结合渐近分析，使构造的相场方程在薄界面厚度的情况下逼近尖锐界面下的物理动力学方程。其分析类似于流体中的边界层问题。

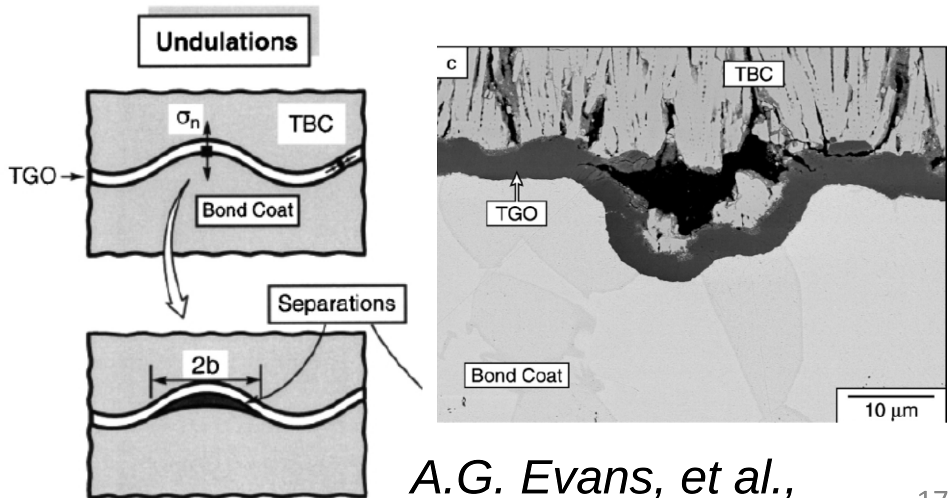
相场方法的特点

1. 相场自由能函数可包含多重相变
2. 扩散界面描述可自适应追踪相边界
3. 动力学方程可描述多物理场耦合和多重时间尺度过程。

Nonlinear mechanical phenomena in layered structures



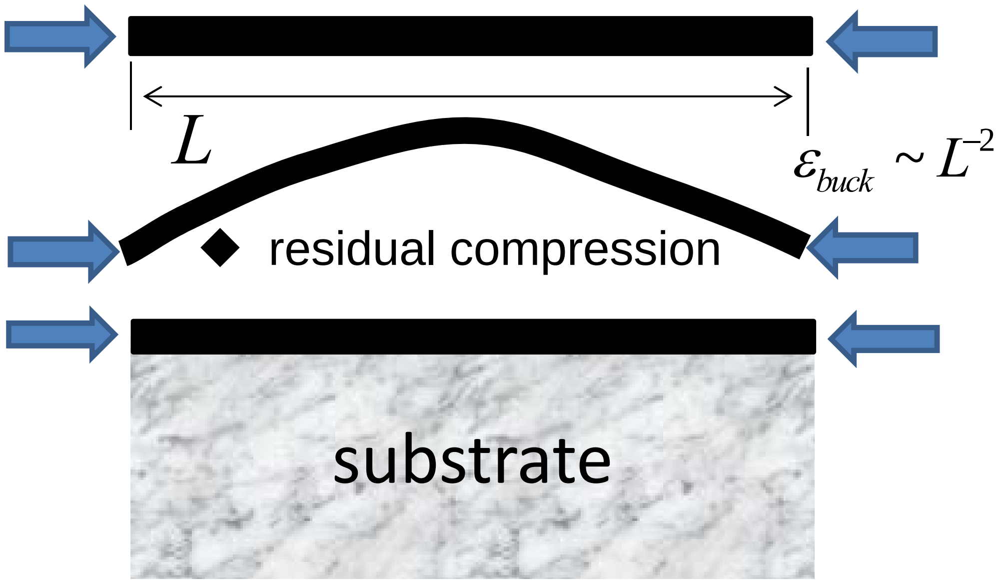
Stopak, *et al., Science,208 (1980)*

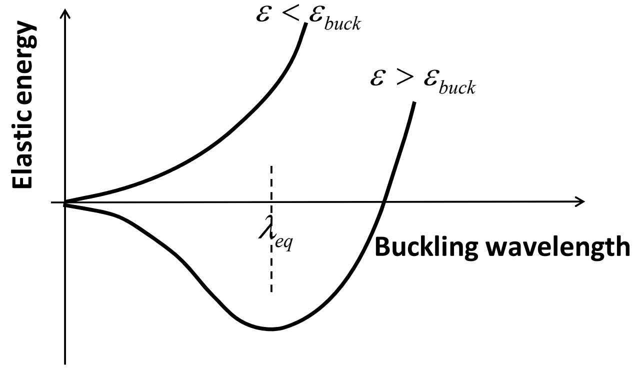


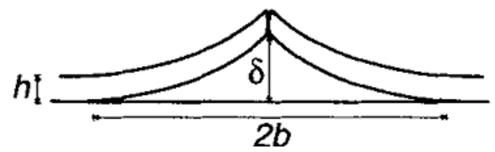
A.G. Evans, et al., Prog. Mater. Sci. 46,505(2001)

Nonlinear buckles in film/substrate systems

Euler Buckling



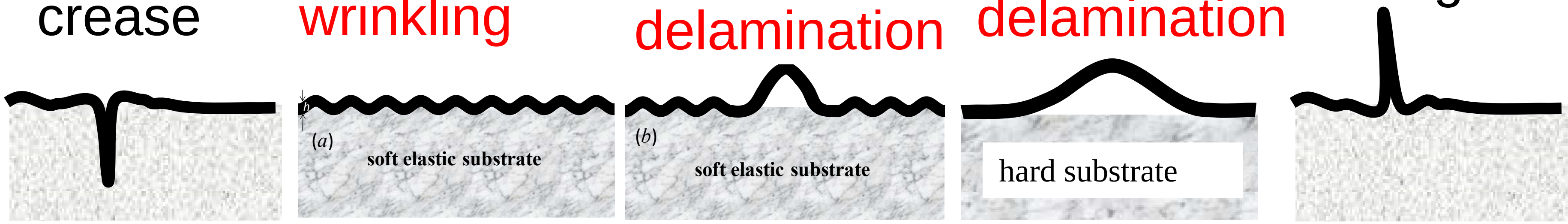




ridge crack

- interface property
- mechanical property of the substrate

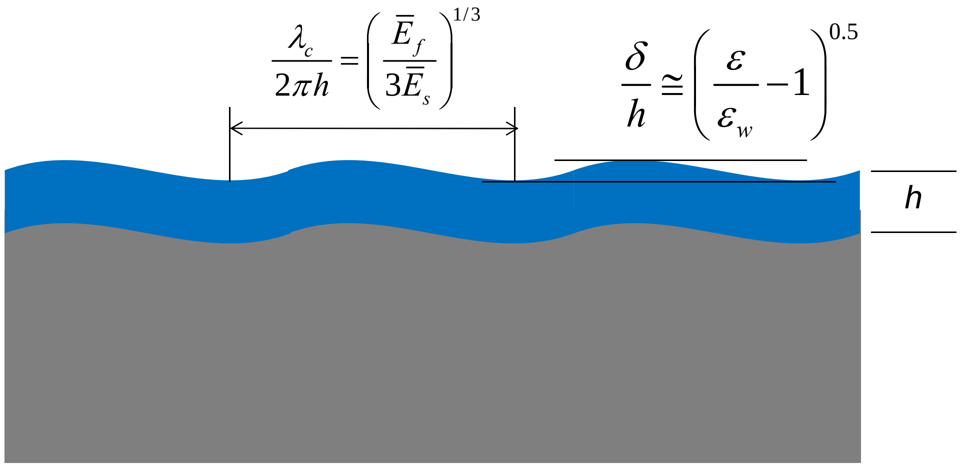
crease | wrinkling | wrinkling-induced delamination | buckle delamination | folding



◆ Homogeneous wrinkling at the onset

$$\varepsilon_w = \frac{1}{4}\left(\frac{3\bar{E}_s}{\bar{E}_f}\right)^{2/3}$$

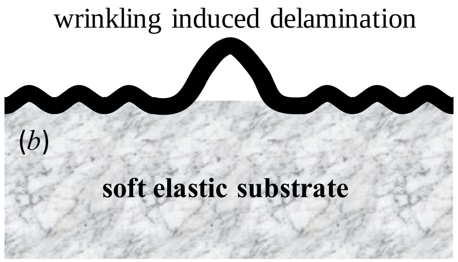
Allen 1969
Groenewolld 2001
Z.Y. Huang et al., 2005
J.Z. Song, et al., 2009
Audoly, JMPS, 2009



◆ Wrinkling-induced delamination

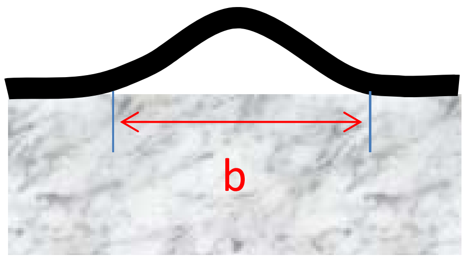
$$\varepsilon_{wd} = \varepsilon_w + \left(\frac{(3-4v_s)\gamma_n}{8(1-v_s)\mu_s e\delta_n}\right)^2$$

H. Mei et al., Mech. Mater., 43,627(2011)



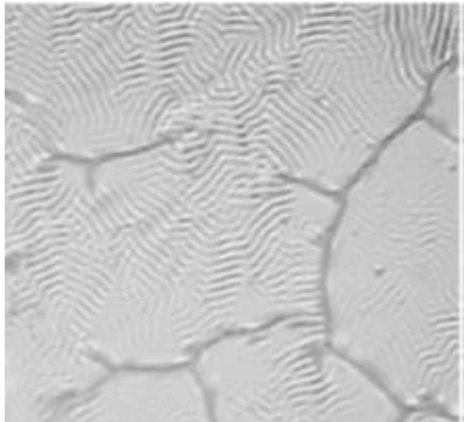
◆ Buckle-delamination

$$\sigma_{B0} = \frac{\pi^2}{12}\left(\frac{h}{b}\right)^2 \bar{E}_f,$$



J. W. Hutchinson and Z. Suo, Adv. Appl. Mech. **29**, 63 (1992).

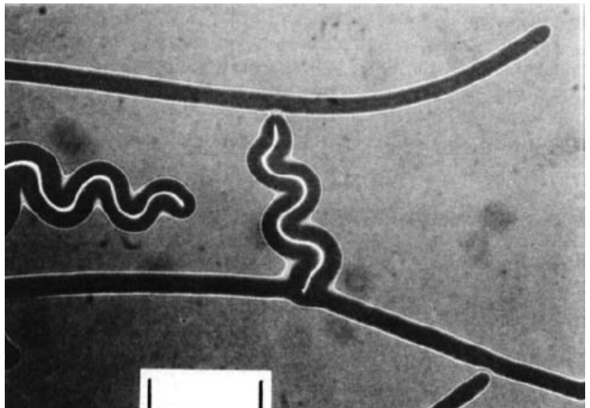
Nonlinear buckling morphology of the film



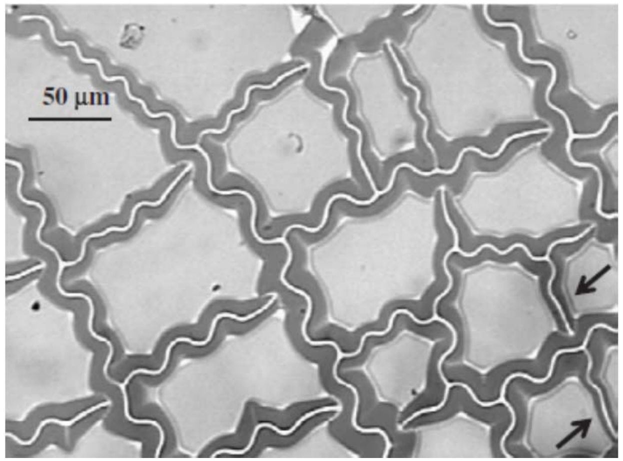
Mei et al. (2007)

complex wrinkling→coexisting wrinkles and buckle-delamination

Vella et al. (2009)



Thouless et al. (1993)

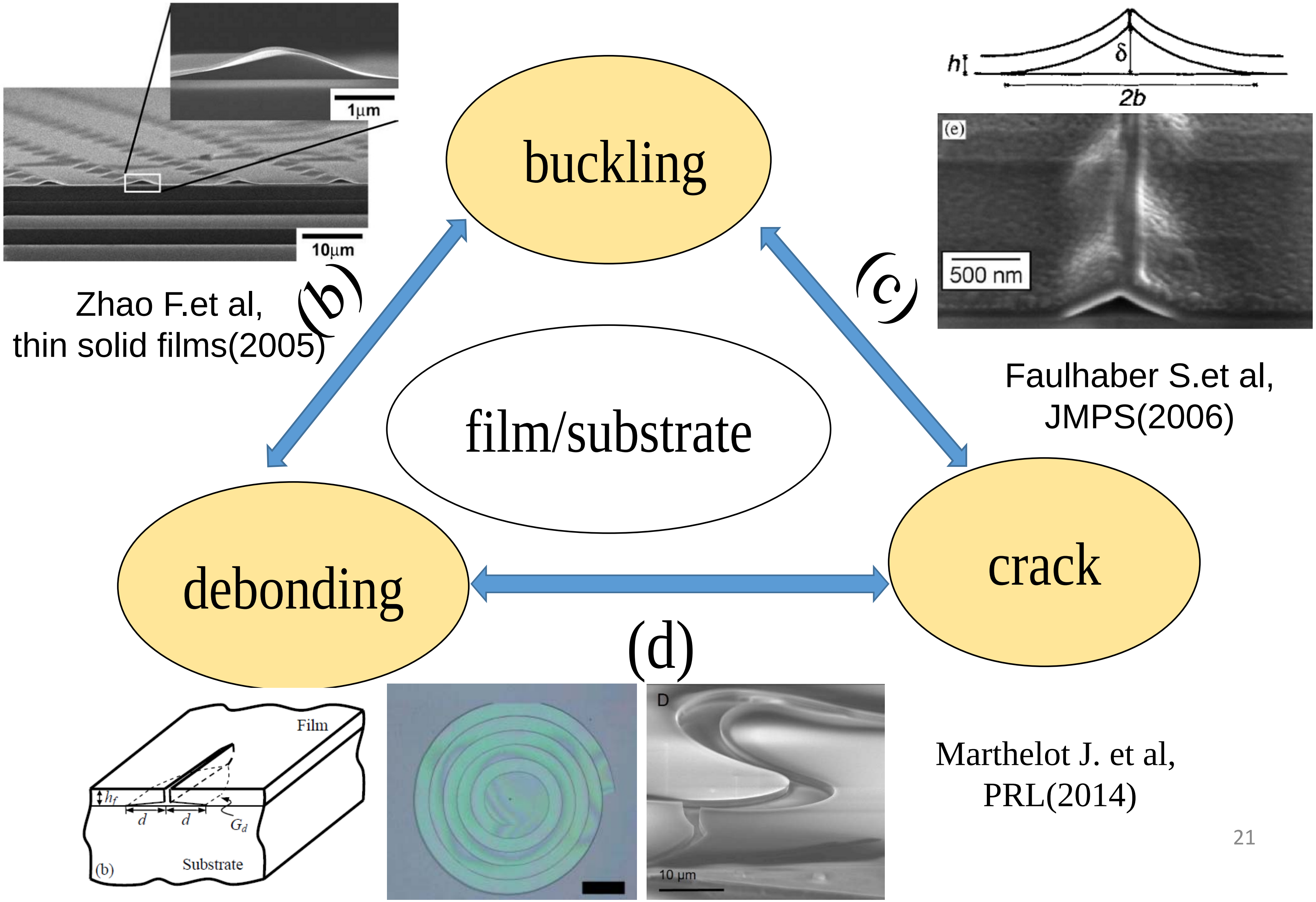


Abdallah et al. (2006)

Buckle-delamination pattern：

straight blister→telephone cord→network-like telephone cord buckles

Microstructural evolution in film/substrate systems



Problems

- ☐ **Complex wrinkling patterns**
- ☐ **Transition from wrinkling to buckle-delamination**
- ☐ **Buckle-delamination patterns**

Phase field modeling of crack, buckle and delamination

$$F^{tot} = F_s^{film} + F_b^{film} + F^{sub} + F_{\text{int}}$$

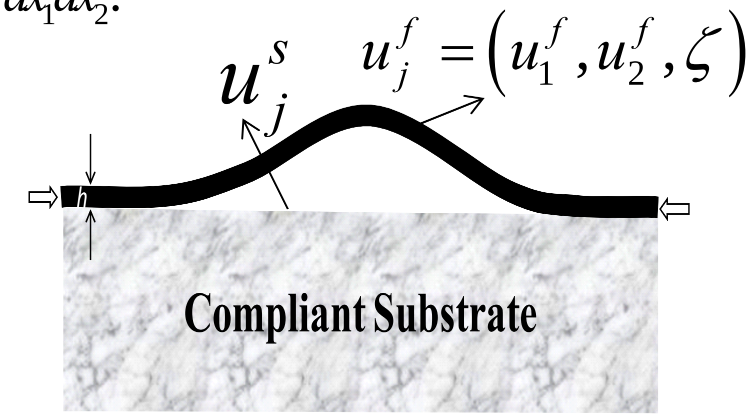
$$F_s^{film} = \frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} N_{\alpha\beta} e_{\alpha\beta} dx_1 dx_2, \quad N_{\alpha\beta} = h\left[C^0_{\alpha\beta\delta\gamma}\phi(r)\left(\varepsilon_{\delta\gamma}(r) - \varepsilon^*_{\delta\gamma}(r)\right)\right] \quad \phi(r) = \begin{cases} 0 & \text{crack} \\ 1 & \text{no crack} \end{cases}$$

$$F_b^{film} = \frac{\mu_f h^3}{12(1-\nu_f)}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left\{\left[(\Delta\zeta)^2 - 2(1-\nu_f)\left[\zeta_{,11}\zeta_{,22} - (\zeta_{,12})^2\right]\right]\right\} dx_1 dx_2.$$

$$F^{sub} = \frac{1}{2}\int M_{ij}\tilde{u}_j^s \tilde{u}_j^{s*} d\xi_1 d\xi_2,$$

$$F^{\text{int}} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\int_0^{\Lambda_3} T_3(\Lambda_i)\, d\Lambda_3 + \int_0^{\Lambda_\alpha} T_\alpha(\Lambda_i)\, d\Lambda_\alpha\right) dx_1 dx_2,$$

Cohesive zone potential



Displacement jump across the interface

$$\Delta_j = u_j^f - u_j^s$$

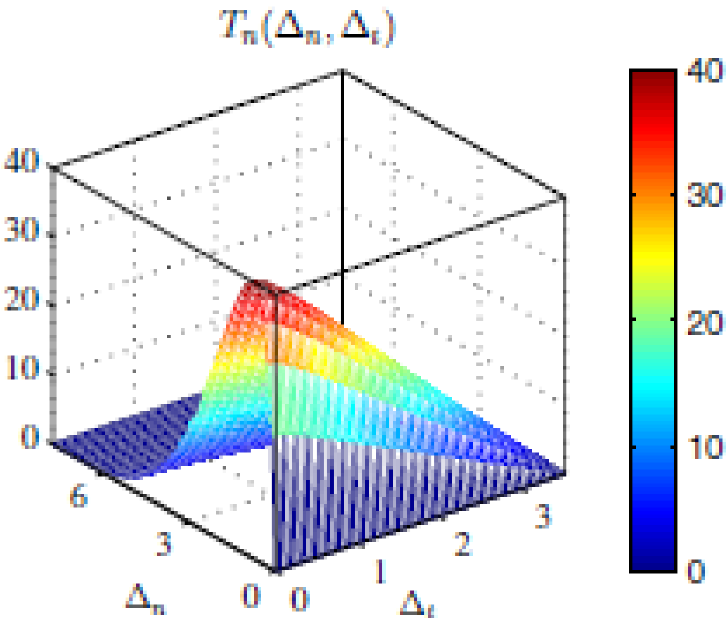
$$F^{tot} = F^{tot}\left(u_i^f, \Lambda_i, \phi\right)$$

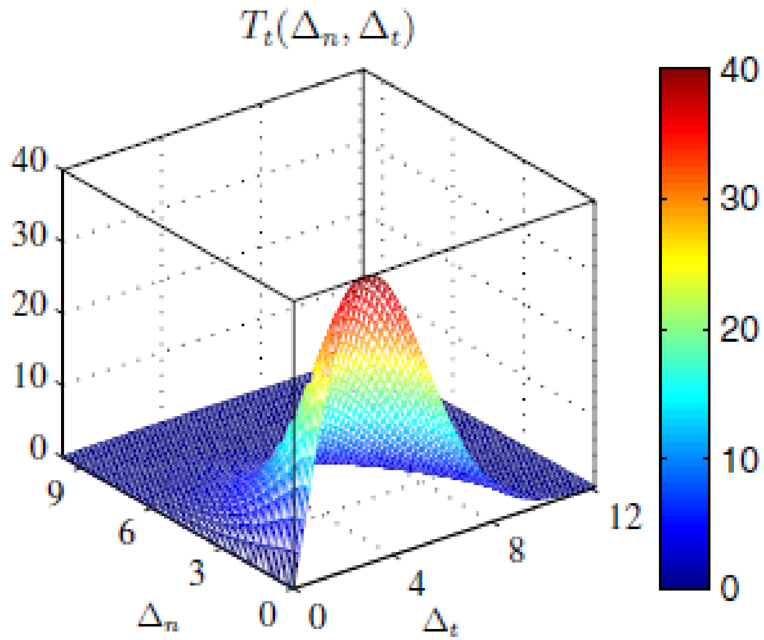
Y. Ni, A.K.Soh, Acta Mater.,(2014)

Cohesive zone potential

$$T_3 = \frac{\gamma_n \Lambda_n}{\delta_n^2} \exp\left(-\frac{\Lambda_n}{\delta_n} - \frac{\Lambda_t^2}{\delta_t^2} \right),$$

$$T_\alpha = \frac{2\gamma_t \Lambda_\alpha}{\delta_t^2} \left(1 + \frac{\Lambda_n}{\delta_n} \right) \exp\left(-\frac{\Lambda_n}{\delta_n} - \frac{\Lambda_t^2}{\delta_t^2} \right),$$





M.J. van den Bosch et al Engineering Fracture Mechanics 73 (2006) 1220–1234

Phase field modeling of crack, buckle and delamination

$$\frac{\partial \zeta}{\partial t} = -\Gamma \frac{\delta F^{tot}}{\delta \zeta} \Longrightarrow D\Delta^2 \zeta - \left(N_{\alpha\beta}\zeta_{,\alpha}\right)_{,\beta} + T_3^s = 0,$$

- Modeling the buckling process

$$\frac{\partial \Lambda_i}{\partial t} = -\Gamma_{\Lambda_i} \frac{\delta F^{tot}}{\delta \Lambda_i} \Longrightarrow T_i - T_i^s = 0.$$

- Modeling the delamination process

$$\frac{\partial u_\alpha}{\partial t} = -\Gamma_{u_\alpha} \frac{\delta F^{tot}}{\delta u_\alpha} \Longrightarrow N_{\alpha\beta,\beta} = h\nabla_\beta \left[C^0_{\alpha\beta\delta\gamma} \phi(r) \left(\varepsilon_{\delta\gamma}(r) - \varepsilon^*_{\delta\gamma}(r) \right) \right] = T^s_\alpha$$

- Modeling the in-plane equilibrium

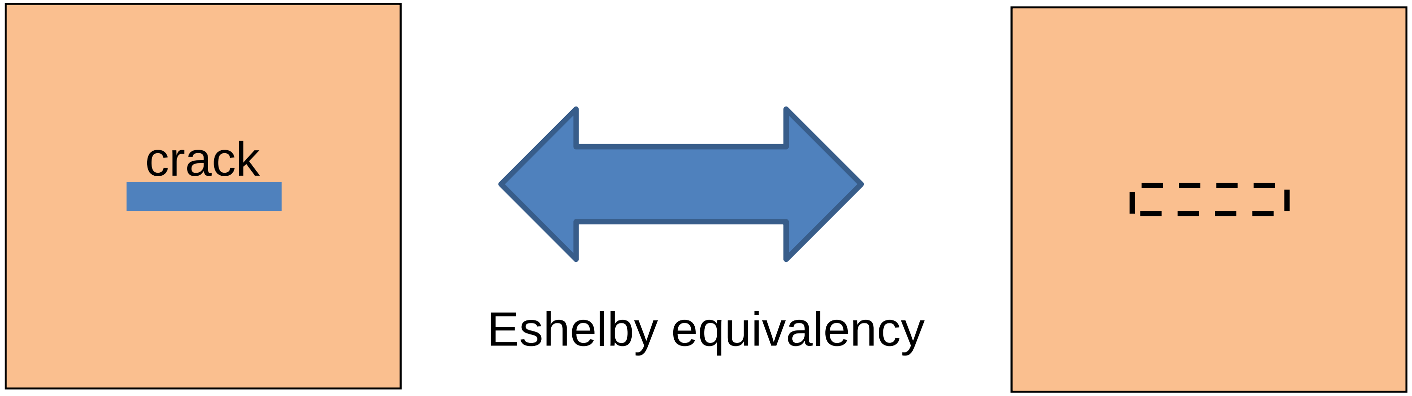
Phase field microelasticity for crack tip field

$$\frac{1}{2}\int_V C_{ijkl}\left(\varepsilon_{ij}(r)-\varepsilon^*_{ij}(r)\right)\left(\varepsilon_{kl}(r)-\varepsilon^*_{kl}(r)\right)d^3r = \frac{1}{2}\int_{|\mathbf{k}|\neq 0} B(\mathbf{e})_{ijkl}\,\tilde{\varepsilon}^*_{ij}(\mathbf{k})\tilde{\varepsilon}^*_{kl}(\mathbf{k})\frac{d^3k}{(2\pi)^3}$$

(Mura 1987; Khachaturyan, 1983, book)

systems with
the inhomogneous moduli
$\mathbf{C}(\mathbf{r}), \varepsilon^*_{ij}(r)$

systems with
homogneous moduli C^0_{ijkl}
distributed $\boldsymbol{\varepsilon}^{\mathrm{o}}(\mathbf{r})$



$$h\nabla_\beta\left[C^0_{\alpha\beta\delta\gamma}\phi(r)\left(\varepsilon_{\delta\gamma}(r)-\varepsilon^*_{\delta\gamma}(r)\right)\right]-T^s_\alpha=0 \rightarrow h\nabla_\beta\left[C^0_{\alpha\beta\delta\gamma}\left(\varepsilon_{\delta\gamma}(r)-\varepsilon^0_{\delta\gamma}(r)\right)\right]=0$$

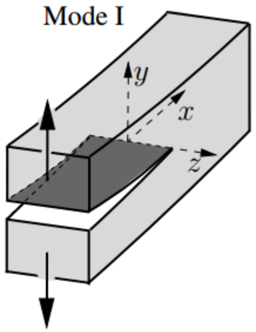
Finding the effective eigenstrain $\varepsilon^0_{ij}(r)$ determined by the above equation

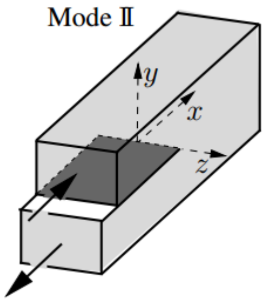
$$\frac{\partial\varepsilon^0_{\delta\gamma}}{\partial t}=-L\frac{\delta\Pi}{\delta\varepsilon^0_{\delta\gamma}(\mathbf{r},t)}$$

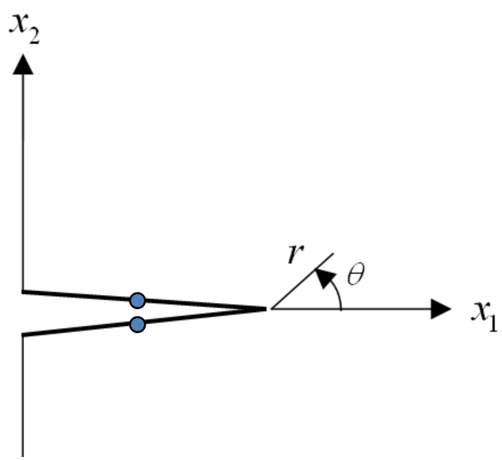
$$\Pi=\frac{1}{2}\int_{|\mathbf{k}|\neq 0} B(\mathbf{e})_{ijkl}\,\tilde{\varepsilon}^0_{ij}(\mathbf{k})\tilde{\varepsilon}^0_{kl}(\mathbf{k})\frac{d^3k}{(2\pi)^3}+\int\frac{1}{2}\left(C^0_{ijpq}(C_{pqmn}-C_{pqmn}(r))^{-1}C^0_{mnkl}-C^0_{ijkl}\right)(\varepsilon^0_{ij}-\varepsilon^*_{ij})(\varepsilon^0_{kl}-\varepsilon^*_{kl})dV$$

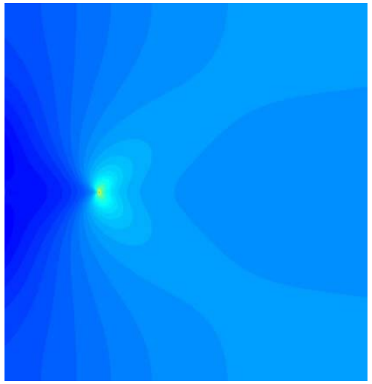
Y.U. Wang et al., JAP, 92,1351 (2002) Y. Ni and Y.M. Chiang JMPS, 55,517 (2007)

Crack tip field in a freestanding film without buckle









$$\begin{Bmatrix} u_1 \\ u_2 \end{Bmatrix} = \frac{(1+\nu)}{2E}\left\{\frac{r}{2\pi}\right\}^{1/2}\begin{Bmatrix} K_{\mathrm{I}}\left[(2\kappa-1)\cos\frac{\theta}{2}-\cos\frac{3\theta}{2}\right]+K_{\mathrm{II}}\left[(2\kappa+3)\sin\frac{\theta}{2}+\sin\frac{3\theta}{2}\right] \\ K_{\mathrm{I}}\left[(2\kappa+1)\sin\frac{\theta}{2}-\sin\frac{3\theta}{2}\right]-K_{\mathrm{II}}\left[(2\kappa-3)\cos\frac{\theta}{2}+\cos\frac{3\theta}{2}\right] \end{Bmatrix}$$

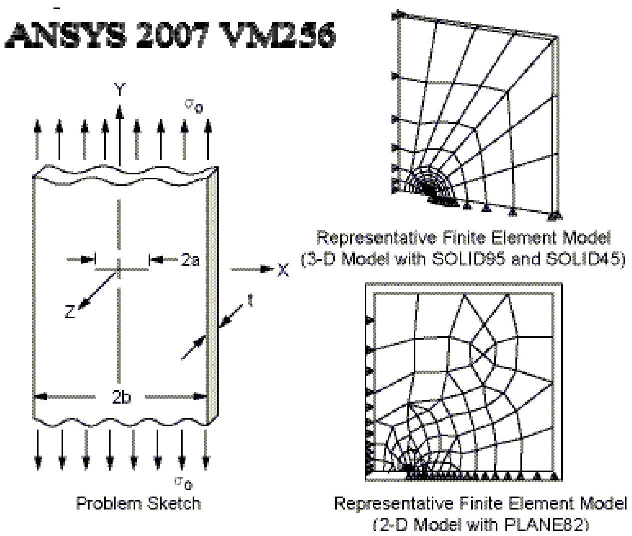
$$K_{\mathrm{I}} = \frac{E}{(1+\nu)(1+\kappa)}\sqrt{\frac{\pi}{2r}}\left(u_2|_{\theta=\pi} - u_2|_{\theta=-\pi}\right)$$

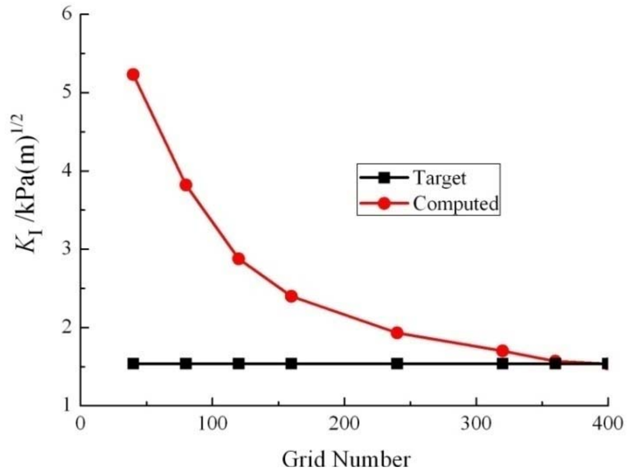
$$K_{\mathrm{II}} = \frac{E}{(1+\nu)(1+\kappa)}\sqrt{\frac{\pi}{2r}}\left(u_1|_{\theta=\pi} - u_1|_{\theta=-\pi}\right)$$

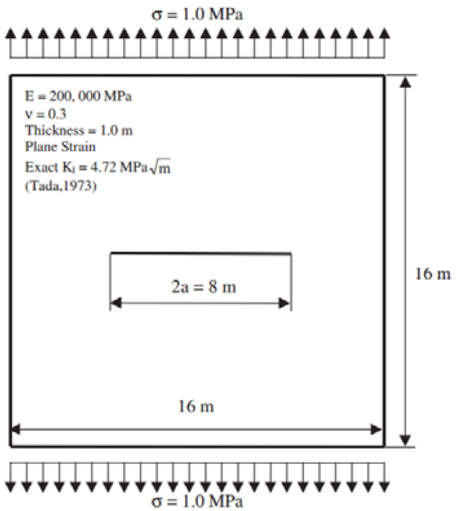
A. Tabiei 2003 Int J Numer Meth Engng

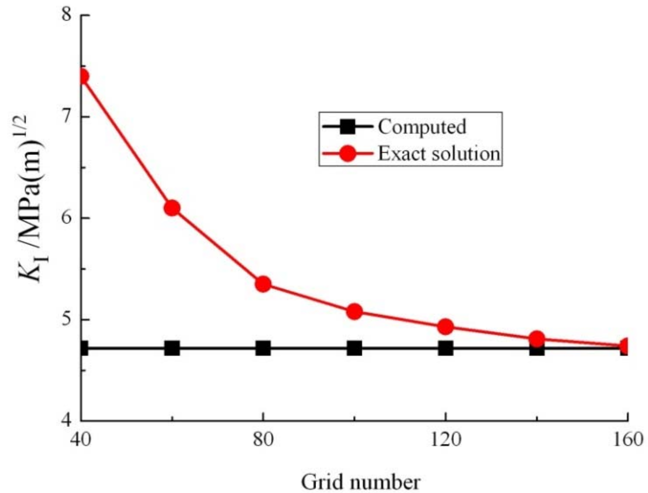
Stress-intensity factor fitted by crack-tip field

ANSYS 2007 VM256









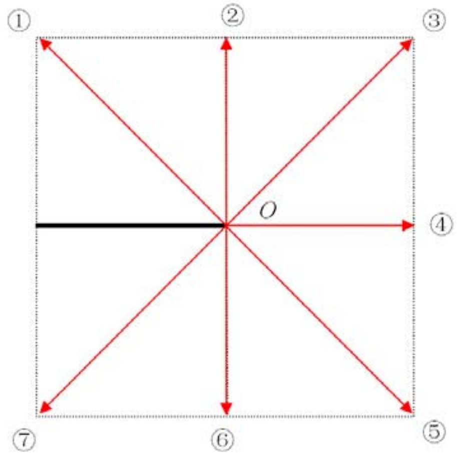
A. Tabiei 2003 Int J Numer Meth Engng

Test of crack growth and deflection

crack growth

E. Wu 1967 J Appl Mech

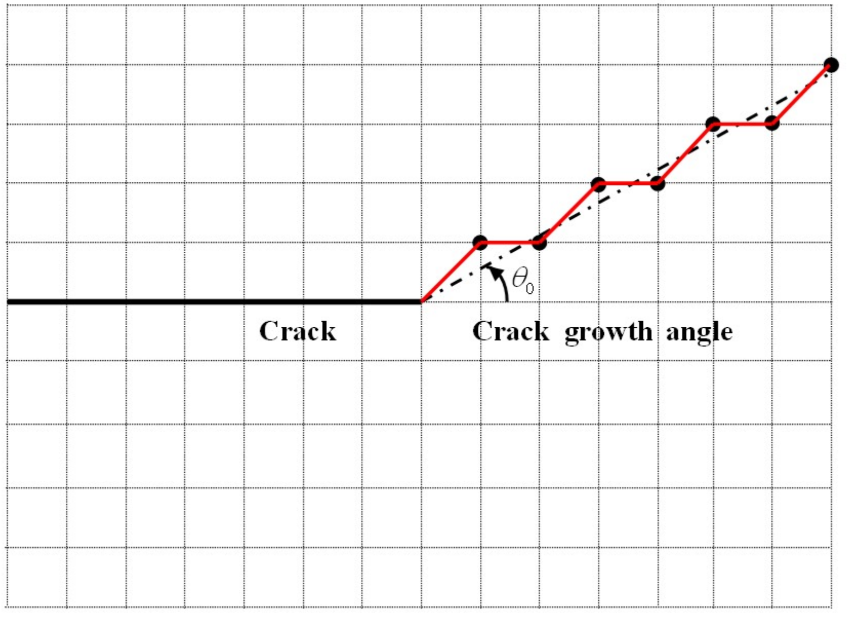
$$\left(\frac{K_I}{K_{Ic}}\right)^2 + \left(\frac{K_{II}}{K_{IIc}}\right)^2 = 1$$



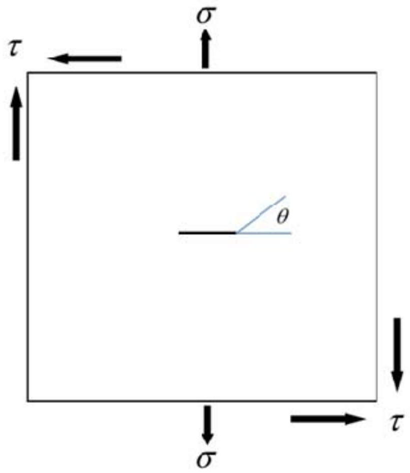
crack deflection

D. Broek 1986 Springer

$$\begin{cases} \theta_0 = 2\tan^{-1}\left(\frac{K_I}{4K_{II}} - \frac{1}{4}\sqrt{\left(\frac{K_I}{K_{II}}\right)^2 + 8}\right) & \text{for } K_{II} > 0 \\ \theta_0 = 2\tan^{-1}\left(\frac{K_I}{4K_{II}} + \frac{1}{4}\sqrt{\left(\frac{K_I}{K_{II}}\right)^2 + 8}\right) & \text{for } K_{II} < 0 \end{cases}$$



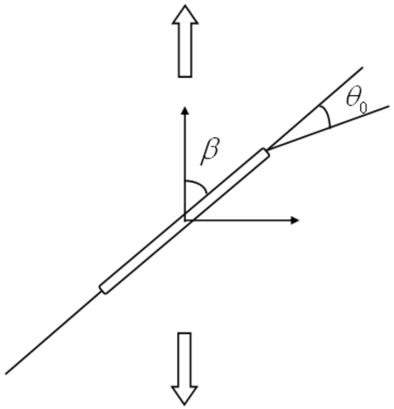
Test of crack growth and deflection



Infinite plate

$$\theta = 2\tan^{-1}\left(-\frac{\sigma}{4\tau} + \frac{1}{4}\sqrt{\left(\frac{\sigma}{\tau}\right)^2 + 8}\right)$$

No.	τ/σ	Theoretical θ_0/deg	Computational θ_0 /deg
1	0.1	11.203	11.202
2	0.2	21.089	21.0875
3	0.3	29.103	29.101
4	0.4	35.357	35.3572
5	0.5	40.208	40.206
6	0.6	44.004	44.003
7	0.7	47.022	47.0204
8	0.8	49.460	49.4587



Theory

$$\sin\theta_0 + (3\cos\theta_0 - 1)\cot\beta = 0,\ \beta \neq 0$$

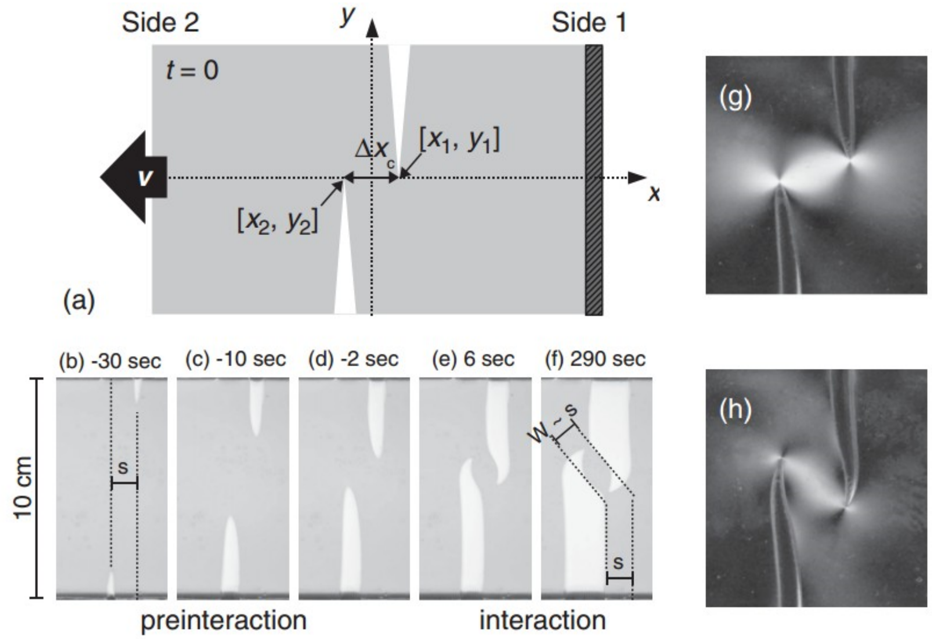
$$\beta = \pi/4 \Rightarrow \theta_0 = -53.1301$$

Simulation

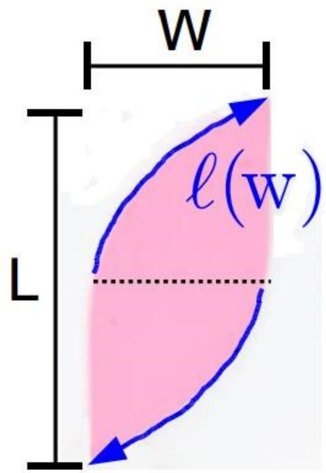
$$\theta_0 = -53.1301$$

A. Tabiei 2003 Int J Numer Meth Engng
G. Sih 1974 Int J Fracture

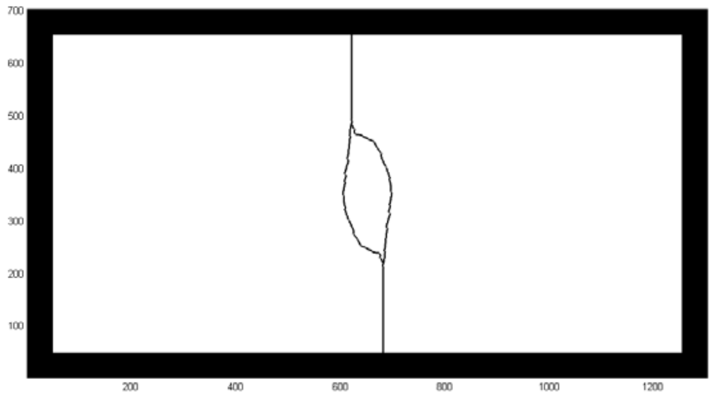
Test of crack growth and deflection



M. Fender 2010 Phys Rev Lett



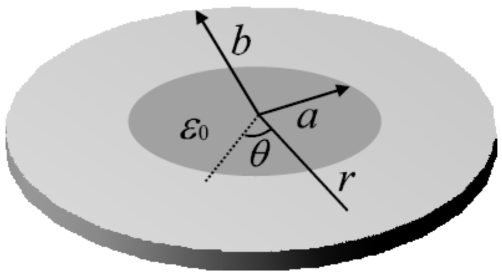
$L/W \approx 2$

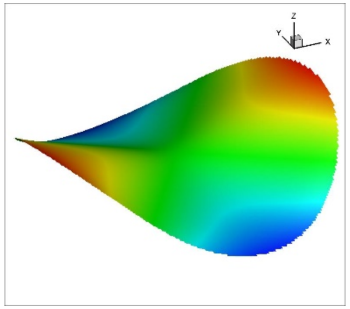


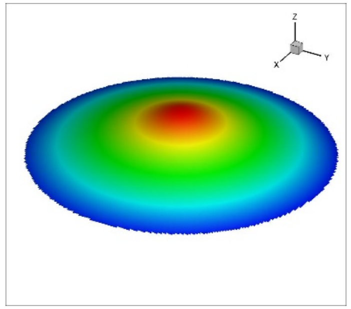
$L/W \approx 2.2$

Our simulation

Test of postbuckling profile of a stressed freestanding film

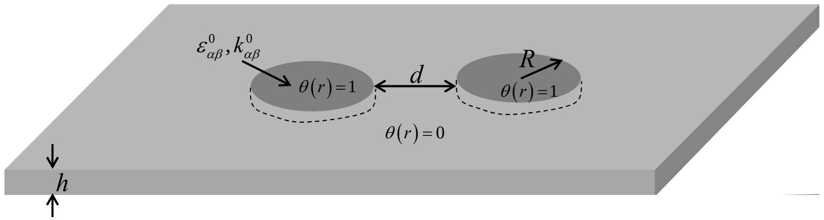


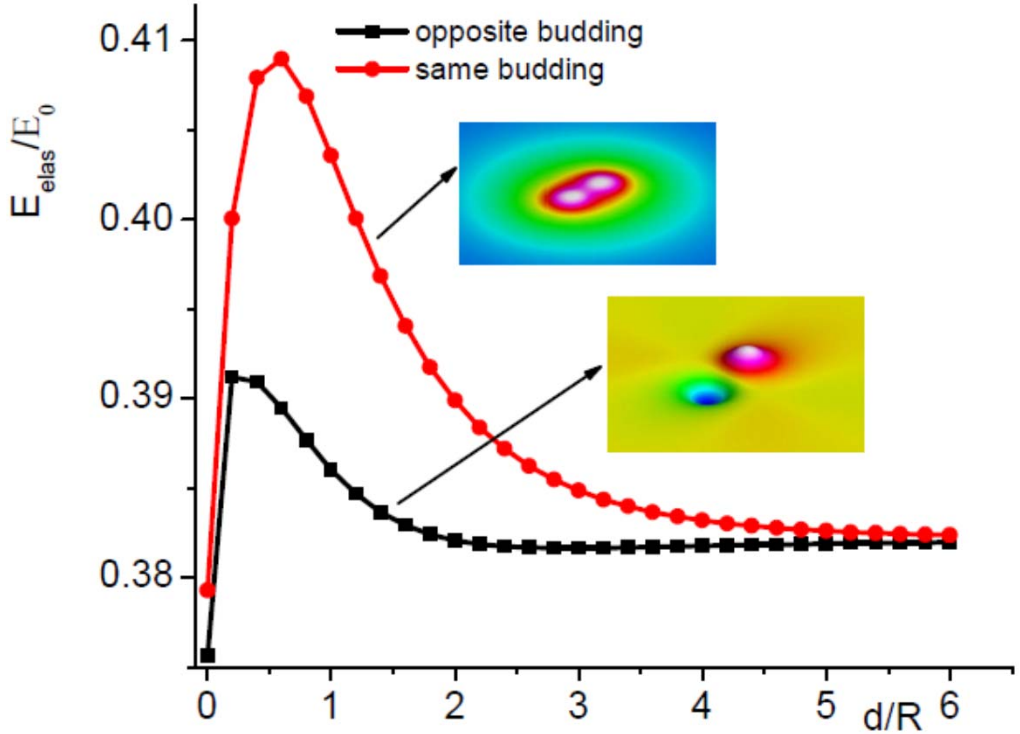




$$\frac{\partial \zeta}{\partial t} = -\Gamma\left[\Delta D(x_i)\Delta\zeta - \left(N_{\alpha\beta}\zeta_{,\alpha}\right)_{,\beta} + \cancel{T_3^s} = 0\right]$$

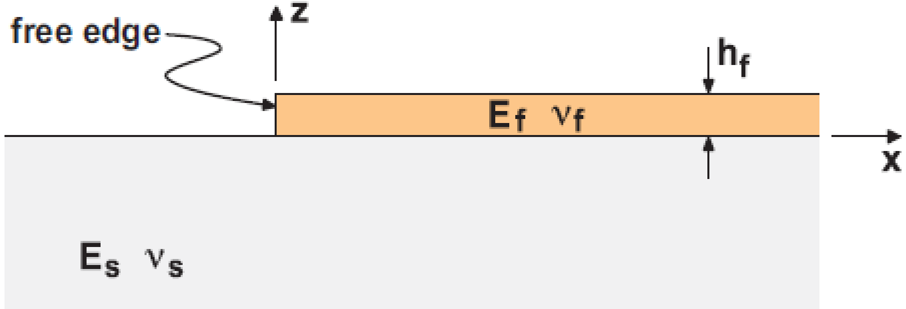
$$h\nabla_{\beta}\left[C^0_{\alpha\beta\delta\gamma}\,\phi(r)\left(\varepsilon_{\delta\gamma}(r) - \varepsilon^*_{\delta\gamma}(r)\right)\right] = 0$$

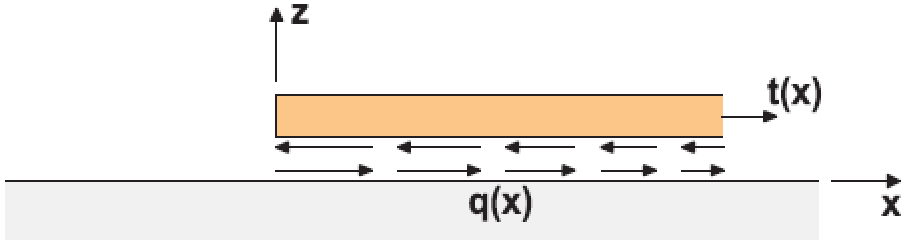




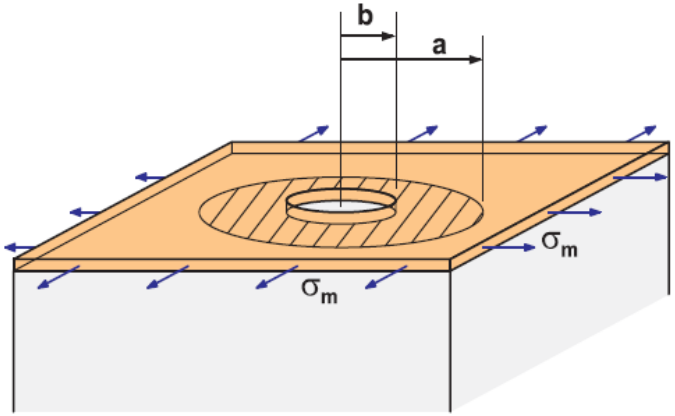
L.Qiao, L.H.He, Y.Ni, IJSS(2013)

Interface debonding





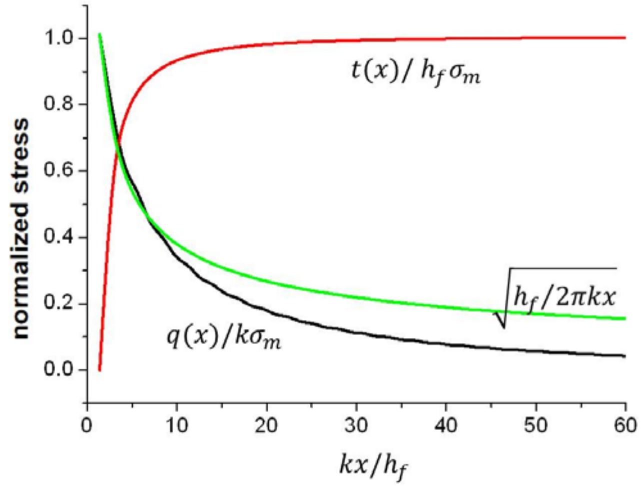
Griffith condition: $\frac{1-\nu_f^2}{2E_f}(\sigma_m - \sigma_a)^2 h_f = \Gamma$

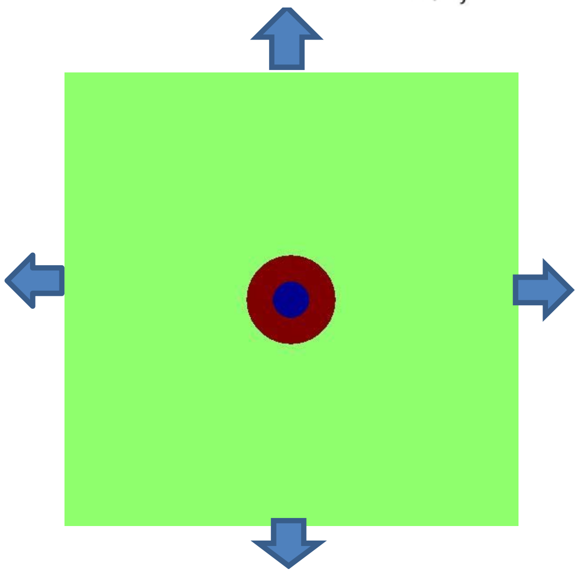


Freund et al, (2003)

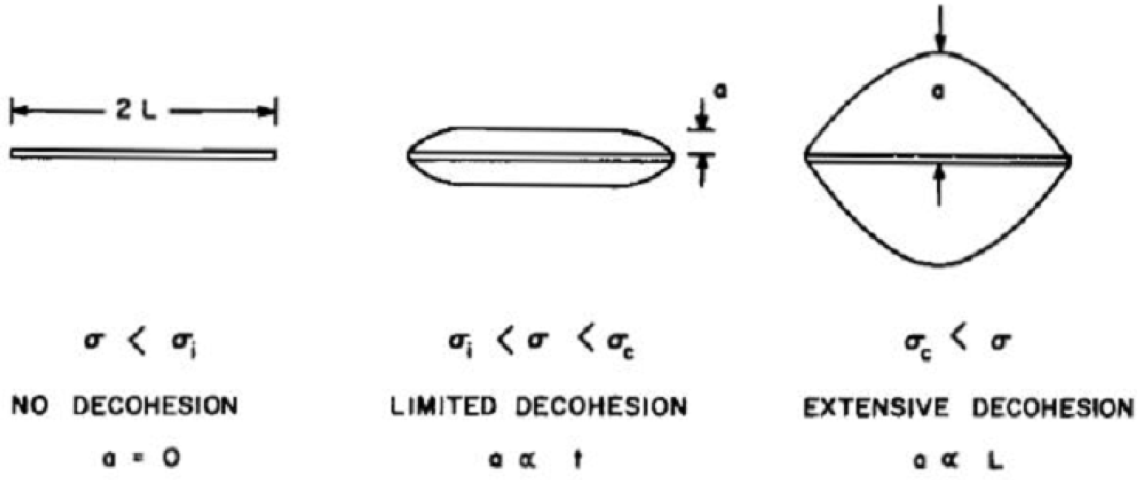
$$\frac{\partial \Lambda_\alpha}{\partial t} = -\Gamma_{\Lambda_\alpha} \frac{\delta F^{tot}}{\delta \Lambda_\alpha}, \alpha = 1, 2$$

Our simulation

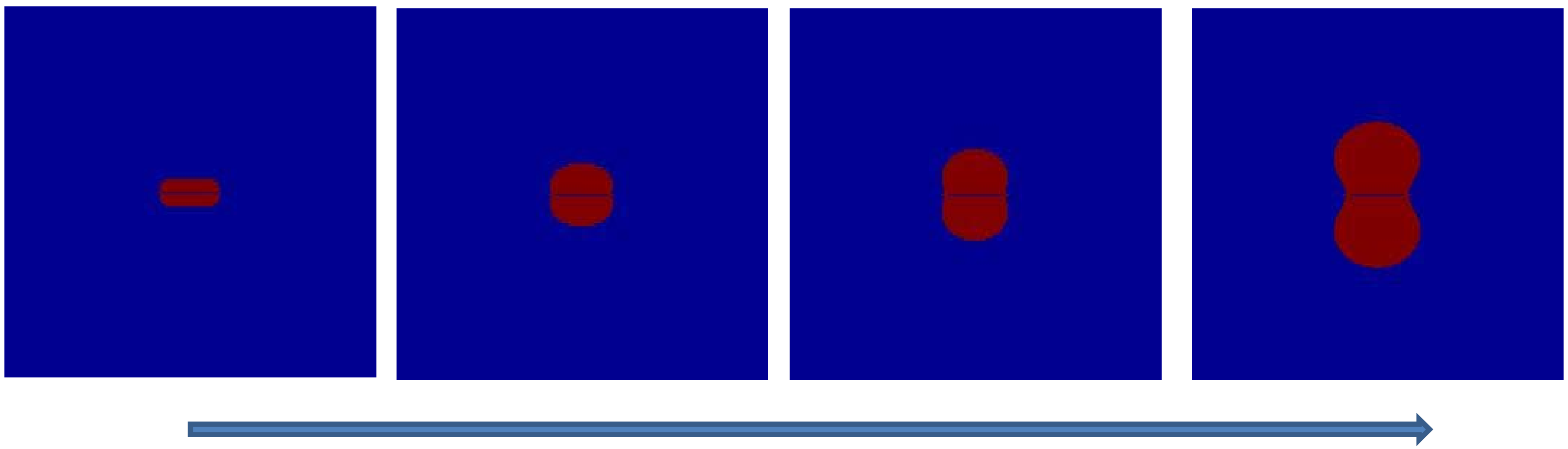




Debonding profile around a crack

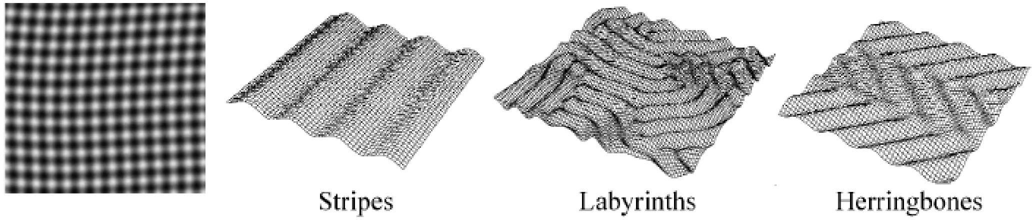


Jessen et al, IJF(1990)

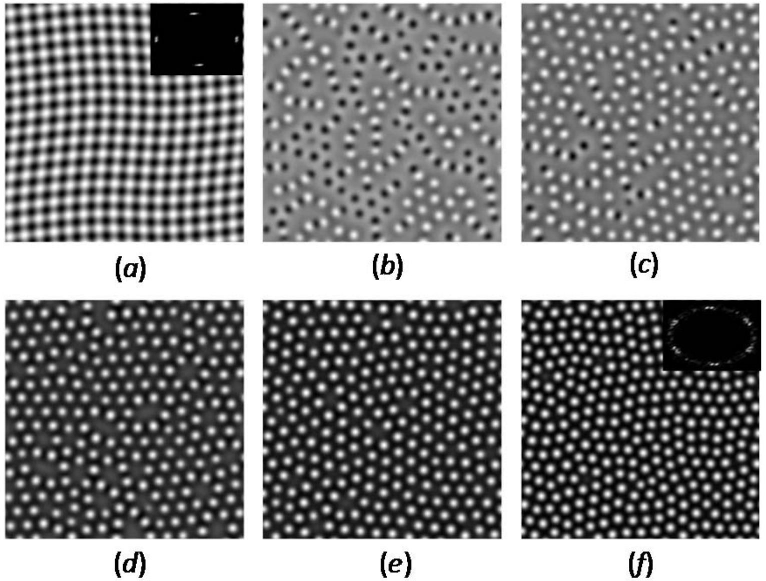


Debonding increases

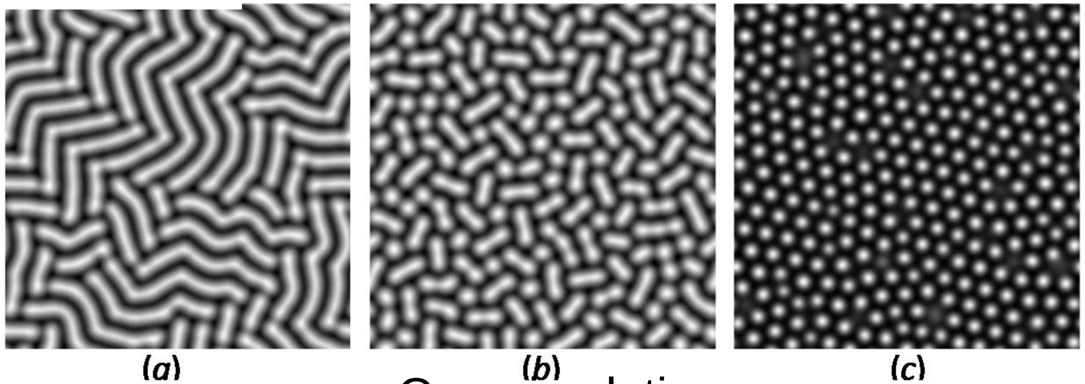
Diffusion-controlled Wrinkles



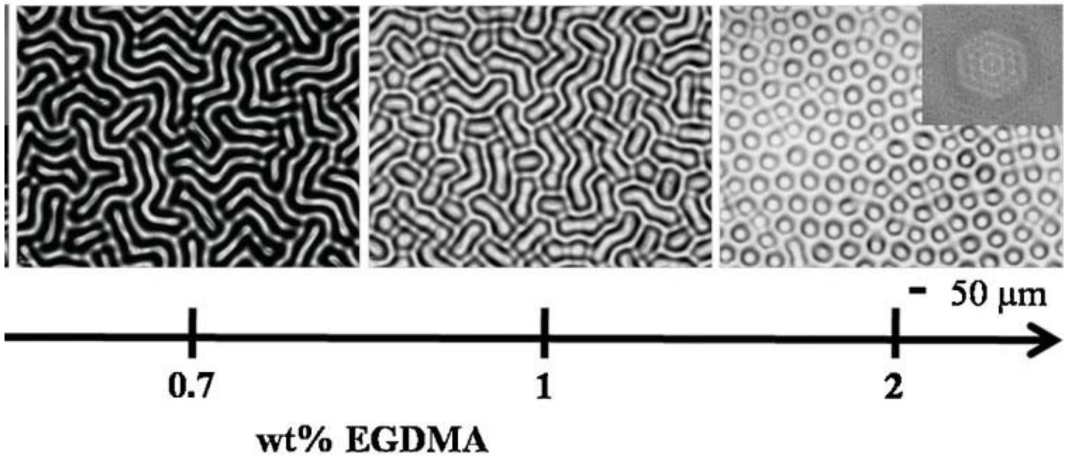
Conventional wrinkling patterns under homogeneous compression



Y. Ni, L.H.He, Q.H. Liu,
Phys. Rev. E, 84,051604(2011)



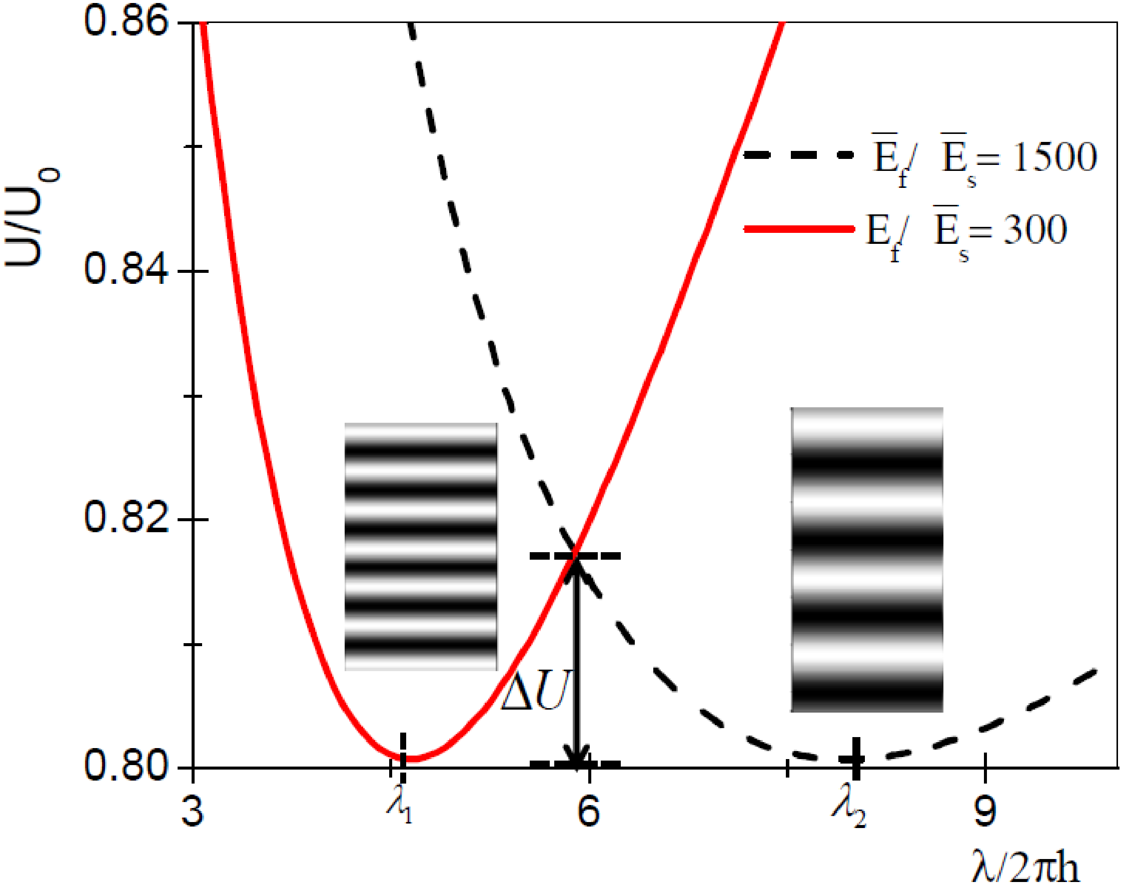
Our simulation

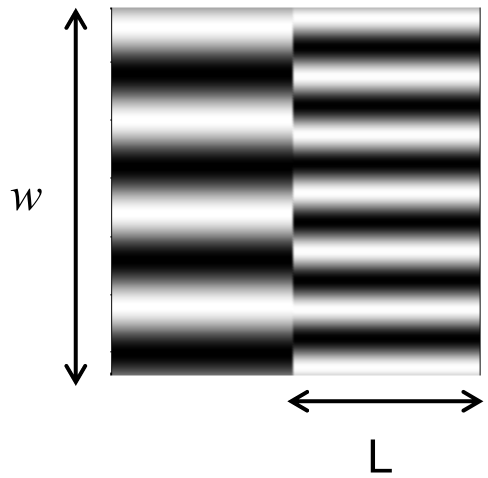


Experimental observation

Guvendiren M., S. Yang, J.A. Burdick,
Adv. Func. Mater., 19,3038(2009)

gradient wrinkling





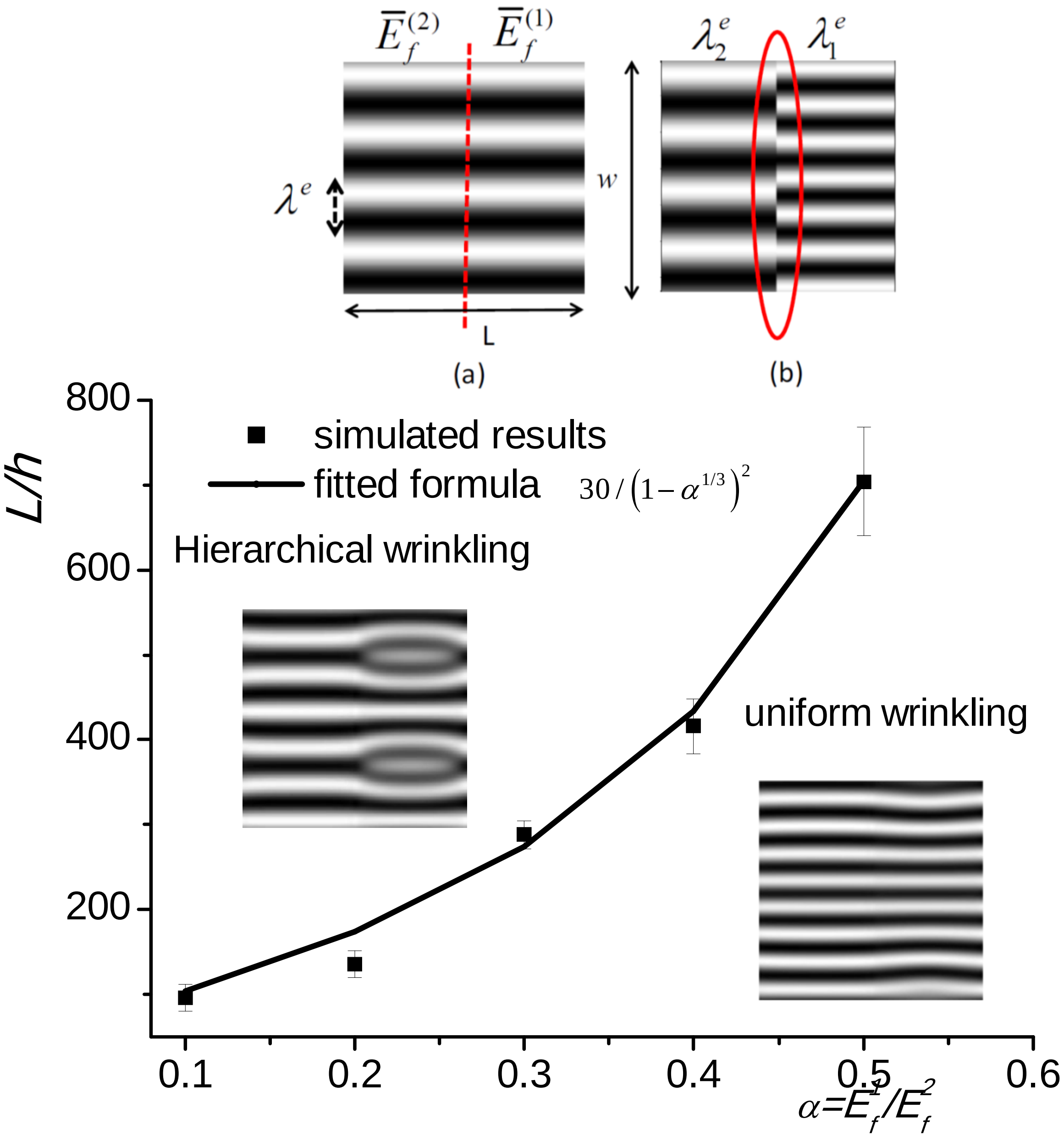
$$\gamma w = \Delta U L_c w$$

$$\gamma \sim \sqrt{\beta \Delta U}$$

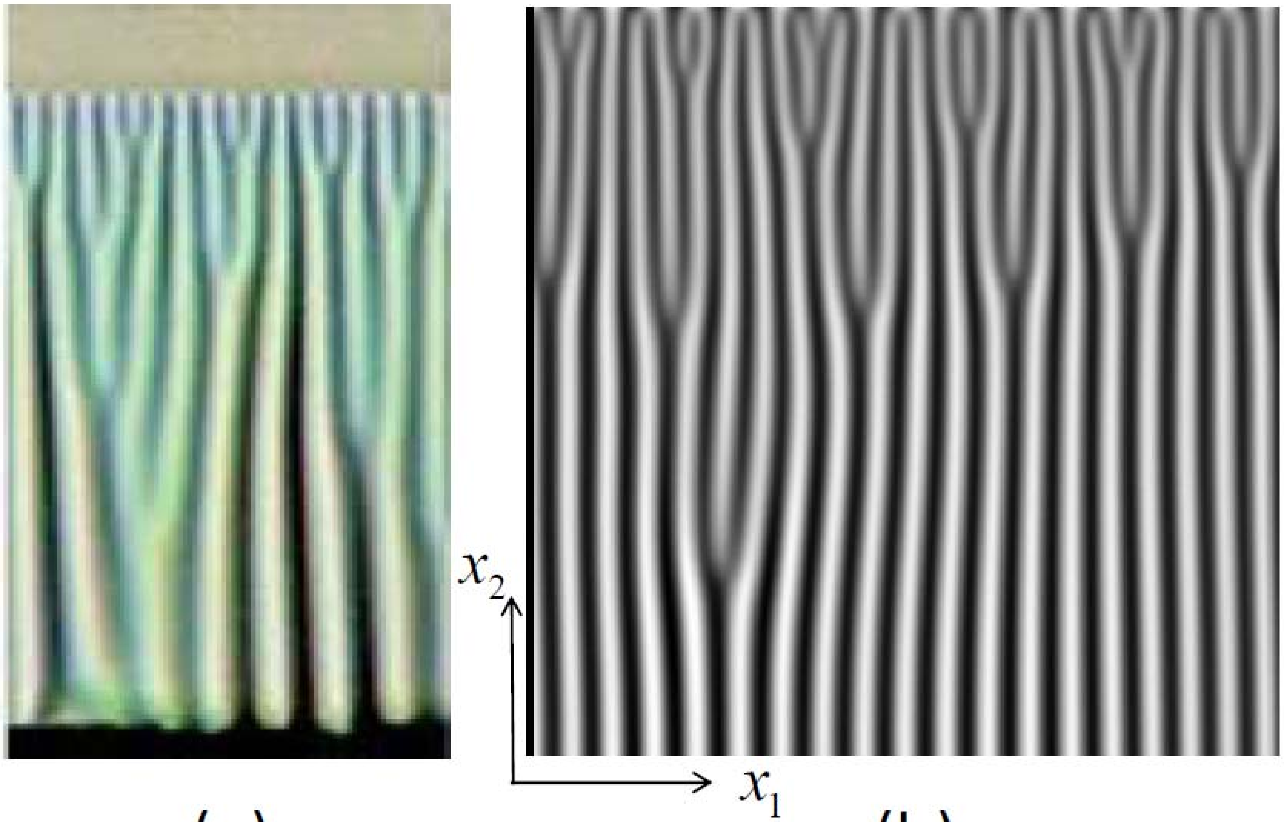
$$\Delta U \approx \Delta U\left(\lambda_1, \lambda_2\right)$$

$$L_c = \frac{\gamma}{\Delta U}$$

$$L \sim (D\eta)^{1/2} > L_c = \frac{C}{\left(1-\alpha^{1/3}\right)^2} \qquad \alpha = E_f^1 \,/\, E_f^2$$



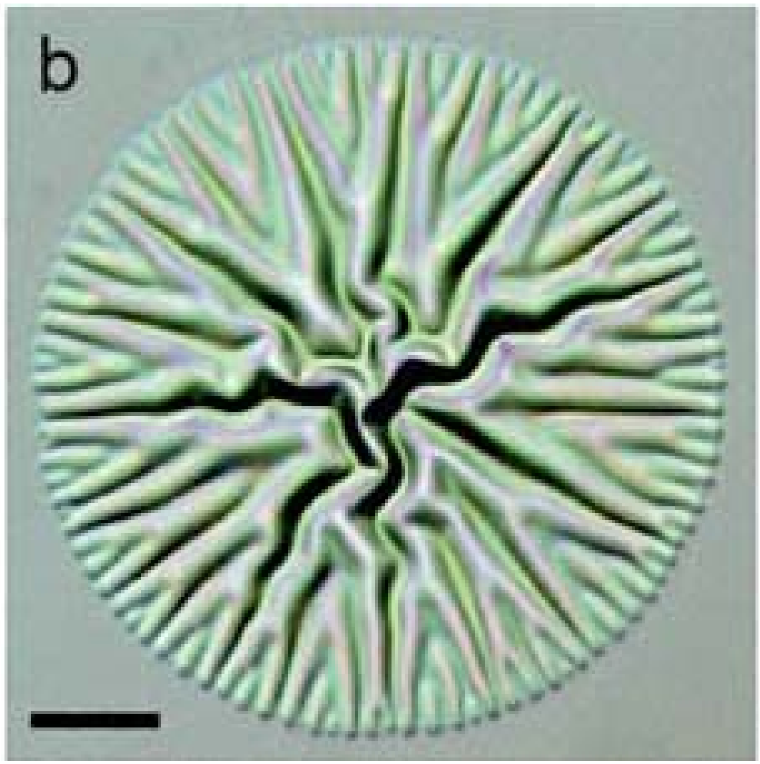
Y. Ni, D. Yang, L.H. He, Phys. Rev. E,86,031604(2012)



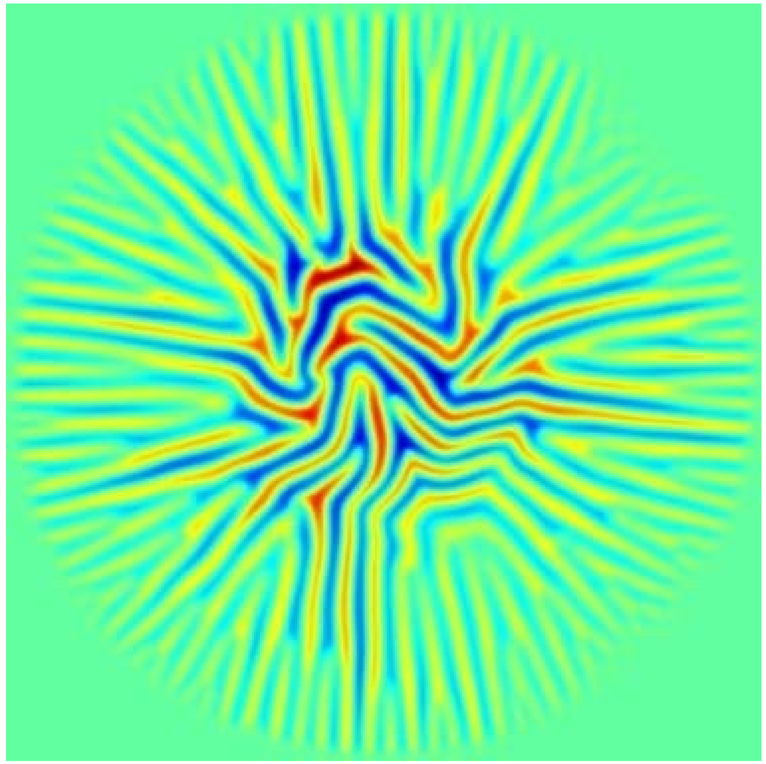
(a) (b)

H. Vandeparre et al,
Soft Matter, 6, 5751(2010)

Our simulated results

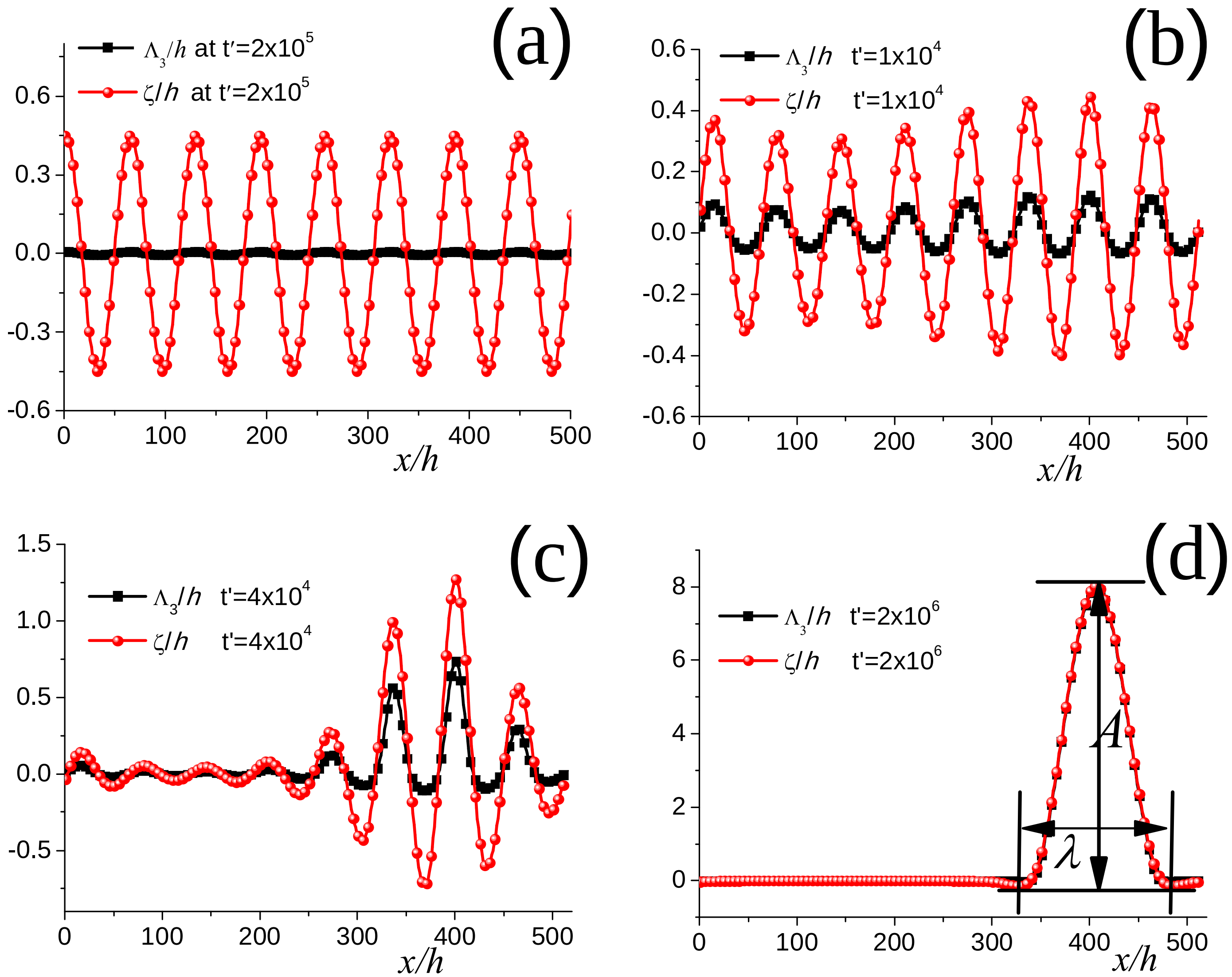


H. Vandeparre et al,
Soft Matter, 6, 5751(2010)

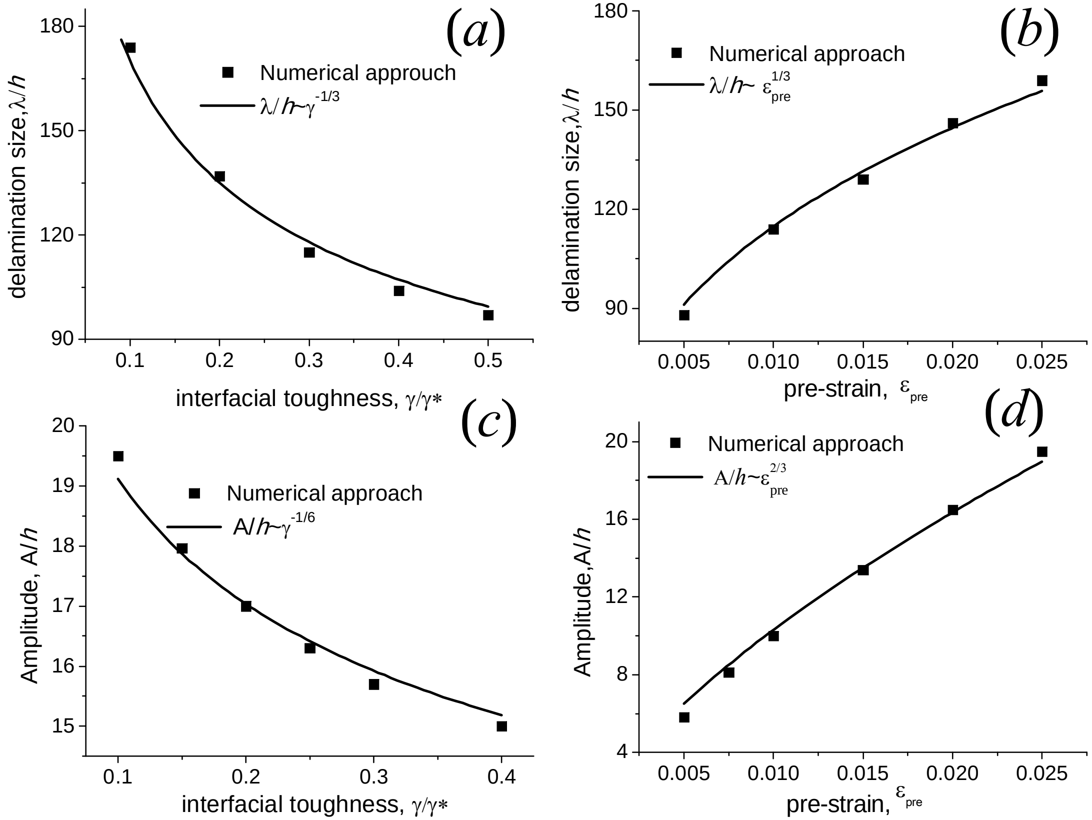


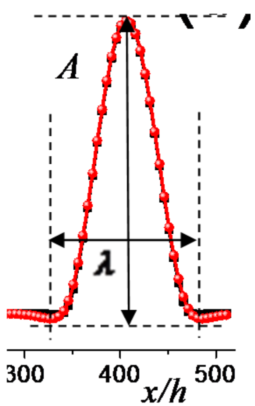
Our simulated results

Transition from wrinkling to buckle-delamination



profile of straight-sided blister

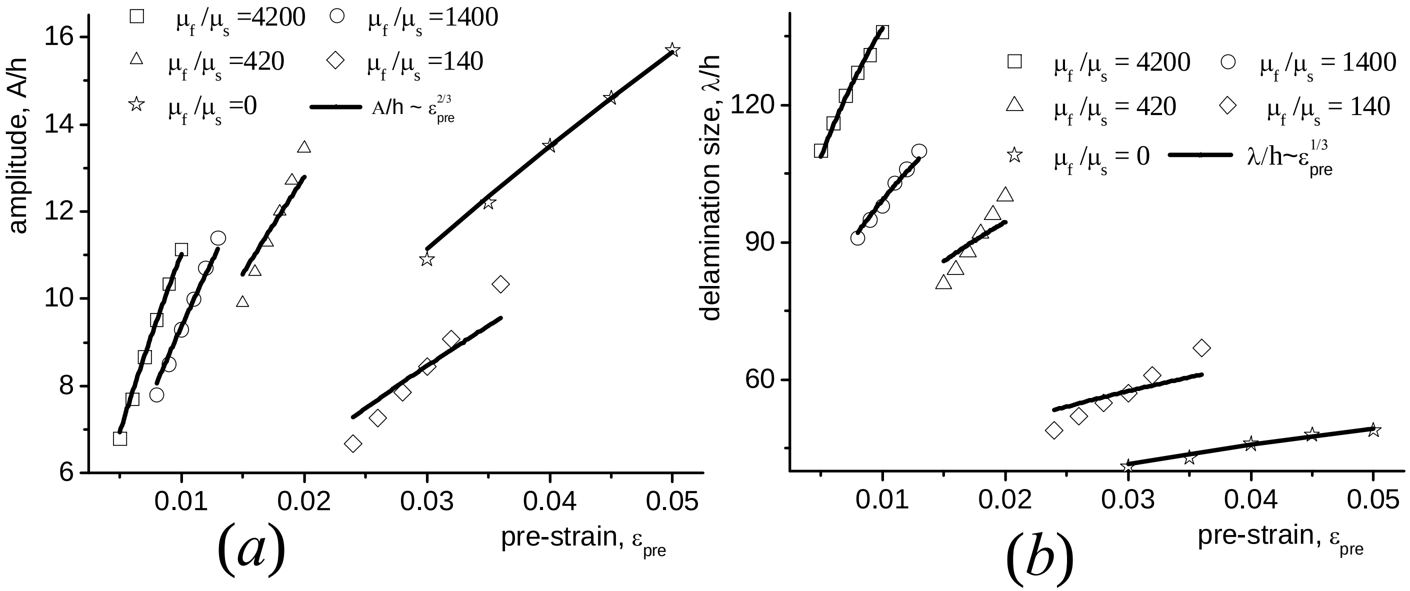




$$A/h \sim \varepsilon_{pre}^{2/3} \quad A/h \sim \gamma_n^{-1/6} \quad \lambda / h \sim \varepsilon_{pre}^{1/3} \quad \lambda / h \sim \gamma_n^{-1/3}$$

K. Pan, Y. Ni, L.H.He, R.Huang, IJSS(2014).

profile of straight-sided blister: scaling law

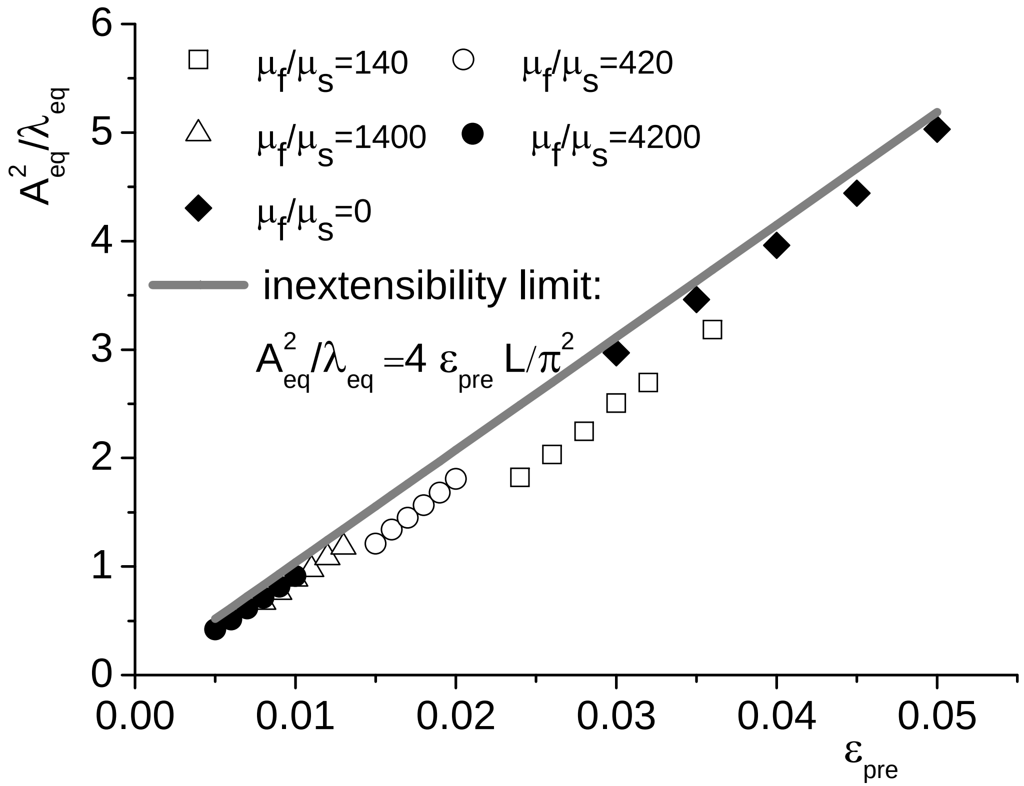


$$E^f_{bend} = DL\pi^4 A^2_{eq} / \lambda^3_{eq} \qquad E_{interface} = \gamma_n \lambda_{eq} L$$

$$U^{total}_{blister} = E^f_{bend} + E_{interface}, \frac{\partial U^{total}_{blister}}{\partial \lambda} = 0$$

$$\mathrm{A}/h \sim \varepsilon^{2/3}_{pre} \quad \mathrm{A}/h \sim \gamma_n^{-1/6} \quad \lambda / h \sim \varepsilon^{1/3}_{pre} \quad \lambda / h \sim \gamma_n^{-1/3}$$

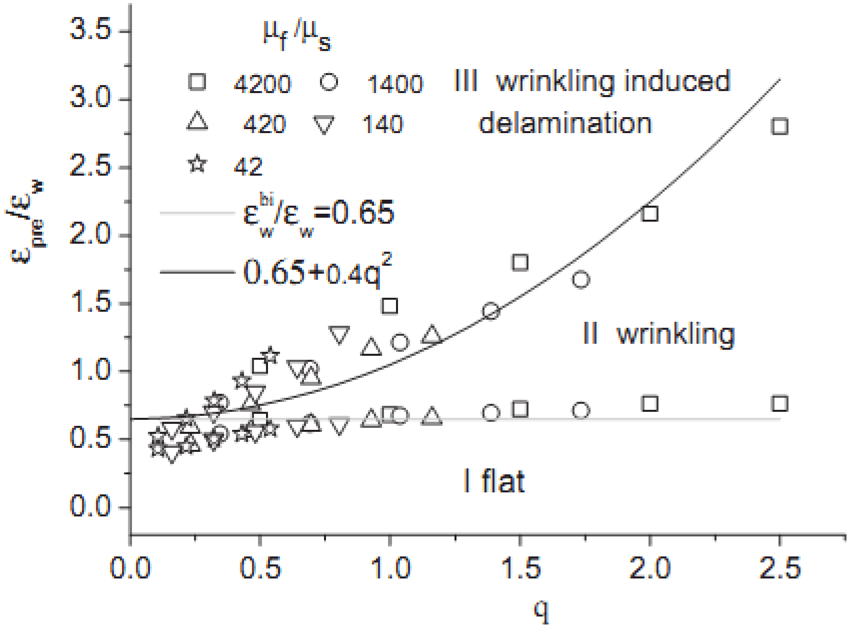
The condition for the valid scaling laws



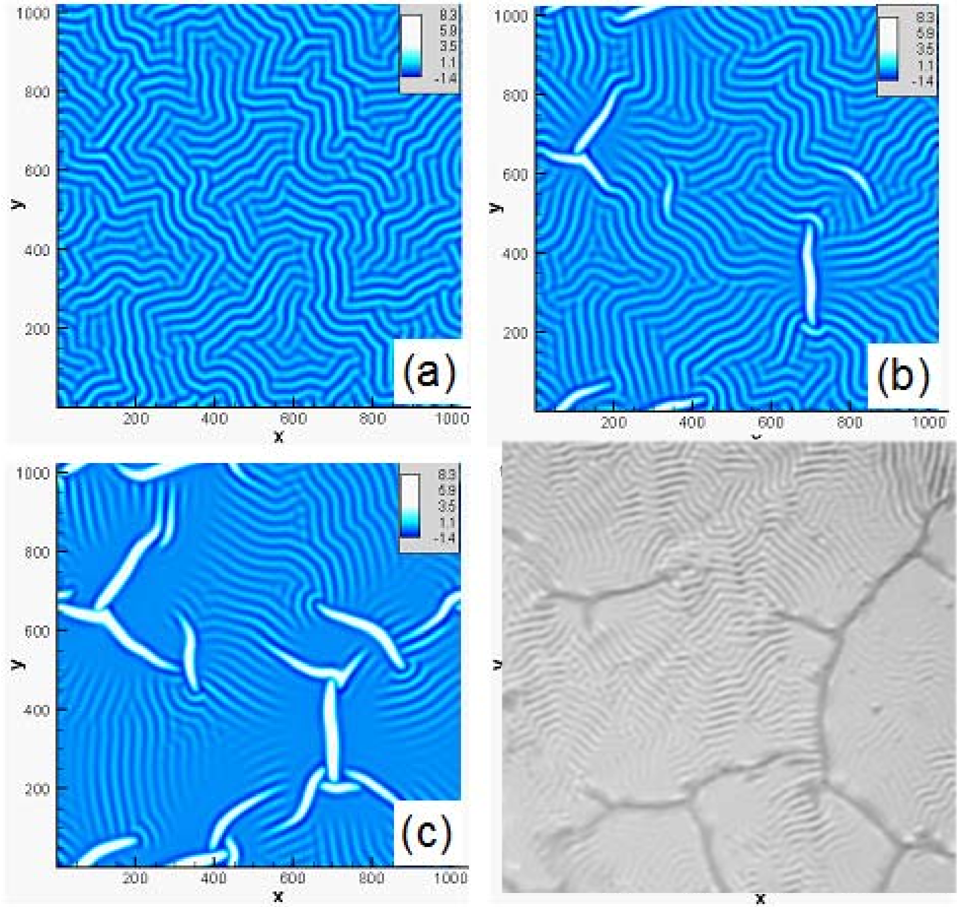
$$A_{eq}^2 / \lambda_{eq} = 4\varepsilon_{pre} L / \pi^2 \quad \Rightarrow \quad U_{stretch}^f = \frac{\mu_f h L^2}{(1-\nu_f)} \left(\frac{\pi^2 A_{eq}^2}{4\lambda_{eq} L} - \varepsilon_{pre} \right)^2 \to 0$$

Transition from wrinkling to buckle-delamination

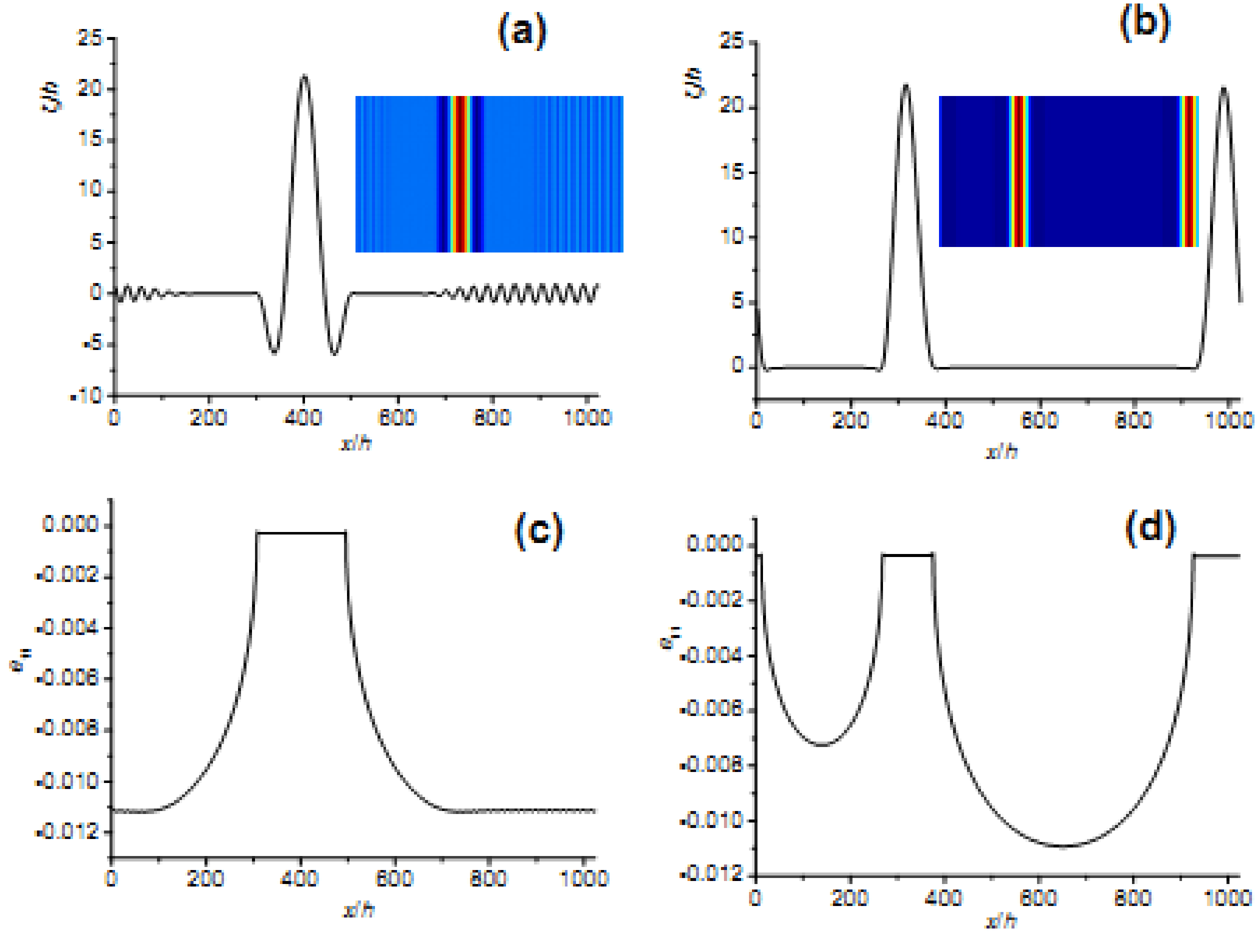
Biaxial compression



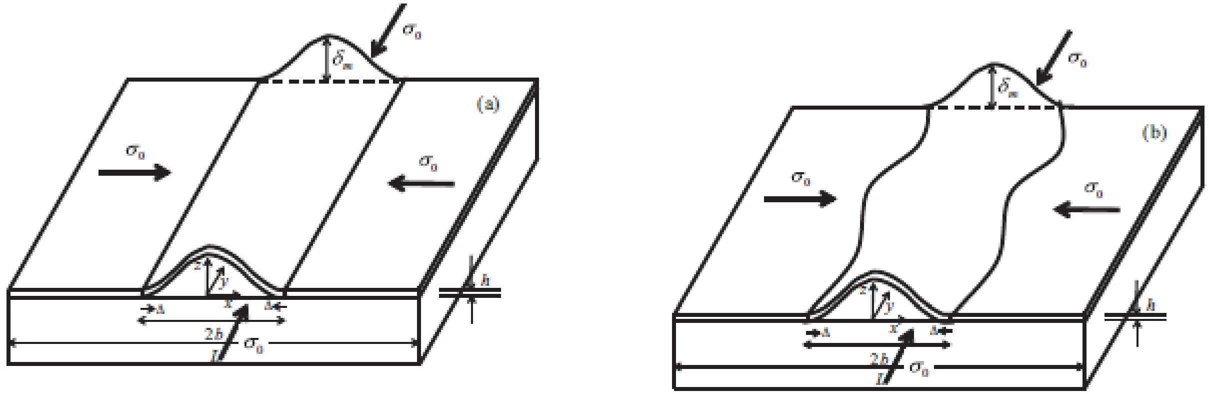
$$q=\frac{5(3-4v_s)\gamma_n}{4(1-v_s)\mu_s eh}\left(\frac{\mu_f(1-v_s)}{3\mu_s(1-v_f)}\right)^{1/3}$$



Coexisting wrinkling and buckle-delamination



Effect of sliding on the stability of straight-sided blister



$$\zeta = \begin{cases} \dfrac{\delta_m}{2}\left(1+\cos\dfrac{\pi x}{b}\right) & 0 \le |x| \le b \\ 0 & b \le |x| \le L/2 \end{cases}, \quad u_x = \mp\Delta,\ u_y = 0,\ \zeta = \zeta_{,x} = 0 \text{ at } x = \pm b.$$

$$u(x) = \frac{\pi\delta_m^2}{32b}\sin\frac{2\pi x}{b} - \frac{\Delta}{b}x, \qquad \delta_m = \frac{4b}{\pi}\sqrt{(1+\nu)\varepsilon_0 - \varepsilon_E + \frac{\Delta}{b}},$$

(A. Ruffini, et al., Acta Mater., 2012)

$$\Delta_m = (\varepsilon_0 - \varepsilon_E)(L/2 - b), \qquad \Delta = \alpha\Delta_m \qquad \alpha \in [0,1]$$

$$\varepsilon_E = \frac{\pi^2}{12}\left(\frac{h}{b}\right)^2$$

ε_0 initial compressive strain in the film

A linear stability analysis of FvK plate equations based on the shooting method

χ Airy potential, D bending stiffness

The FvK equations:

$$\nabla^4 \chi + E\left[\frac{\partial^2 \zeta}{\partial x^2}\frac{\partial^2 \zeta}{\partial y^2} - \left(\frac{\partial^2 \zeta}{\partial x \partial y}\right)^2\right] = 0,$$

$$D\nabla^4 \zeta + h\sigma_0 \nabla^2 \zeta - h\{\chi, \zeta\} = 0,$$

$$\frac{\partial u_x}{\partial x} = \frac{1}{2\mu(1+\nu)}\left(\frac{\partial^2 \chi}{\partial y^2} - \nu \frac{\partial^2 \chi}{\partial x^2}\right) - \frac{1}{2}\left(\frac{\partial \zeta}{\partial x}\right)^2,$$

$$\frac{\partial u_y}{\partial y} = \frac{1}{2\mu(1+\nu)}\left(\frac{\partial^2 \chi}{\partial x^2} - \nu \frac{\partial^2 \chi}{\partial y^2}\right) - \frac{1}{2}\left(\frac{\partial \zeta}{\partial y}\right)^2,$$

$$\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} = \frac{-1}{\mu}\frac{\partial^2 \chi}{\partial x\, \partial y} - \frac{\partial \zeta}{\partial x}\frac{\partial \zeta}{\partial y}.$$

$$\chi_b = \left(\frac{E\pi^2 \delta_m^2}{32 b^2 \left(1-\nu^2\right)} - \frac{E\Delta}{b}\right)\left(y^2 + \nu x^2\right)$$

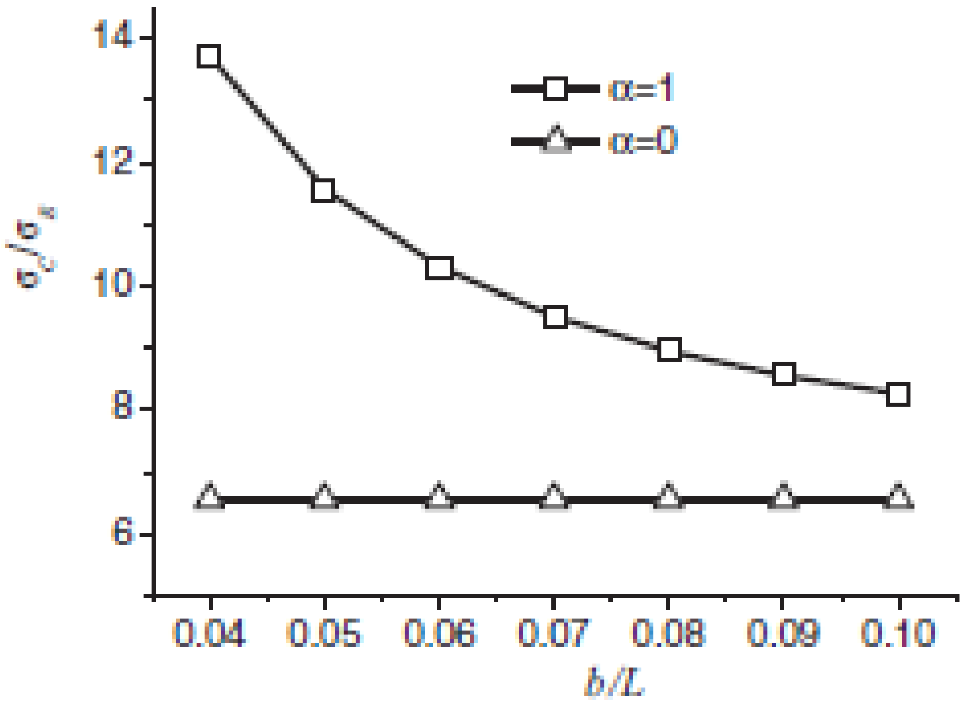
$$\zeta_b = \begin{cases} \frac{\delta_m}{2}\left(1 + \cos\frac{\pi x}{b}\right) & 0 \le |x| \le b \\ 0 & b \le |x| \le L/2 \end{cases},$$

perturbation

$$\left(\zeta_b + \zeta_{lin}, \chi_b + \chi_{lin}\right)$$

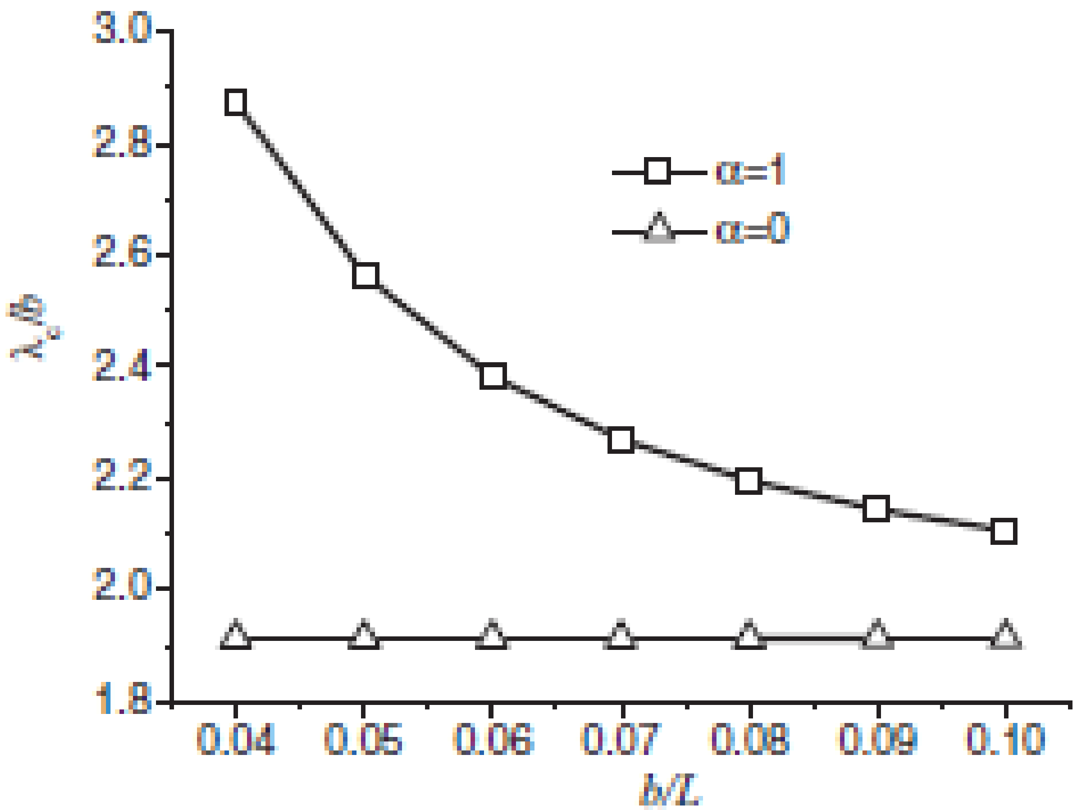
Pan & Ni & He, PRE (2013)

Critical stress changes with the changes of α and b / L



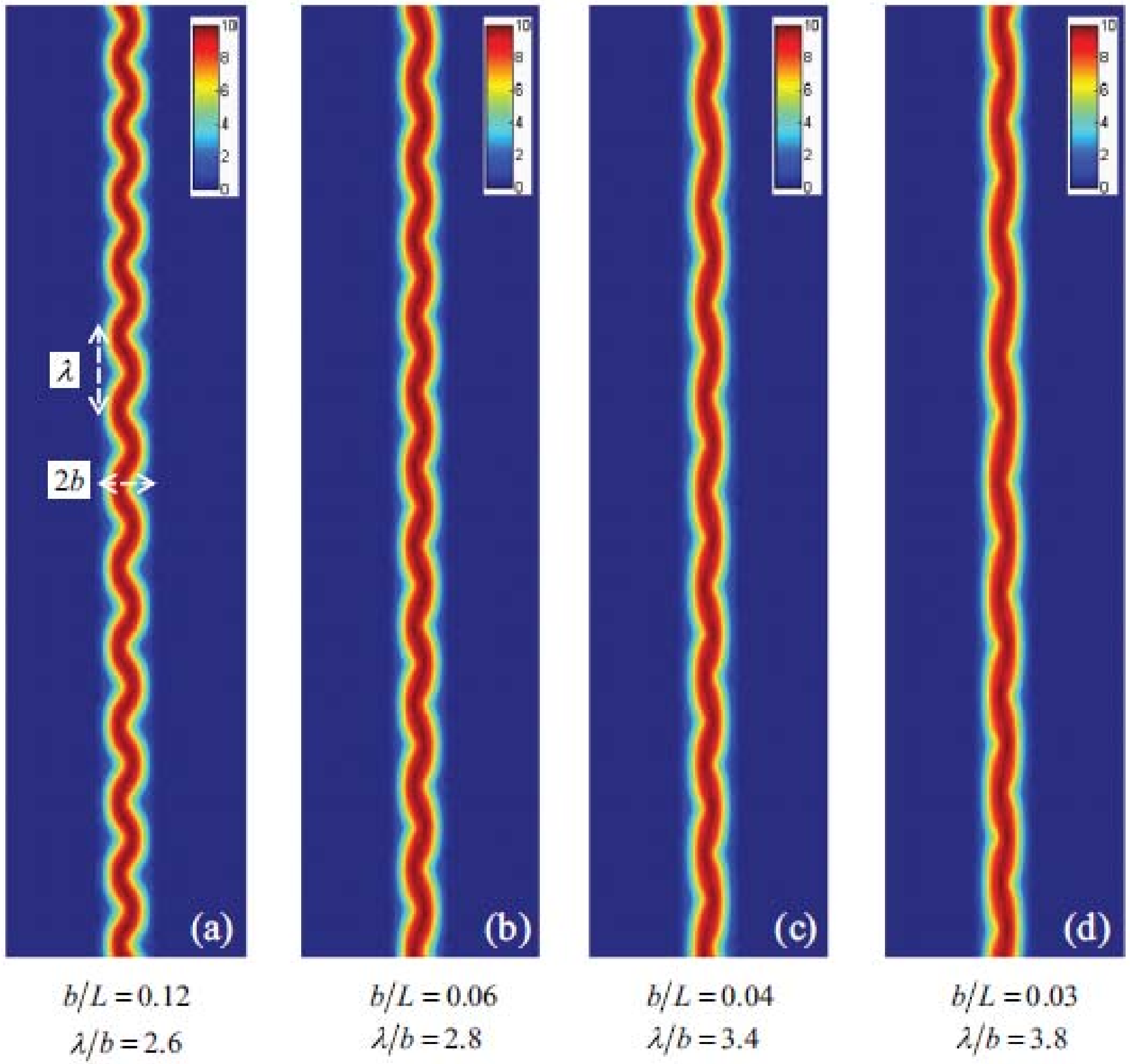
$$\sigma_E = \frac{Eh^2}{12(1-\nu^2)b^2} \qquad \upsilon = 0.3, \mathrm{L} = 1000\mathrm{h}$$

Critical wavelength changes with the changes of α and b / L



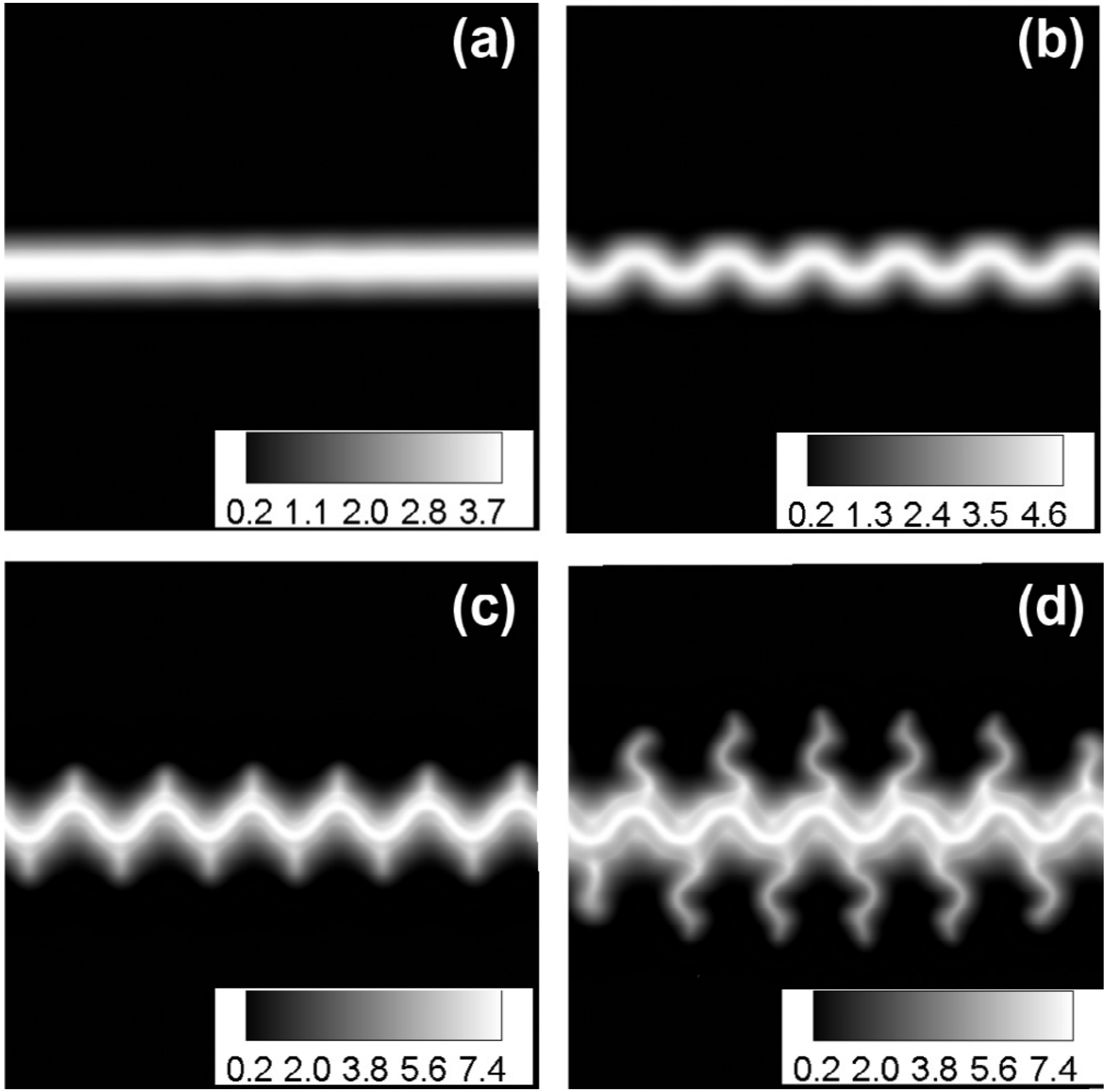
$\upsilon = 0.3, \mathrm{L} = 1000\mathrm{h}$

Simulated result: effect of interface sliding



Pan K, et al, 2013, PRE

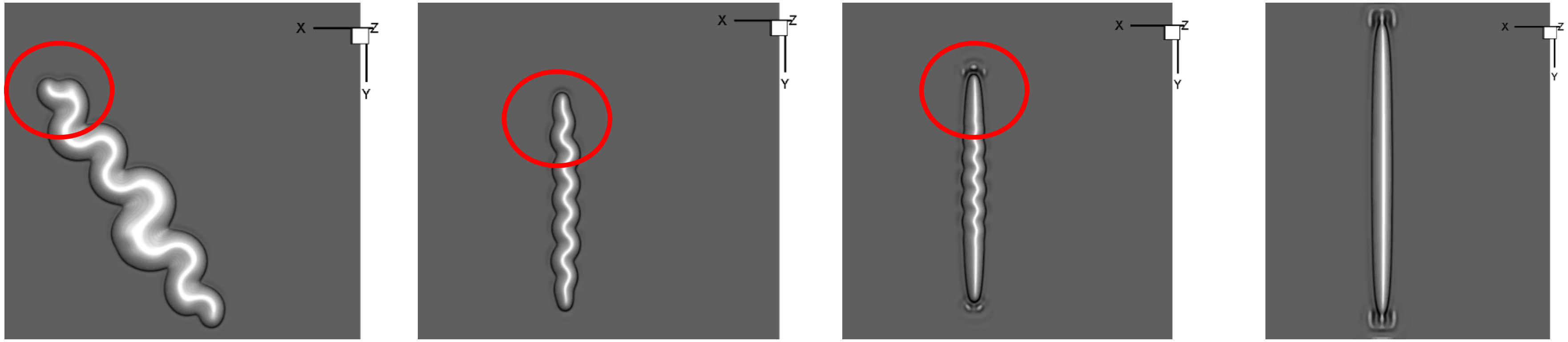
buckle branching induced by high compression

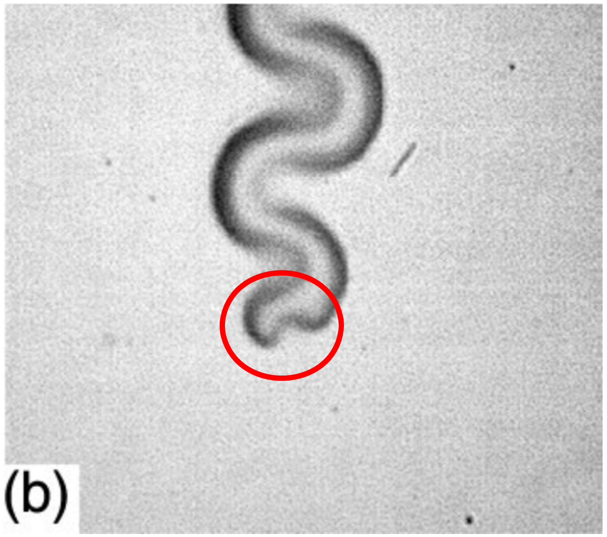


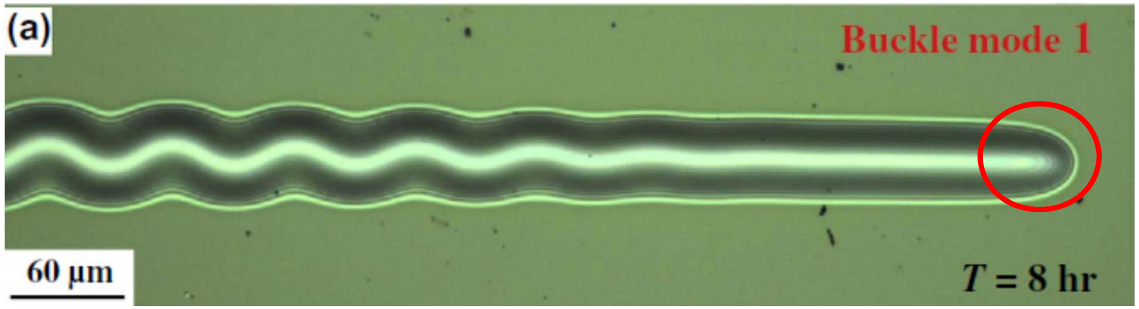
Substrate compliance on the buckle-delamination growth

$$\frac{\mu_f}{\mu_s} = 5, 20, 40, 100$$

Our simulation



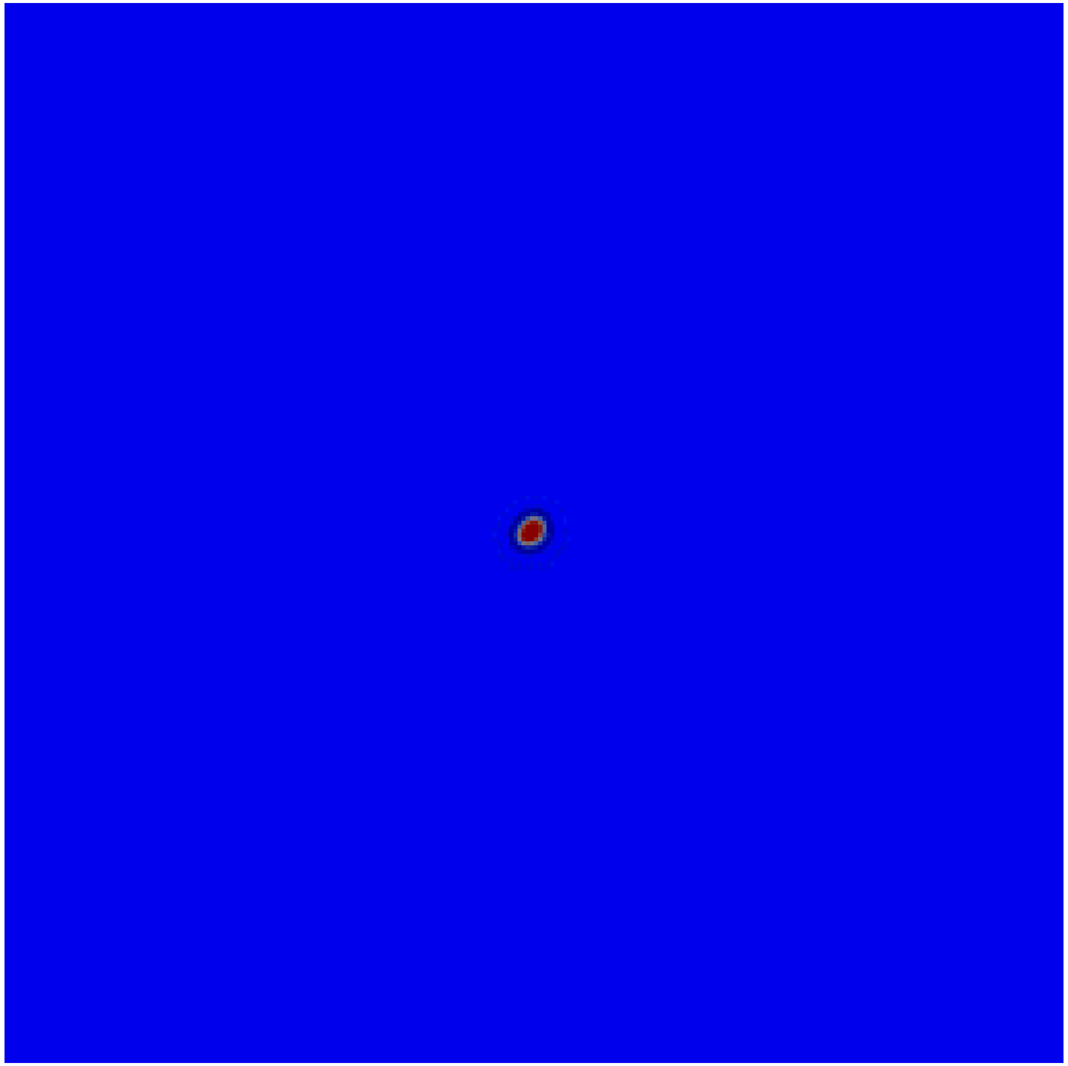


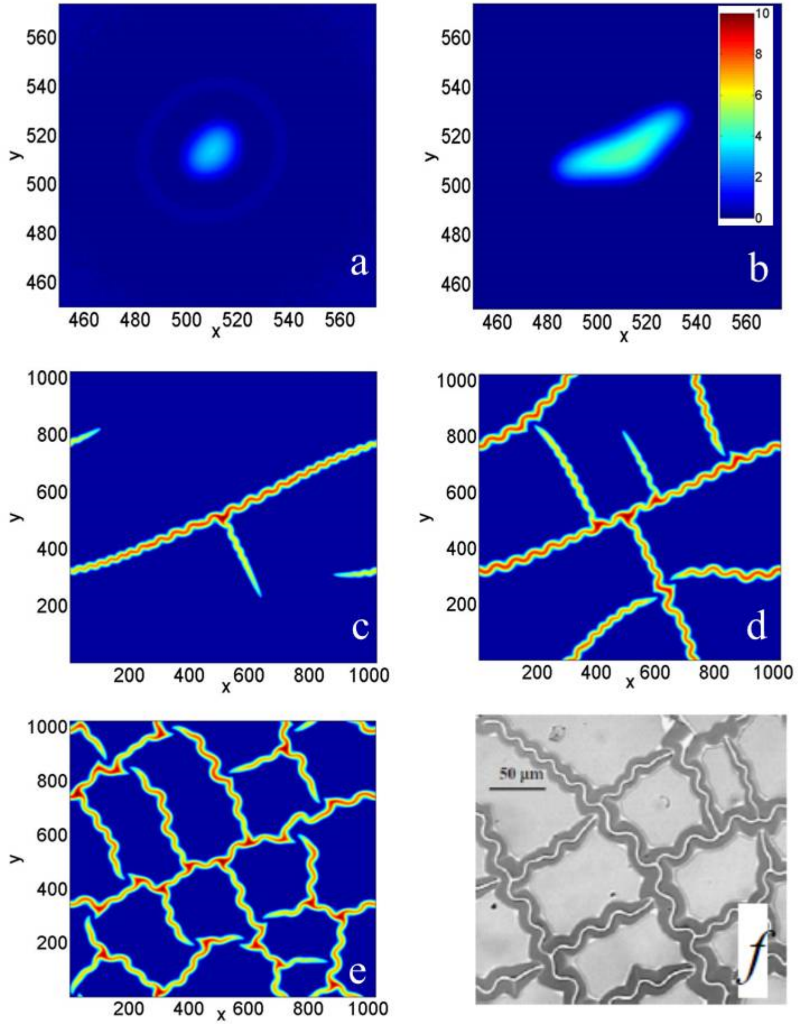


Yu SJ, et al, 2013, Surf.Coat,Tech.

Faou JY, et al, PRL (2012)

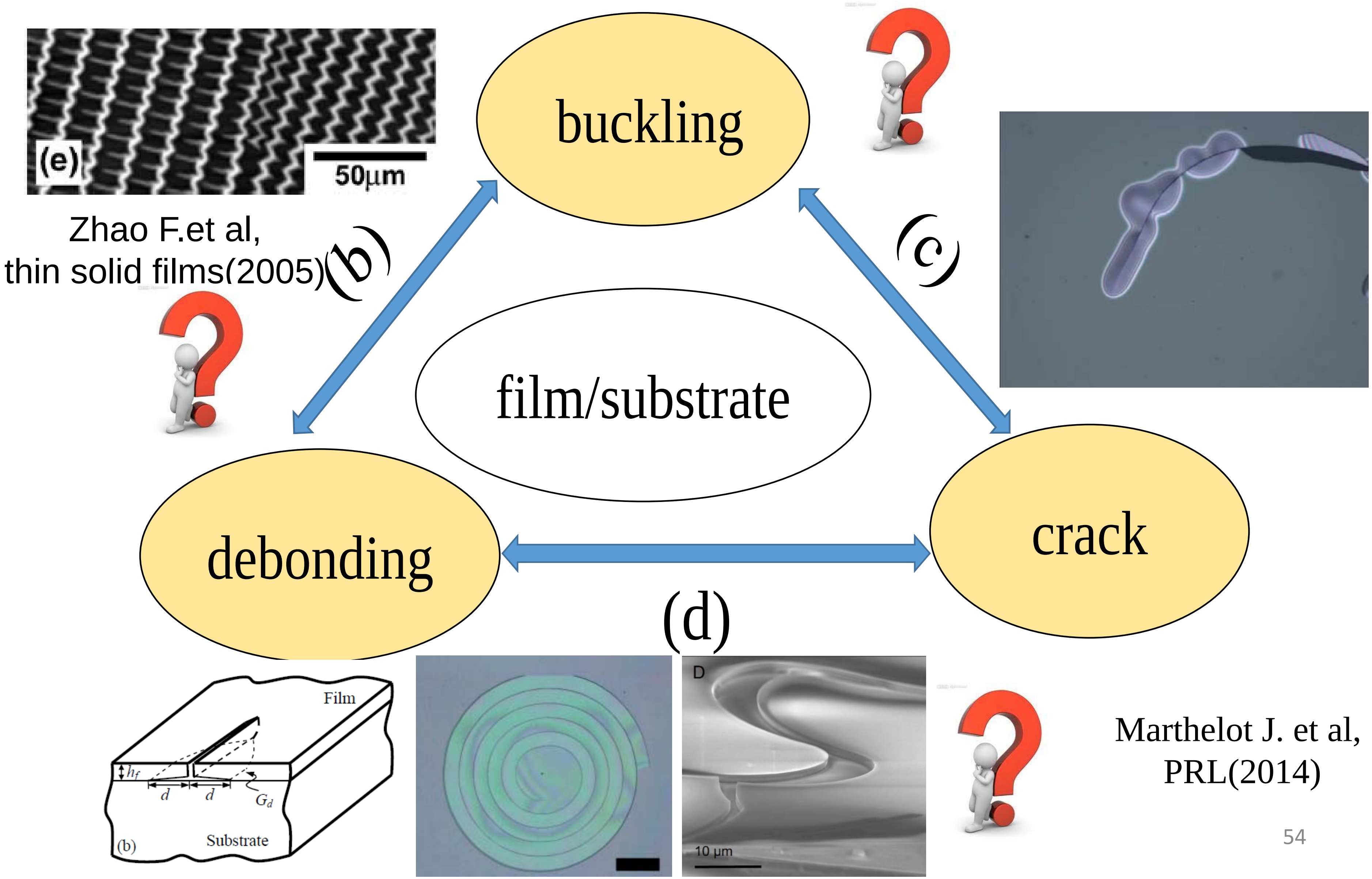
Formation of network-like blisters





Y. Ni, and Soh AK, 2014 Acta Mater

Microstructural evolution in film/substrate systems



Conclusions

- A phase field modeling of combined buckling, delamination and cracking of layered materials is developed.
- Complex wrinkling patterns comparable with experiments are recovered.
- Transition from wrinkling to buckle-delamation can be fully tracked.
- The effects modulus ratio, interface adhesion and compression amplitude on the buckle-delamination are discussed.

Thanks

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