

固体力学与计算材料

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捞车的尴尬

















◆ 结构受力平衡与稳定性

理论力学，一般力学与控制

湖南桃源，石门米糖制作过程



<http://blog.sina.com.cn/xiaoboheng19930121>

湖南桃源，石门米糖制作过程

麦芽和发酵的米熬制后







龙须酥

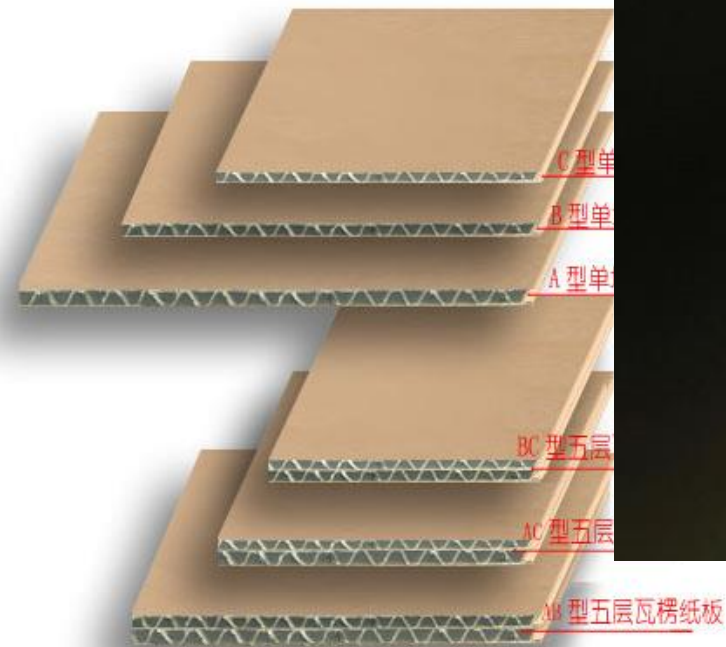
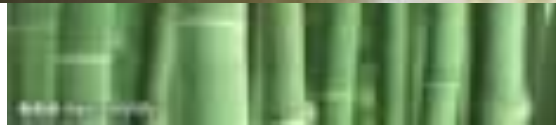


◆ 你会切米糖吗？

A: 用手掰 B 用刀切 C 用木头敲

◆ 炼糖与炼钢的相似性

固体变形的学问



材料
高性能化

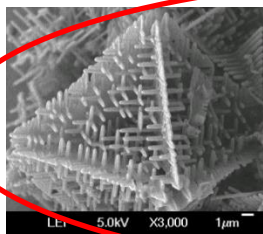
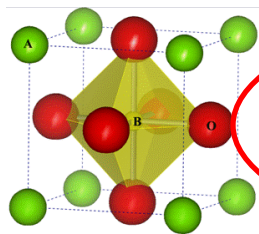
原子层次

纳米

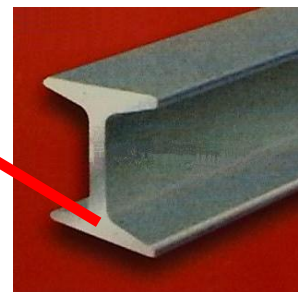
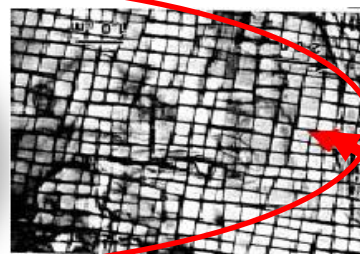
细观层次

微米

宏观



微结构
调控



定量化



材料制备

评估设计



Integrated computational Materials
Science and Engineering (ICMSE)

材料微结构演变与
性能调控的计算材料研究

计算材料
微结构力学

提纲

□ 计算材料简介

□ 固体力学简介

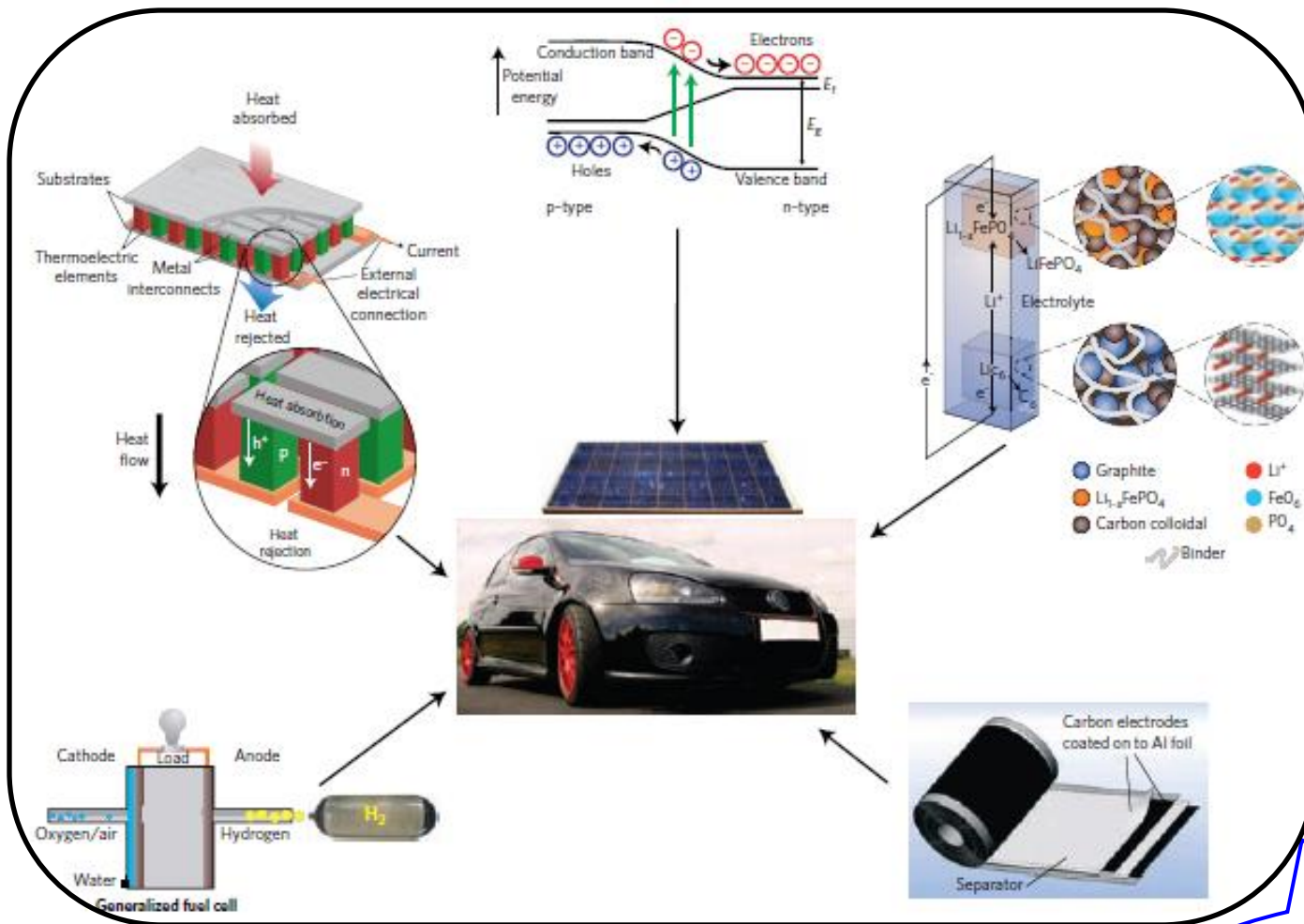
□ 固体力学在材料中的应用

1. 超材料、材料强韧化设计举例

2. 功能材料的力学稳定性与寿命分析举例

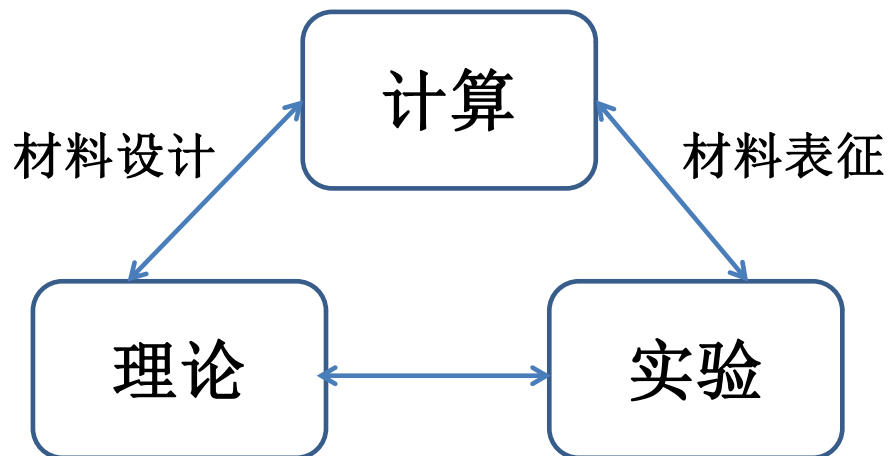
3. 基于变形耦合的功能材料设计举例

4. 微结构演化调控的应力工程举例



Materials for sustainable energy, edited by V. Dusastre, world scientific, 2010

构筑并研究复杂材料体系是物质科学和技术发展的一个重要趋势



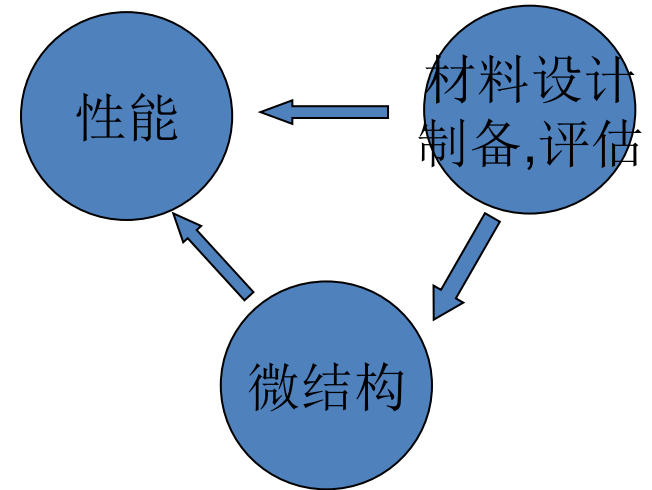
计算日益成为独立的重要科学手段，与理论和实验形成三足鼎立之势

材料设计（Materials by Design）

Meeting [2012 TMS Annual Meeting & Exhibition](#)

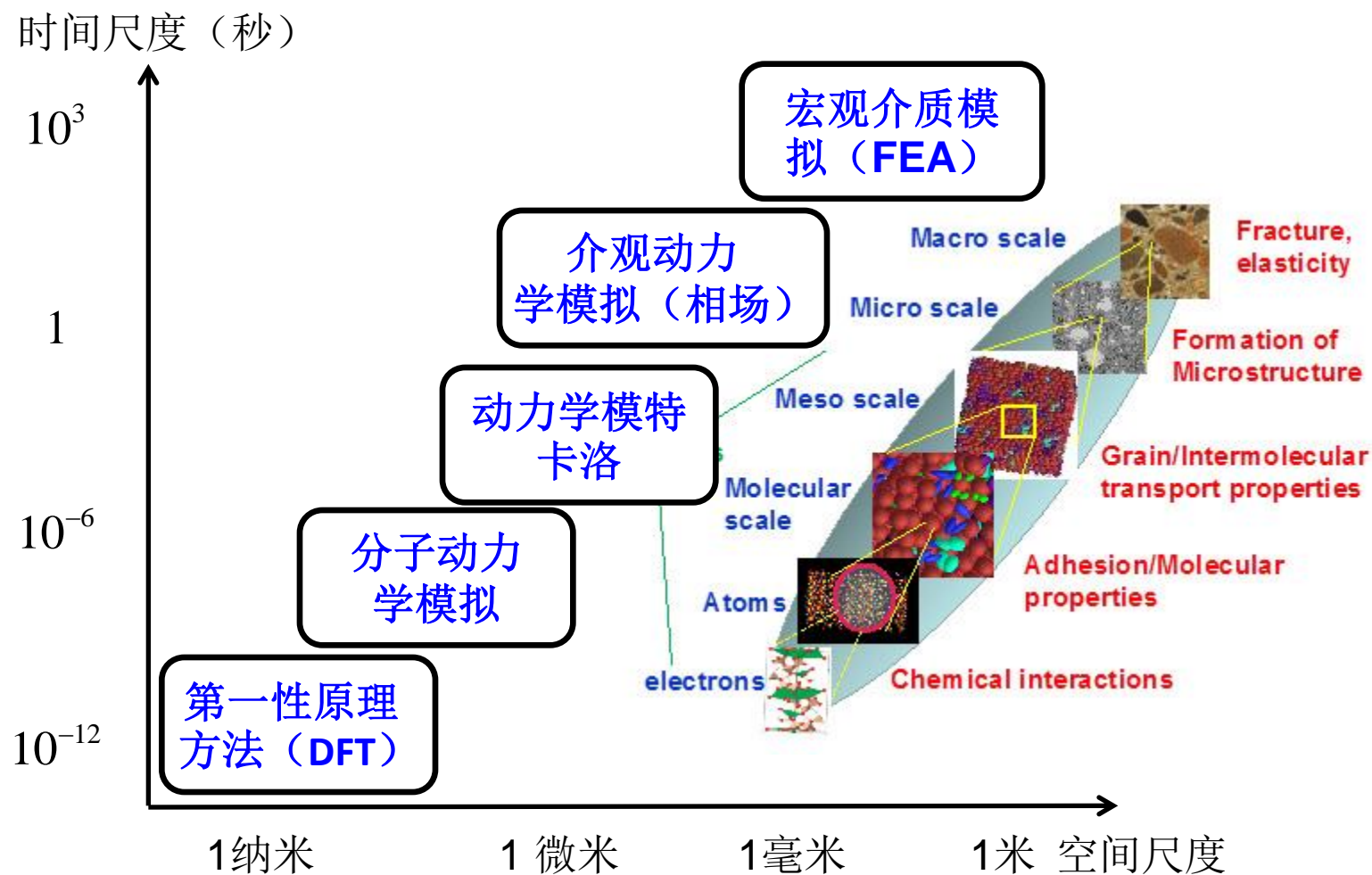
Symposium **Computational Thermodynamics and Kinetics**

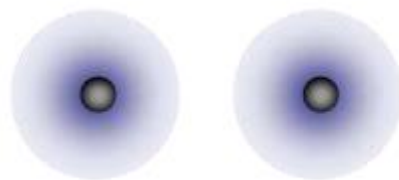
Sponsorship The Minerals, Metals and Materials Society
TMS Electronic, Magnetic, and Photonic Materials Division
TMS Materials Processing and Manufacturing Division
TMS Structural Materials Division
TMS: Alloy Phases Committee
TMS: Chemistry and Physics of Materials Committee
TMS/ASM: Computational Materials Science and Engineering Committee
TMS: Integrated Computational Materials Engineering Committee
TMS/ASM: Phase Transformations Committee
TMS: Process Technology and Modeling Committee



- 发展有效的计算材料学工具
- 理解材料性能与微结构的定量关联
- 微结构演化的预测
- 有序微纳米结构的可调控性

各个尺度的模拟方法





离子键

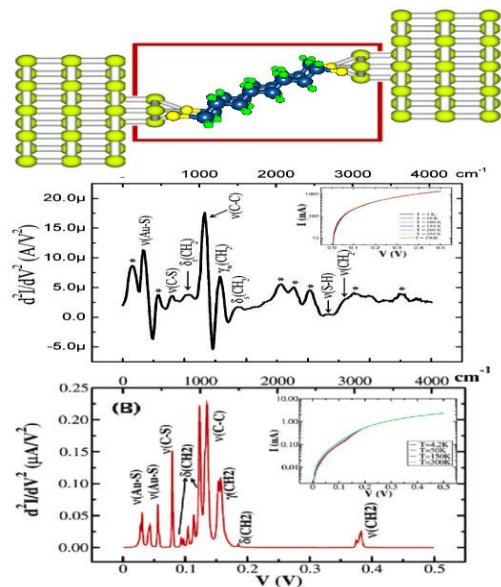


共价键

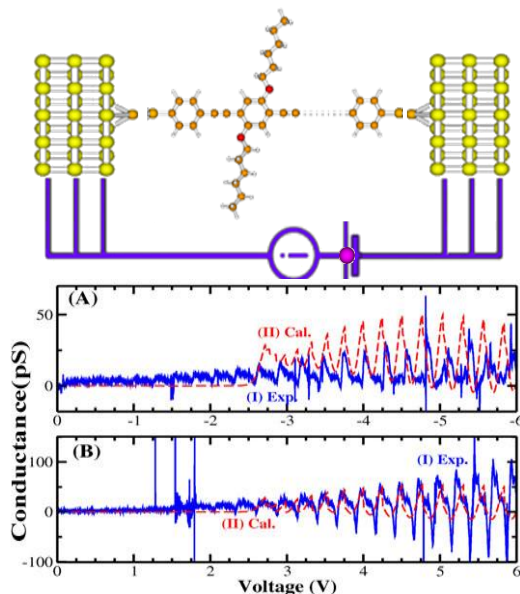
- ◆ 基于量子力学
- ◆ 电子结构计算
- ◆ 基态均匀体系的热力学性质与其它基本物性
- ◆ 结合统计方法计算激发态的性质：如相图等
- ◆ 分子尺度的材料与器件性质模拟与预测

分子尺度材料与器件性质表征

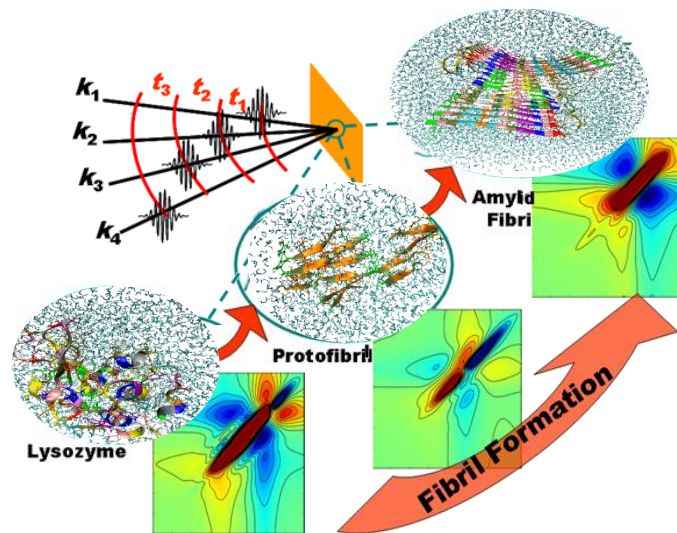
分子器件非弹性散射谱



大纳米尺度 polymer 电导谱



生物大分子溶液 多维光谱

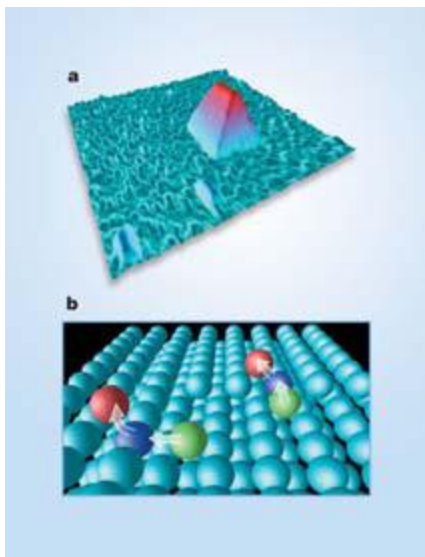


分子器件模拟：
描述分子结与
金属块材料耦合

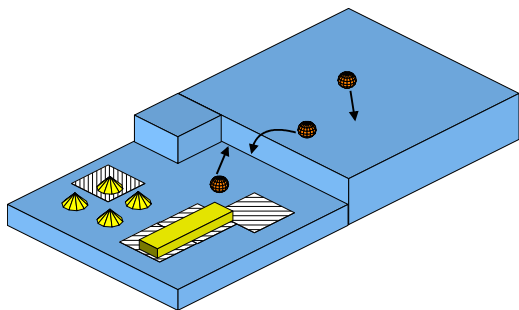
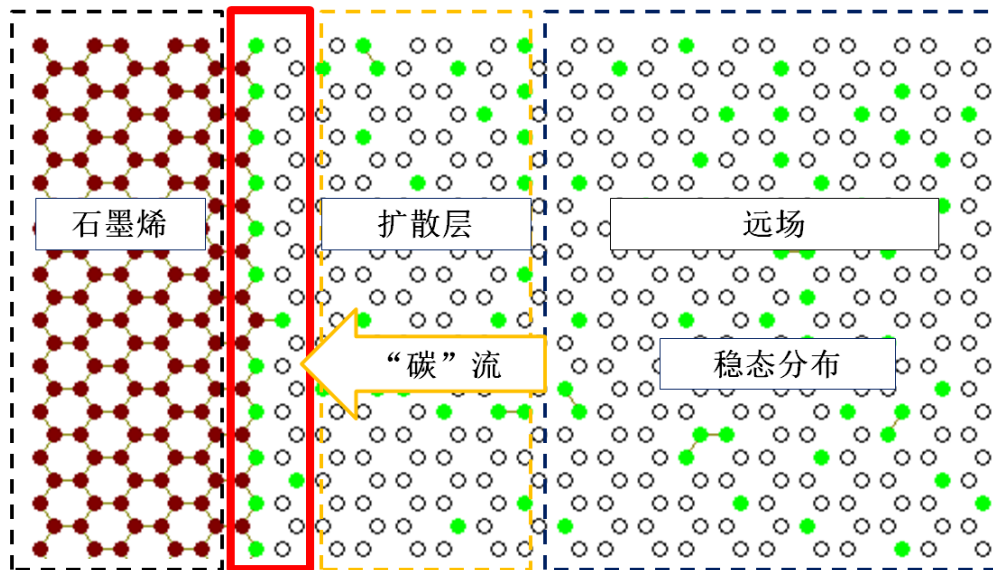
纳米材料科学：
连接小分子和
延展体系

生物分子光学：
微观分子性质的
宏观环境涨落效应

动力学Monte carlo 模拟：表面生长

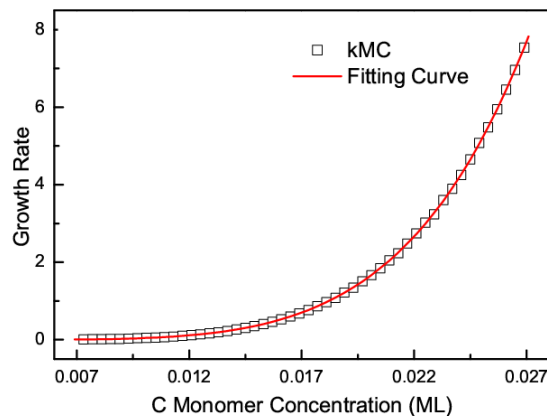


石墨烯非线性生长

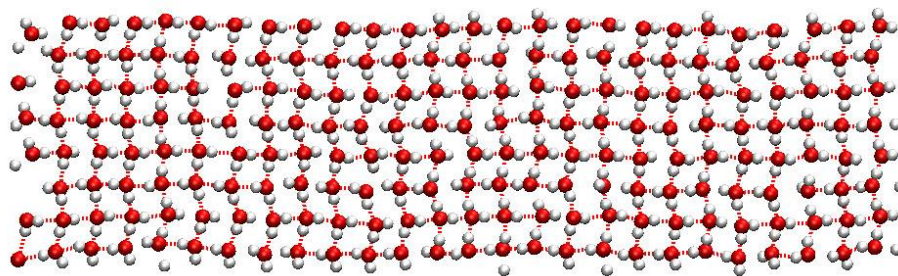
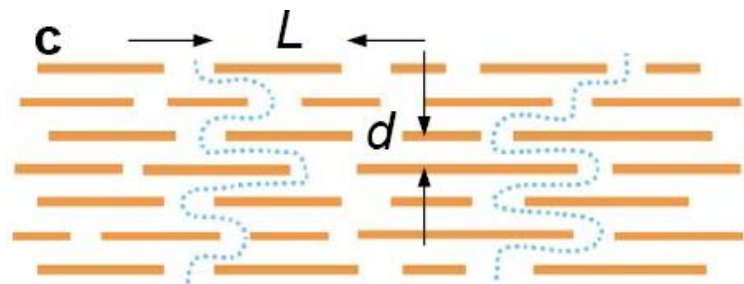
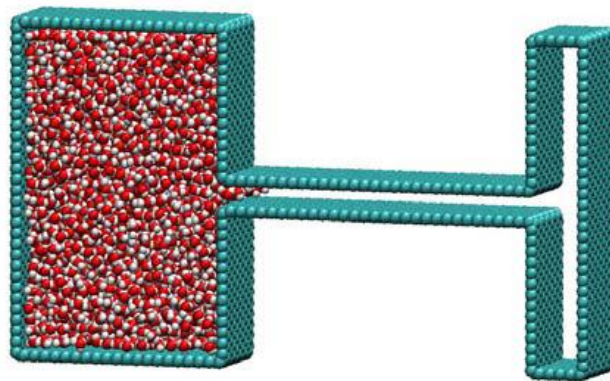
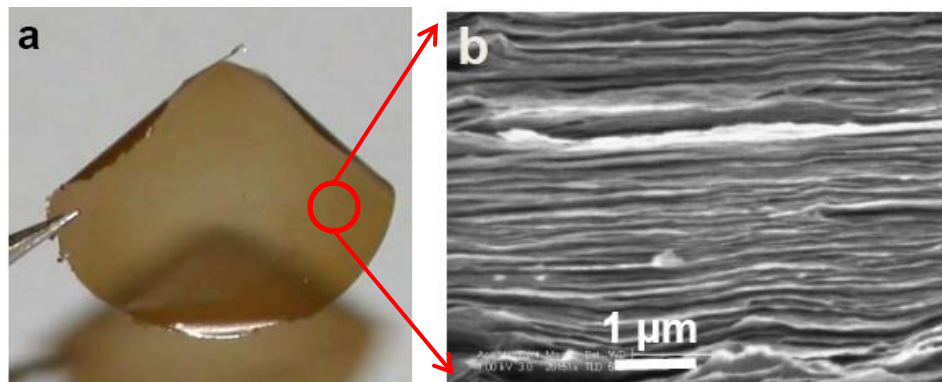


铝110表面形成巨型纳米岛的机理

完美重现实验
观察到的5次非
线性行为！

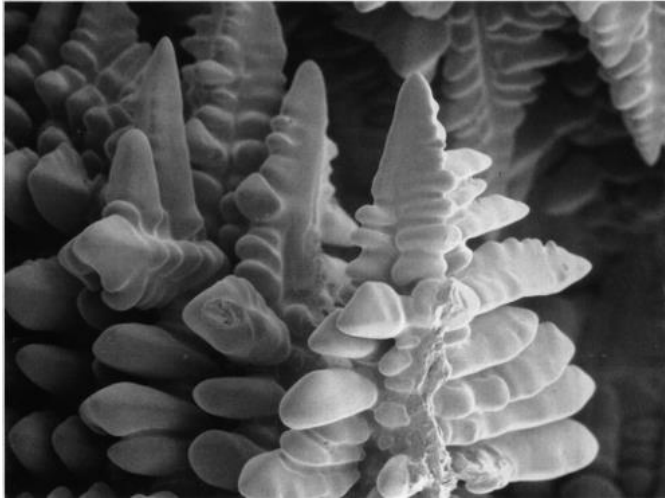


分子动力学模拟：界面微流动

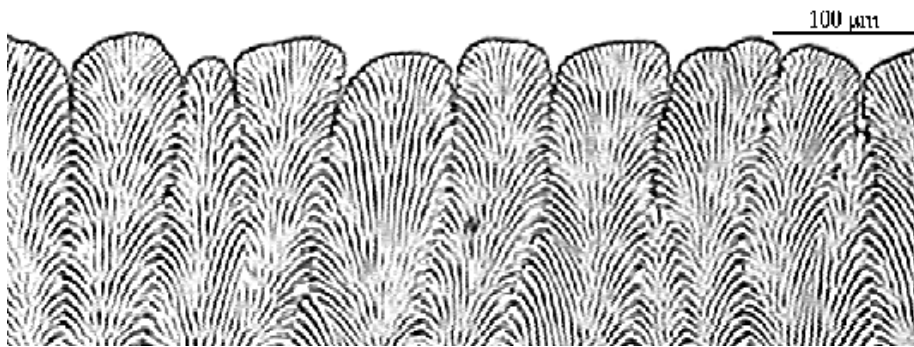
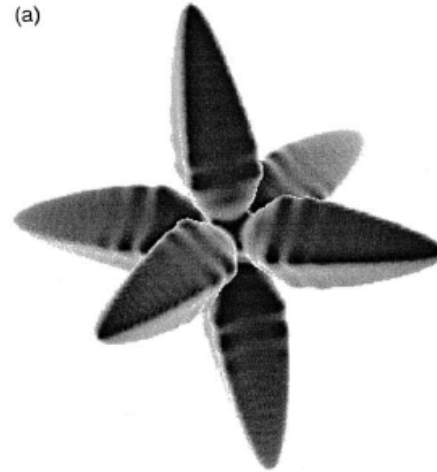


揭示氧化石墨烯薄膜的超透水机理：分子动力学模拟发现水分子可以自发进入到间隙只有0.35nm左右的两层石墨烯形成的纳米通道中，水分子在石墨烯纳米通道自发形成二维的网络状类固体结构，水分子的快速定向运动是蒸发和纳米通道毛细作用联合驱动。

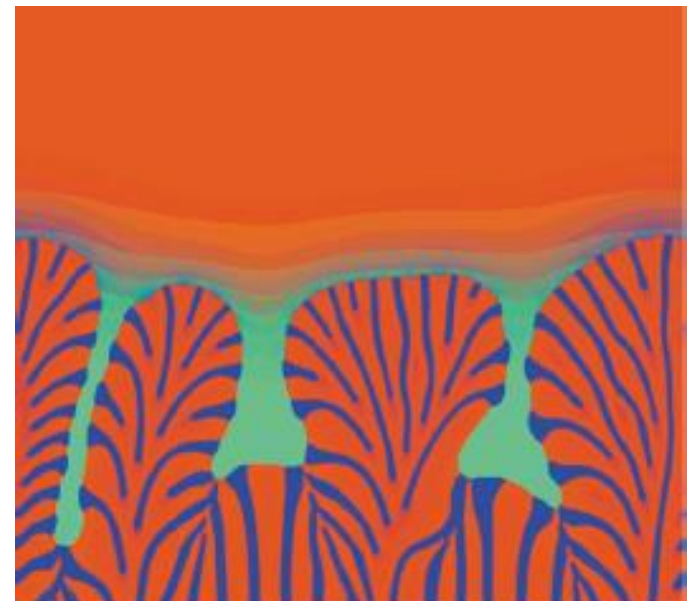
介观相场模拟:固化微结构



Dendrites (Co-Cr)



Eutectic colonies



W. J. Boettinger et al 2002

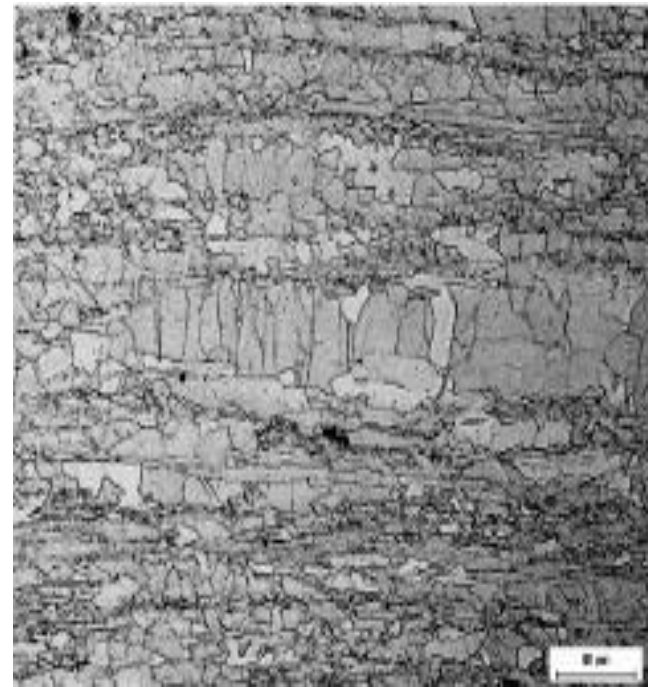
固体力学

- **固体力学研究内容**

研究固体在一定条件下的变形和破坏现象。

- **基本方法**

均匀化、连续化。



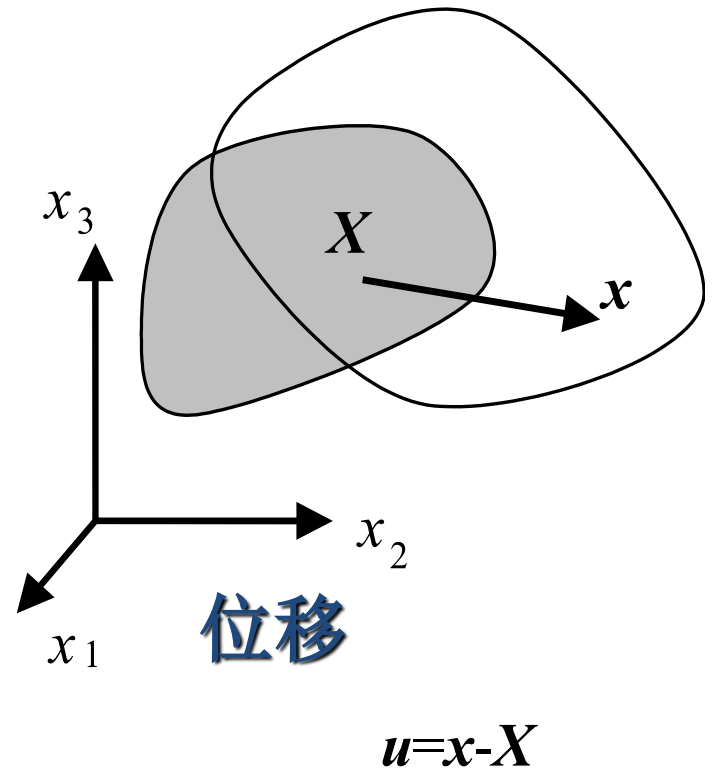
一种钢的微结构

固体变形的描述

应变张量

$$\boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{bmatrix}$$

$$\varepsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i} + u_{k,i} u_{k,j})$$



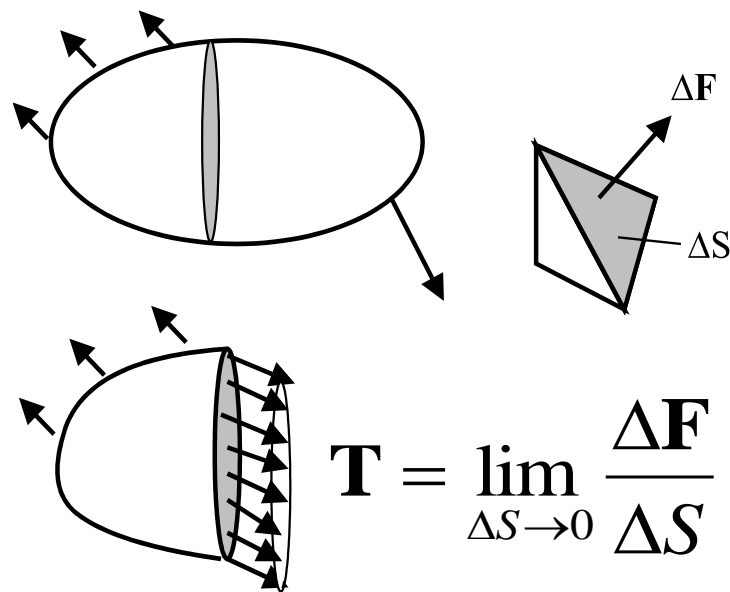
固体中的内力描述

应力张量

$$T = \sigma n$$

$$\sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} \end{bmatrix}$$

$$\sigma_{ij,j} + X_i = \rho \ddot{u}_i$$

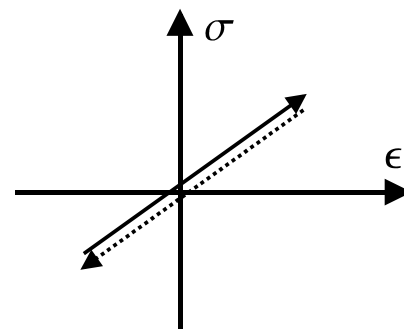


Cauchy应力

应力-应变关系 (本构方程)

$$\sigma = f(\varepsilon, \dots)$$

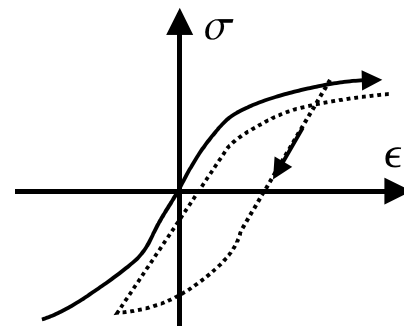
弹性



客观性条件
局部作用原理

弹性力学、塑性力学、
粘弹性力学、粘塑性力学。。。

塑性

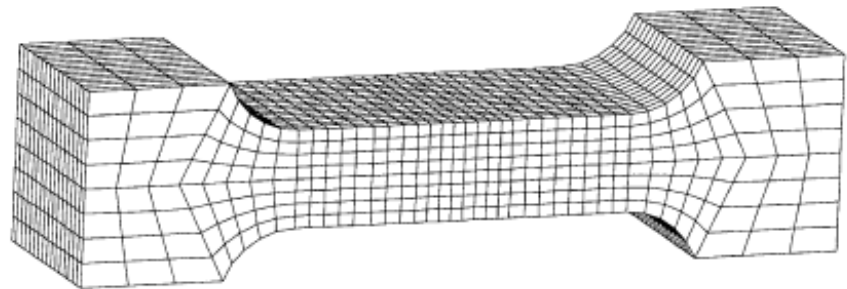
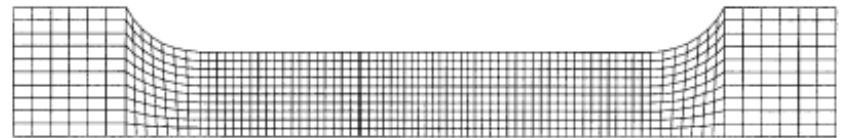
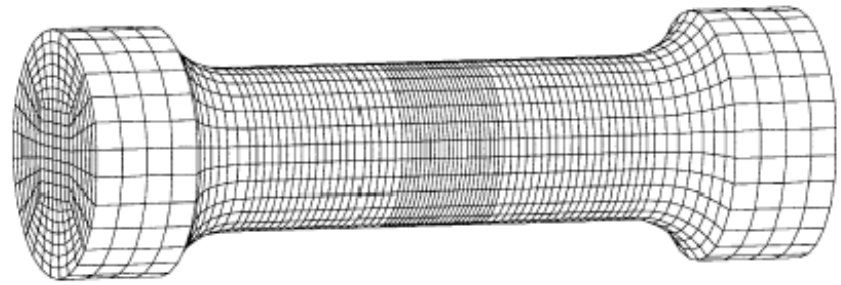


边值问题的求解

有限元法

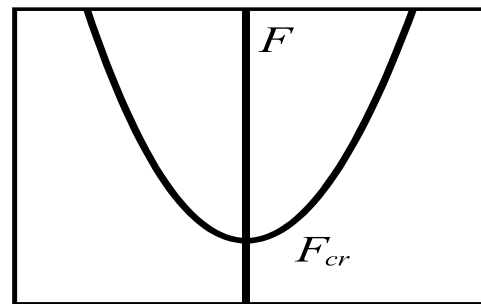
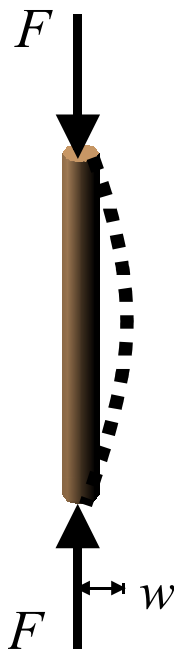
已有 **Abaqus, Ansys**
COMSOL
等商业软件

广泛用于各种宏观结构的变形与
受力设计,多场耦合问题求解

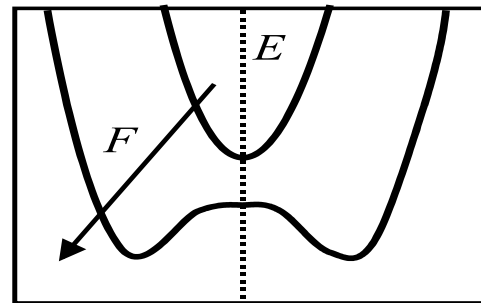


分叉与不稳定性

受压固体
一定条件
下出现多
个平衡状
态



w



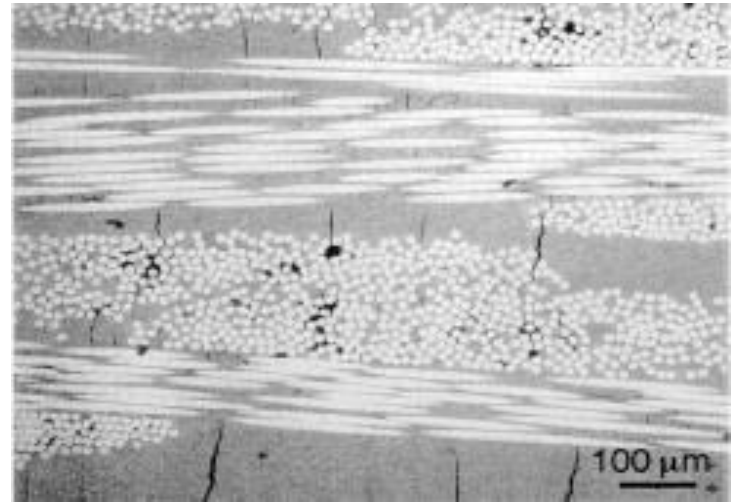
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Euler压杆

固体的破坏

固体 损伤 裂纹 扩展 断裂

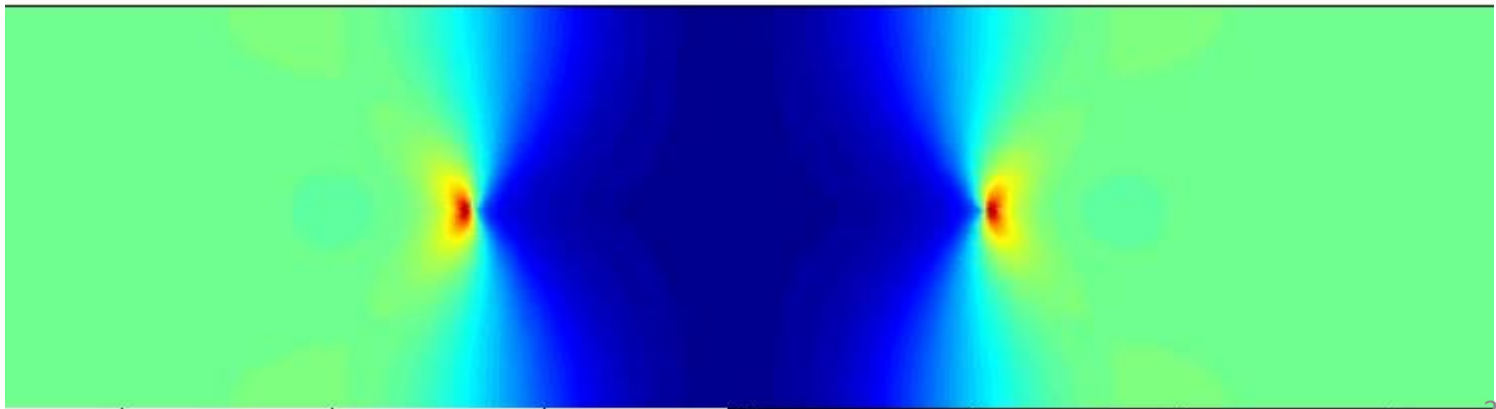
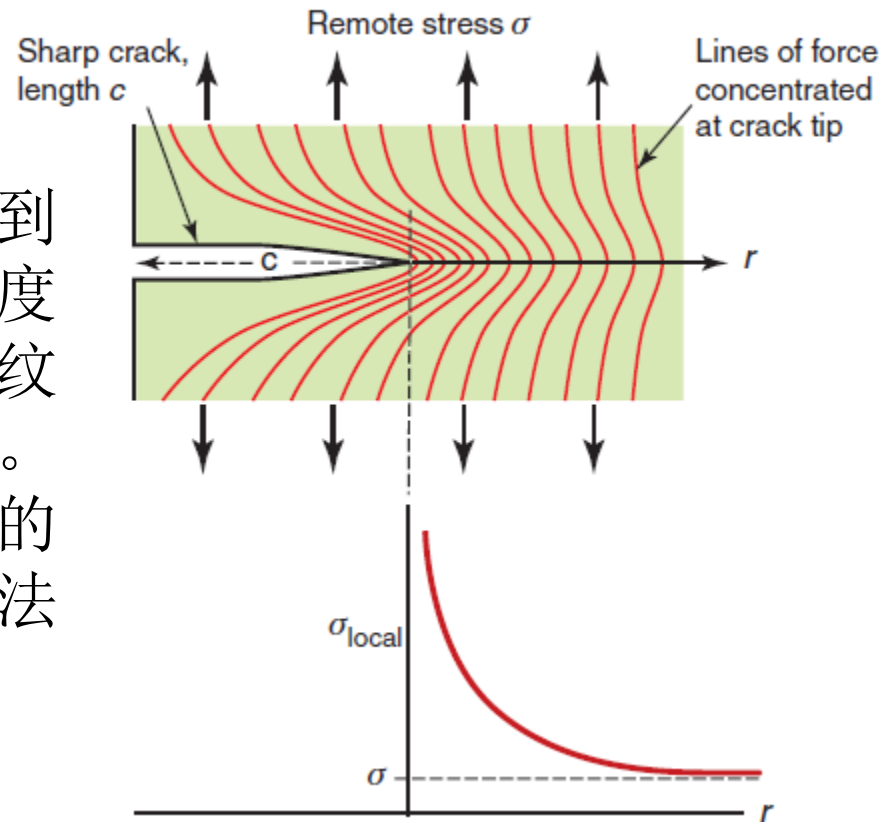
损伤力学
断裂力学



复合材料中的裂纹

应力集中

裂尖处应力集中揭示了外载传递到裂尖的现象，然而裂尖的断裂强度不确定，除非是原子层次尖锐裂纹，裂尖断裂强度为原子键合强度。另外裂尖处的应力集中与裂尖处的曲率有关，不容易确定。因而无法用应力准则研究裂纹扩展规律。



□ 裂纹形核与扩展

Griffith能量平衡原理1921

裂纹扩展导致的外载依赖的**机械能释放**提供了裂纹扩展的驱动力，裂尖扩展产生的新表面能等能量耗散提供了裂纹扩展**阻力**。裂纹处于热力学平衡时驱动力与阻力相等。

扩展条件

$$\frac{d(U_m + U_s)}{dA} < 0$$

或

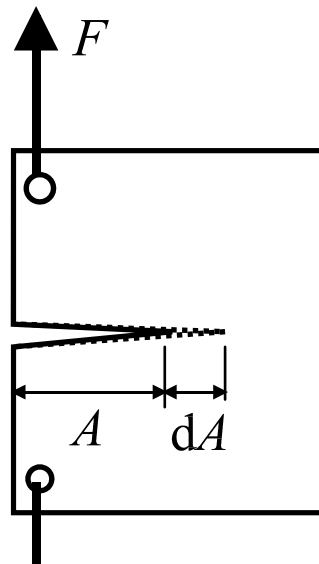
$$-\frac{dU_m}{dA} > \frac{dU_s}{dA}$$

驱动力

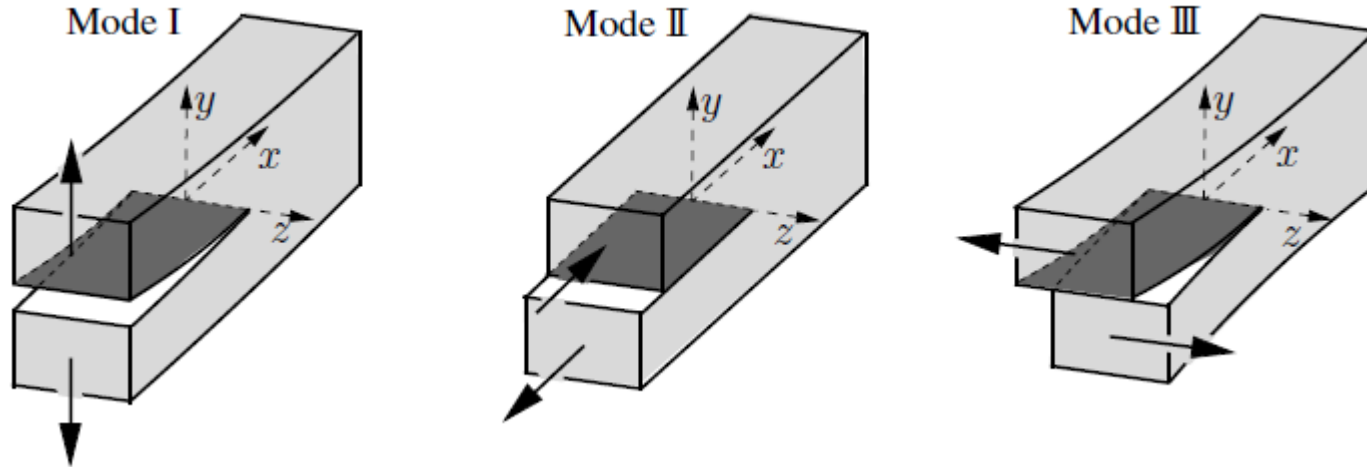
$$G = -\frac{dU_m}{dA}$$

阻力

$$R = \frac{dU_s}{dA}$$



线性断裂力学



三类典型裂纹

裂尖弹性场的普适解---K 场

$$\sigma_{ij} = \frac{K_m}{\sqrt{2\pi r}} f_{ij}^{(m)}(\theta) \text{ and } u_i = \frac{K_m}{2E} \left(\frac{r}{2\pi} \right)^{1/2} g_i^{(m)}(\theta)$$

$$K_m = \psi \sigma^{exit} \sqrt{a}$$

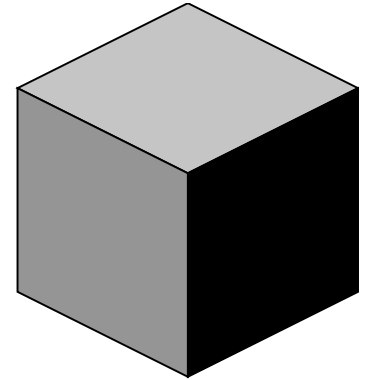
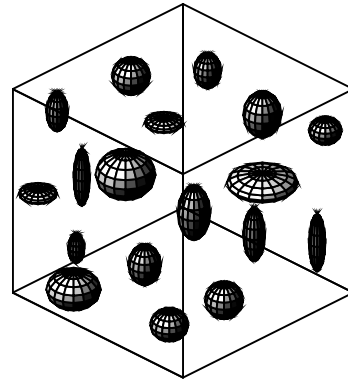
应力强度因子反映了裂尖场的奇异性强度，由外部边界条件、裂纹几何等决定。

细观力学

- 宏-细观物理量的关系:

$$Q = \frac{1}{V} \int_V q dV$$

- 建立考虑细观结构的宏观本构理论



体积元代表性

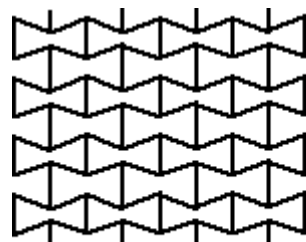
□ 固体力学在材料中的应用

1. 超材料、材料强韧化设计举例

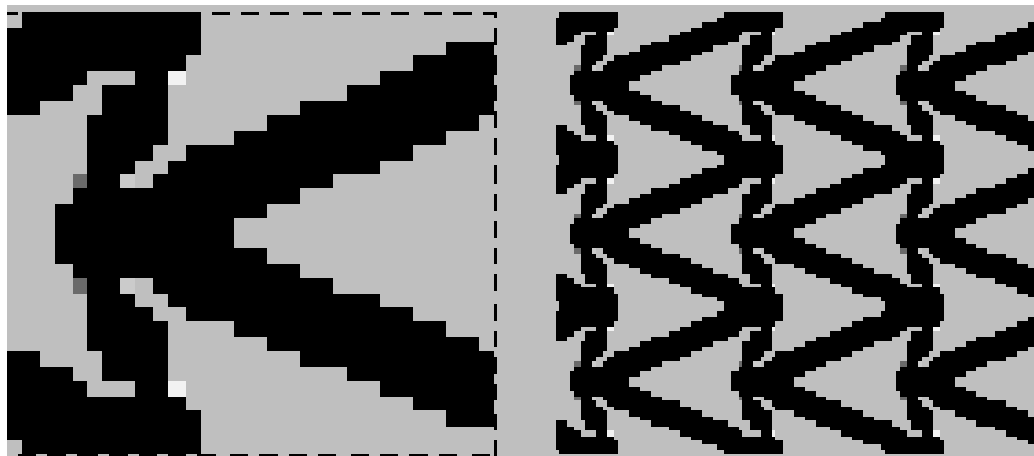
负泊松比材料



$$\nu = -\frac{d\varepsilon_{\text{trans}}}{d\varepsilon_{\text{axial}}} = -\frac{d\varepsilon_y}{d\varepsilon_x} = -\frac{d\varepsilon_z}{d\varepsilon_x}$$



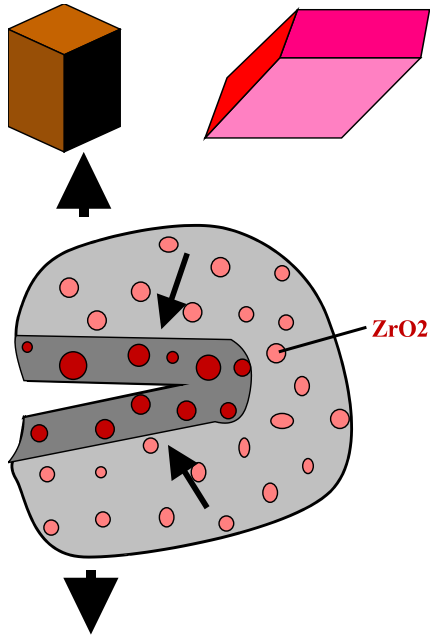
大部分传统材料: [0,0.5]



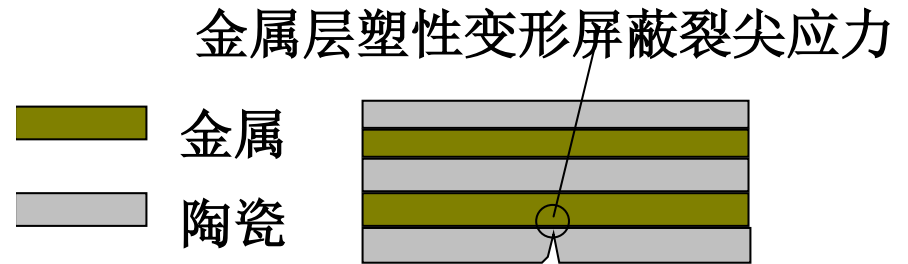
<http://silver.neep.wisc.edu/~lakes/>

Lakes, R. S., "Negative Poisson's ratio materials", *Science*, 238 551 (1987)

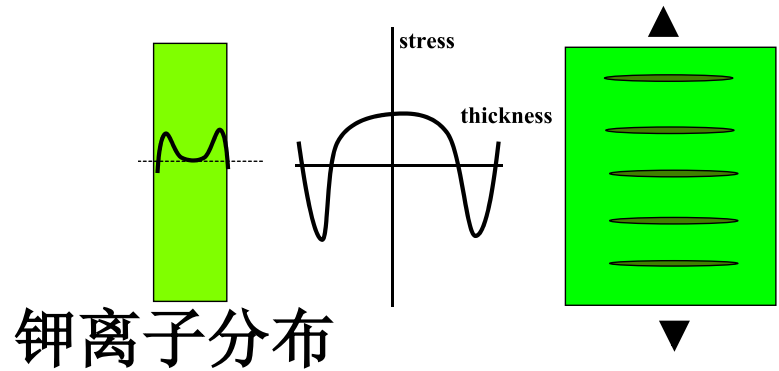
材料增韧



相变增韧陶瓷断裂

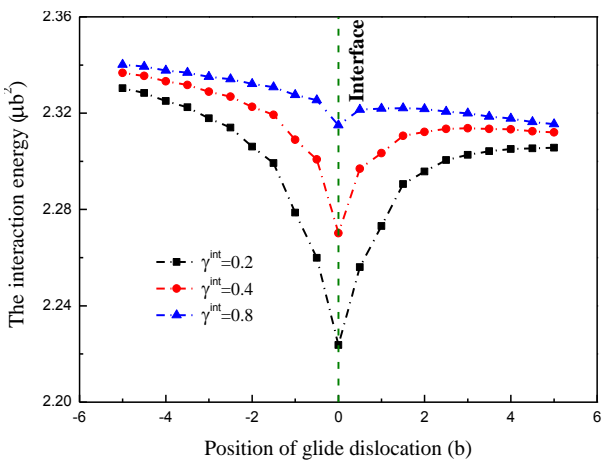
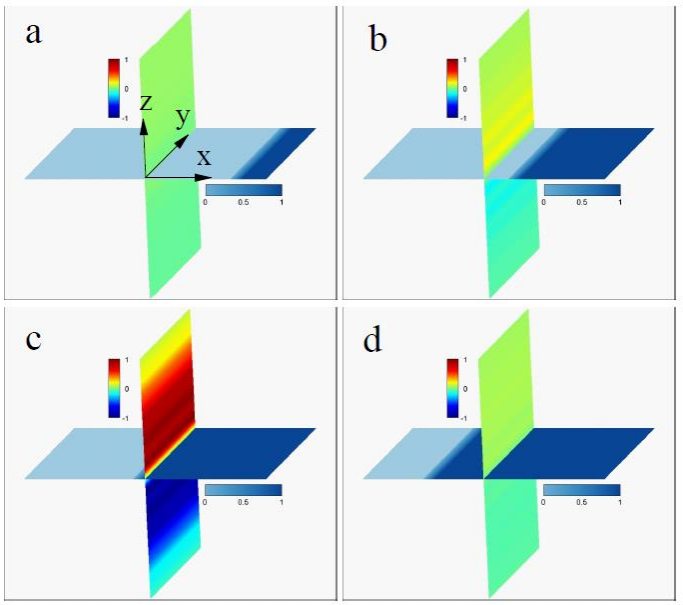
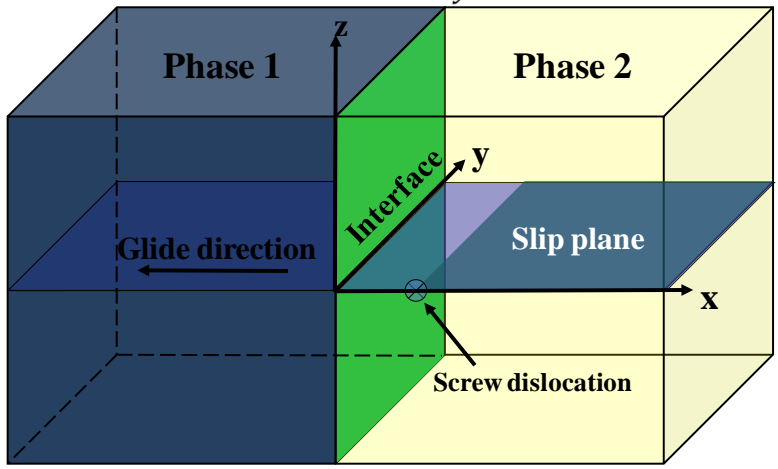
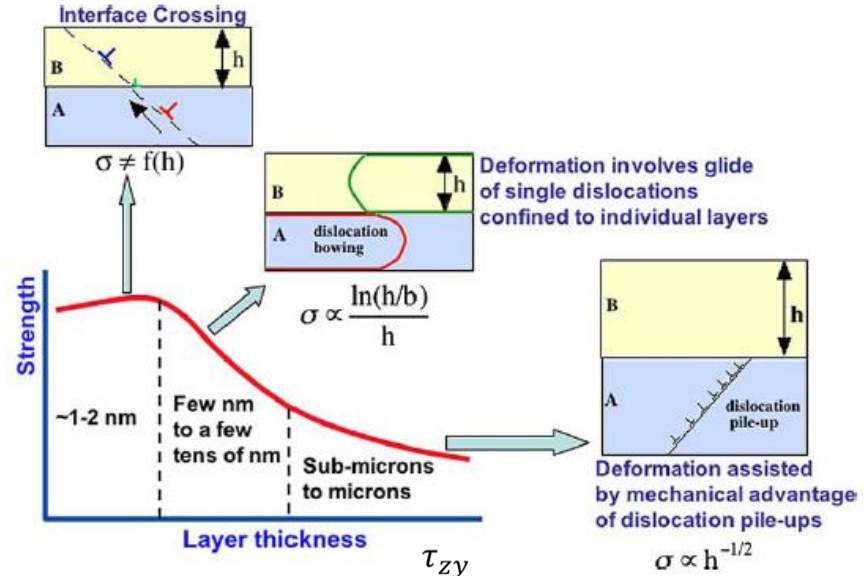


金属陶瓷多层材料



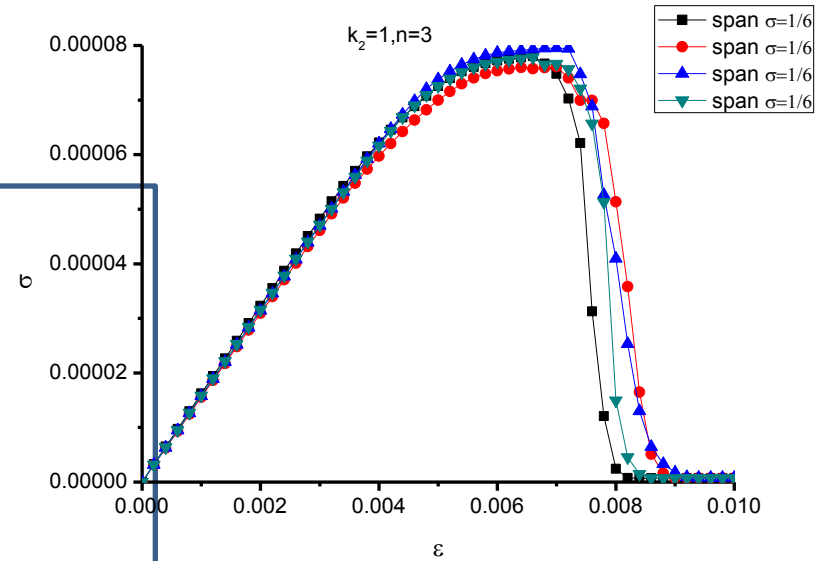
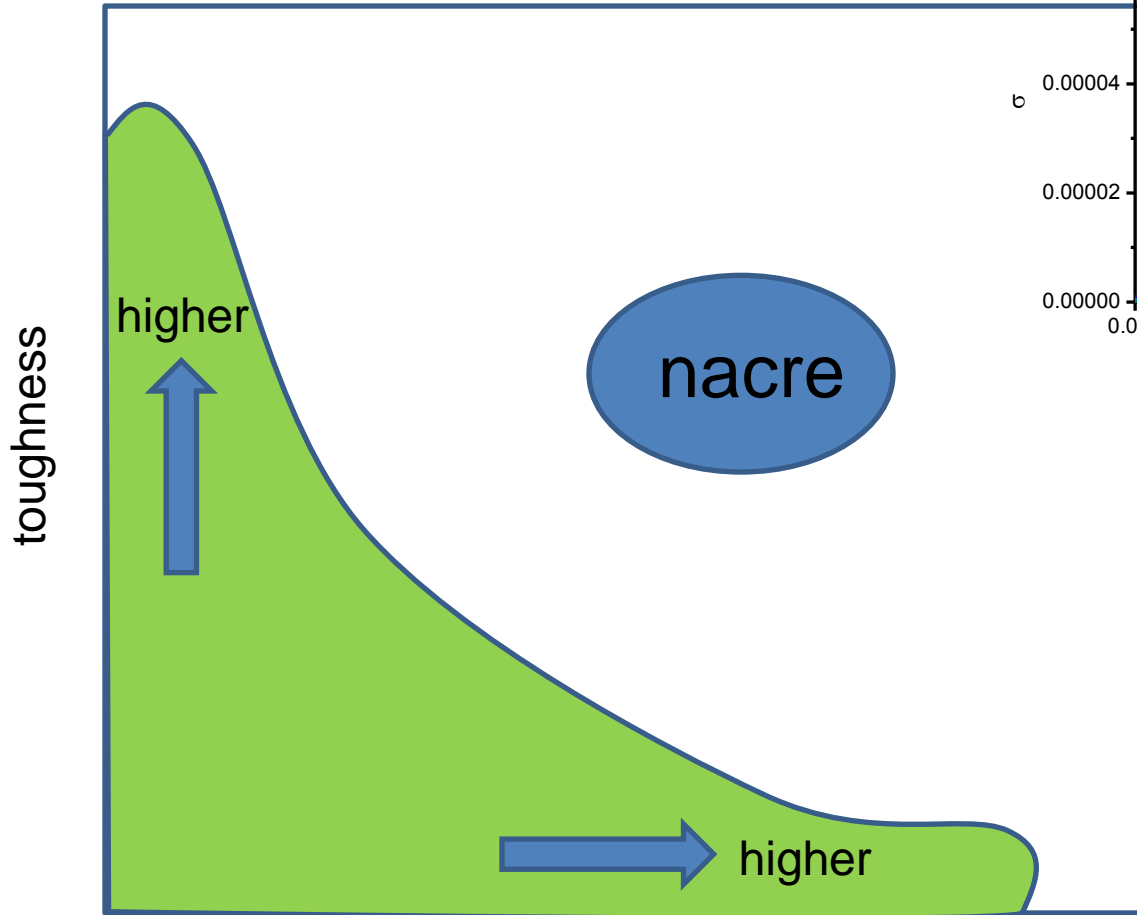
离子交换增韧玻璃

金属多层结构强化的弱界面阻碍位错穿越的能量阱机制

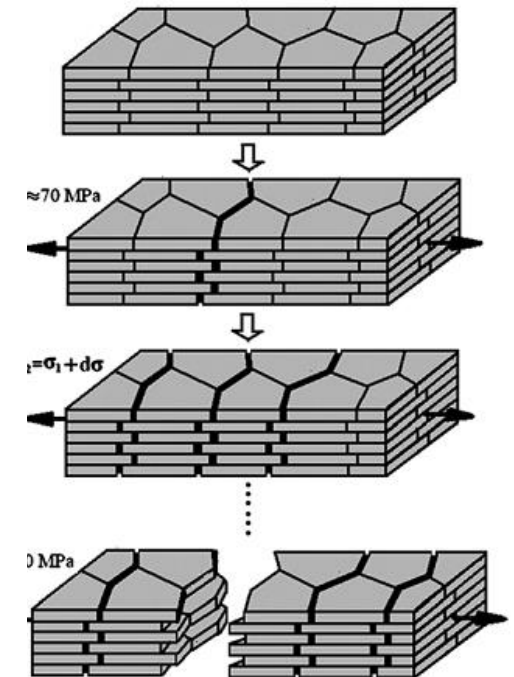
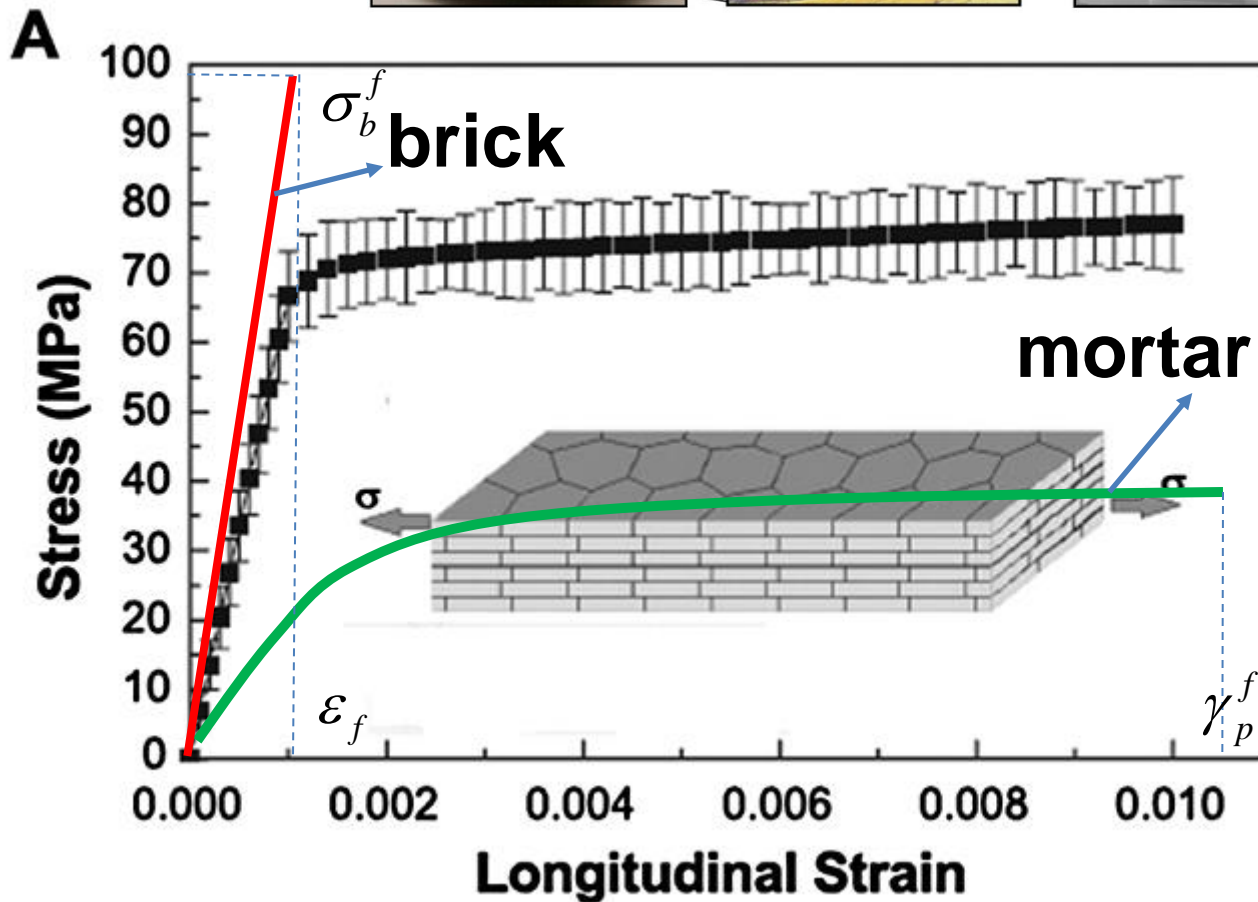
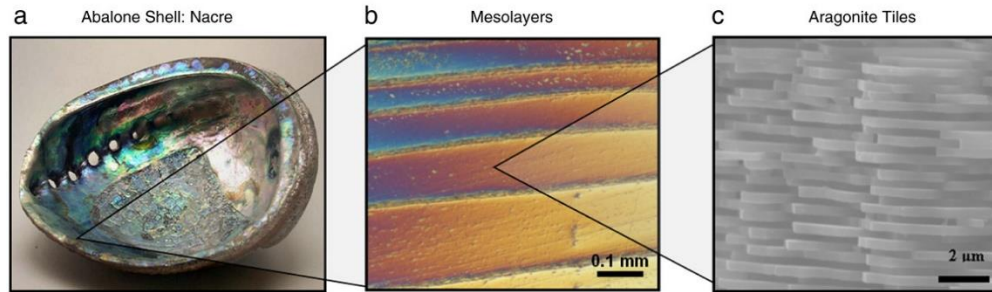


Strength and toughness are usually exclusive in single phase materials

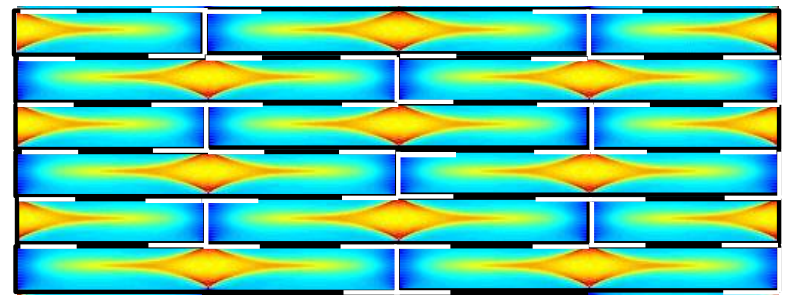
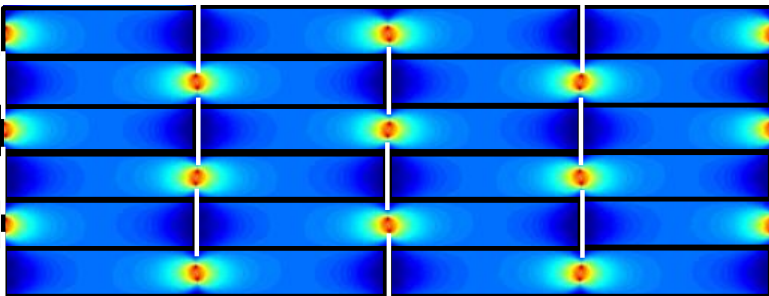
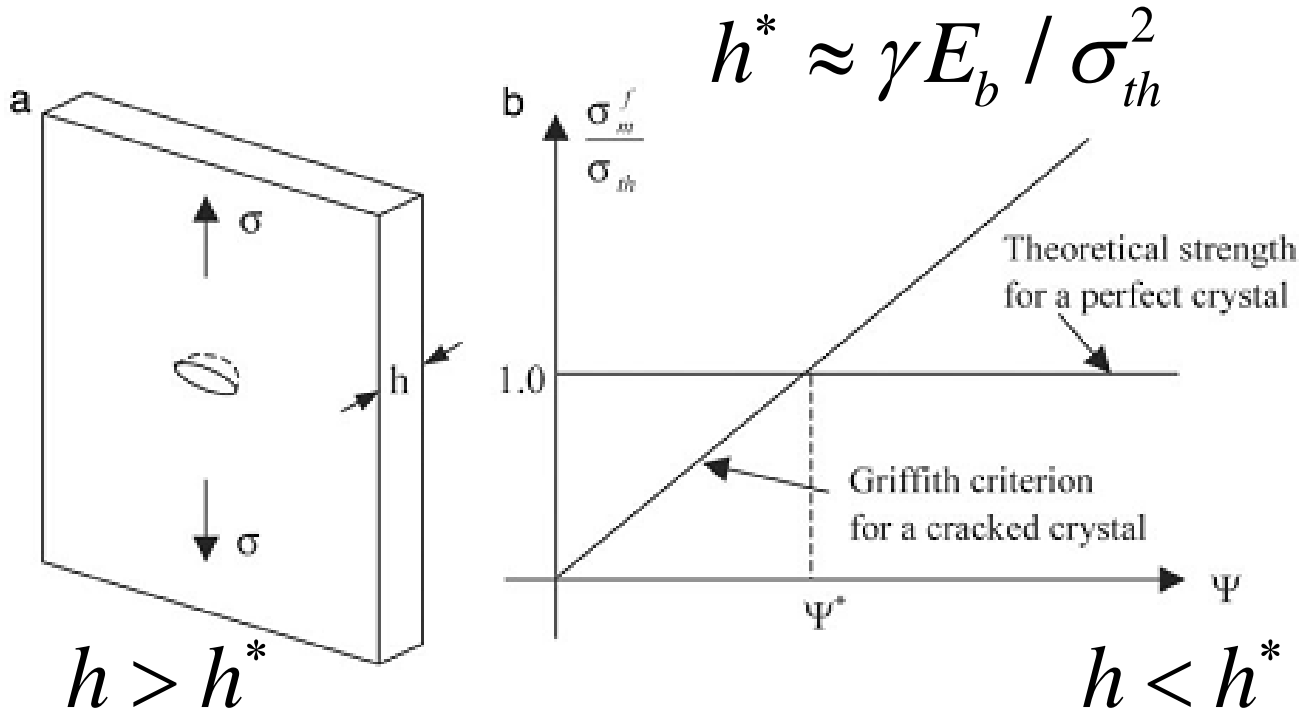
仿生力学



Nacre as a prime example holding optimal strength and toughness

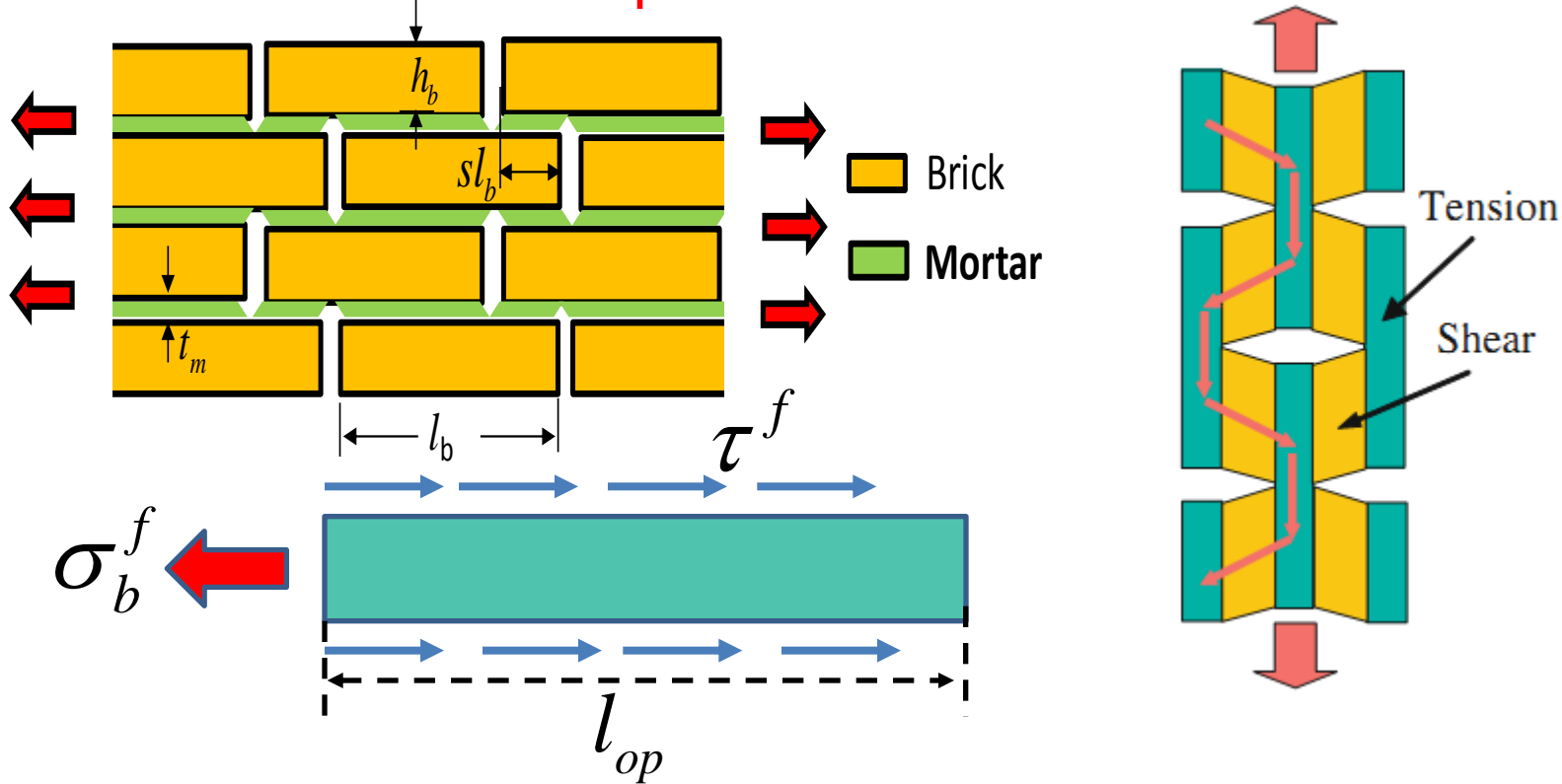


Size effect: flaw tolerance state



Mechanisms for optimal strength and toughness of nacre

Tension-shear chain: optimal size ratio



$$l_{op} \approx 0.5 \sigma_b^f h_b / \tau^f$$

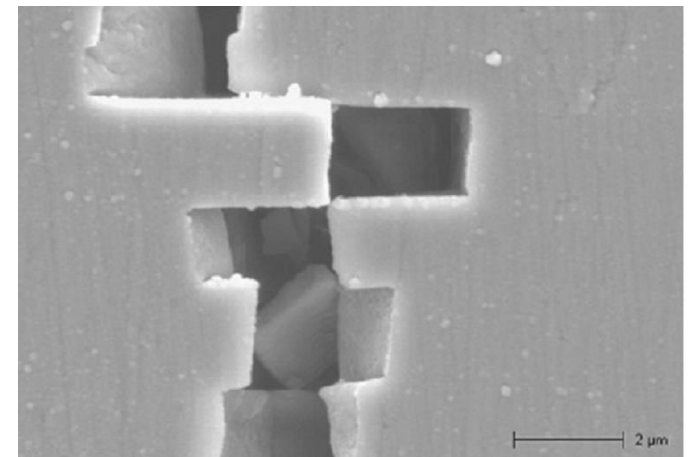
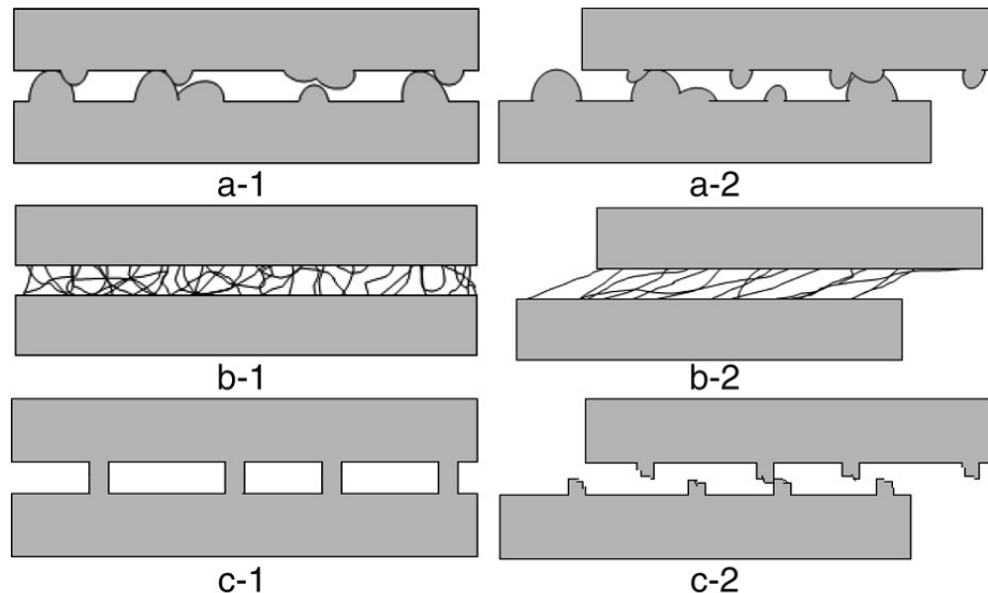
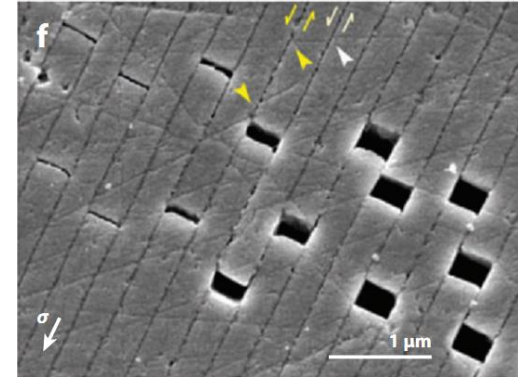
$$\sigma_c^f = 0.5 \sigma_b^f$$

Jäger I., and Fratzl P., Biophys. J. **79**, 1737(2000)

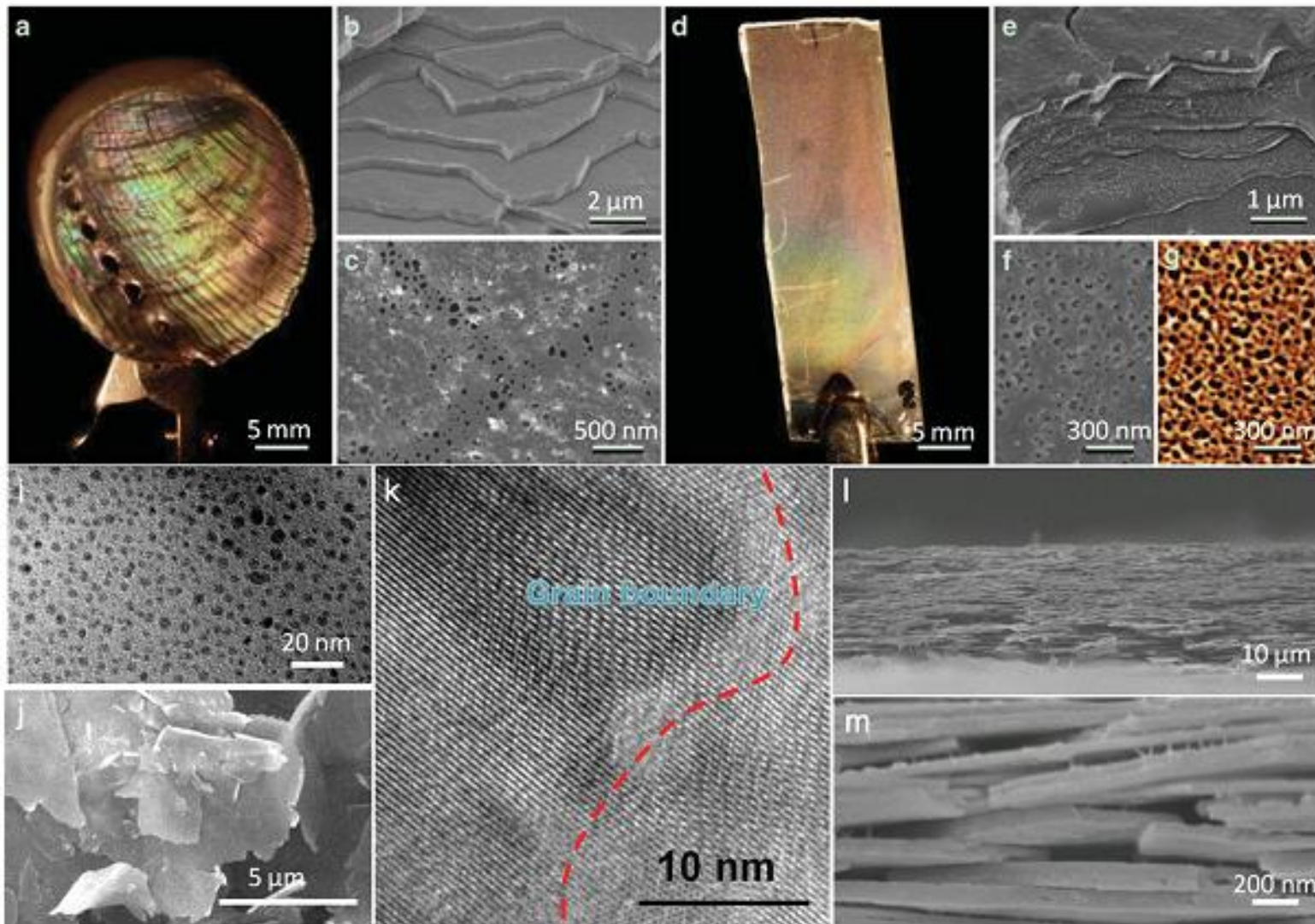
Gao H.J., et al, PNAS, 100,5597(2003)

High toughness via controlled interface feature

- ✓ Weak organic interface sliding
- ✓ Interlocking of nano-asperities
- ✓ Inter-lamellar mineral bridges
- ✓ Plastic deformation of individual tile
- ✓ Multiple cracking and large-scale crack bridging



Successful fabrication of nacreous composites



Finnemore A., et al., Nat. Commun. 3, (2012)

Data of nacreous composites

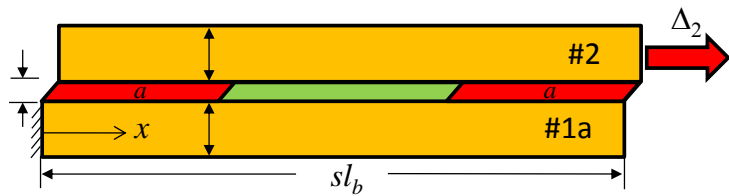
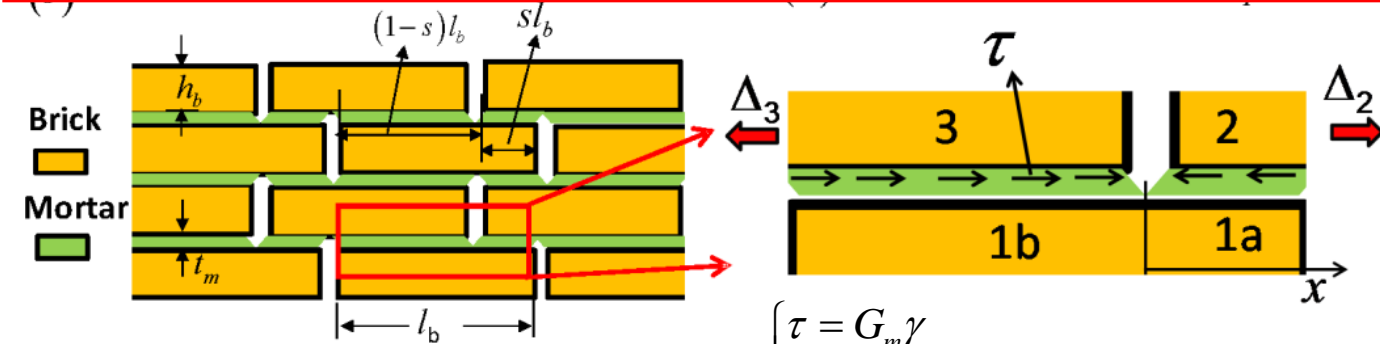
Materials	E_b (GPa)	G_m (MPa)	τ_m (MPa)	ϕ	σ_m^b (GPa)	σ_c^f (MPa)	$\frac{\sigma_m^b}{\tau_m} \sqrt{\frac{G_m \phi}{E_b (1-\phi)}}$	γ_p^f / γ_e^c
Nacre[3,8]	30	30	25	0.9	1	100~150	5.5	5
PVA/MTM[23,24]	270	70	1.5	0.3	9	90~110	63	5~6
PVA / MTM + Al^{3+} [28]	270	600	25	0.5	9	200~300	17	<4
PVA / MTM + Cu^{2+} [28]	270	600	25	0.5	9	280~360	17	<4
PVA/MTM+borate[28]	270	600	25	0.5	9	229~267	17	<4
PVA/MTM+GA[24]	270	600	25	0.5	9	151~187	17	1~2
MTM/chitosan[28]	270	1000	40	0.7	9	86~112	21	2~3
Al_2O_3 / Chitosan [28]	370	1000	40	0.2	12	220~410	6.3	2~3
Bone[4]	120	480	173	0.5	4	500~600	1.3	3~4

Optimal nacreous composites:

- ◆ component selection
- ◆ size and arrangement tailoring of building blocks
- ◆ interface design

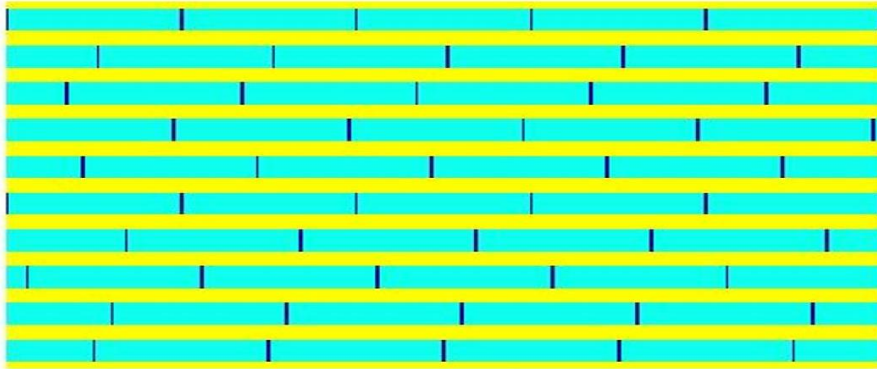
$$\sigma_c^f < 0.5\sigma_b^f$$

Nonlinear shear-lag model



$$\begin{cases} \tau = G_m \gamma \\ \frac{\partial \sigma}{\partial x} + \frac{\partial \tau}{\partial y} = 0 \end{cases} \quad a < x < sl_b - a$$

$$\tau^f = \begin{cases} -\frac{1}{2} h_b E_b u_{1a}''(x) & 0 \leq x \leq a \text{ and } sl_b - a \leq x \leq sl_b \\ \frac{1}{2} h_b E_b u_2''(x) & \end{cases}$$



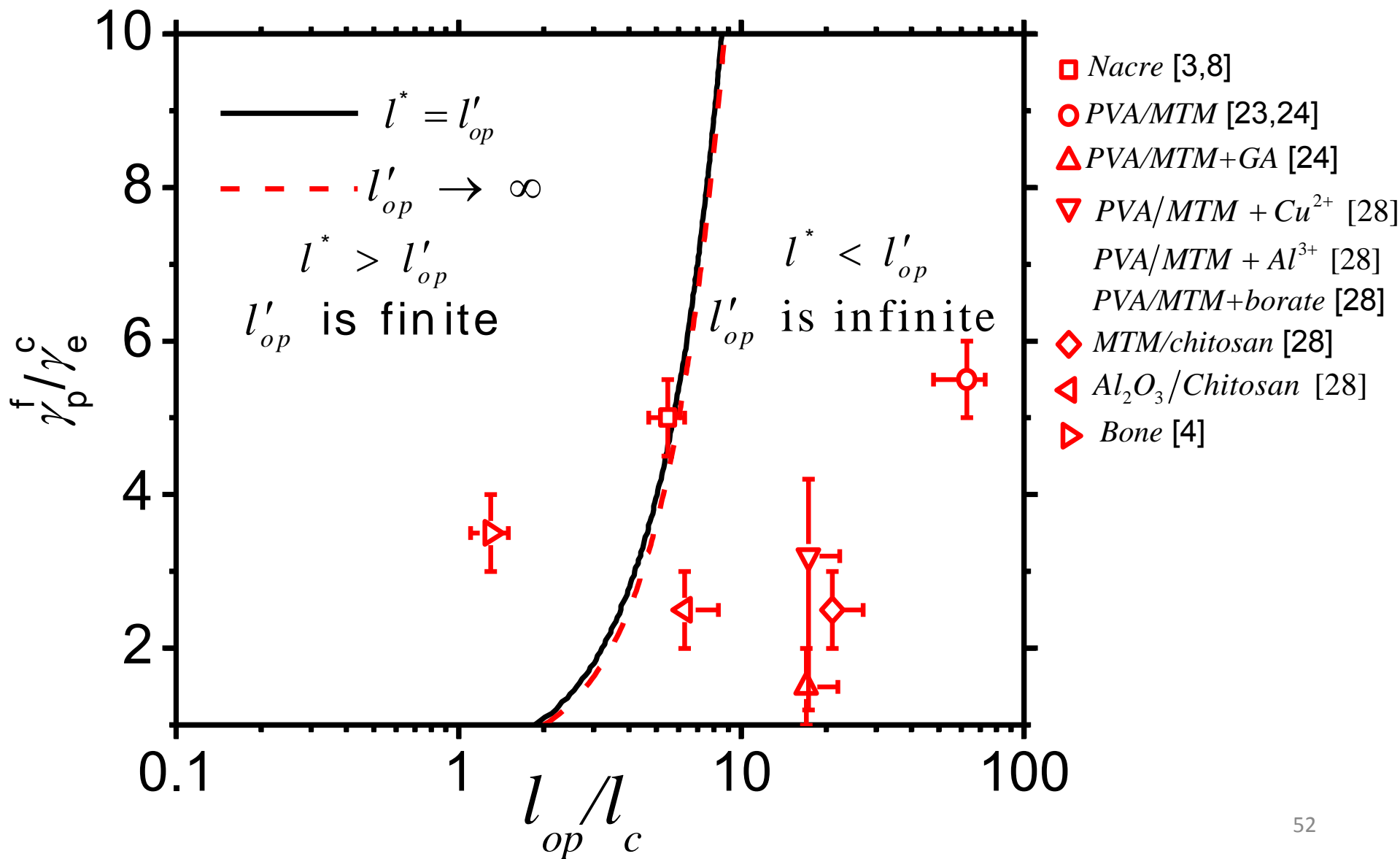
$$E_{el}^{(i)} = \int \sigma^{(i)} d\varepsilon^{(i)} dx dy = \frac{1}{2} \int c^{(i)} (\varepsilon^{(i)})^2 h_b dx$$

$$\begin{aligned} E_{int}^{(i)} &= \frac{1}{2} \left[\int \tau^{(i+1)} d(\delta^{(i+1)}/t_m) dx dy + \int \tau^{(i)} d(\delta^{(i)}/t_m) dx dy \right] \\ &= \frac{1}{2} \left[\int \tau^{(i+1)} d\delta^{(i+1)} dx + \int \tau^{(i)} d\delta^{(i)} dx \right] \end{aligned}$$

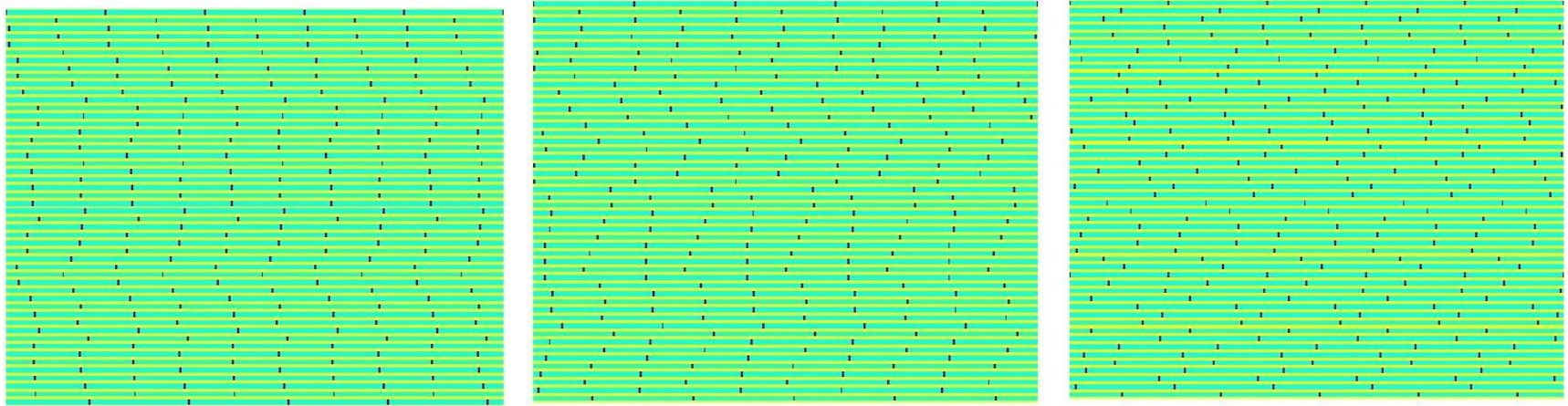
$$E^{tot} = \sum (E_{el}^{(i)} + E_{int}^{(i)})$$

$$\frac{\partial u^{(i)}}{\partial t} = -\kappa \frac{\delta E^{tot}}{\delta u^{(i)}}$$

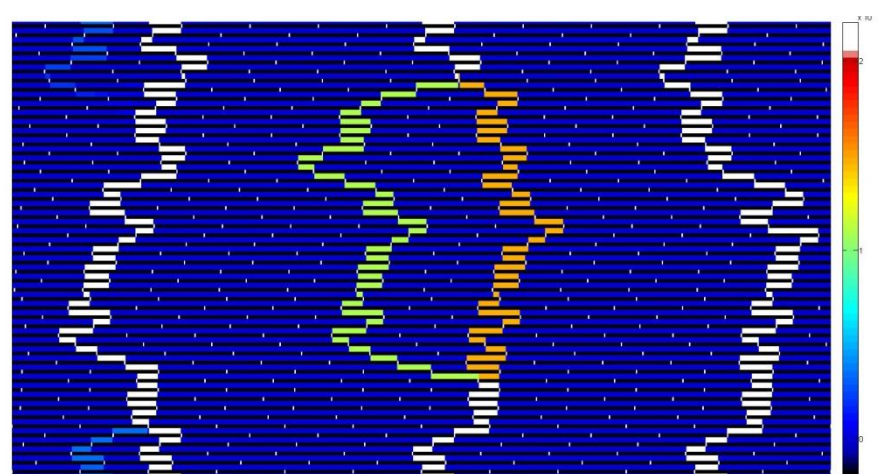
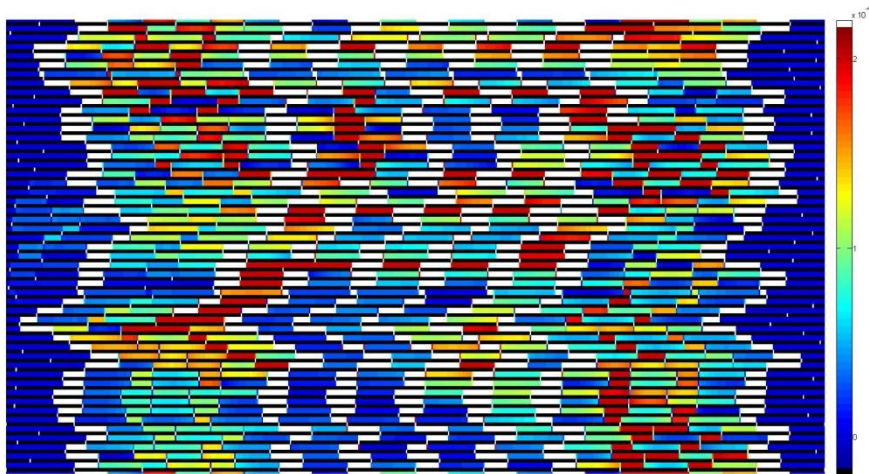
Map for optimal strength and toughness of nacreous composites



Effect of staggering randomness



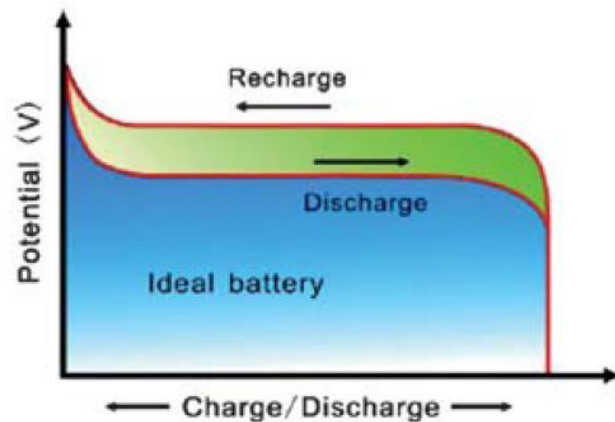
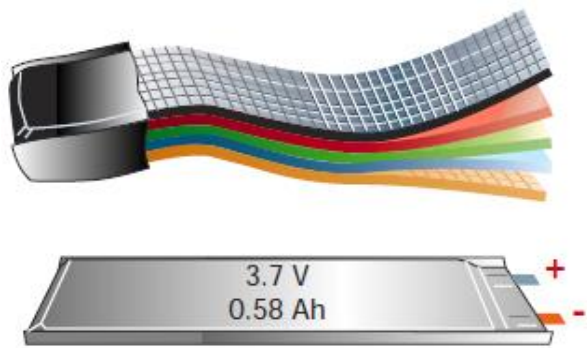
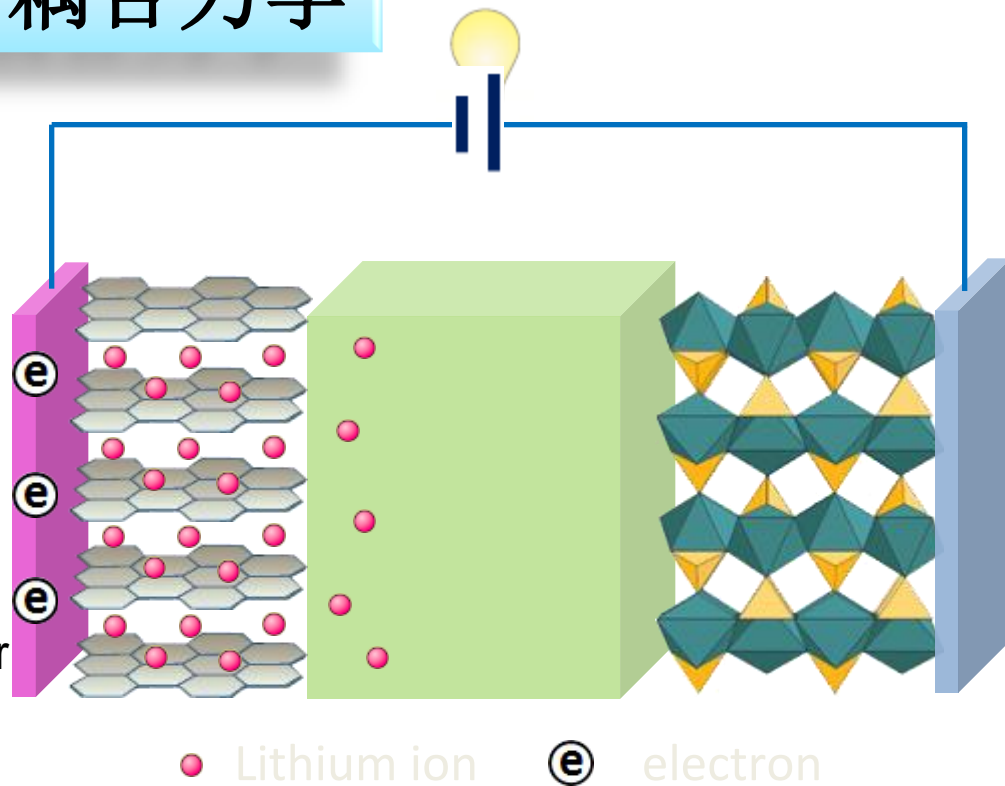
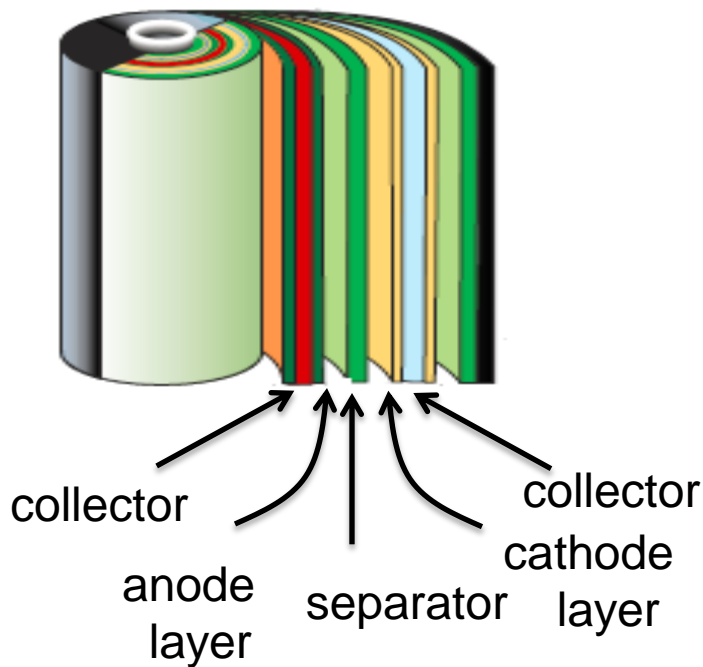
increase staggering randomness



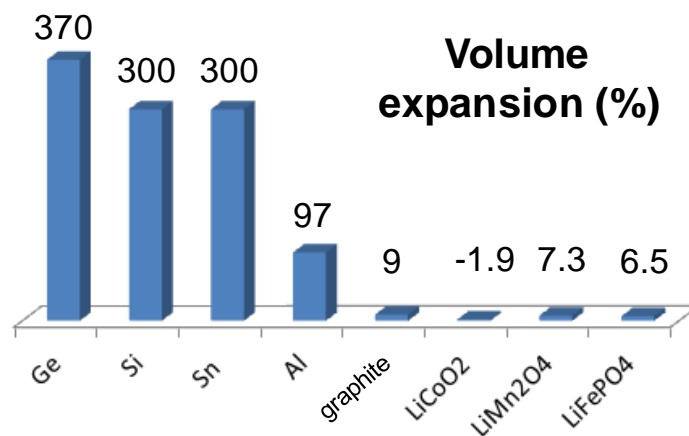
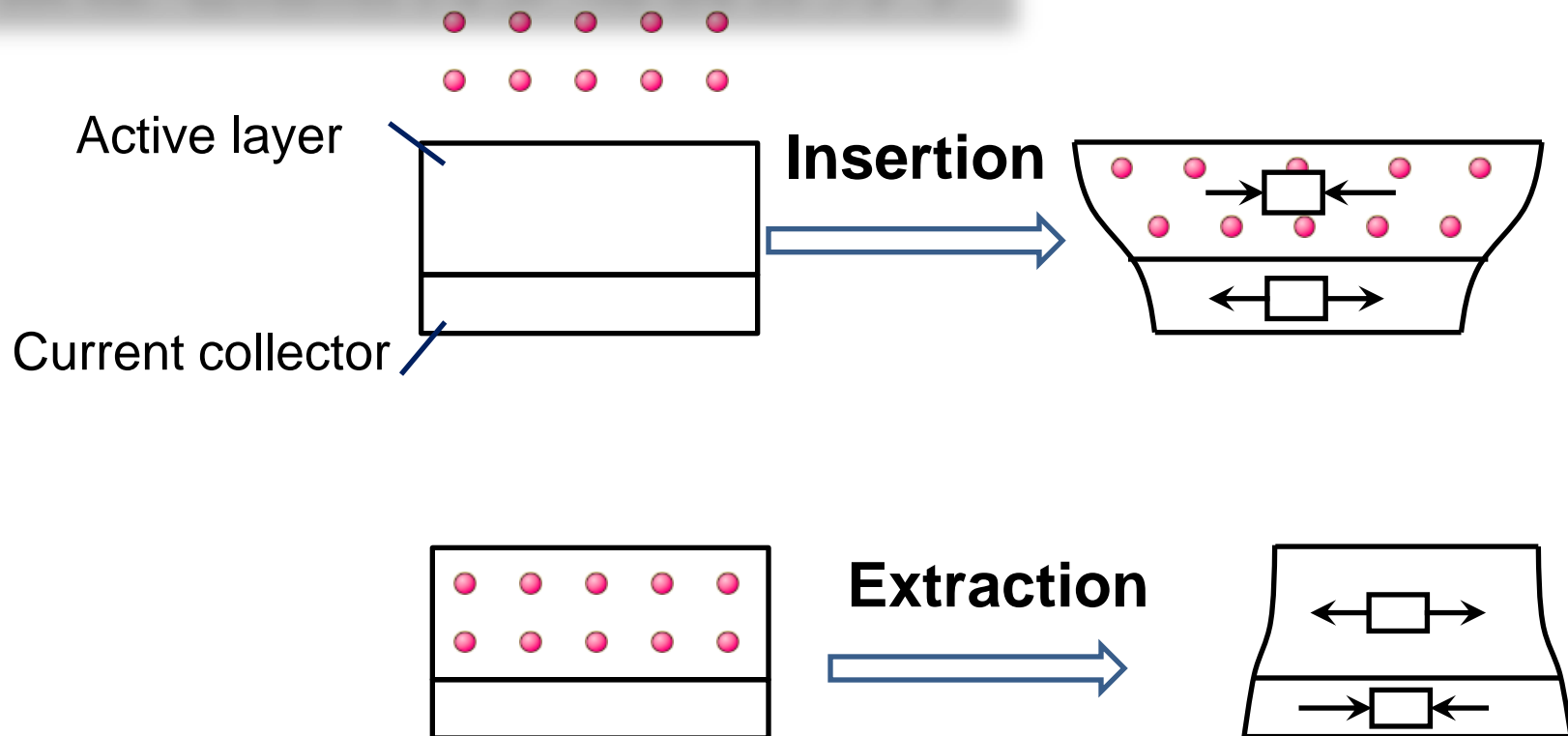
□ 固体力学在材料中的应用

2. 功能材料的力学稳定性与寿命分析举例

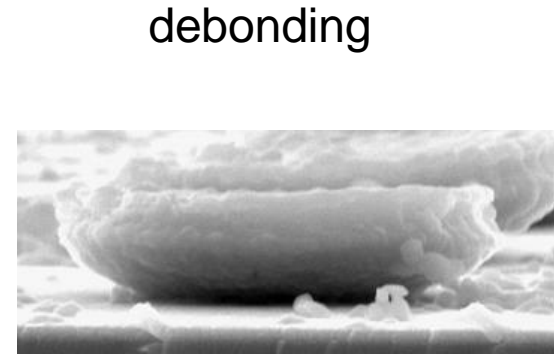
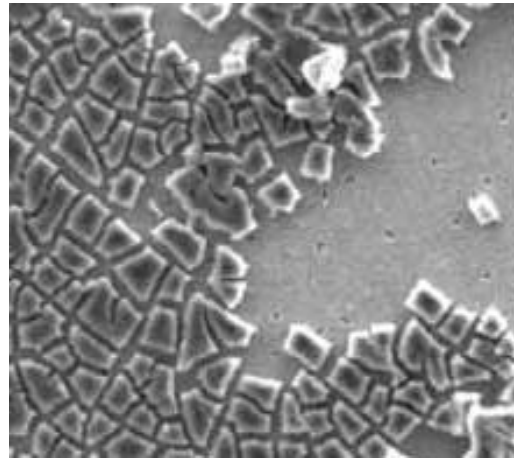
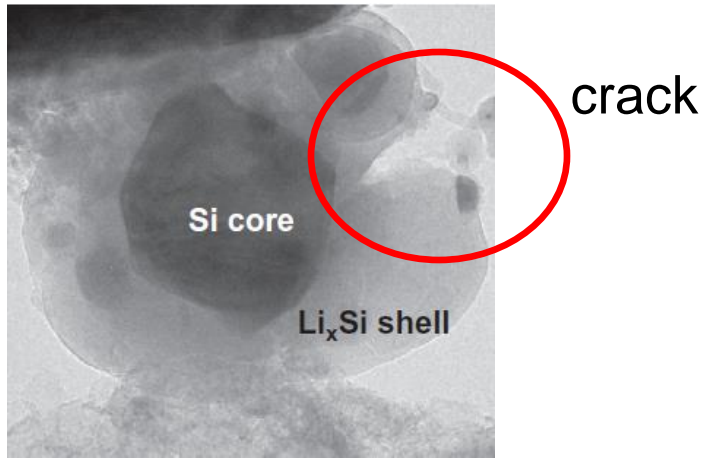
微锂电池结构多场耦合力学



微锂电池结构多场耦合力学

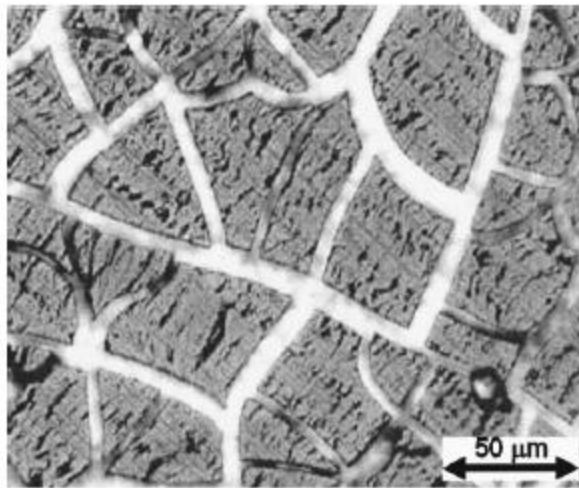


扩散应力导致的破坏

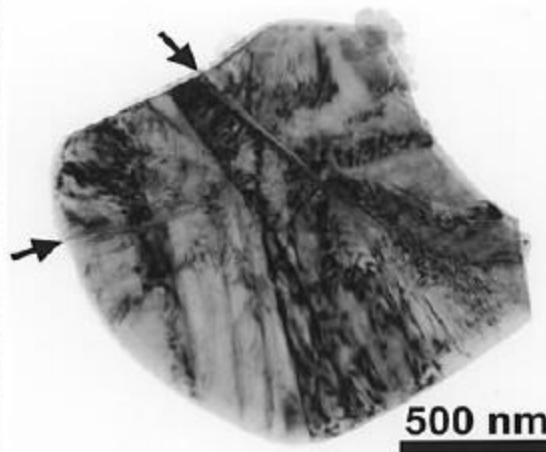


Liu XH et al, ACS Nano (2012)

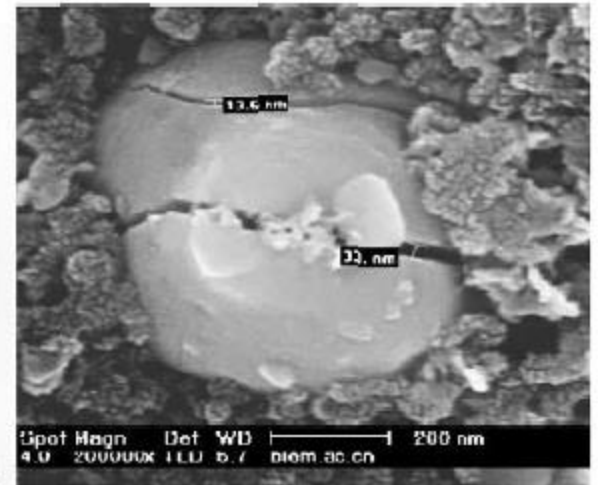
He Y, JPS (2012)



(a) SiSn thin film



(b) LiCoO₂ particle



(c) LiFePO₄ particle

Beaulieu et al, ESSL (2012) Wang HF et al, JES (1999)

Wang DY et al, JPS (2005)

扩散应力调控与优化

材料选择

正极

负极

集电层

电解质

结构设计

尺寸

形状

拓扑

充放电优化

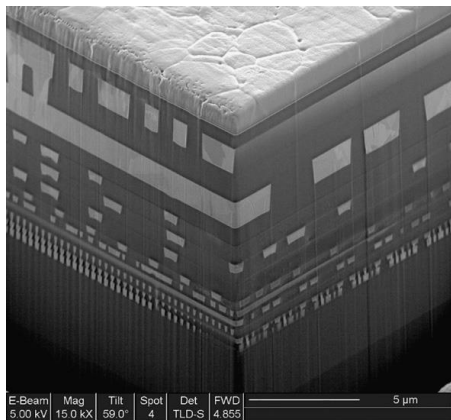
速率

时间

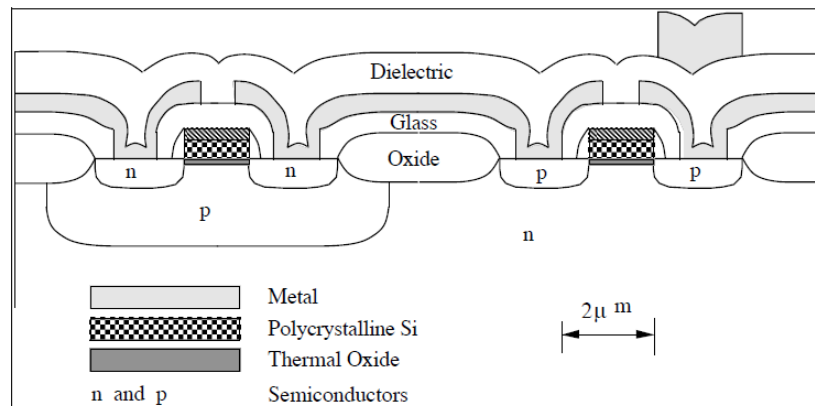
恒流、恒压

.....

薄膜器件结构的细观非均匀性

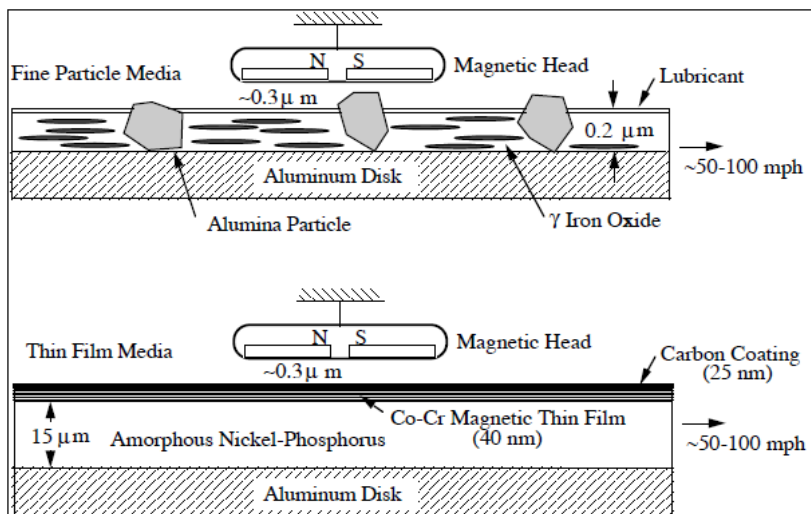


Complimentary Metal-Oxide-Semiconductor Transistor



Copper and low-k interconnect structures in IBM CMOS microprocessor (Edelstein et al., 2004).

Magnetic Head-Disk Interactions



Thin Films in Technology

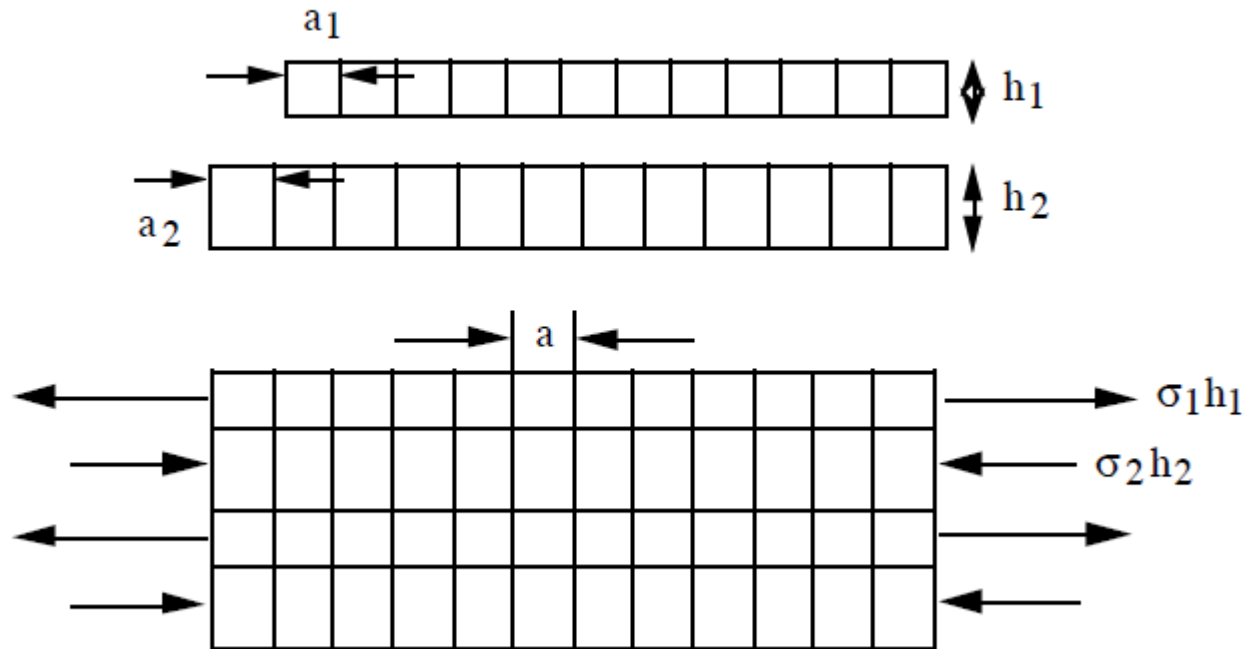
- * Microelectronic IC's
- * Magnetic Storage
- * Optical Filters
- * Wear Resistant Coatings
- * Corrosion Resistant Coatings

From Prof. W. D. Nix's lecture

薄膜器件结构的应力与变形

热失配应力、晶体相变失配应力、晶格失配应力

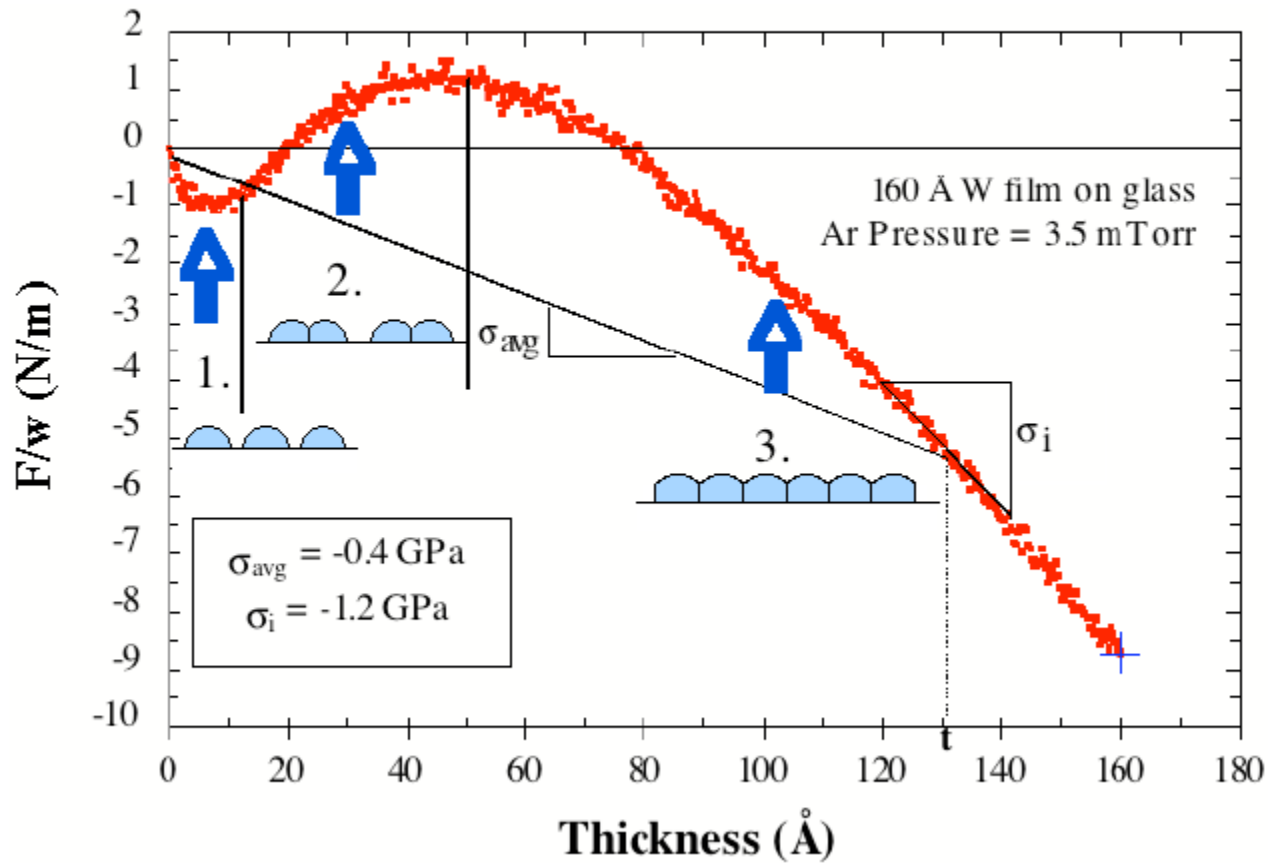
Coherent multilayer



Film 1 is biaxially stretched, and Film 2 biaxially compressed.

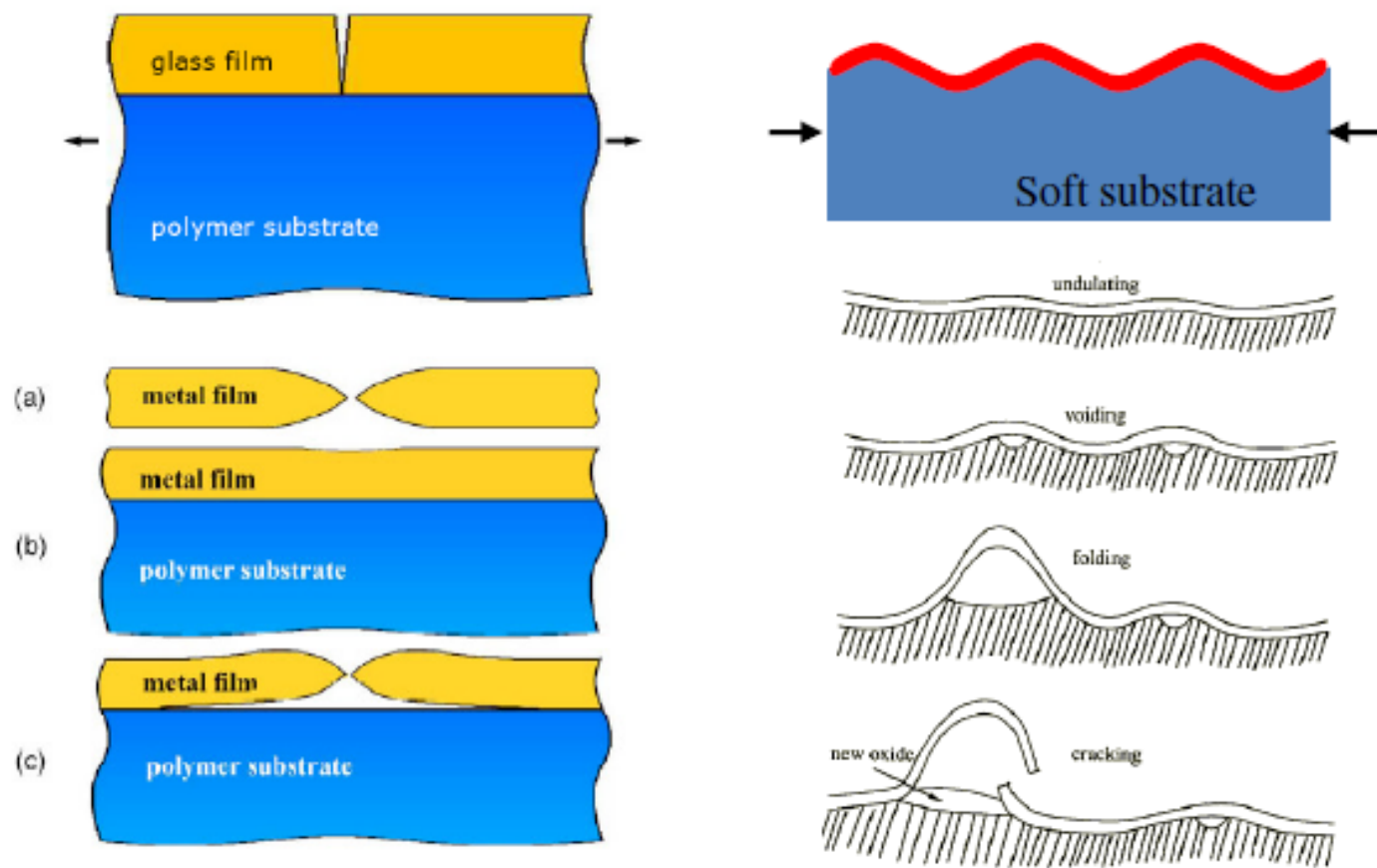
薄膜生长应力

Stress Evolution for a sputtered Pt film on a thin glass substrate



From Prof. W. D. Nix's lecture

Mechanics of Thin Films: Stretch and Compress



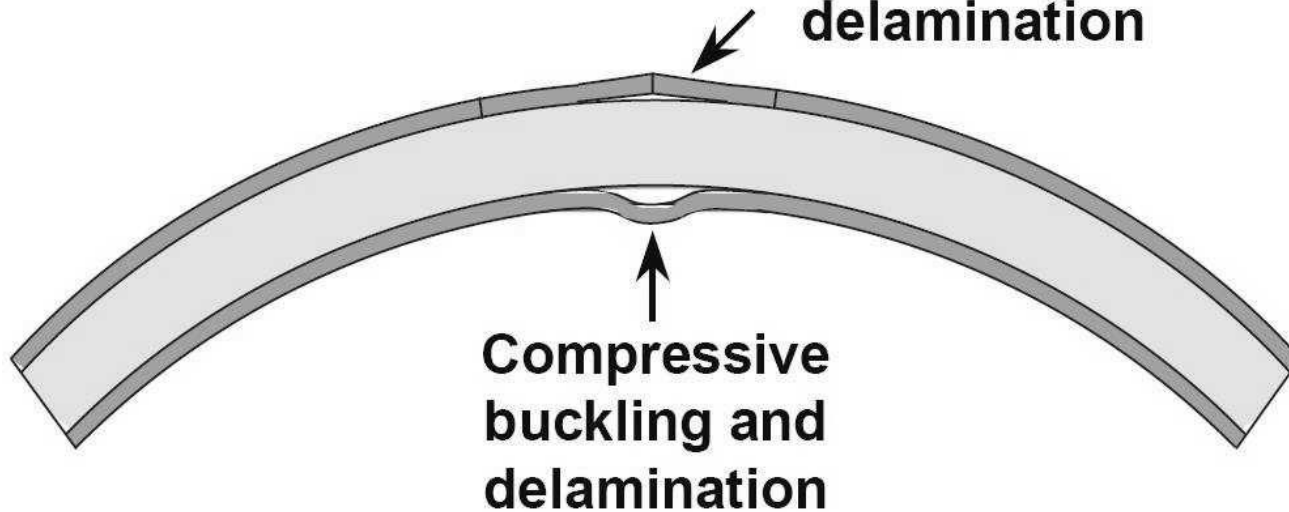
Li et al, 2005

Suo, 1995

Flexible Electronics

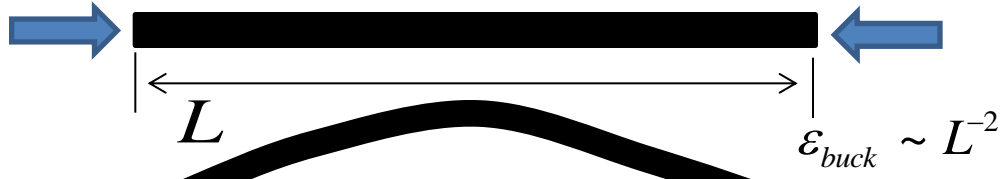


Tensile failure and delamination

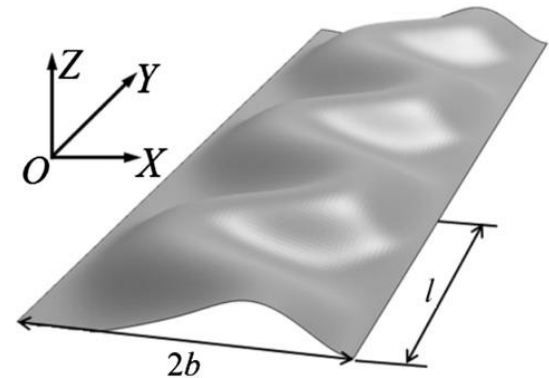
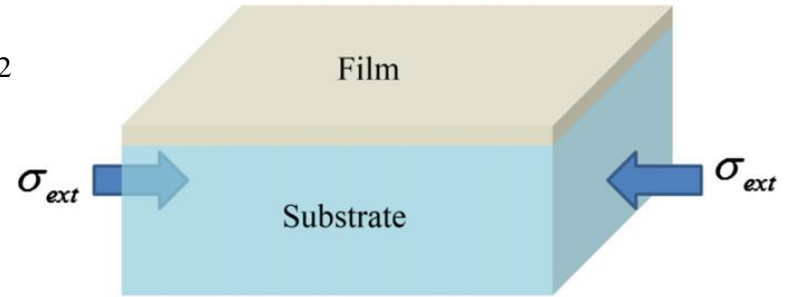
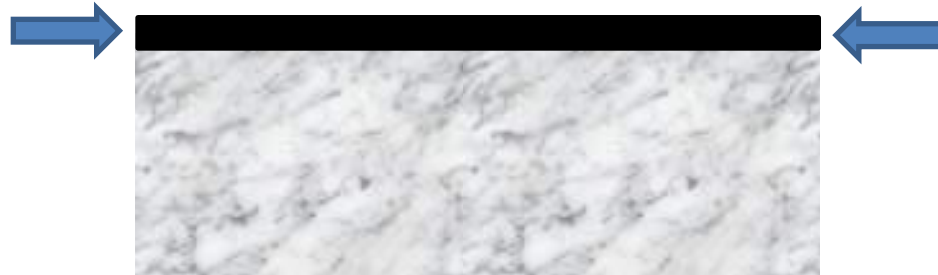


多层薄膜结构中的非线性屈曲

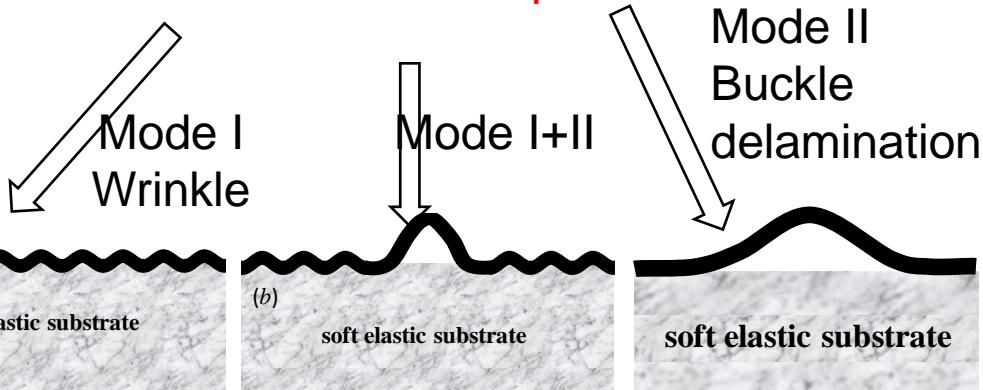
Euler Buckling



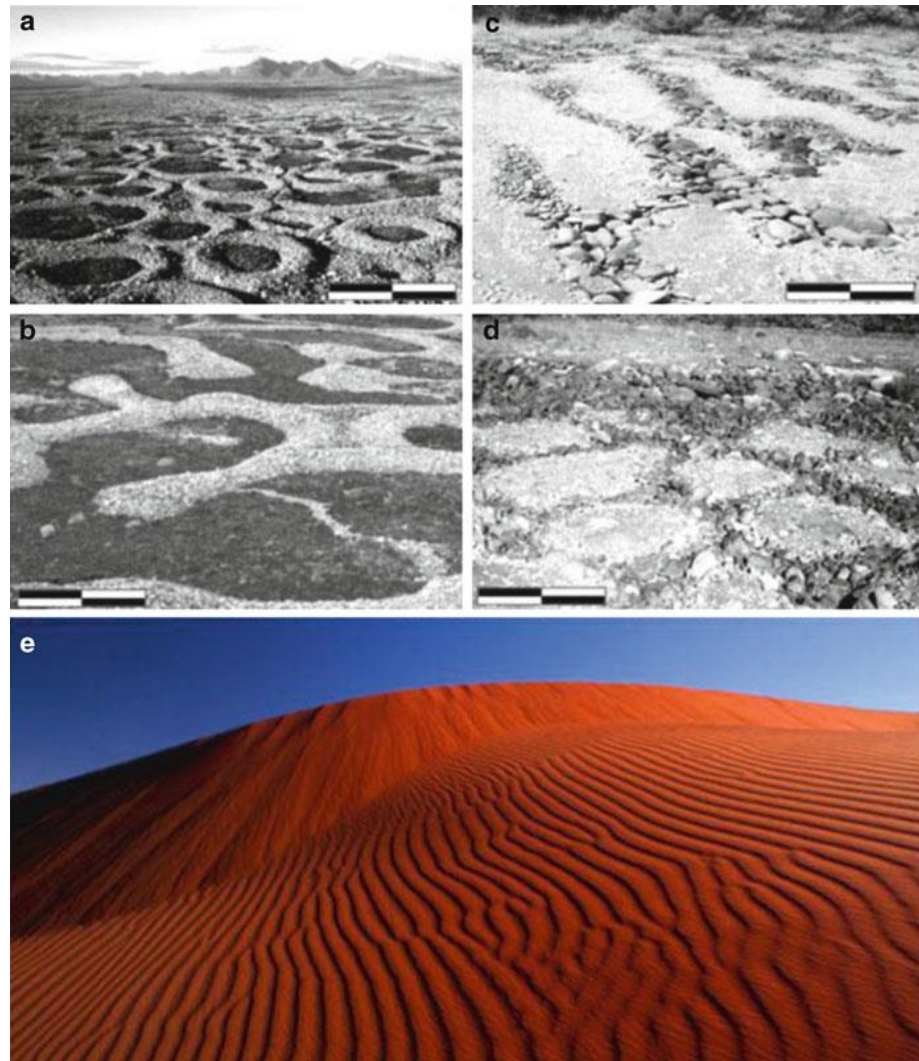
◆ The role of pre-strain



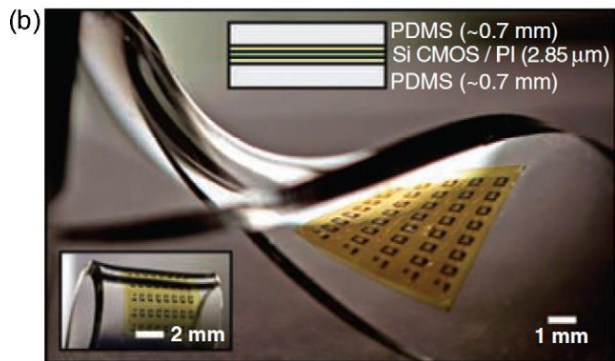
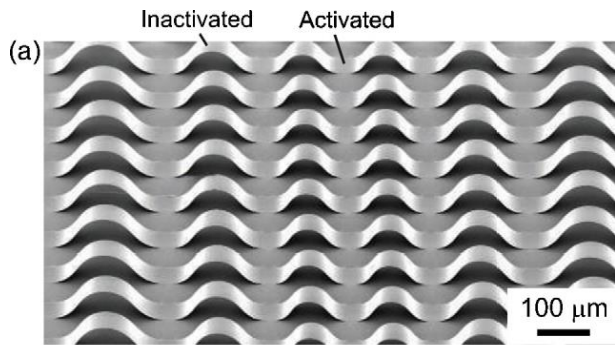
◆ The role of interfacial adhesion and substrate compliance

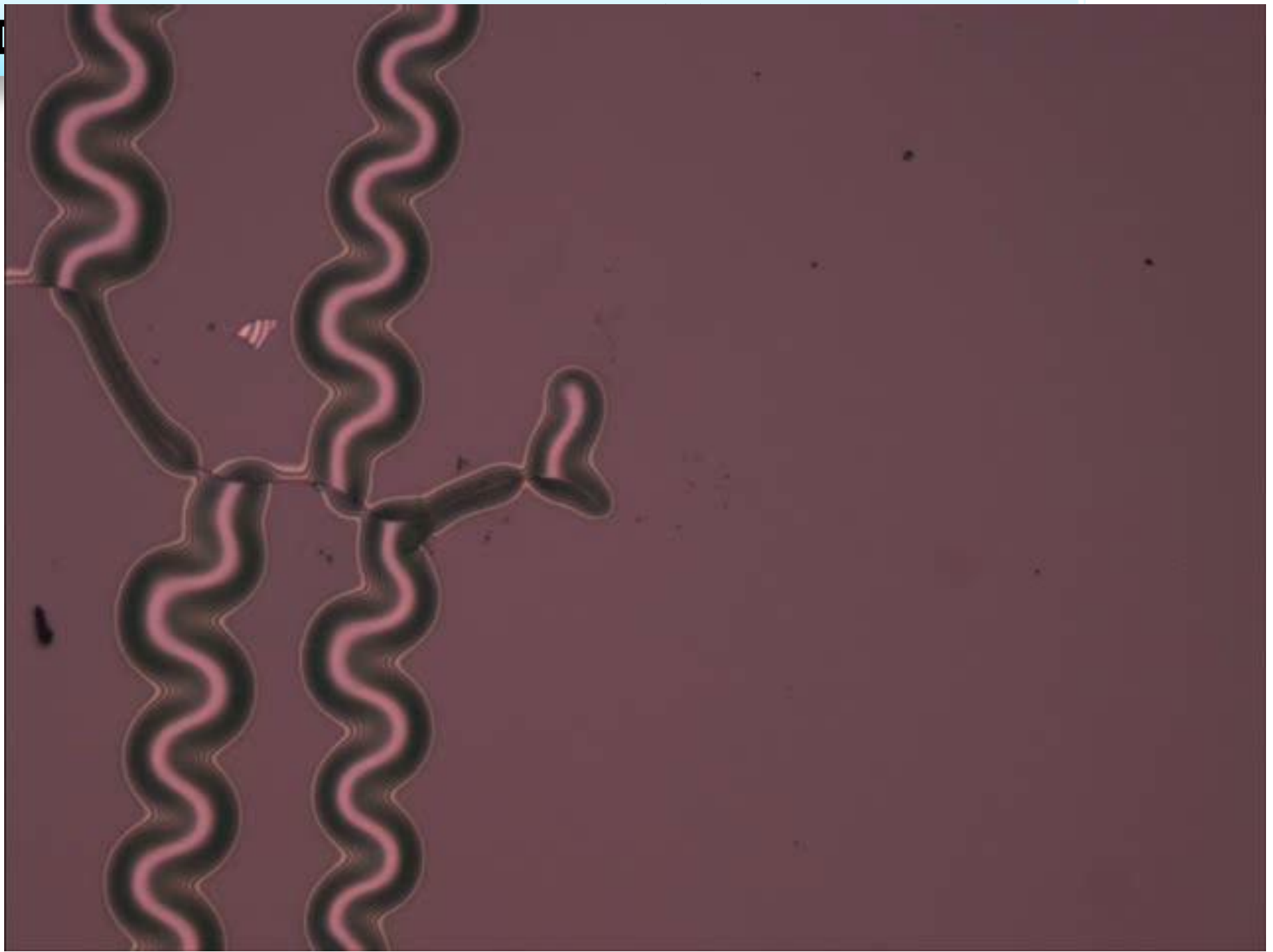


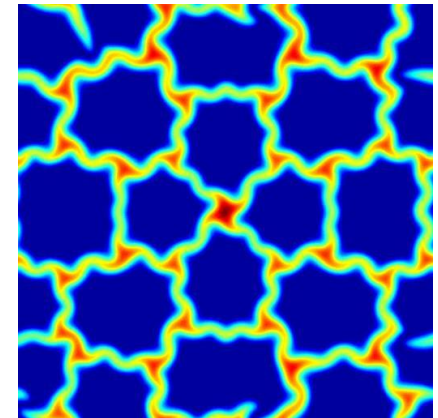
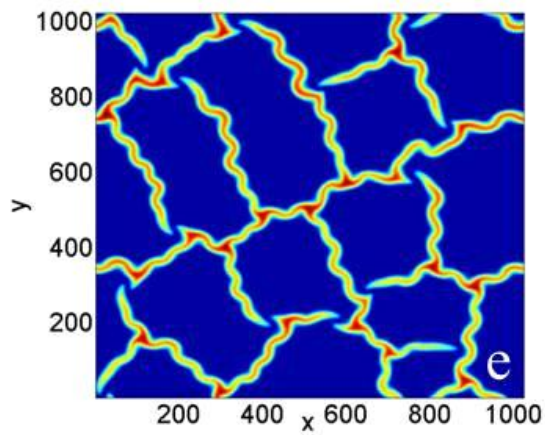
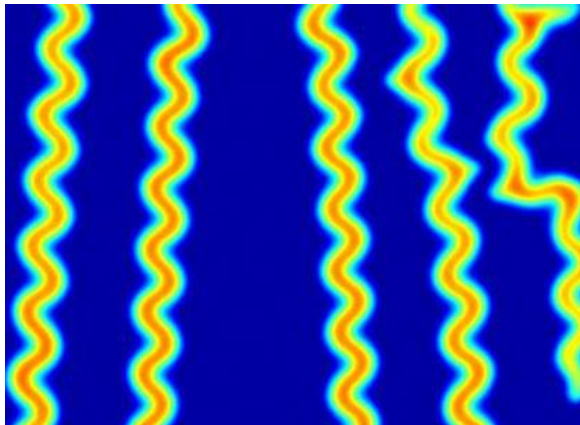
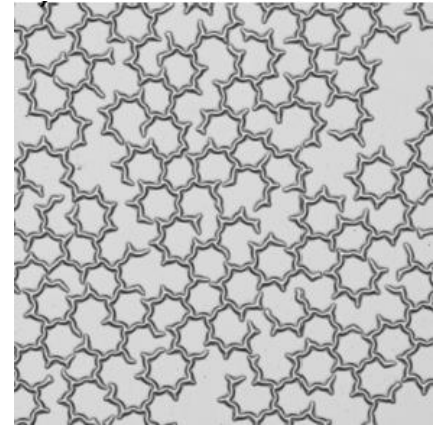
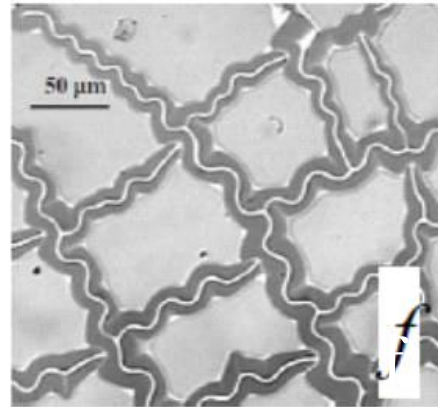
□非平衡演化：失稳→微结构演化→斑图



□非平衡演化：失稳→微结构演化→斑图



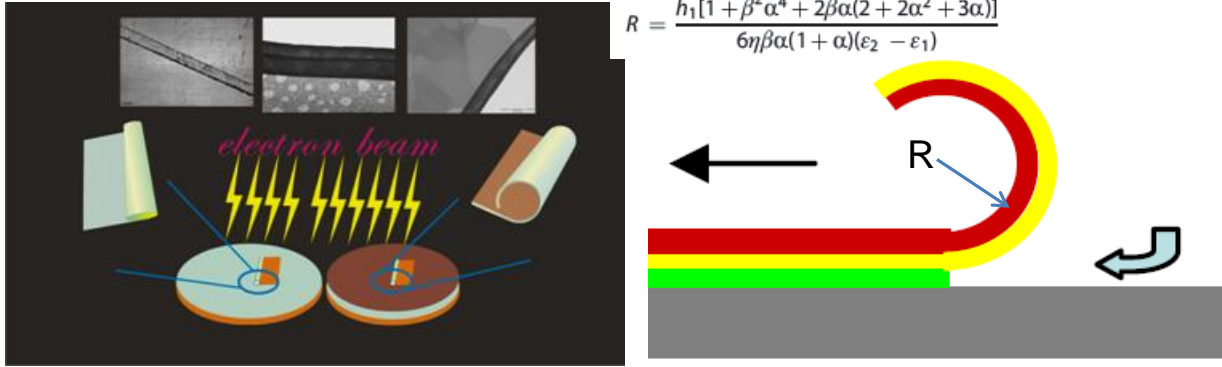




□ 固体力学在材料中的应用

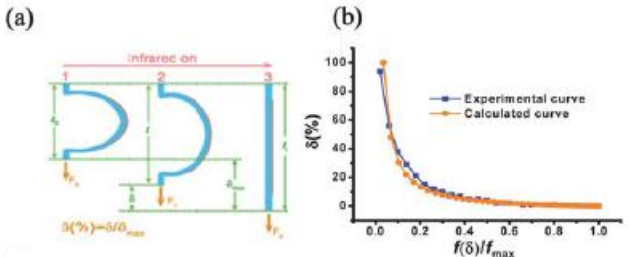
3. 基于变形耦合的功能材料设计举例

多层膜成管和红外驱动的应力机制



$$R = \frac{h_1[1 + \beta^2\alpha^4 + 2\beta\alpha(2 + 2\alpha^2 + 3\alpha)]}{6\eta\beta\alpha(1 + \alpha)(\epsilon_2 - \epsilon_1)}$$

J. W. Liu, et al. ACS Nano, 6,4500,2012

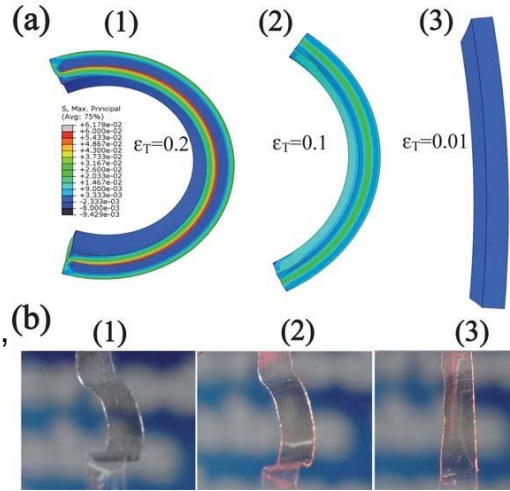


$$f(\delta) = \frac{Ak^2}{\frac{L}{\pi} \left(\delta - \frac{\pi}{2} \cos \frac{Lk}{2} \right)}$$

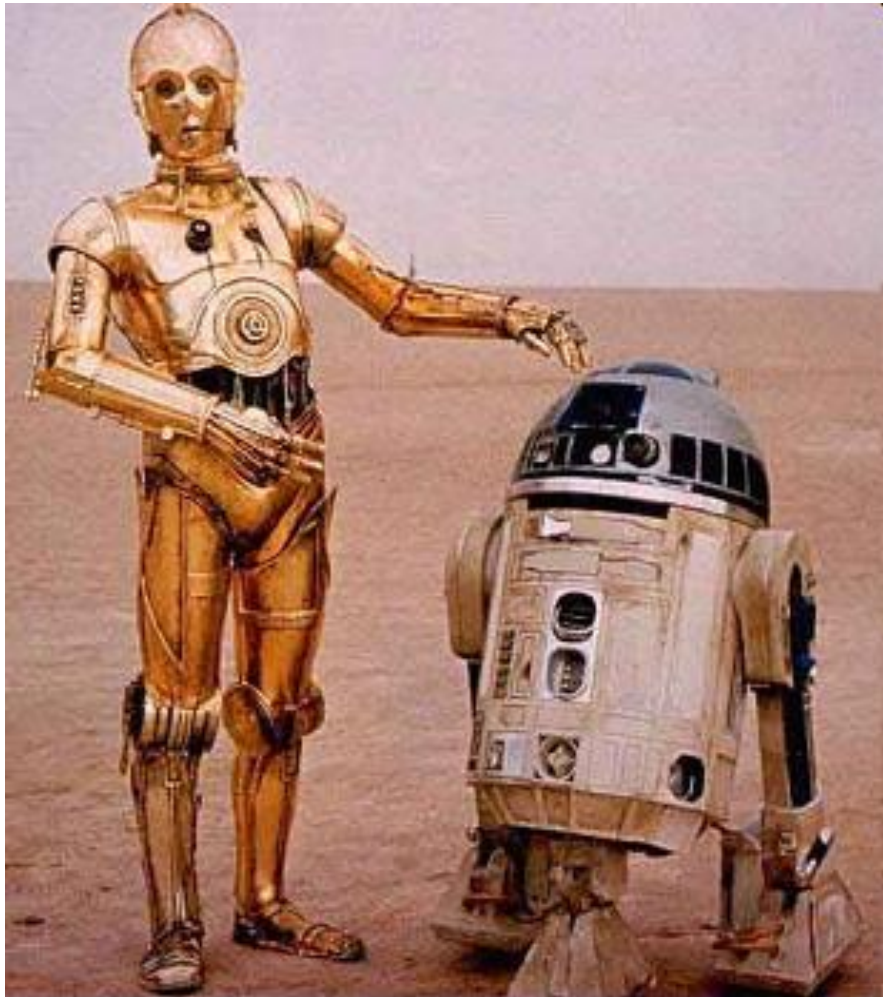
with

$$A = LWh_1^2 M_1 - \left[\frac{M_2^2}{2M_1^2} \left(\frac{h_2^2}{h_1^2} + \frac{h_2}{h_1} \right)^2 \left(1 + \frac{h_2}{h_1} \frac{M_2}{M_1} \right)^{-1} + \frac{1}{6} \left(1 + \frac{4M_2}{M_1} + \frac{4h_2}{h_1} \frac{M_2}{M_1} + \frac{6h_2^2}{h_1^2} \frac{M_2}{M_1} \right) \right]$$

C. Z. Wu, et al., J. Mater. Chem., 21,18584,2011

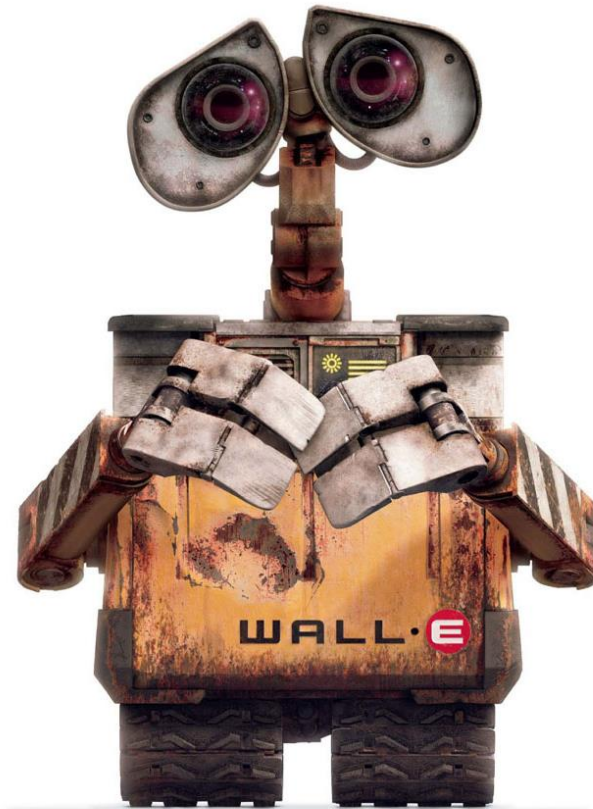


Hard Machines



C-3PO

R2-D2



2008

Disney • PIXAR

From Professor Suo's lecture

Soft Machines

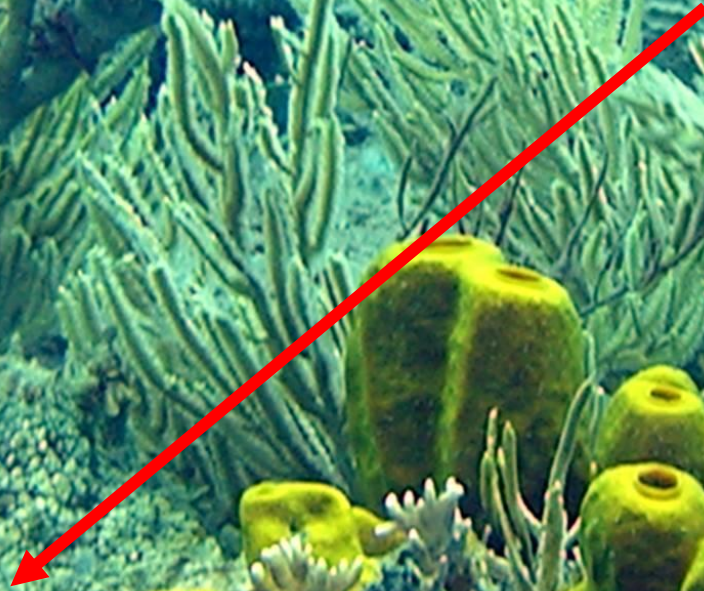


Angelina Jolie



Octopus

octopus

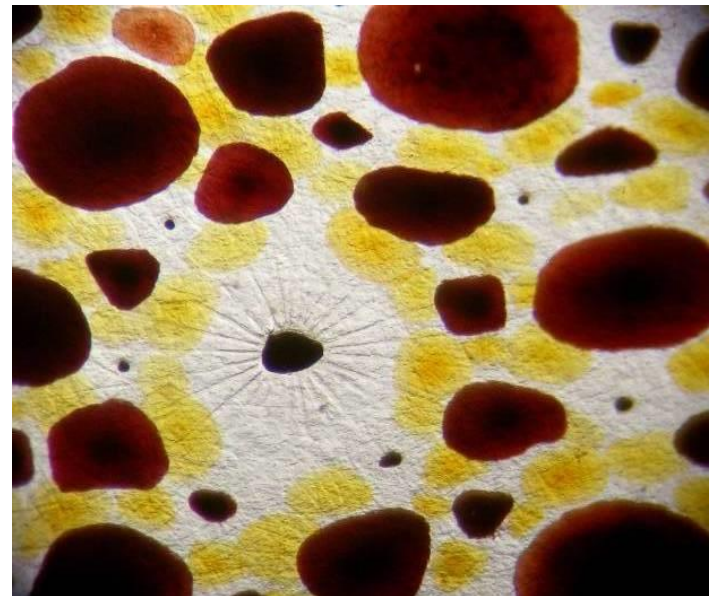
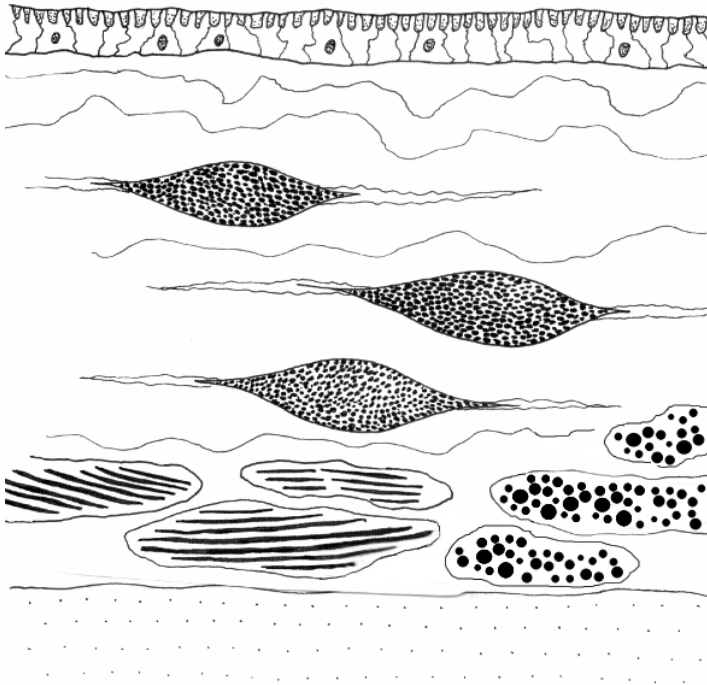


Mäthger, Hanlon, Kuzirian – Marine Biological Laboratory, Woods Hole MA

Squid changes color



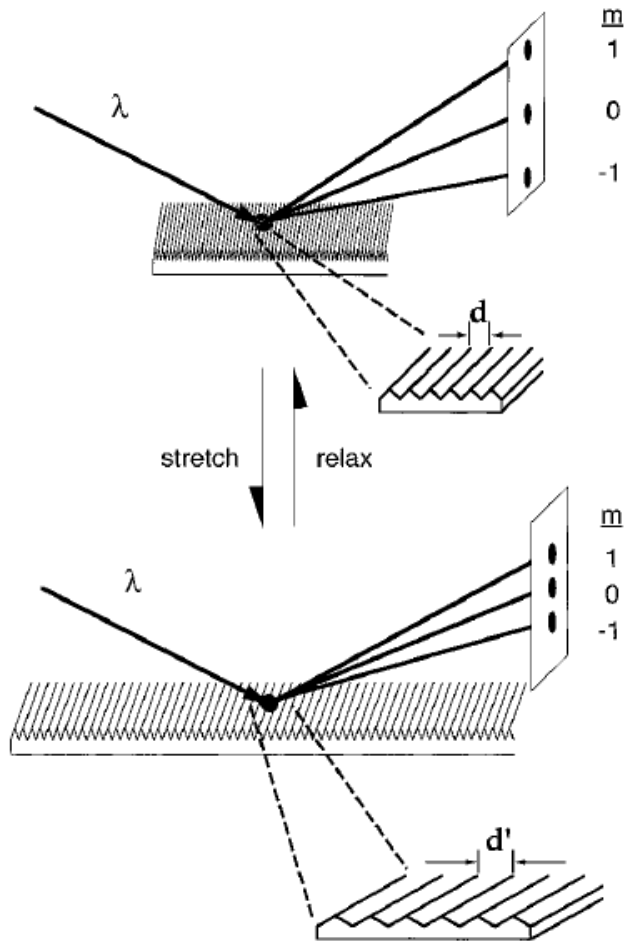
Expand pigmented sacs by contracting muscles



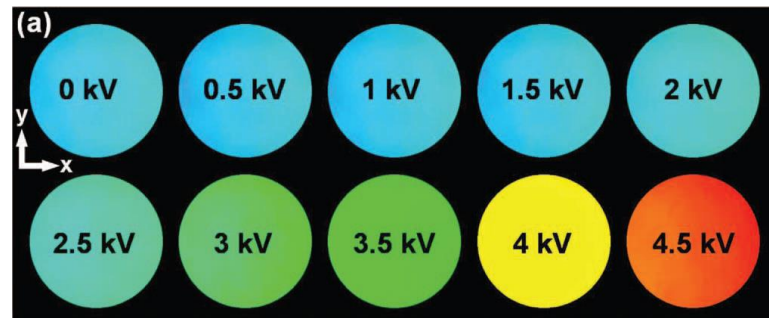
Elastomeric Optics



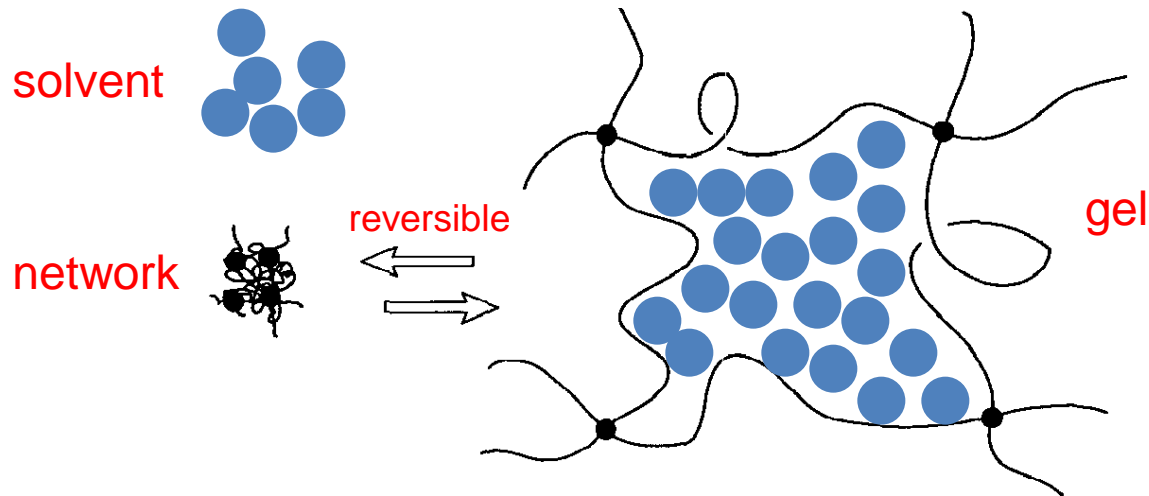
George Whitesides



- Many stimuli cause deformation.
- Deformation affects optics.



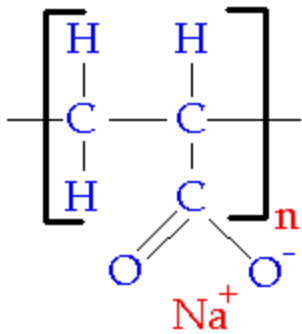
elastomer = network
gel = network + solvent



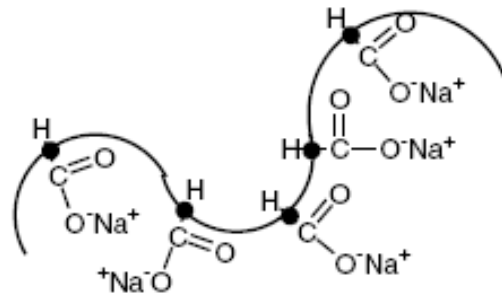
Super absorbent diaper



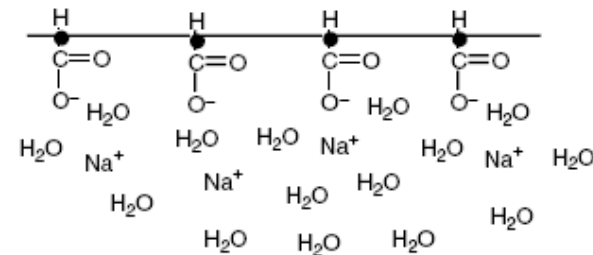
Sodium polyacrylate



Dry



in Water



Oil Spill...Hair

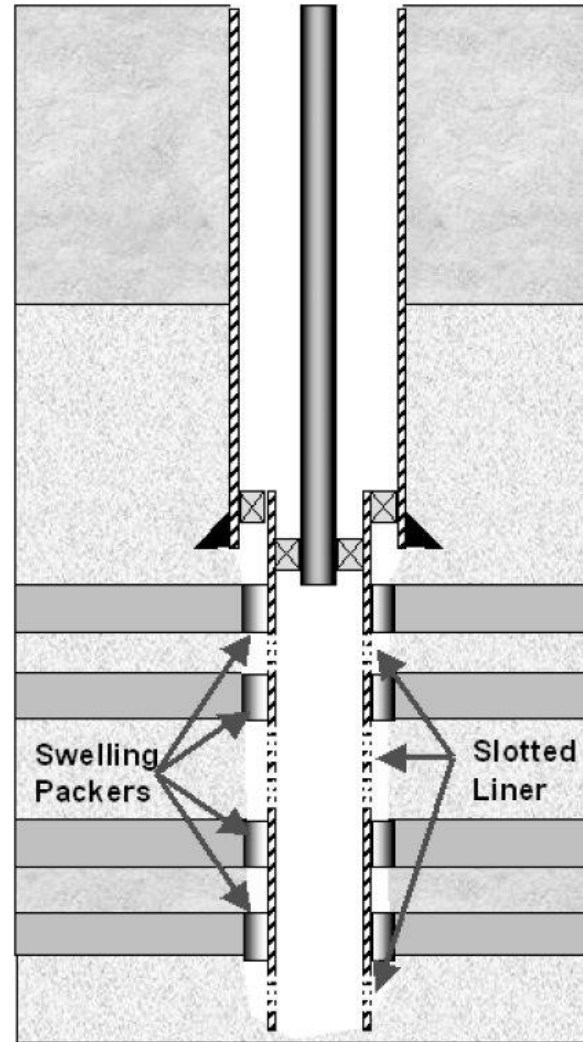
- Hair **adsorbs** oil (~3g oil/1g hair)
- Polypropylene fibers **absorb** oil (~10g oil/1g polypropylene)



Phil McCrory, Inventor of the hairmats
Lisa Gautier, Founder of Matter of Trust



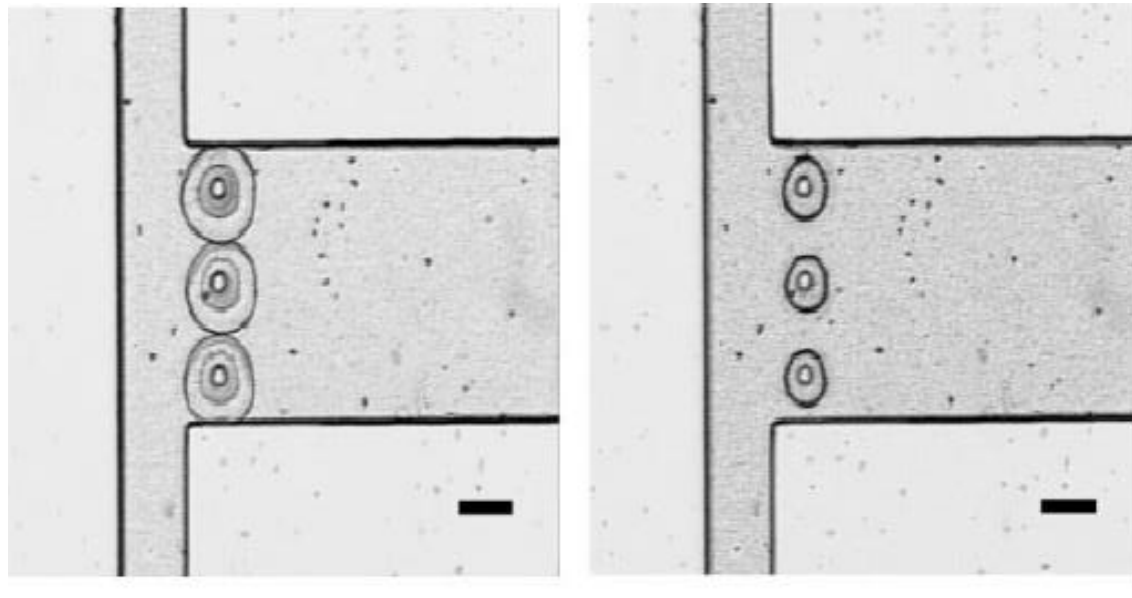
Swelling packers in oil wells



Self-regulating fluidics



David Beebe



Responsive to
Physiological variables:

- pH
- Salt
- Temperature
- light

- Many stimuli cause deformation.
- Deformation regulates flow.

Soft Active Materials

Soft: capable of large and reversible deformation
(rubbers, gels,...)

Active: response to diverse stimuli
(electric field, temperature, pH, salt,...)

A stimulus causes deformation.

Deformation provides a function.

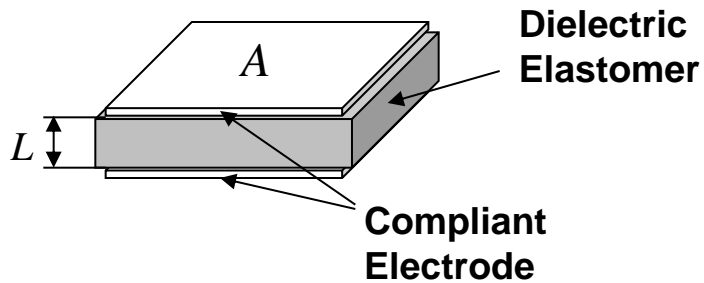


<http://www.seas.harvard.edu/suo/>

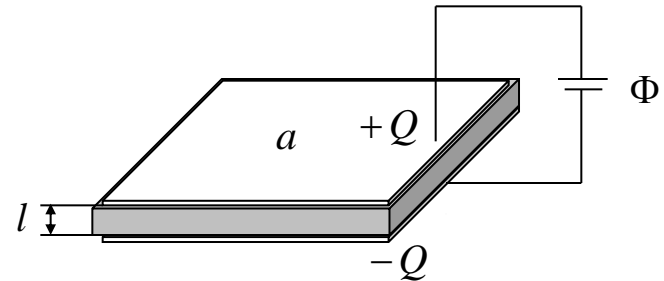
Better life through deformation

Dielectric elastomer

Reference State

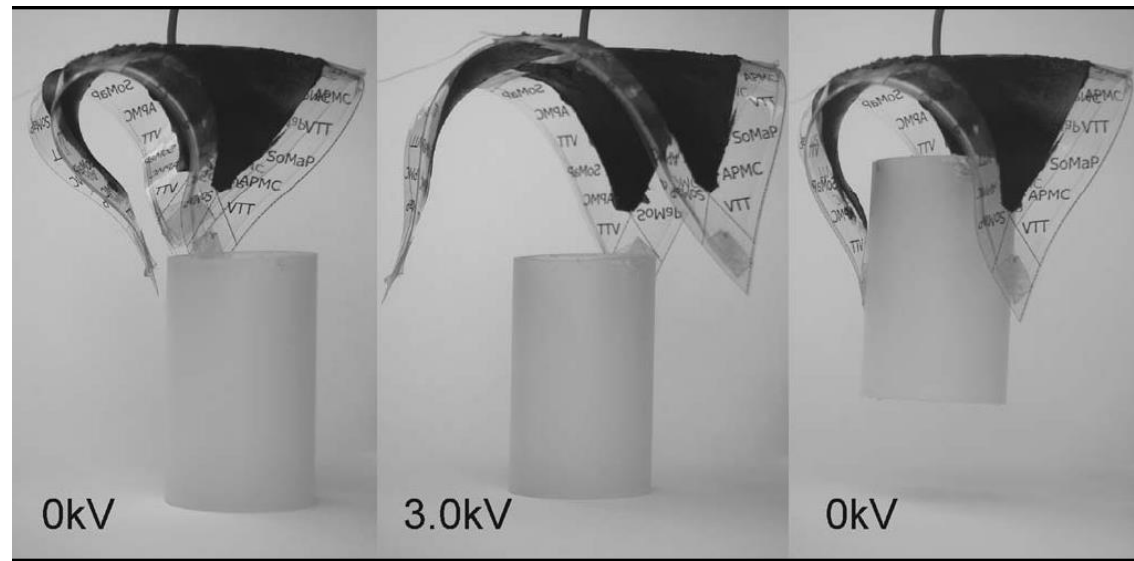
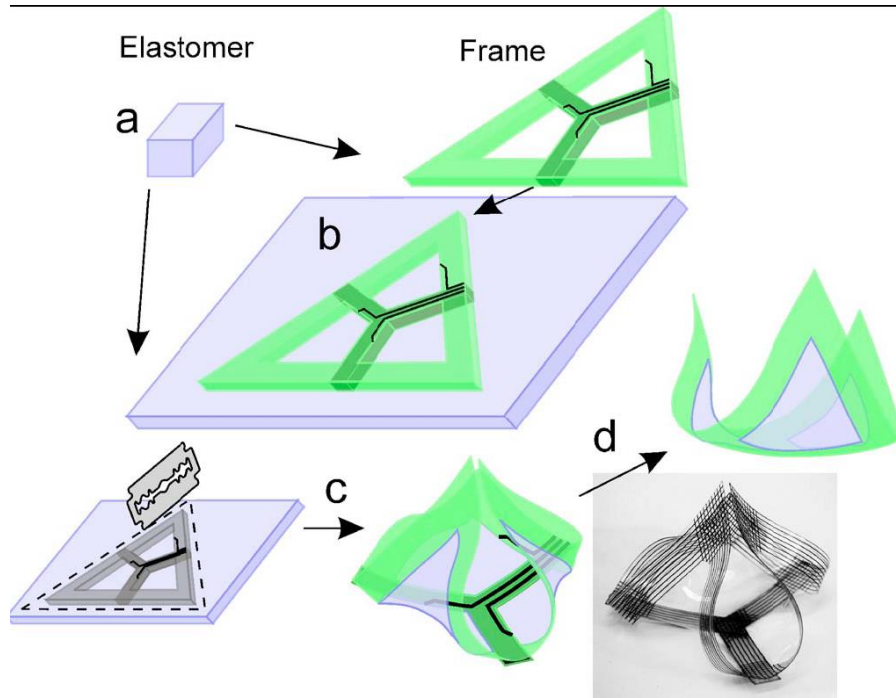


Current State



- Large strain
- Noise-less
- Cheap

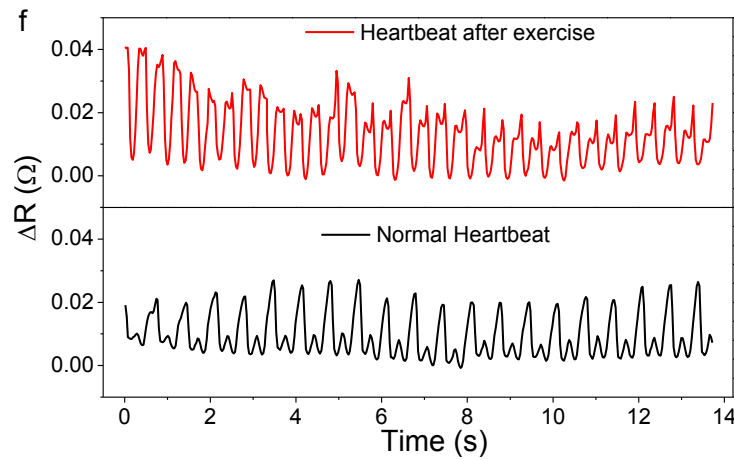
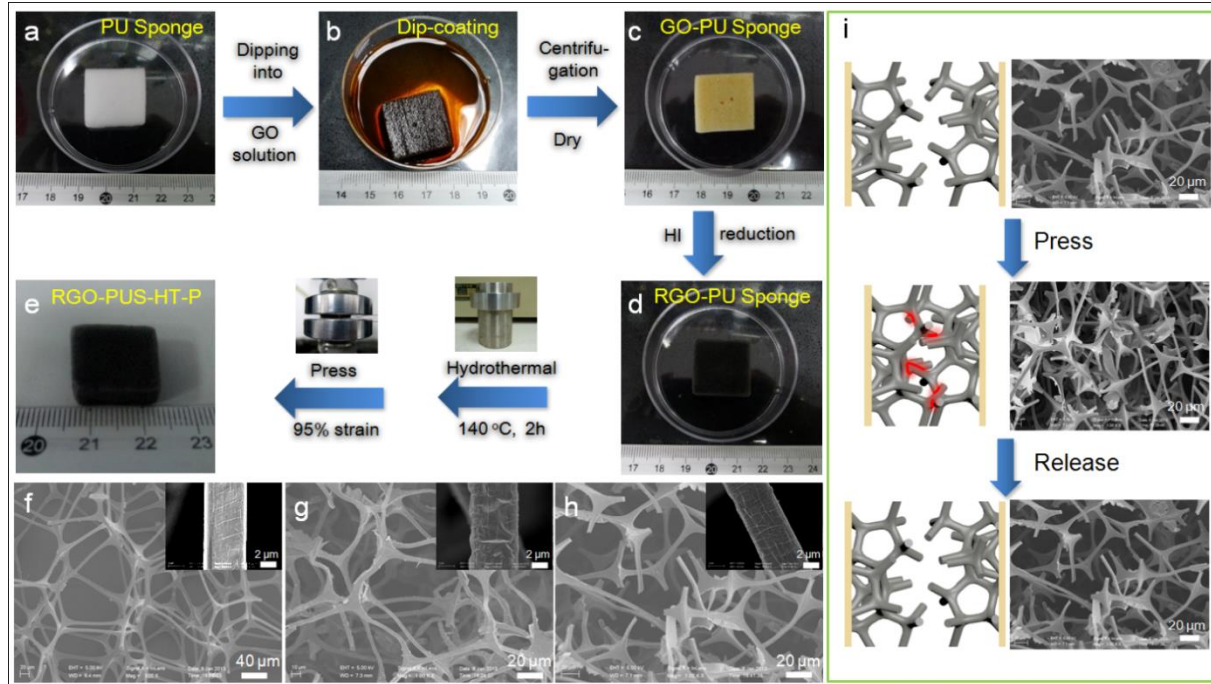
Programmable deformation



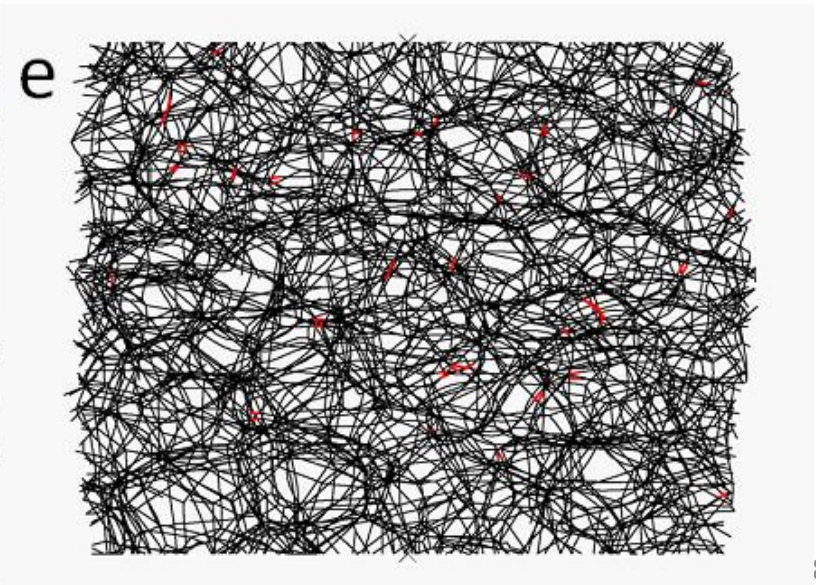
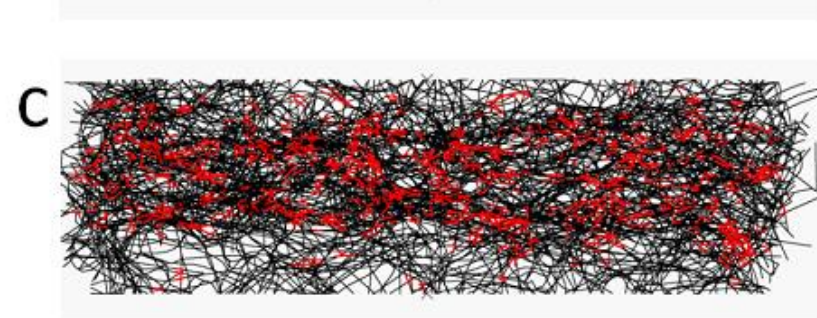
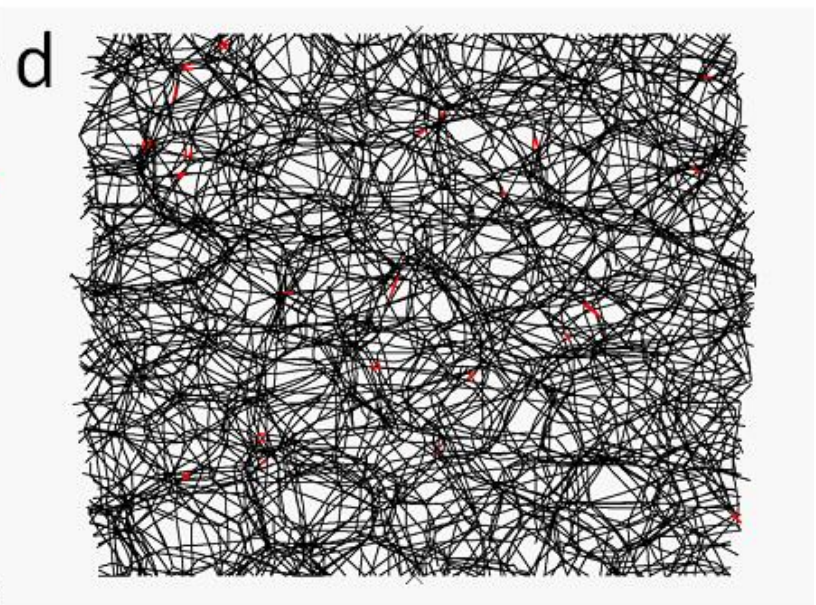
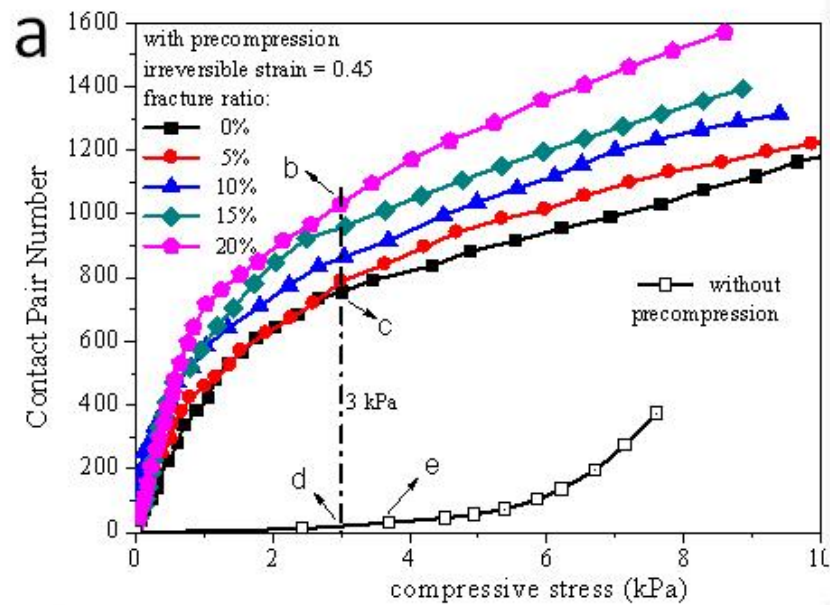
Design:
Kofod, Wirges, Paajanen, Bauer
APL **90**, 081916 (2007)

Simulation:
Zhao, Suo
APL **93**, 251902 (2008)

巨压阻传感器



From Professor Yu's lab
<http://staff.ustc.edu.cn/~yulab/>

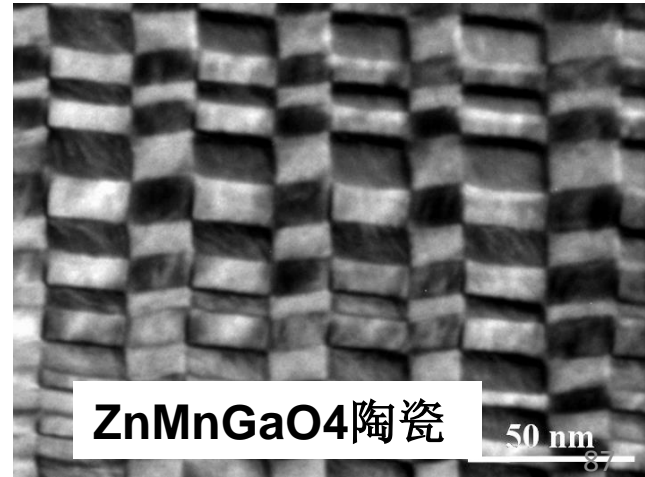
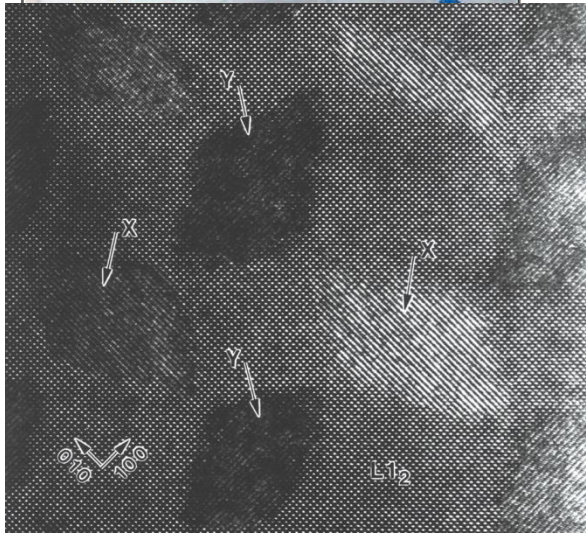
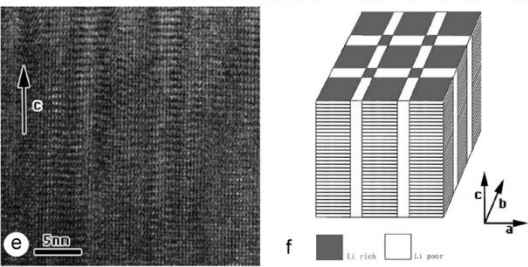
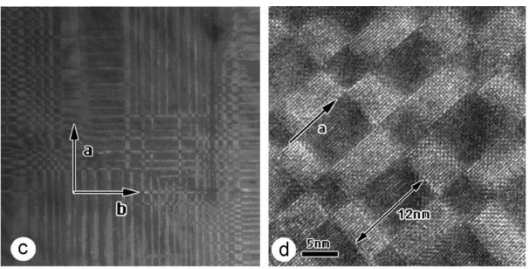
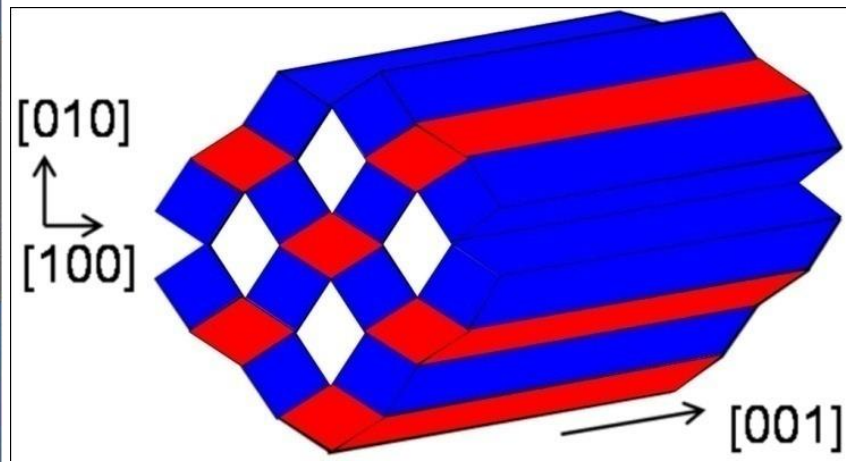
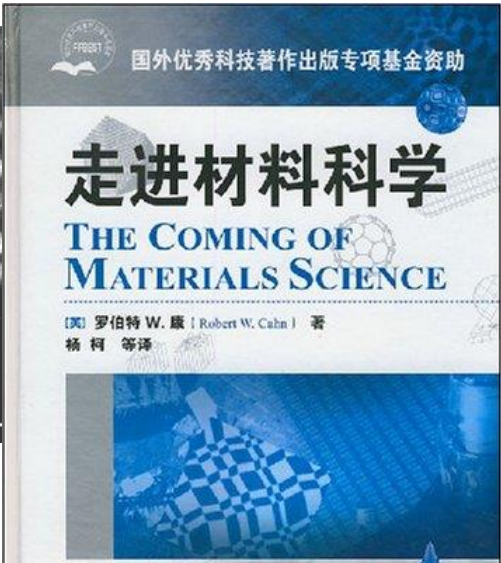
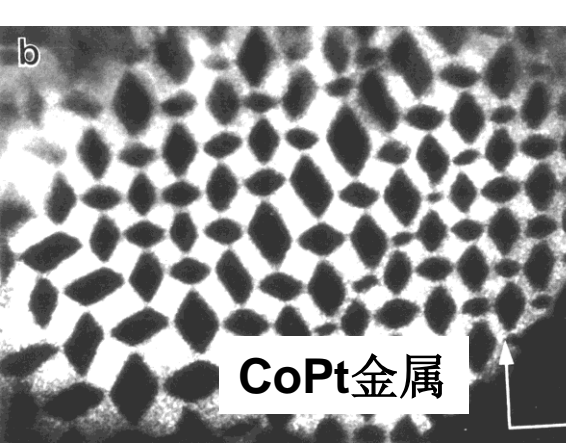


提纲

□ 固体力学在材料中的应用

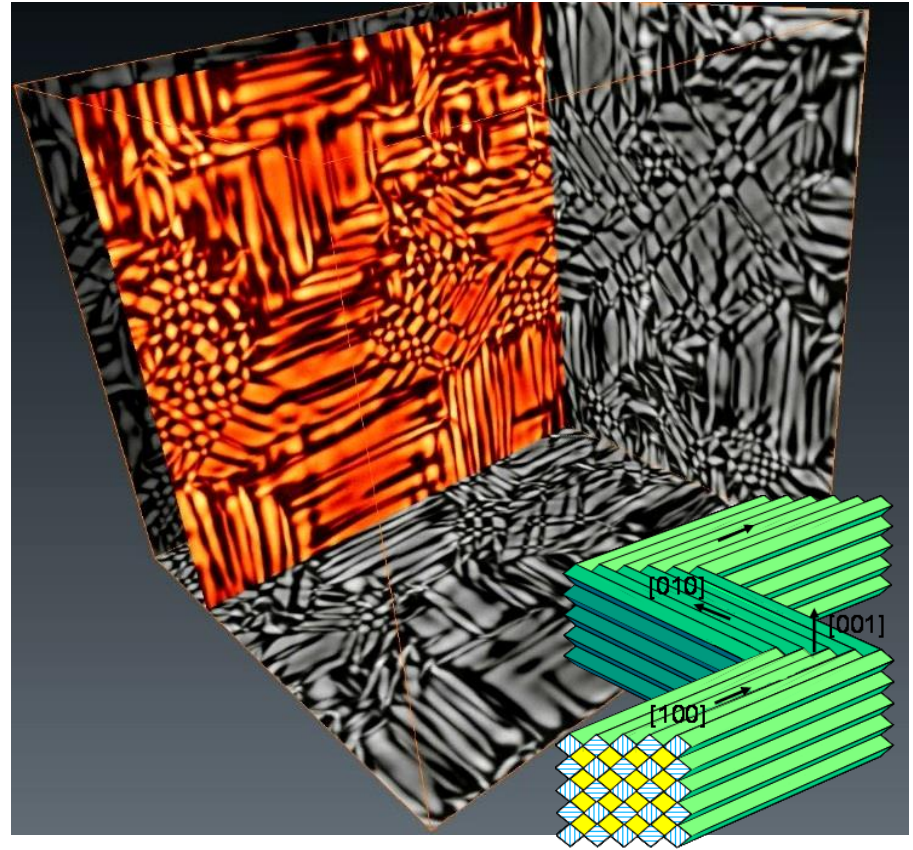
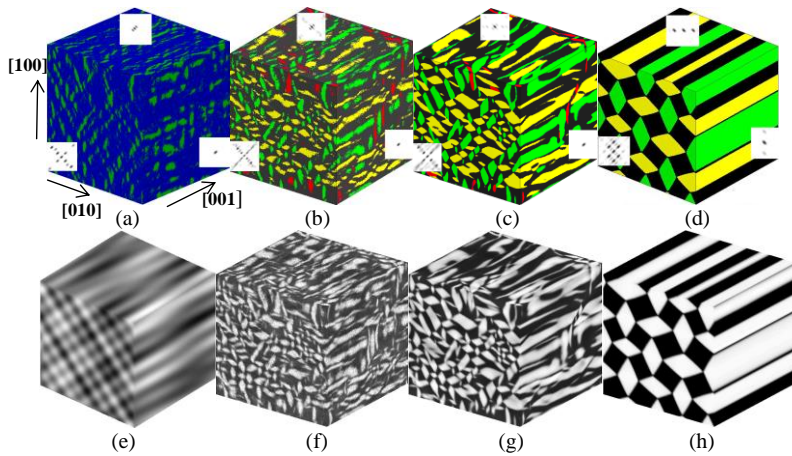
4. 微结构演化调控的应力工程举例

自组装的棋盘状纳米线束



Nd_{2/3-x}Li_{3x}TiO₃陶瓷

自组装的棋盘状纳米线束：演化模拟



棋盘状纳米线束薄膜:优化的生长条件

优化温度与组分

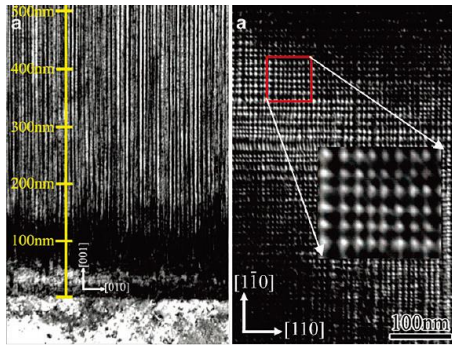
$$c \sim c_0(T) \quad \text{and} \quad c < c_0(T)$$

优化晶体学参数一

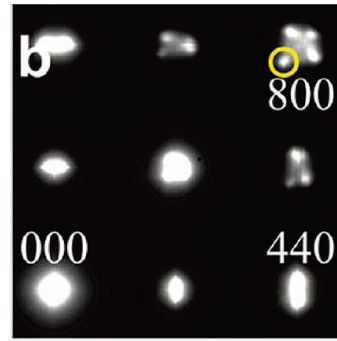
$$\xi_0 = \frac{a_c - a_t}{c_t - a_t} = \frac{1 + 4\nu}{11 + 8\nu}$$

优化晶体学参数二

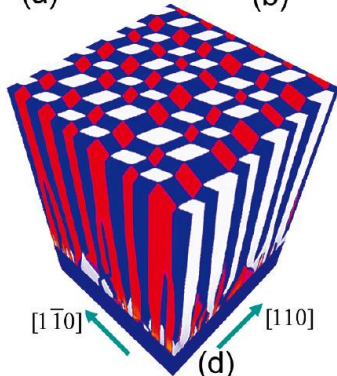
$$\rho = \frac{\bar{a}^f}{a_s} = \frac{2a_c + c_t + a_t}{4a_s} \rightarrow 1$$



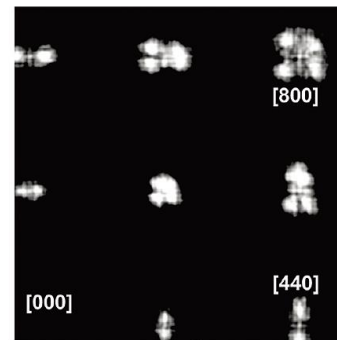
(a) (b)



(c)



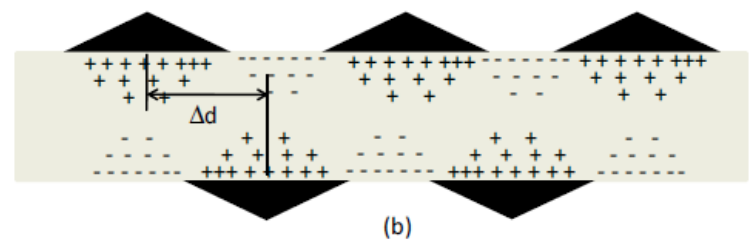
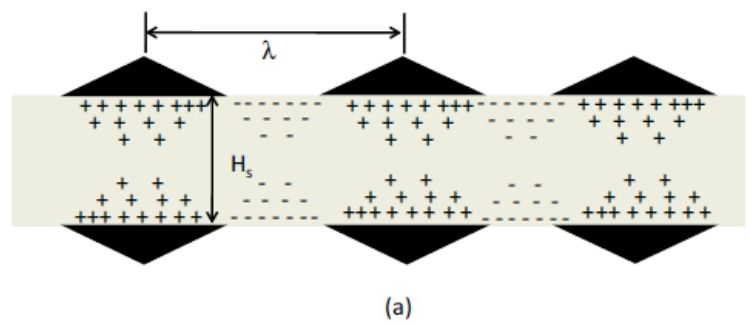
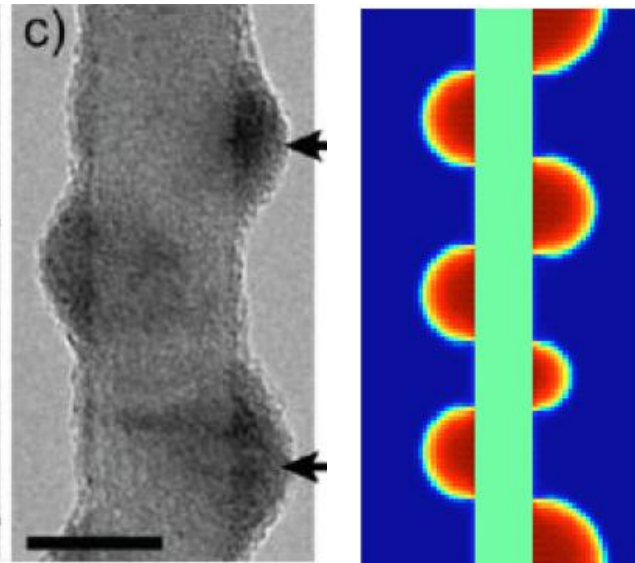
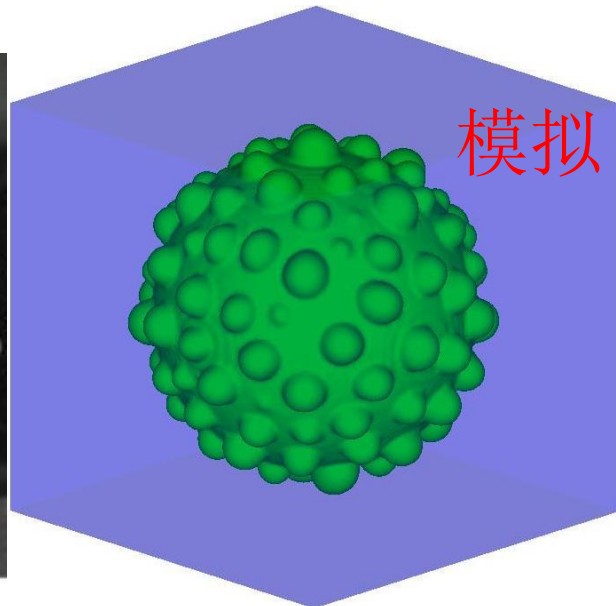
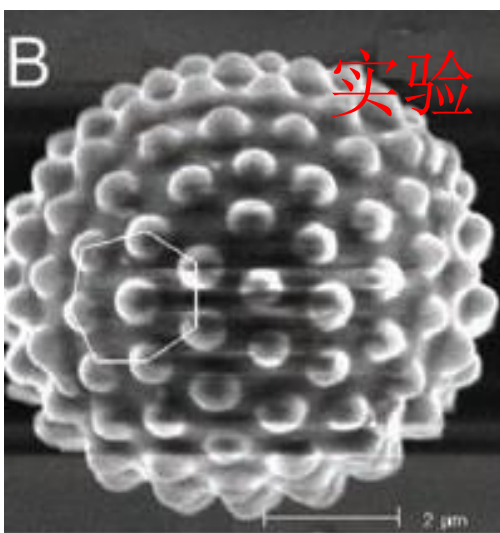
(d)



(e)

Yong Ni, et al, Nano Letter, 9,3275(2009)

量子点与应变自组装生长



远场弹性对表界面
形态演化的影响

Y. Ni, L.H.He, *APL.*, 2010, **97**, 261911.
Y. Ni, D. Yang, L.H.He, *PRE.*, 2012, **86**, 031604.

总结

□ 计算材料简介

□ 固体力学简介

□ 固体力学在材料中的应用

1. 超材料、材料强韧化设计举例

2. 功能材料的力学稳定性与寿命分析举例

3. 基于变形耦合的功能材料设计举例

4. 微结构演化调控的应力工程举例