



西安交通大学
XI'AN JIAOTONG UNIVERSITY

复合材料多尺度力学分析

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工业中的多尺度力学方法讲习班

2021.1.15



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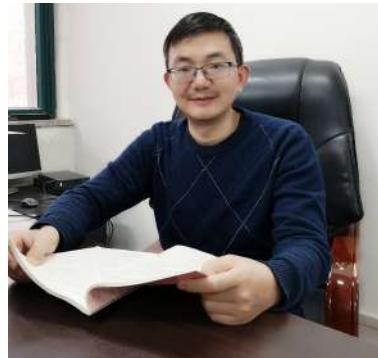
2019. 3—至今：西安交通大学 航天学院，教授



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王刚锋
杰青



刘益伦



徐光魁



欢迎青年才俊加入
共同发展多尺度力学！



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1. 碳纤维增强复合材料多尺度力学行为
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3. 碳纤维增强复合材料宏观力学行为

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- 1.1. 碳纤维增强复合材料多级结构
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- 1.3. 纤维增强复合材料多尺度优化设计



历史曾用材料来划分人类的文明时代的四次重大突破

天然材料：新石器时代

人工材料：铜器和铁器时代

合成材料：塑料（1924）、橡胶（1931）

复合材料：玻璃纤维（1942）



世界最长的LM 88.4米风电叶片

•复合材料是指由有机高分子、无机非金属或金属等几类不同材料通过复合工艺组合而成的新型材料，它既能保留原有组分材料的主要特色，又通过材料设计使各组分的性能互相补充并彼此关联，从而获得新的优越性能，与一般材料的简单混合有本质的区别

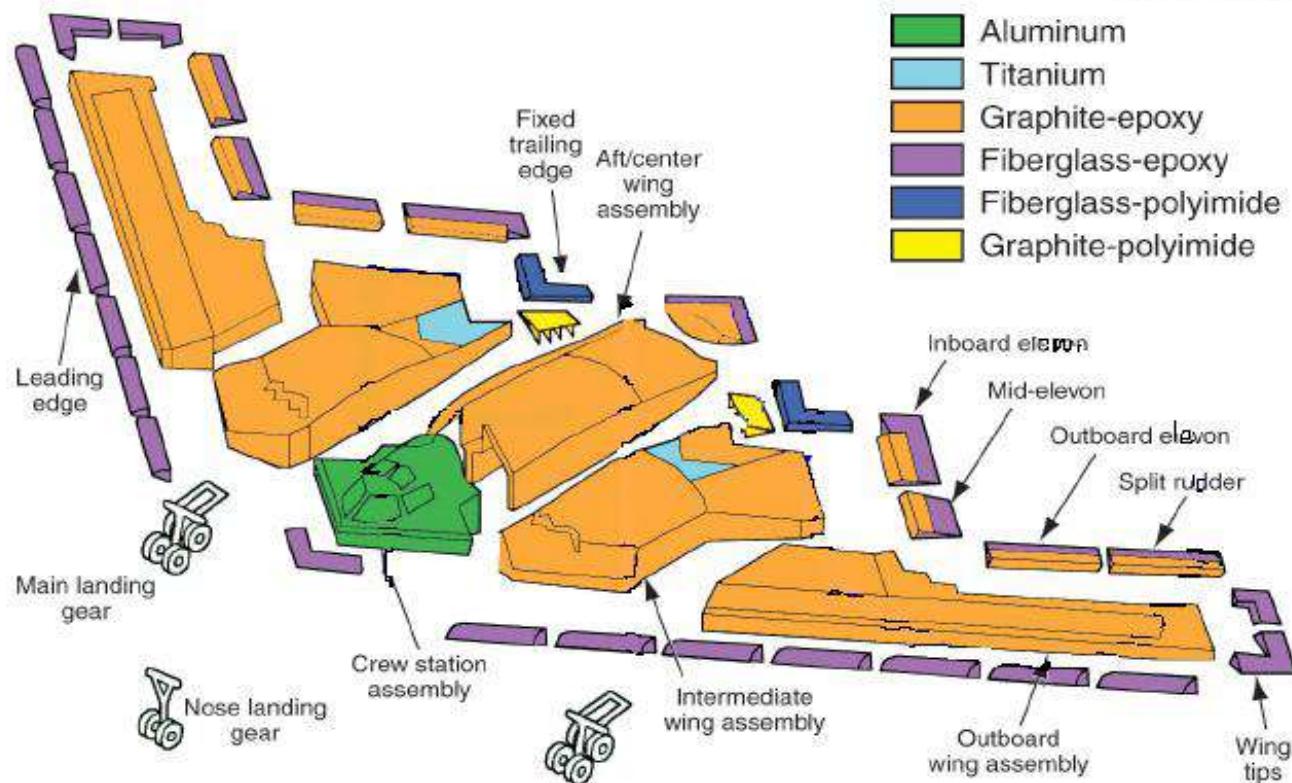
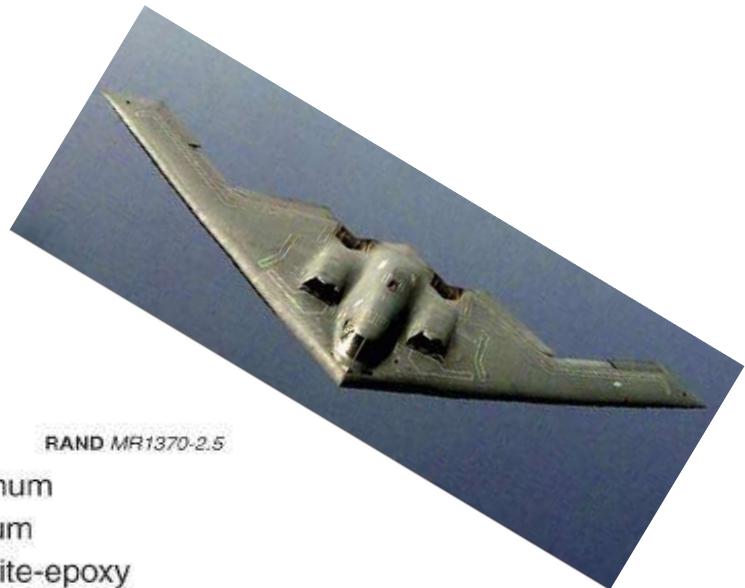
• (1994年出版，师昌绪主编《材料大辞典》)

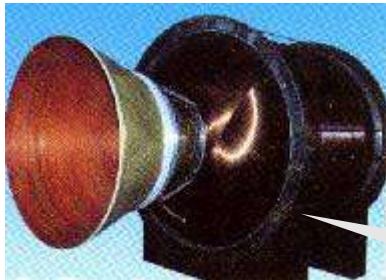


复合材料的三要素



B-2隐形轰炸机，当今世界上已公开的唯一一种隐形战略轰炸机。其机身结构，除主梁和发动机采用了钛合金外，其余部分皆由碳纤维复合材料构成。



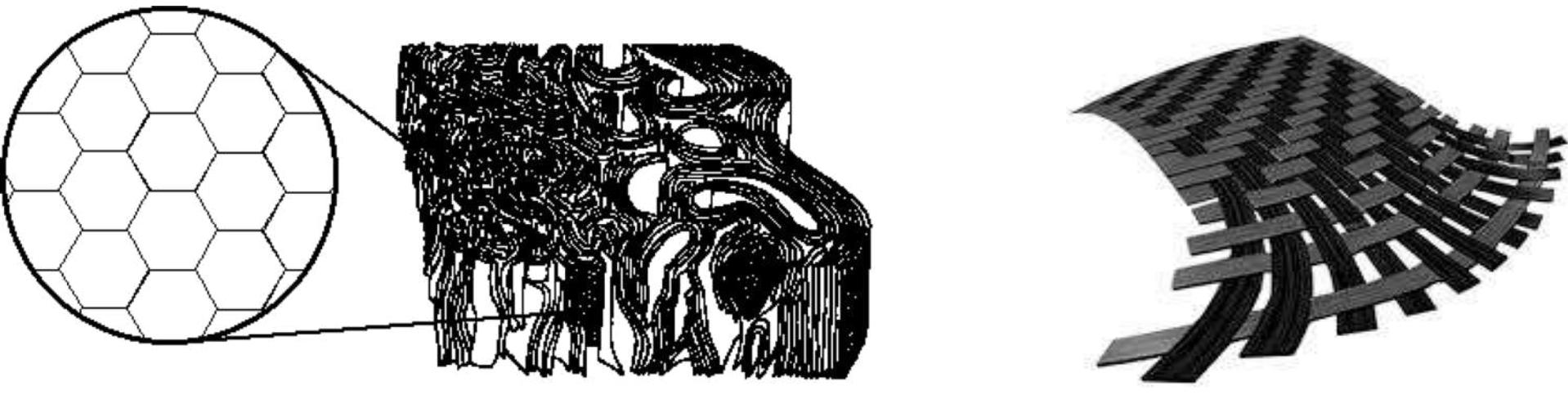


战略导弹弹头减少1Kg结构重量，增加射程20Km

战略导弹三级固体火箭发动机减少1Kg结构重量，增加射程16Km

某第三级固体发动机壳体采用碳/环氧复合材料后，结构质量由原来的116千克降为46千克，仅此就将导弹射程提高1000Km以上

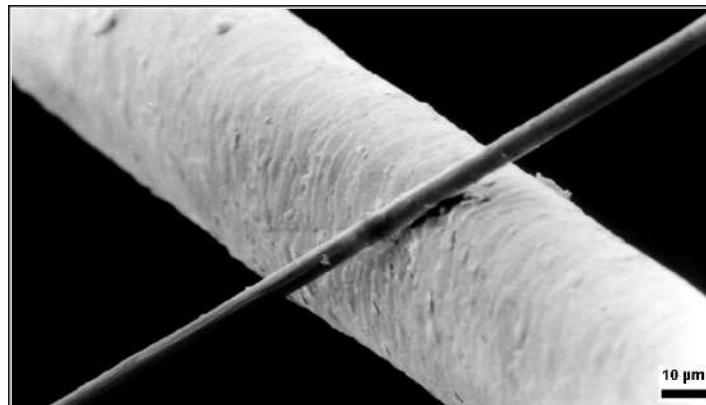
现阶段的先进复合材料主要是以碳纤维、硼纤维、芳纶纤维等高性能增强材料，使用高性能树脂、金属与陶瓷等为基体。



多层石墨烯

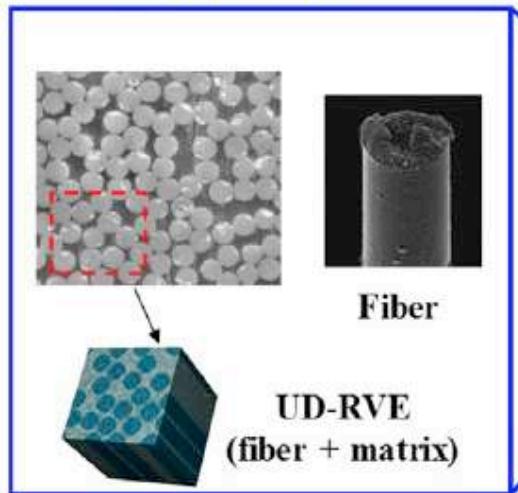
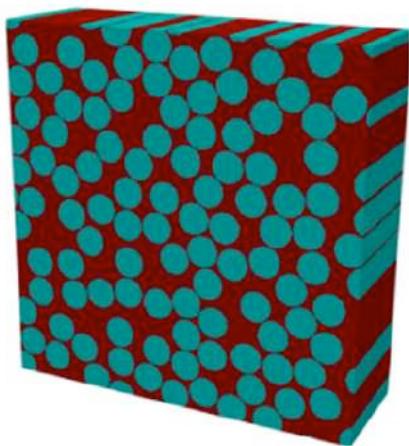
碳纤维

碳纤维布



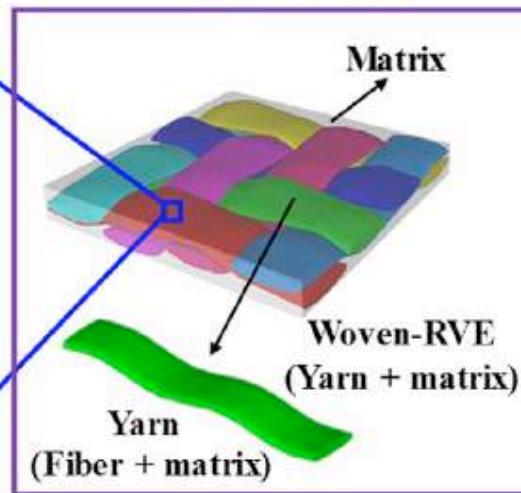
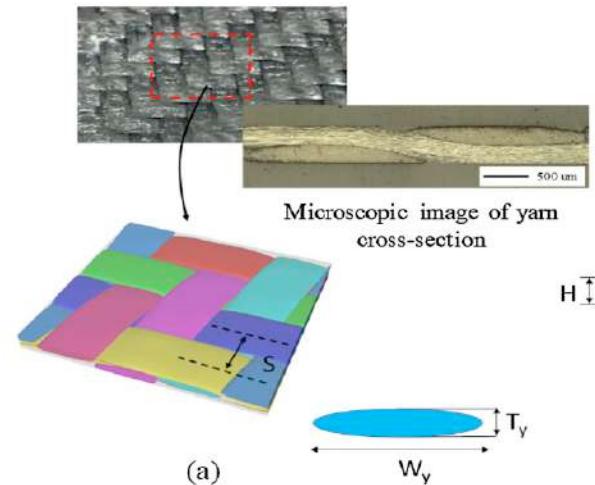


Micro-scale

 $\sim 10^{-6} \text{ m}$ 

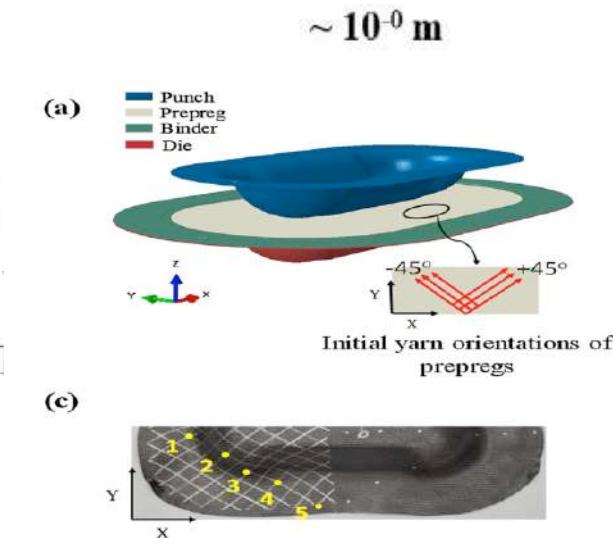
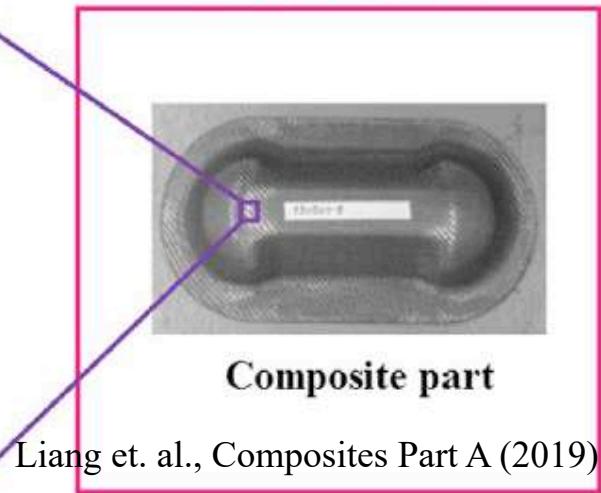
碳纤维束

Meso-scale

 $\sim 10^{-3} \text{ m}$ 

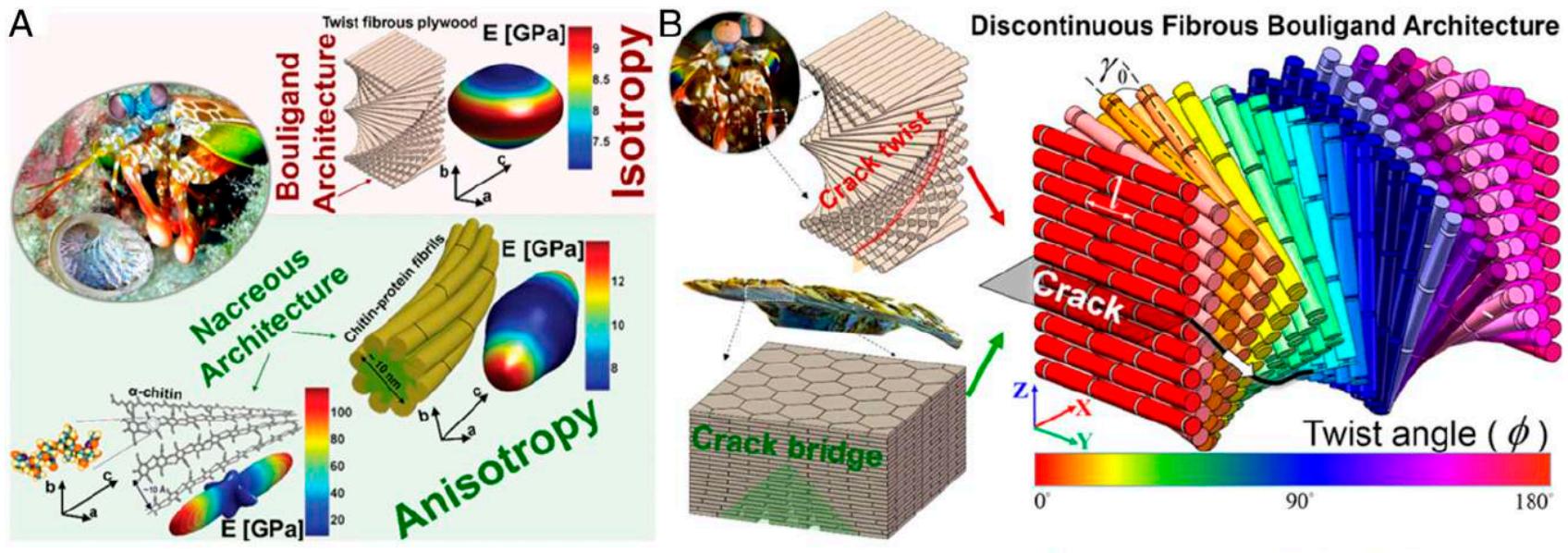
细观胞元

Macro-scale



宏观结构

生物材料矛和盾的竞争

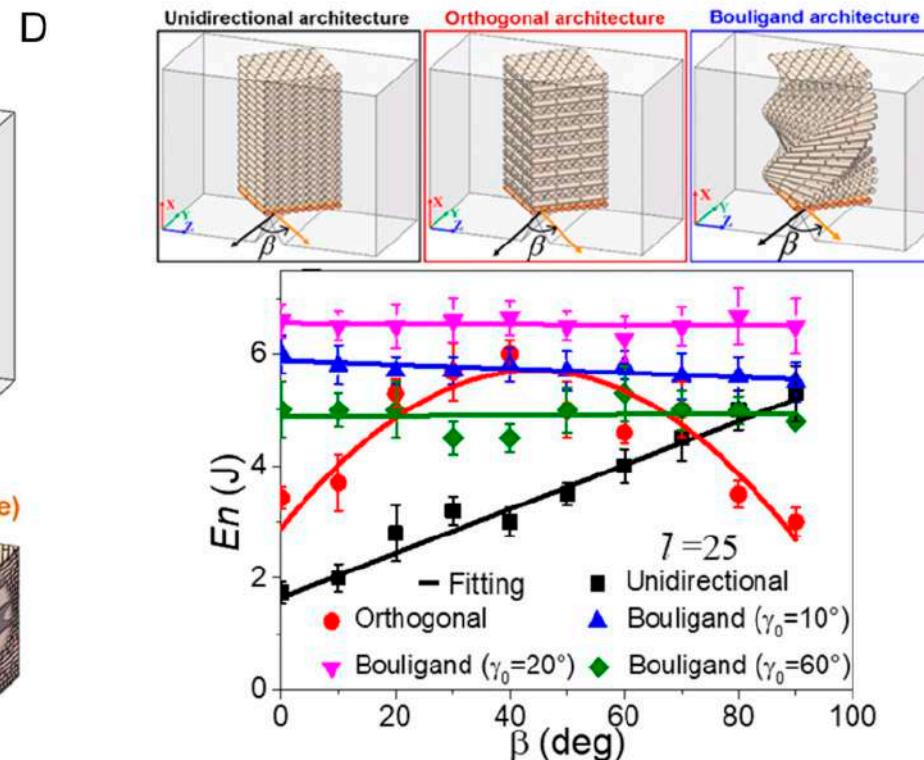
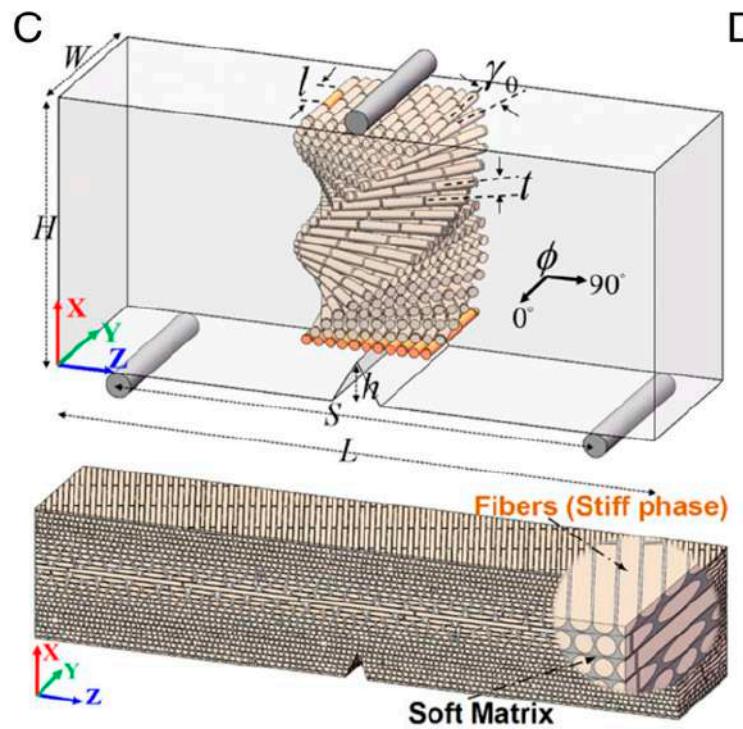


(A) 蟑螂虾和鲍鱼，甲壳动物表皮中不同结构的杨氏模量的3D图，其中具有珍珠阵列的甲壳素-蛋白质纳米纤维显示出高各向异性，而具有Bouligand结构的纤维胶合板显示出面内各向同性。

(B) DFB结构特征，结合了球型结构和珍珠状结构。



受侵略性甲壳类动物(如螃蟹、龙虾或螳螂虾)外骨骼结构排列的启发，具有有限特征长度的几丁质-蛋白质纳米纤维以重叠阵列排列，形成薄片和几丁质-蛋白质



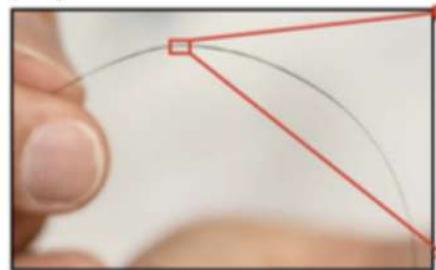
(C) 带有DFB结构的3D印刷单边缺口弯曲试样的几何配置。

(D) 初始裂纹尖端 β 的取向对单向、正交和不连续纤维布里甘结构中总能量耗散的影响。

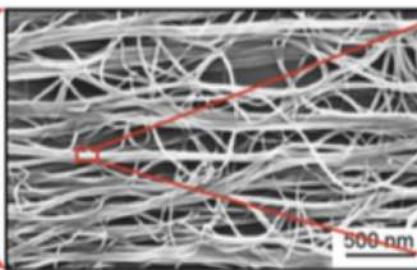
1.2 复合材料多尺度力学分析

多尺度力学分析

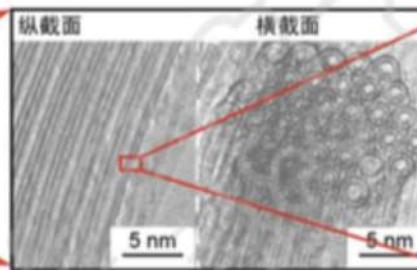
碳纳米管纤维



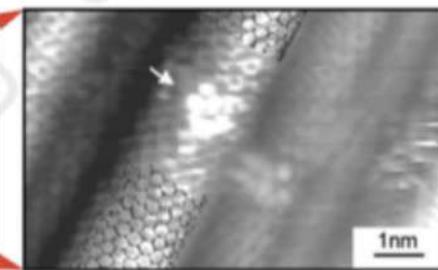
管束网状结构



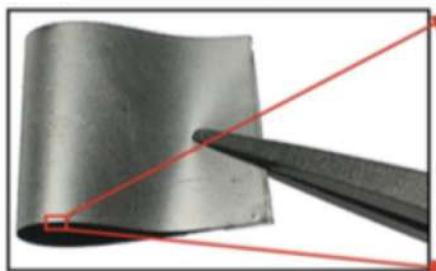
束状结构



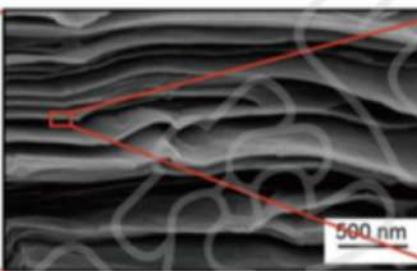
碳纳米管



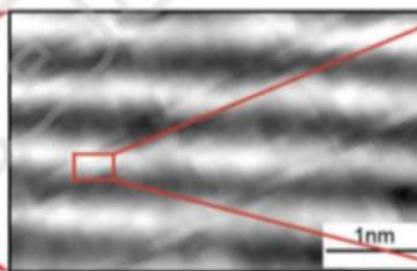
石墨烯薄膜



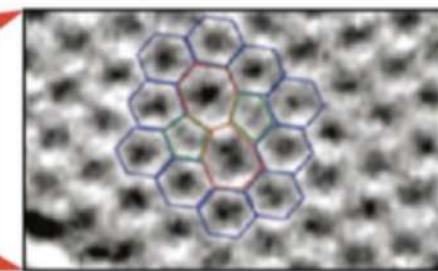
片层褶皱结构



层状结构

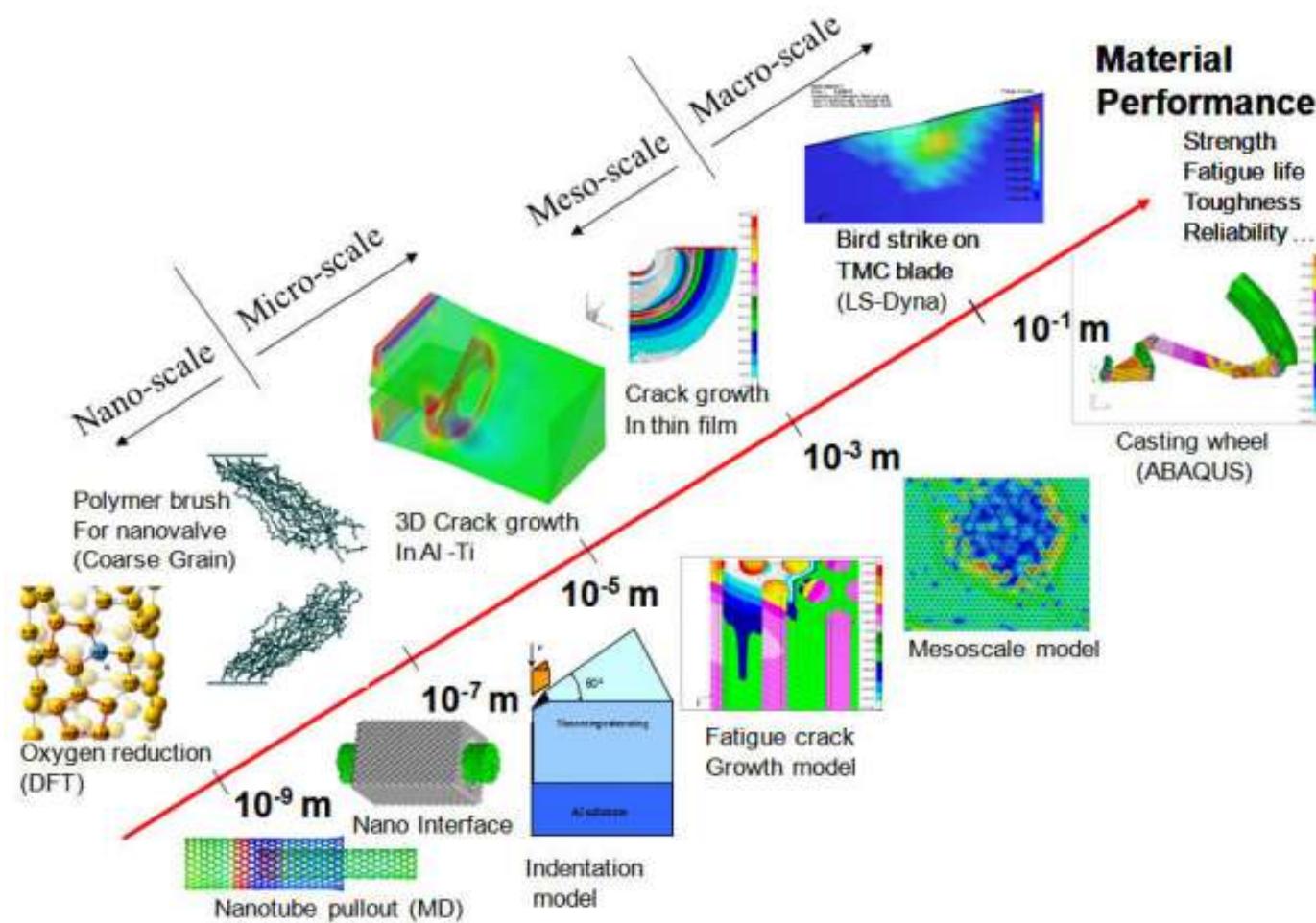


石墨烯



多层次结构 → 多尺度力学分析

多尺度力学分析



量子力学

分子力学

细观力学

宏观力学

From Xia's group@uakron



表1 多尺度复合材料分析的主要理论和模拟方法

Table 1 Theoretical and simulational methods of multiscale analysis

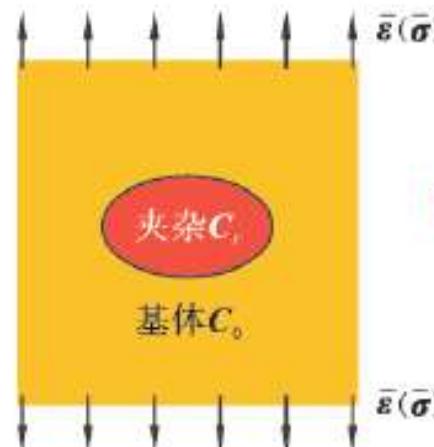
		非均质→均质	离散→连续
多层次分析方法	理论		
		Voigt 近似, Reuss 近似, Hashin-Shtrikman 上下限法, 稀疏方法, 自洽法, 广义自洽法, 微分法, 有效自洽法, IDD 方法, Mori-Tanaka 方法, 剪滞理论, 内聚力模型, 等	Cauchy-Born 准则, 非局部理论, 等

陈玉丽, 固体力学学报, 2018

	非均质→均质	离散→连续
多层次分析方法	<p>有限元(FEM), 扩展有限元法(XFEM), 边界元(BEM), 有限体积法(FVM), 离散元(DEM), 无网格方法, 渐近展开均匀化方法, 胞元法, Voronoi 单元有限元法(VCFEM), 快速傅里叶变换模型(FFT Model),等</p>	<p>密度泛函理论(DFT), 从头算分子动力学(AIMD), 蒙特卡洛模拟(MC), 分子动力学(MD), 原子尺度有限元方法(AFEM), 近场动力学(PD), 粗粒化方法(CG), 分子结构力学方法(MSM), 分子统计热力学方法(MST), 集团统计热力学方法(CST), 广义均匀化方法(GMH),等</p>
并发多尺度分析方法	<p>双尺度有限元法(FE^2), 多尺度有限元法(MsFEM), 多尺度有限体积法(MsFV), 扩展多尺度有限元方法(EMsFEM),等</p>	<p>FEAt, MAAD, CADD, AFEM-FEM, 连续介质-分子动力学交叠层方法, 桥接尺度方法(BSM), 桥接区域方法(BDM), 三层网格桥接区域模型(TBDM), 准连续方法(QC), 粗粒化分子动力学(CGMD), 混合分子/集团统计热力学方法(HMCST), 异质多尺度方法(HMM),等</p>

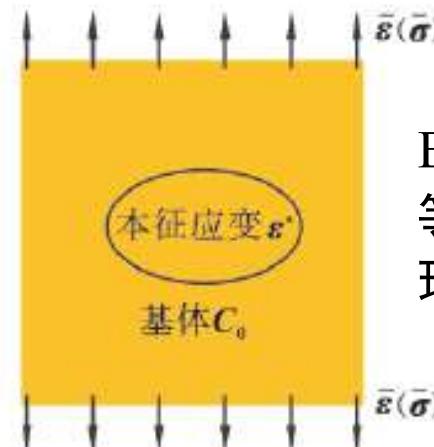


复合材料理论分析方法



(a) 单夹杂问题

假想相变
→



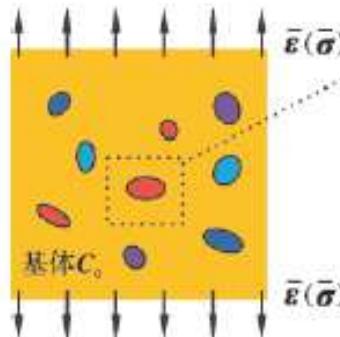
(b) 本征应变问题

Eshelby
等效夹杂
理论

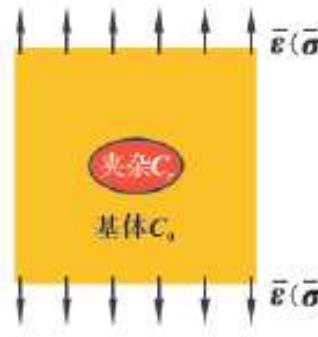
$$\boldsymbol{\varepsilon}_{in} = \mathbf{S}^E : \boldsymbol{\varepsilon}^*$$

$$\langle \boldsymbol{\varepsilon} \rangle_r = [\mathbf{I} + \mathbf{S}_r^E : \mathbf{C}_0^{-1} : (\mathbf{C}_r - \mathbf{C}_0)]^{-1} : \bar{\boldsymbol{\varepsilon}}$$

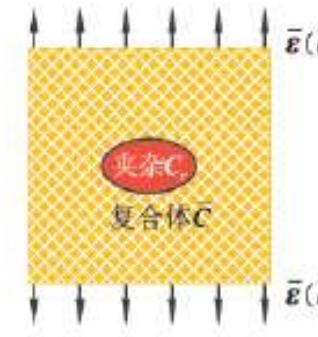
$$\langle \boldsymbol{\sigma} \rangle_r = \mathbf{C}_r : [\mathbf{C}_0 + \mathbf{C}_0 : \mathbf{S}_r^E : \mathbf{C}_0^{-1} : (\mathbf{C}_r - \mathbf{C}_0)]^{-1} : \bar{\boldsymbol{\sigma}}$$



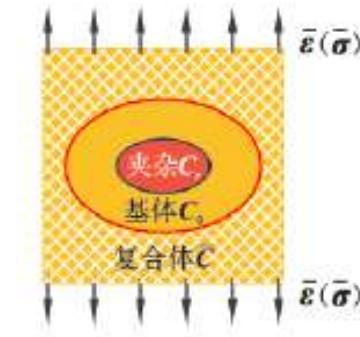
(a) 多平杂问题



(b) 稀疏法



(c) 自治法

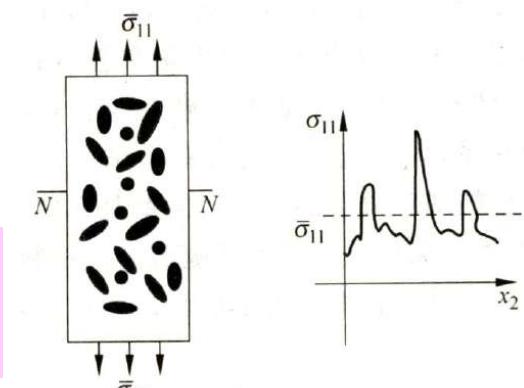


(d) 广义自治法



渐进均匀化方法

$$u^\varepsilon(x) = u^0(x, y) + \varepsilon u^1(x, y) + \varepsilon^2 u^2(x, y) + \dots, \quad y = \frac{x}{\varepsilon}$$



$$\begin{aligned} \text{应变张量 } e_{kl}^\varepsilon &= \frac{1}{2} \left(\frac{\partial u_k^\varepsilon}{\partial x_l^\varepsilon} + \frac{\partial u_l^\varepsilon}{\partial x_k^\varepsilon} \right) = \frac{1}{2} \left(\frac{1}{\varepsilon} \left(\frac{\partial u_k^0}{\partial y_l} + \frac{\partial u_l^0}{\partial y_k} \right) + \left(\frac{\partial u_k^0}{\partial x_l} + \frac{\partial u_l^0}{\partial x_k} + \frac{\partial u_k^1}{\partial y_l} + \frac{\partial u_l^1}{\partial y_k} \right) \right. \\ &\quad \left. + \varepsilon \left(\frac{\partial u_k^1}{\partial x_l} + \frac{\partial u_l^1}{\partial x_k} + \frac{\partial u_k^2}{\partial y_l} + \frac{\partial u_l^2}{\partial y_k} \right) + \varepsilon^2 \left(\frac{\partial u_k^2}{\partial x_l} + \frac{\partial u_l^2}{\partial x_k} + \frac{\partial u_k^3}{\partial y_l} + \frac{\partial u_l^3}{\partial y_k} \right) + \dots \right) \\ &= \frac{1}{\varepsilon} e_{kl}^{-1}(x, y) + e_{kl}^0(x, y) + \varepsilon e_{kl}^1(x, y) + \varepsilon^2 e_{kl}^2(x, y) + \dots \end{aligned}$$

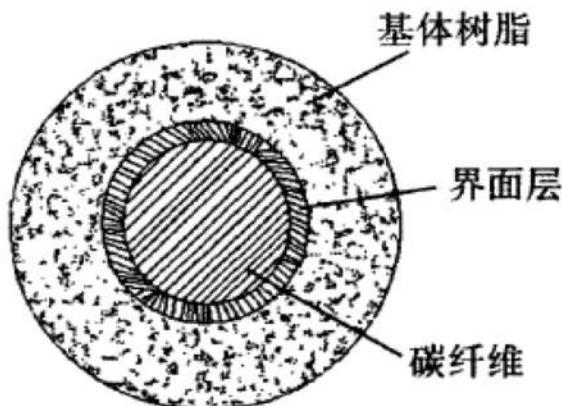
将应力的渐进展开式代入平衡方程，有

$$\begin{aligned} &\frac{1}{\varepsilon} \left[\frac{\partial \sigma_{ij}^{-1}(x, y)}{\partial x_j} + \frac{1}{\varepsilon} \frac{\partial \sigma_{ij}^{-1}(x, y)}{\partial y_j} \right] + \left[\frac{\partial \sigma_{ij}^0(x, y)}{\partial x_j} + \frac{1}{\varepsilon} \frac{\partial \sigma_{ij}^0(x, y)}{\partial y_j} \right] + \\ &\varepsilon \left[\frac{\partial \sigma_{ij}^1(x, y)}{\partial x_j} + \frac{1}{\varepsilon} \frac{\partial \sigma_{ij}^1(x, y)}{\partial y_j} \right] + \varepsilon^2 \left[\frac{\partial \sigma_{ij}^2(x, y)}{\partial x_j} + \frac{1}{\varepsilon} \frac{\partial \sigma_{ij}^2(x, y)}{\partial y_j} \right] + \dots + f_i = 0 \end{aligned}$$

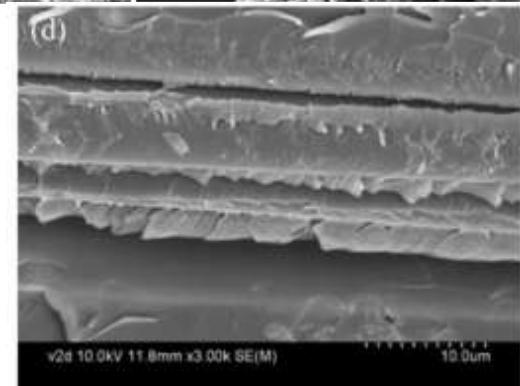
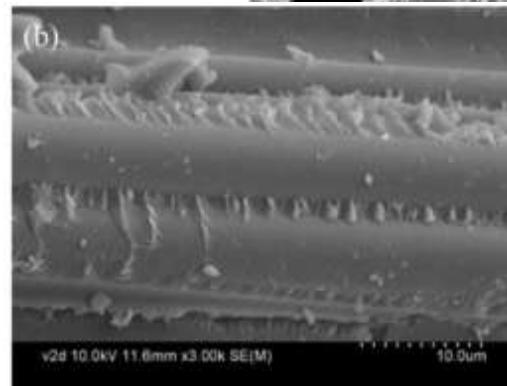
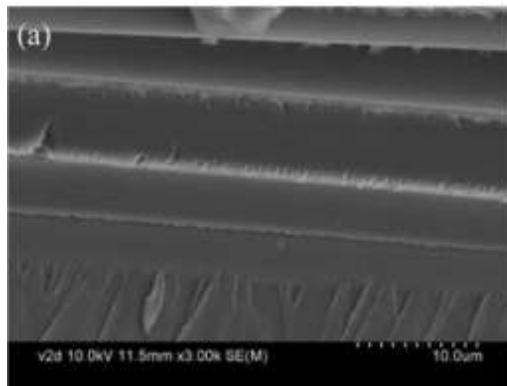
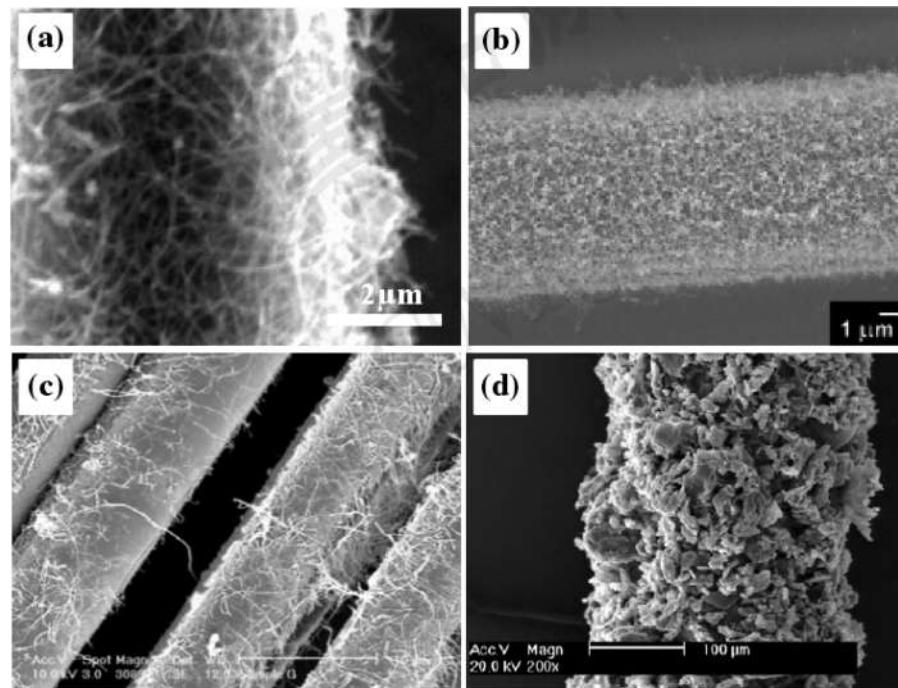
1.3 纤维增强复合材料多尺度优化设计 ----复合材料界面设计

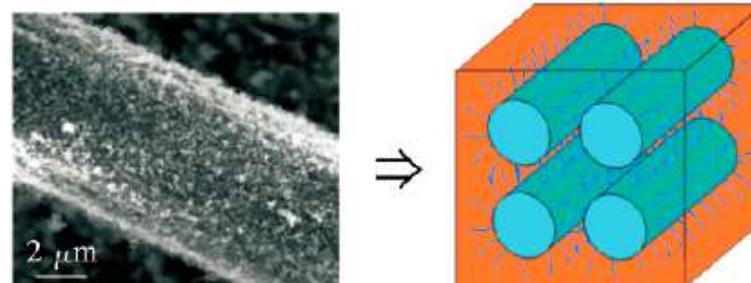


由于碳纤维表面表现为非极性和化学惰性，有疏水、光滑、吸附性能低等缺点，导致碳纤维与树脂基体间的界面粘结性差。

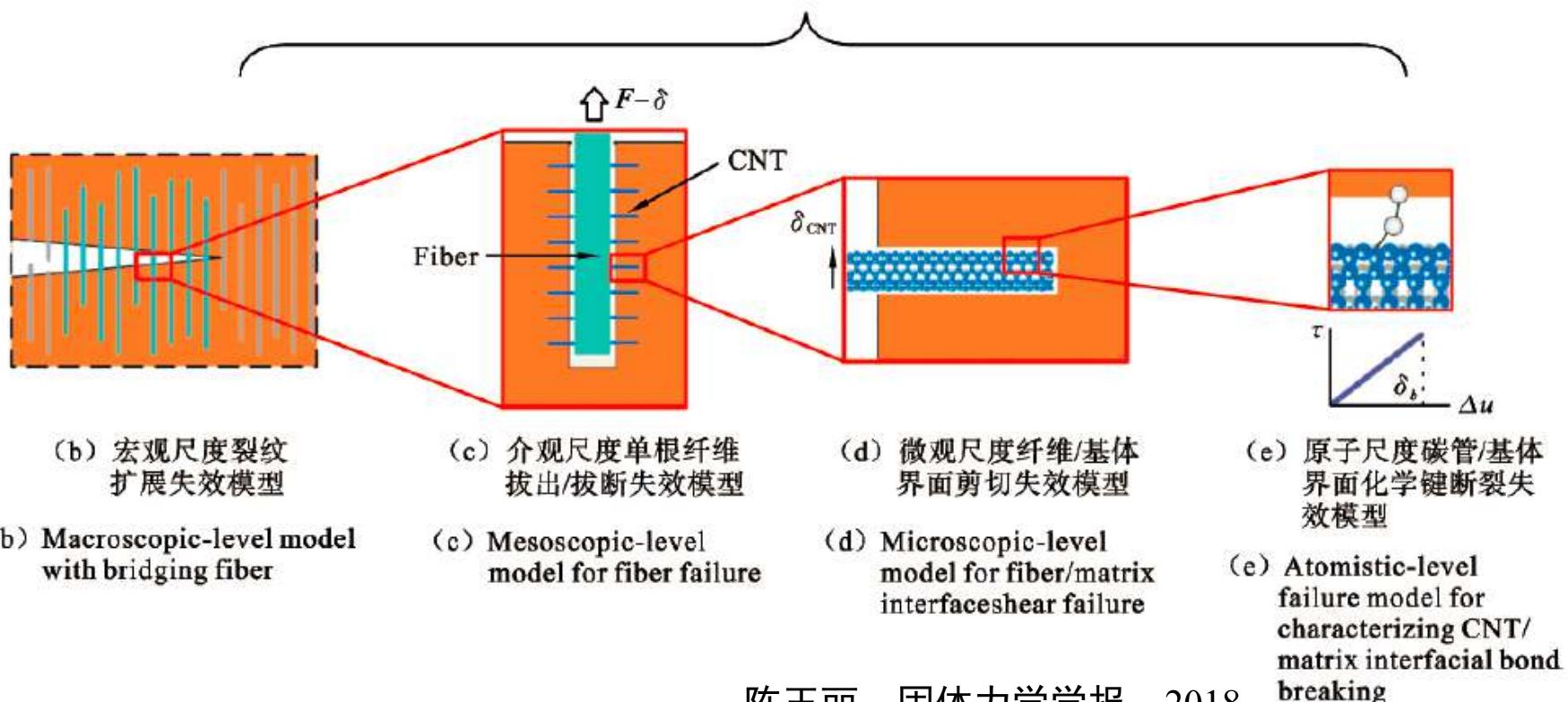


碳纤维增强树脂基复合材料界面层示意图





(a) 碳纳米管改性碳纤维的SEM照片^[425]及等效复合材料模型
(a) SEM picture^[425] and equivalent model of CNT-grafted fiber



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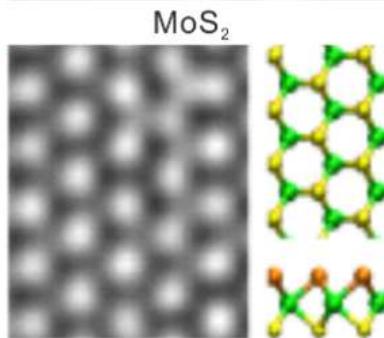
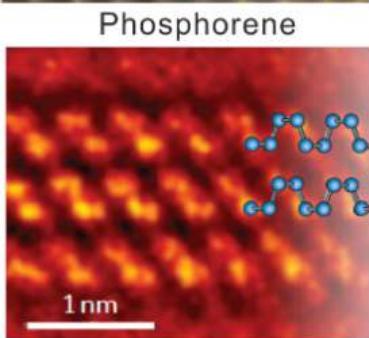
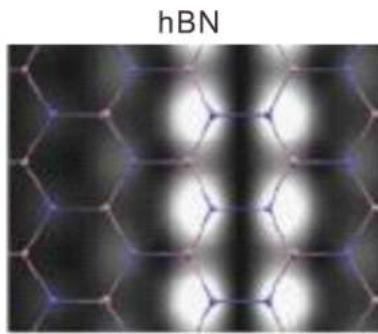
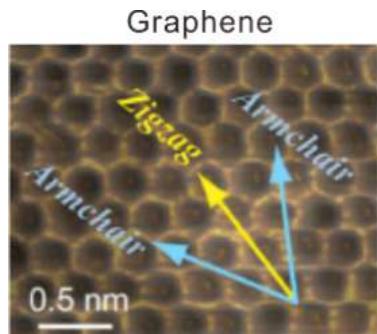
2.2 层状材料类贝壳结构力学行为

2.3 界面力学行为

目录

2.1 层状材料类层合板结构力学行为

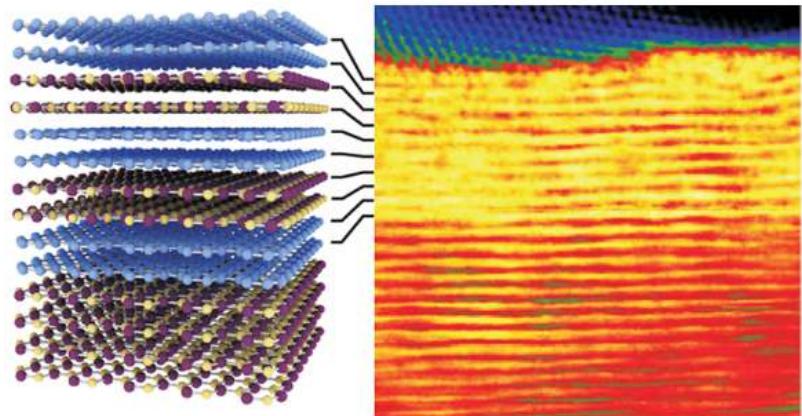
层状材料微结构



二维材料

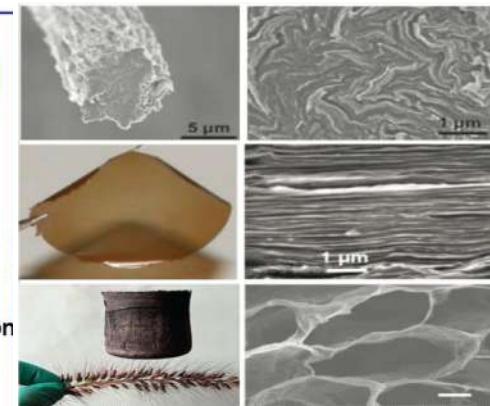
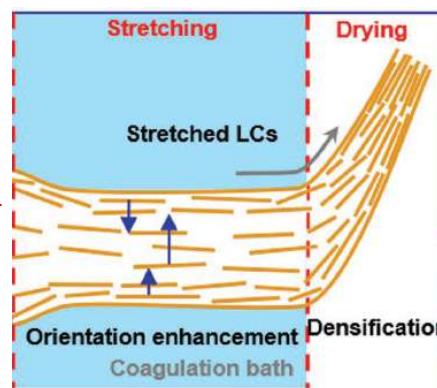
Qin, PhD (2020), Rutter et al. *PRB* (2010), Liu et al. *ACS Nano* (2012), Carvalho et al. *Nat. Rev. Mat.* (2016), Komsa et al. *PRB* (2013)

连续



类层合板材料

间断

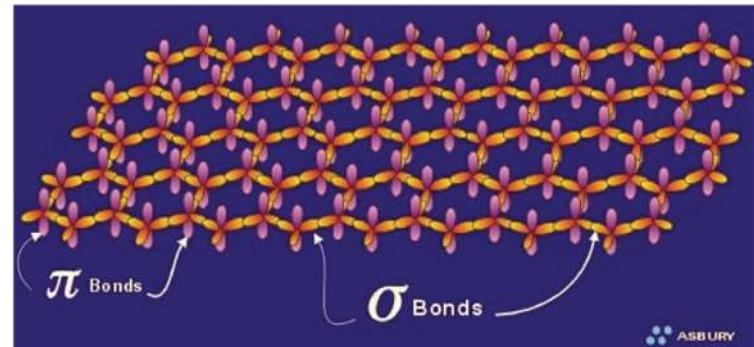


Z Xu et al., *Adv. Mater.* (2016)

类贝壳材料

石墨烯层状材料极端各向异性

- ✓ 面内强：刚度和强度极高
- ✓ 层间弱：剪切模量和强度极低



$$\begin{Bmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \\ \tau_{yz} \\ \tau_{xz} \\ \tau_{xy} \end{Bmatrix} = 10^9 \times \begin{bmatrix} 1060 & 15 & 180 & 0 & 0 & 0 \\ 15 & 36.5 & 15 & 0 & 0 & 0 \\ 180 & 15 & 1060 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2.25 & 0 & 0 \\ 0 & 0 & 0 & 0 & 220 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2.25 \end{bmatrix} \begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \gamma_{yz} \\ \gamma_{xz} \\ \gamma_{xy} \end{Bmatrix}$$

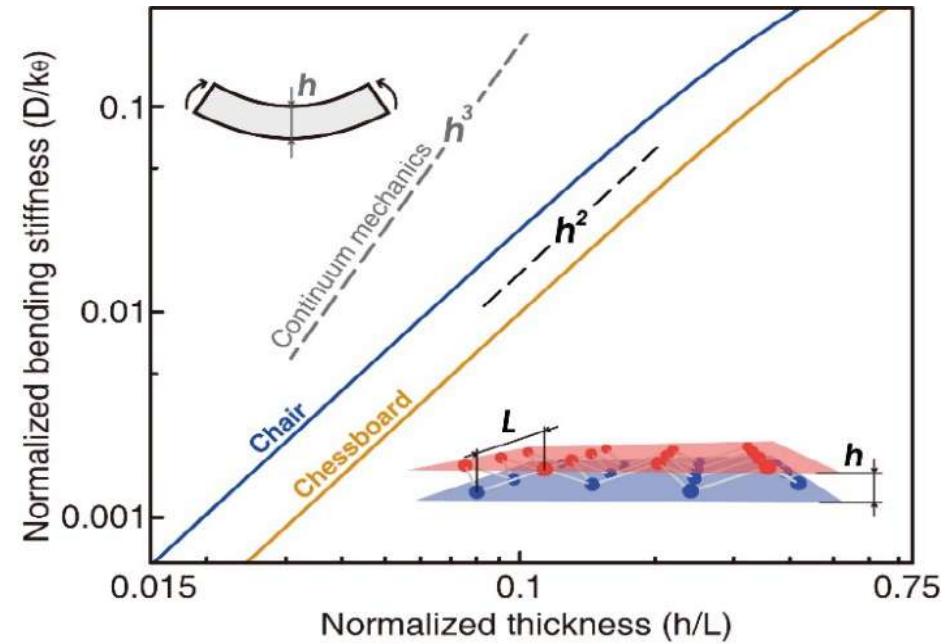
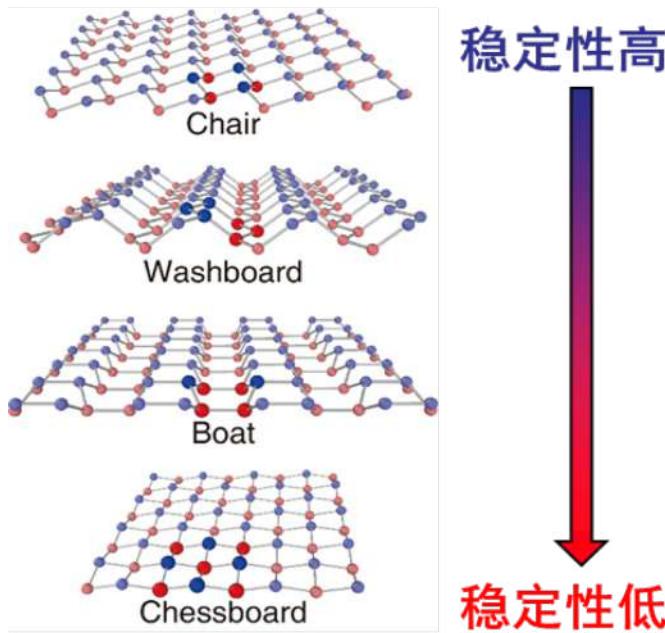
钢
各向同性

$$C_{44} / C_{33} = 0.345$$

石墨
各向异性

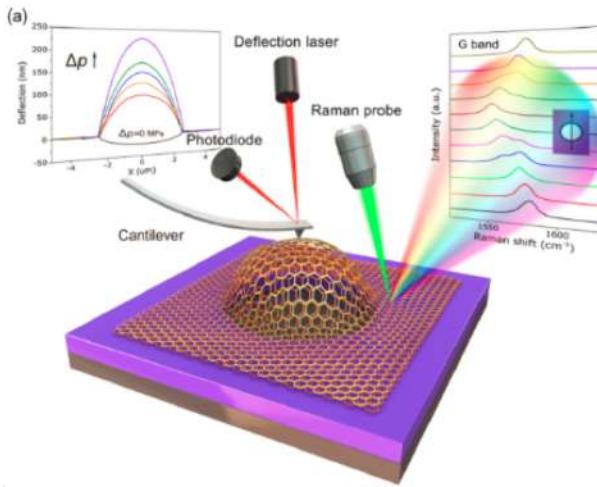
$$C_{44} / C_{33} = 0.002$$

二维材料弯曲刚度

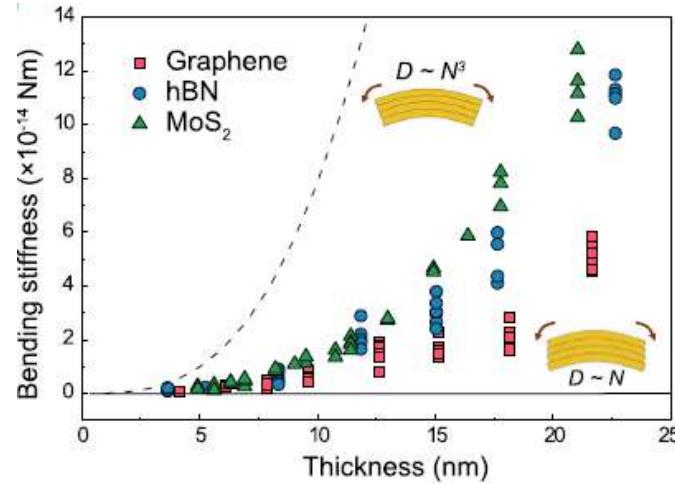


二维材料面内杨氏模量 E 、弯曲刚度 h 、弯曲刚度 D 都是独立材料常数，需要独立确定。

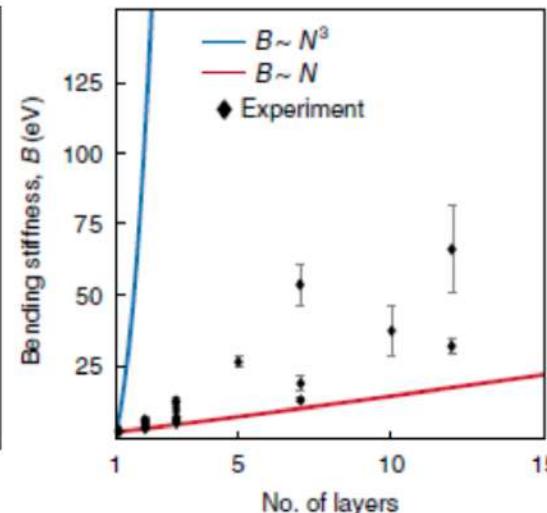
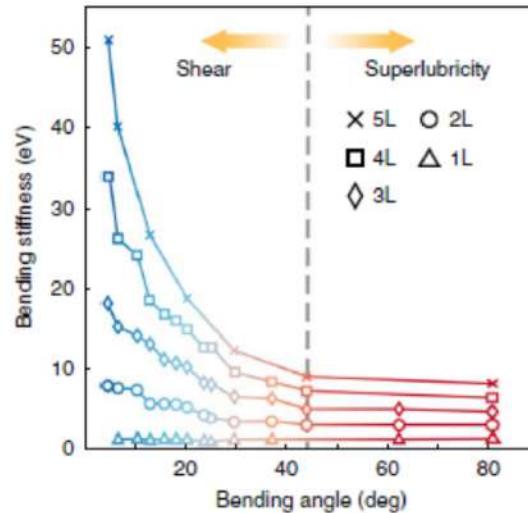
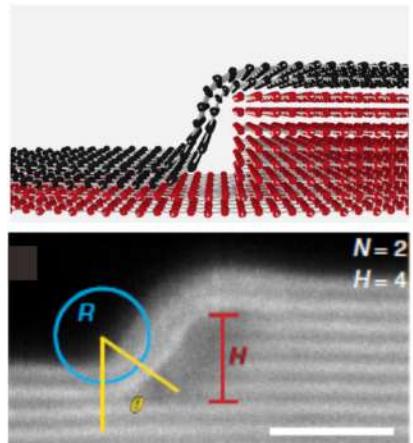
奇异弯曲行为



Wang et al. *PRL* (2019)
Wang et al. *PRL* (2017)



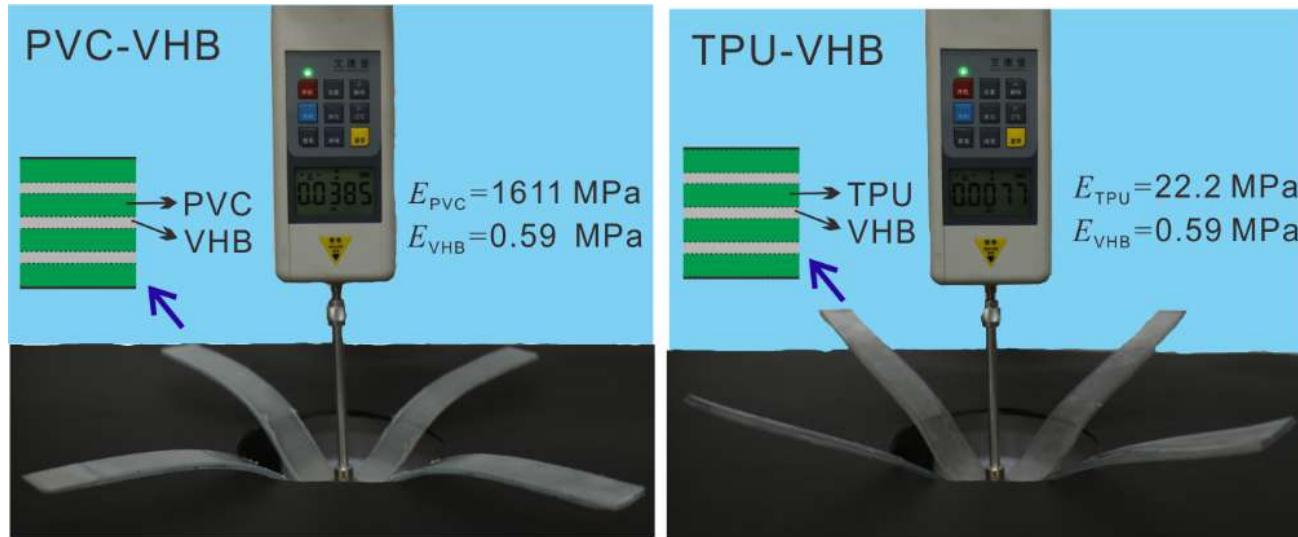
理想束缚状态
无层间剪切变形
理想滑移状态
层间剪切力为零



弯曲刚度随变
形增加而降低

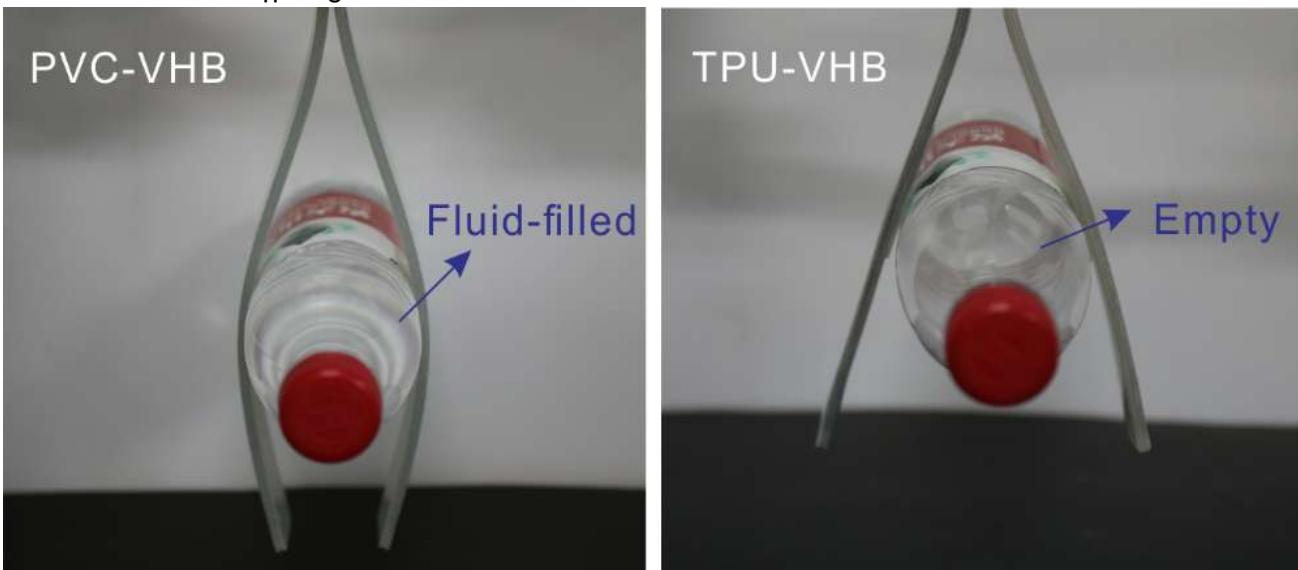
Han et al. *Nat. Mater.*
(2019)

奇异弯曲行为



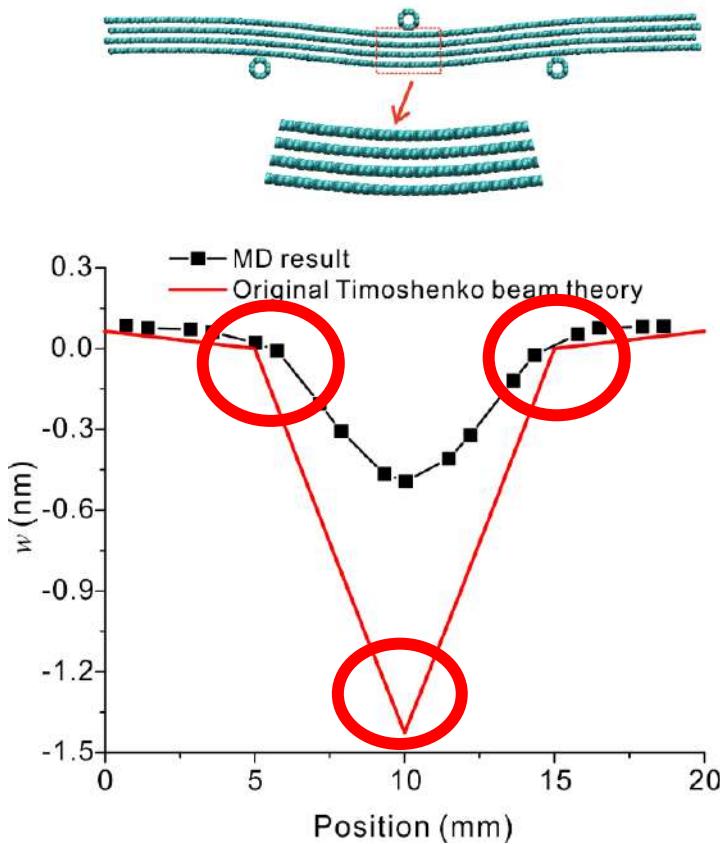
$$E_h/E_s \sim 10^3$$

$$E_h/E_s \sim 10^2$$



层状材料弯曲

Graphene layered materials



铁木辛柯梁模型

$$w(x) = \begin{cases} \frac{P}{2} \left(\frac{1}{6D_0} x^3 - \frac{L^2}{8D_0} x + \frac{x}{kGA} \right) & (0 \leq x \leq \frac{L}{2}) \\ \frac{-PL^2}{16D_0} x & (s \leq x < 0) \end{cases}$$

Bending effect Shear effect

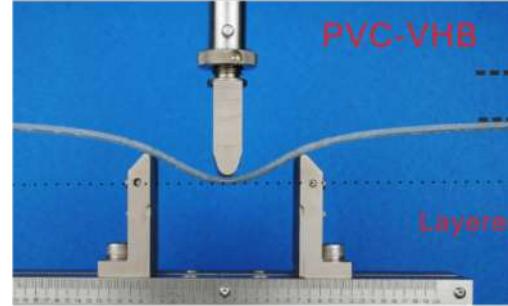
(1) As $G \rightarrow 0$, $w \rightarrow \infty$

(2) w' discontinuity

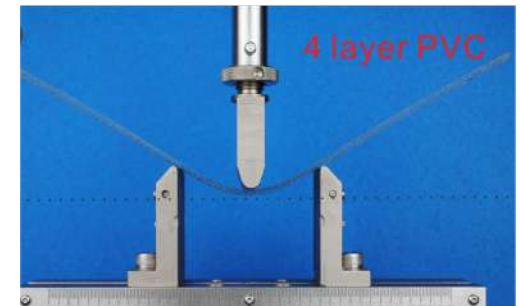
层状结构弯曲



$$E_1/E_2 \sim 10$$



$$E_1/E_2 \sim 1000$$



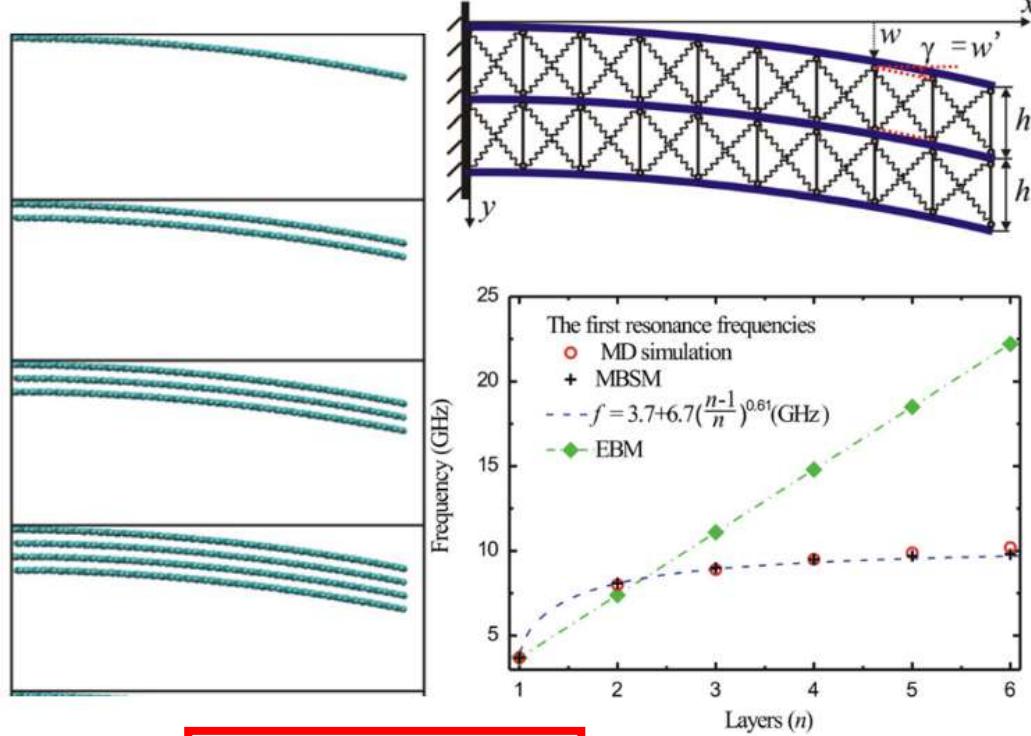
$$E_2 \rightarrow 0, E_1/E_2 \rightarrow \infty$$

$$w(x) = \begin{cases} \frac{P}{2} \left(\frac{1}{6D_0} x^3 - \frac{L^2}{8D_0} x - \frac{x}{kGA} \right) & (0 \leq x \leq \frac{L}{2}) \\ \frac{-PL^2}{16D_0} x & (s \leq x < 0) \end{cases}$$

(1) As $G \rightarrow 0, w \rightarrow \infty$
(2) w' discontinuity

层状材料弯曲模型

均匀化模型



$$\Pi(w) = n \frac{D_{\text{bend}}}{2} \int_0^L (w'')^2 dx + (n-1) \frac{D_{\text{shear}}}{2} \int_0^L (w')^2 dx - \int_0^L q w dx - \int_0^L m \varphi dx$$

单层弯曲能

JMPS (2011)

多梁结构模型

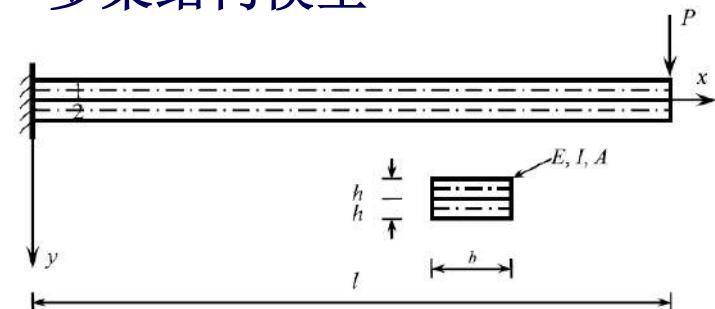


Fig. 1. Cantilever bilayer graphene nanoribbon subjected to a tip force.

$$M \begin{pmatrix} Q \\ F \end{pmatrix} = \begin{pmatrix} M_1 & N_1 \\ M_2 & N_2 \end{pmatrix} \begin{pmatrix} Q_1 & \tau \\ Q_2 & \tau \end{pmatrix} \begin{pmatrix} M_1+dM_1 & N_1+dN_1 \\ M_2+dM_2 & N_2+dN_2 \end{pmatrix} = \begin{pmatrix} F \\ Q+dQ \end{pmatrix}$$

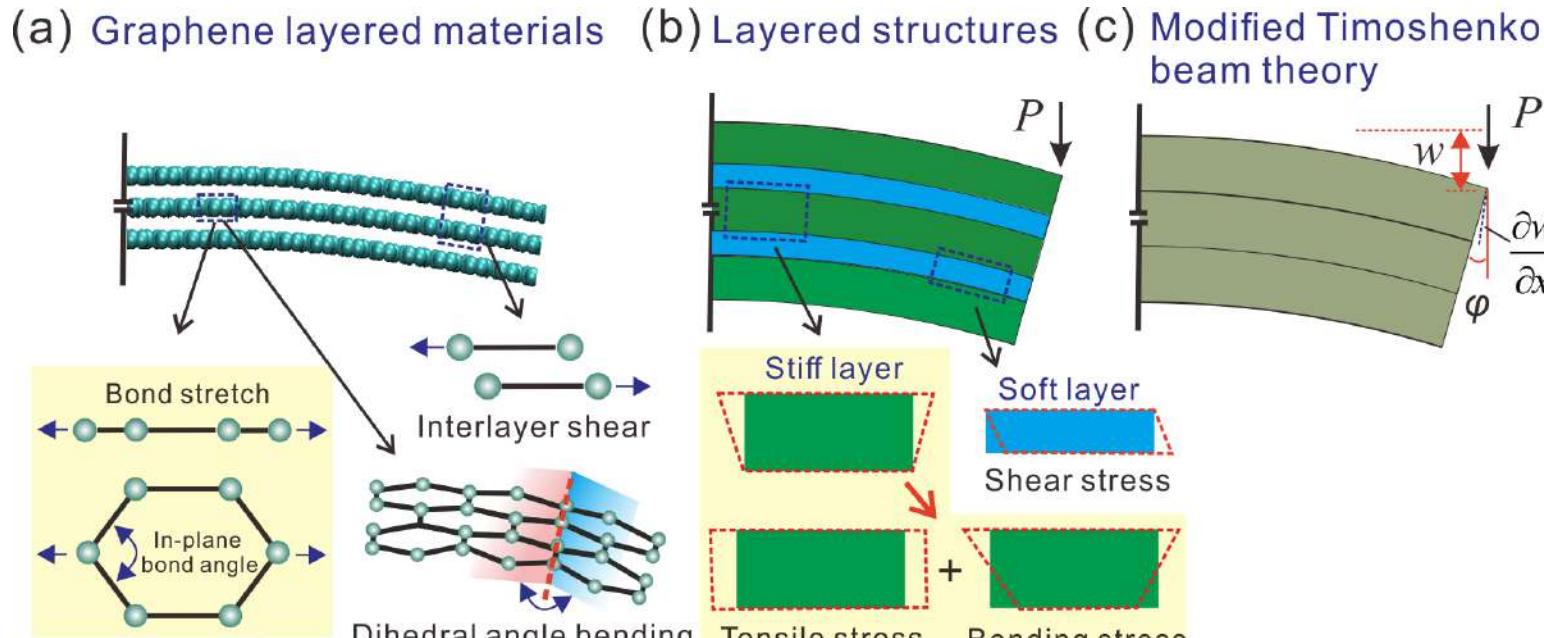
$$F = N_1 + N_2 + N_3 = 0,$$

$$Q = Q_1 + Q_2 + Q_3,$$

$$M = M_1 + M_2 + M_3 - N_1 h + N_3 h.$$

Chen, Physics Letters A (2013)

改进铁木辛柯梁模型



Total potential energy:

$$\Pi(w, \phi) = \frac{D_0}{2} \int_0^L \phi'^2 dx + \frac{kGA}{2} \int_0^L (\phi - w')^2 dx + n \frac{D_{\text{bend}}}{2} \int_0^L (w'')^2 dx - \int_0^L qwdx - \int_0^L m\phi dx$$

Monolayer bending energy

Treating layered material or layered structure as a homogenous solid.

改进铁木辛柯梁模型

Govern equation:

$$-D_0\phi'' + kGA(\phi - w') = 0$$

$$nD_{bend}w''' + kGA(\phi' - w'') = q$$

Monolayer bending Effect

D_{bend} : Monolayer bending rigidity

$$\lambda = \sqrt{\frac{kGA}{D_0} + \frac{kGA}{nD_{bend}}}$$

Important parameter determining the bending behaviors of layered materials and structures with inverse length unit.

General solution for point force P

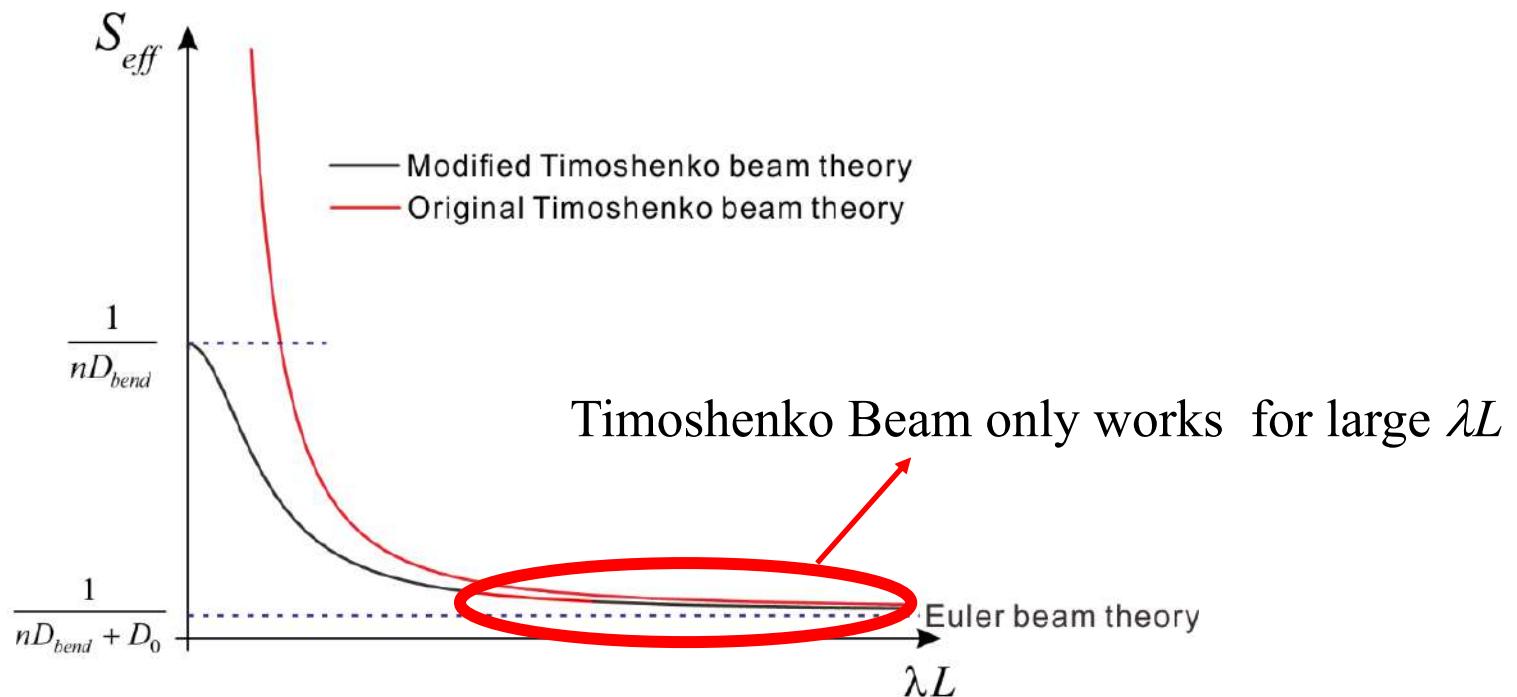
$$w = \frac{1}{nD_{bend} + D_0} \left(\frac{1}{12} Px^3 + \frac{1}{2} cx^2 + dx \right) + \frac{D_0}{nD_{bend} + D_0} \left[\frac{1}{\lambda} ae^{\lambda x} - \frac{1}{\lambda} be^{-\lambda x} - \frac{P}{2kGA(1 + \frac{nD_{bend}}{D_0})} x \right] + g$$

$$\phi = \frac{1}{nD_{bend} + D_0} \left(\frac{1}{4} Px^2 + c_1 x + d_1 \right) - \frac{nD_{bend}}{nD_{bend} + D_0} \left[a_1 e^{\lambda x} + b_1 e^{-\lambda x} - \frac{P}{2kGA(1 + \frac{nD_{bend}}{D_0})} \right]$$

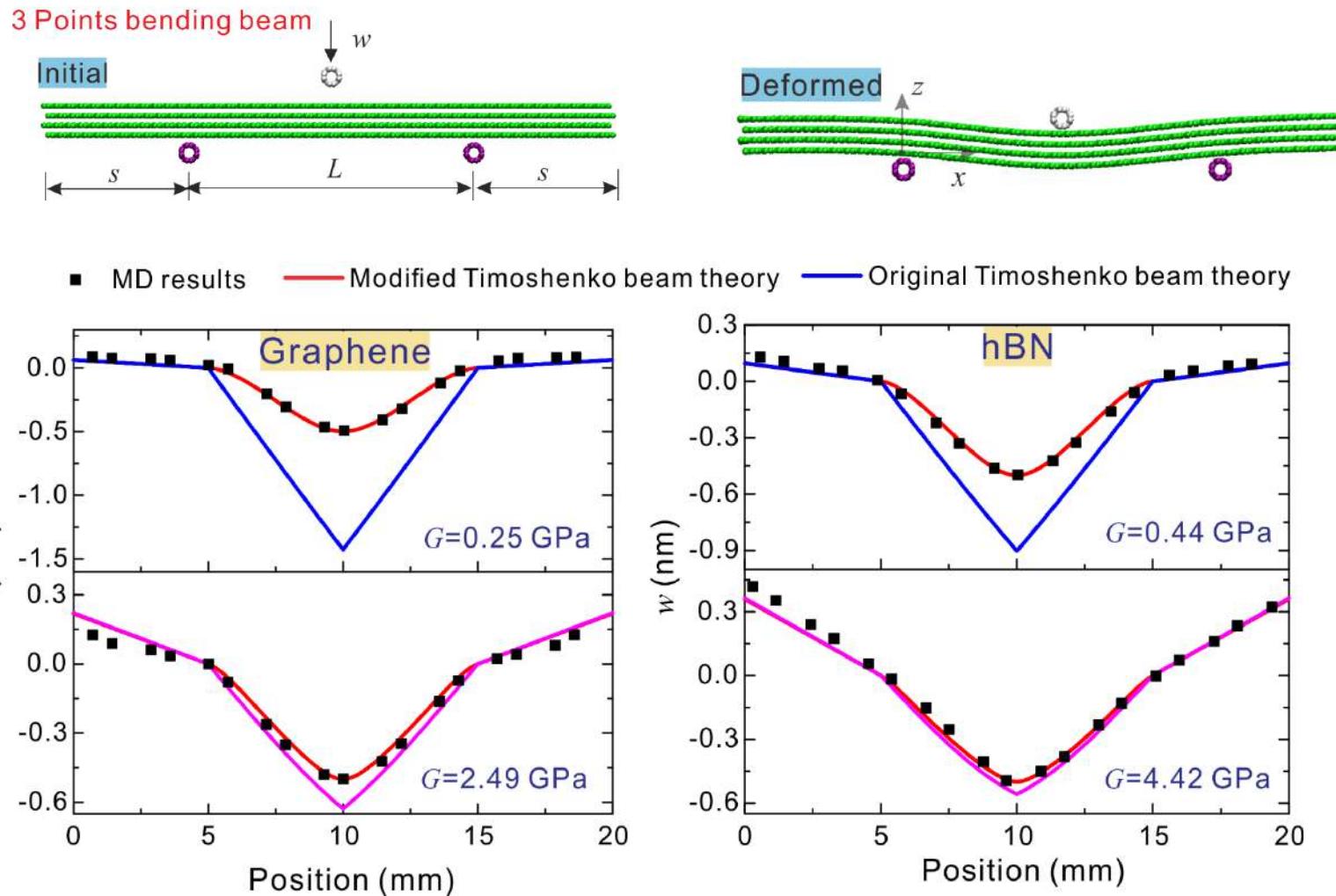
改进铁木辛柯梁模型

$$w = \frac{P}{nD_{bend} + D_0} \left(\frac{x^3}{12} - \frac{Lx^2}{16} \right) - \frac{Px}{2kGA \left(1 + \frac{nD_{bend}}{D_0} \right)^2} + \frac{1}{\lambda L} \frac{PL}{2kGA \left(1 + \frac{nD_{bend}}{D_0} \right)^2} \frac{\left(e^{\lambda x} - e^{\frac{\lambda L}{2}} e^{-\lambda x} + e^{\frac{\lambda L}{2}} - 1 \right)}{\left(1 + e^{\frac{\lambda L}{2}} \right)}$$

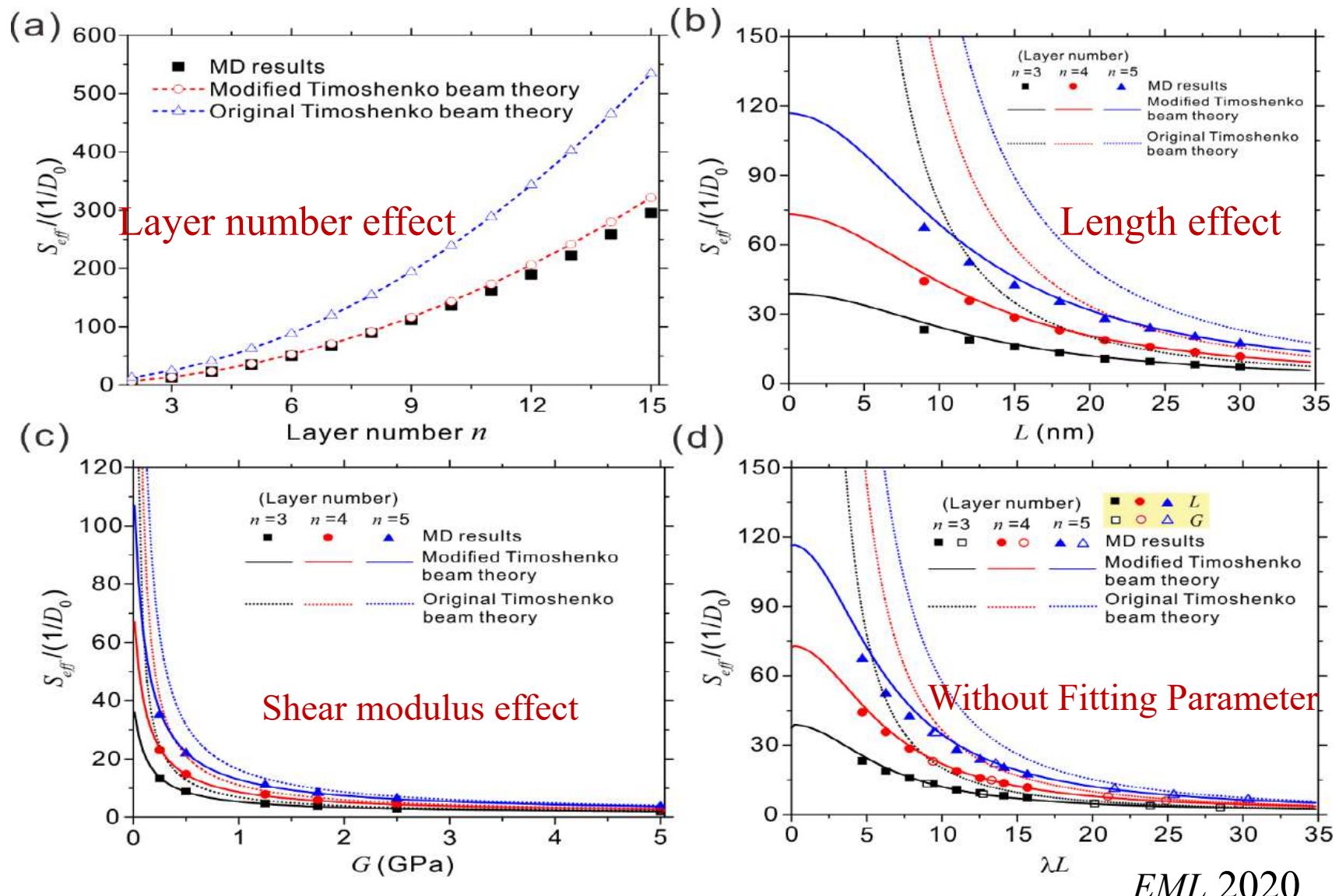
Effective bending flexibility: $S_{eff} = 192w(L/2)/PL^3$



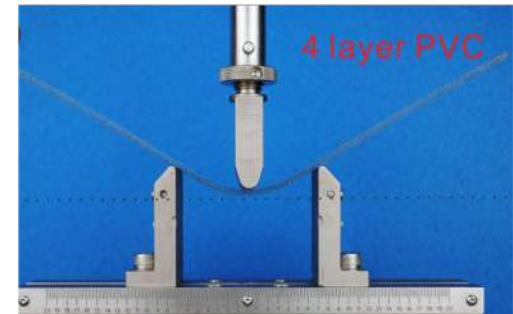
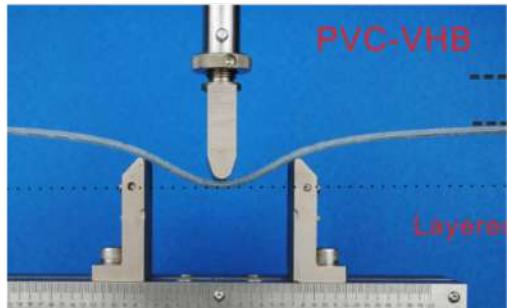
模拟验证



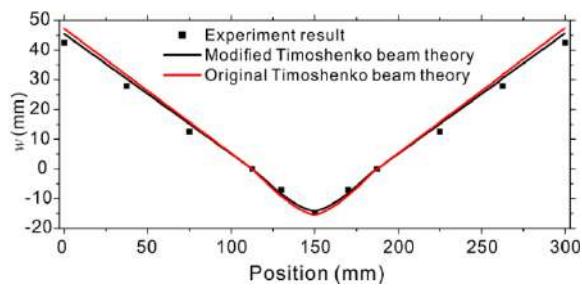
多层石墨烯弯曲柔度



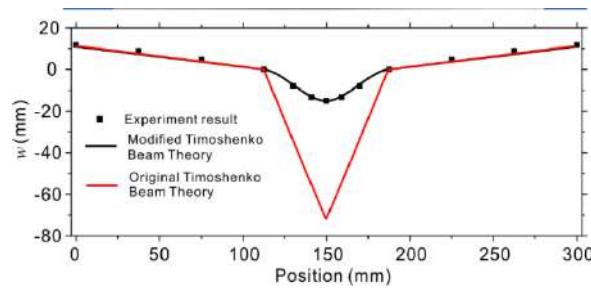
层状结构弯曲行为



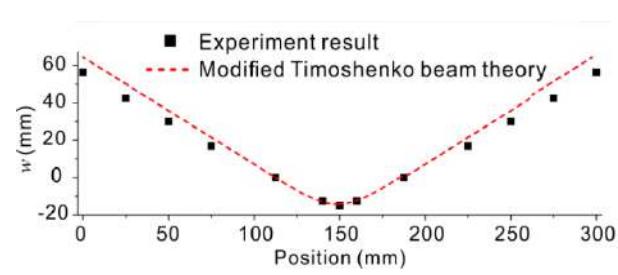
$$E_1/E_2 \sim 10$$



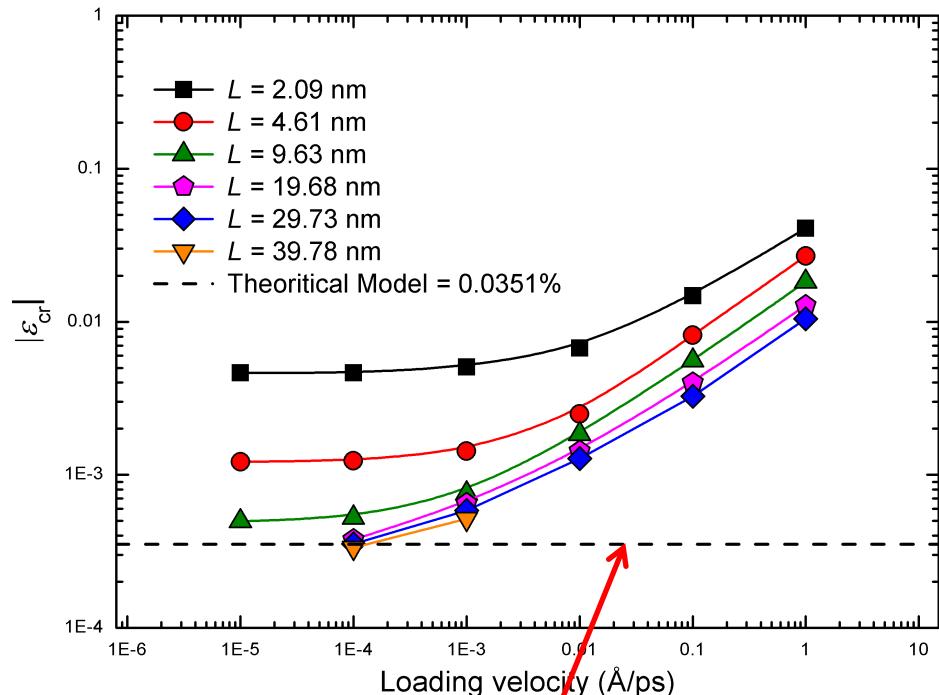
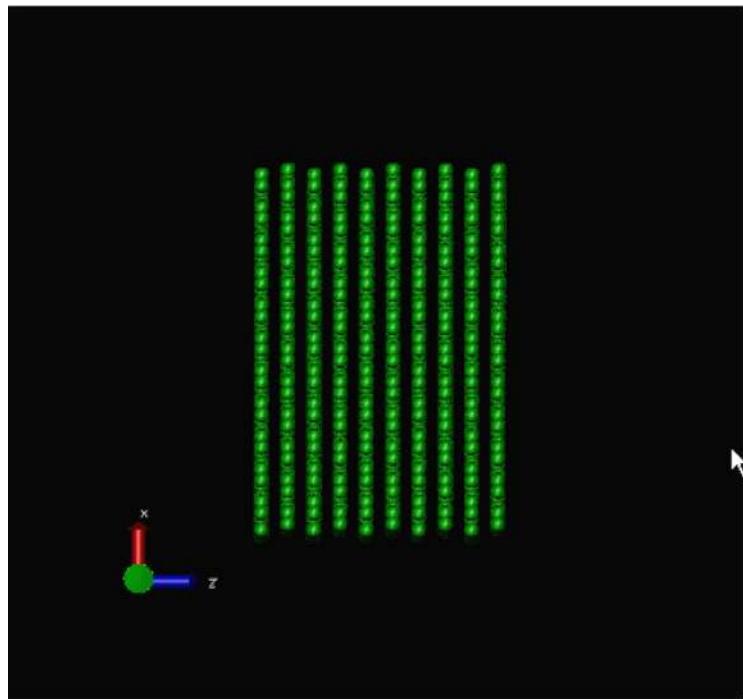
$$E_1/E_2 \sim 1000$$



$$E_2 \rightarrow 0, \quad E_1/E_2 \rightarrow \infty$$

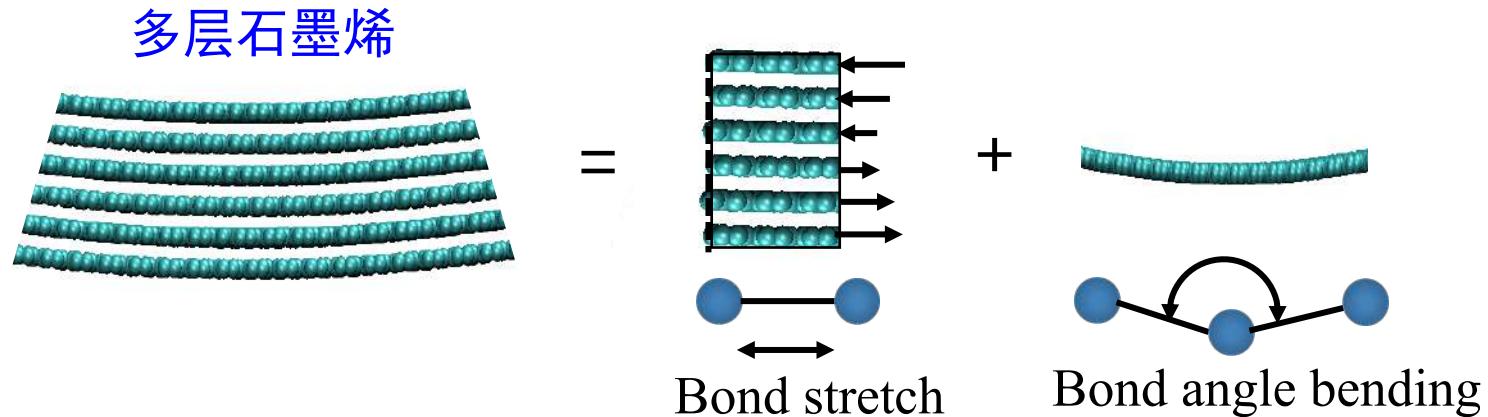


压缩失稳应变



$$\varepsilon_{\text{cr}} = \frac{C_{44}}{C_{11} - (2C_{44} + C_{13})C_{13}/C_{33}}$$

弯-剪耦合模型



- 应变能

$$W = \boxed{\int_V \frac{1}{2} \boldsymbol{\epsilon} : \mathbf{C} : \boldsymbol{\epsilon} dV} + \boxed{\int_V \frac{1}{2} \mathbf{k} : \mathbf{D} : \mathbf{k} dV}$$

经典弹性能 局部弯曲能

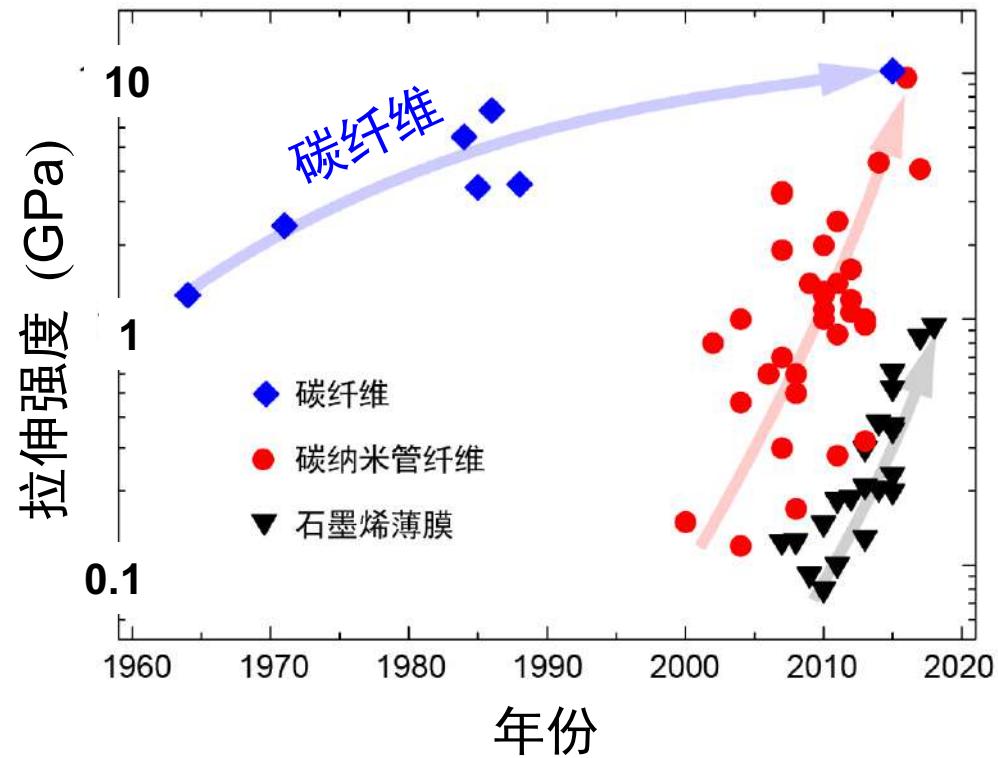
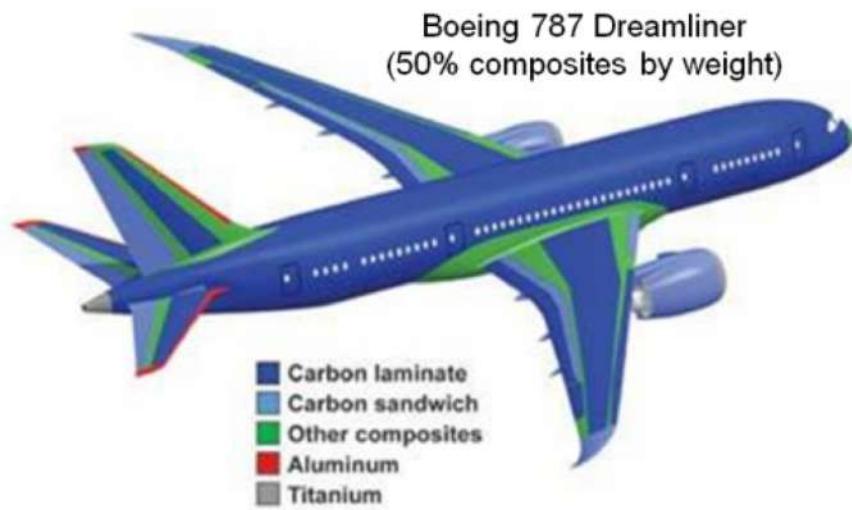
$$\sigma_{aj,j} + f_a = 0$$

$$\sigma_{3j,j} + f_3 - m_{ab,ab} = 0$$

目录

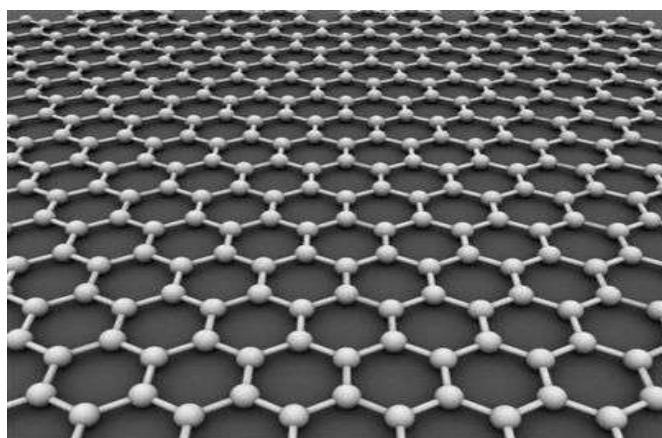
2.2 层状材料类贝壳结构力学行为

碳纳米复合材料

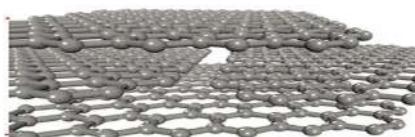
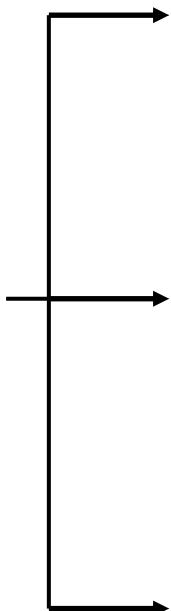


轻质高强复合材料在各行各业都有重要的用途，科学家和工业界投入大量资源研发高性能碳纳米复合材料。

类石墨烯层状材料力学性质



石墨烯 $\sigma_y \sim 109$ GPa



缺陷处理石墨烯纤维 $\sigma_y \sim 2$ GPa
Xu et al., *Adv. Mater.* (2016)



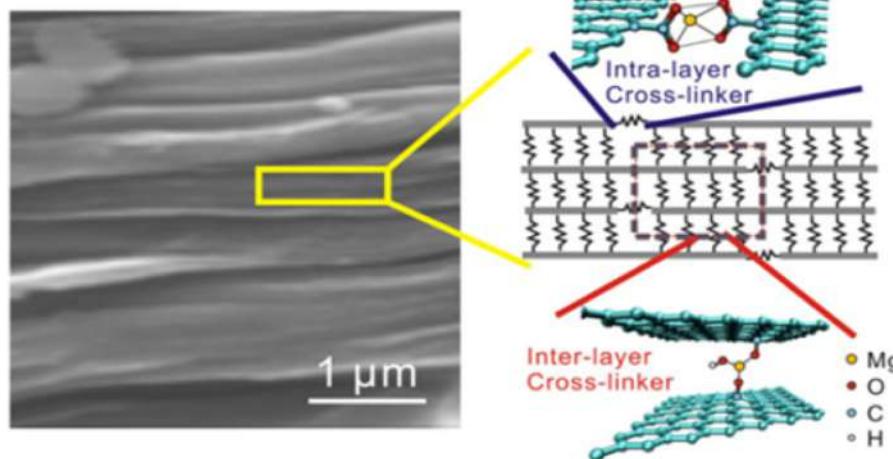
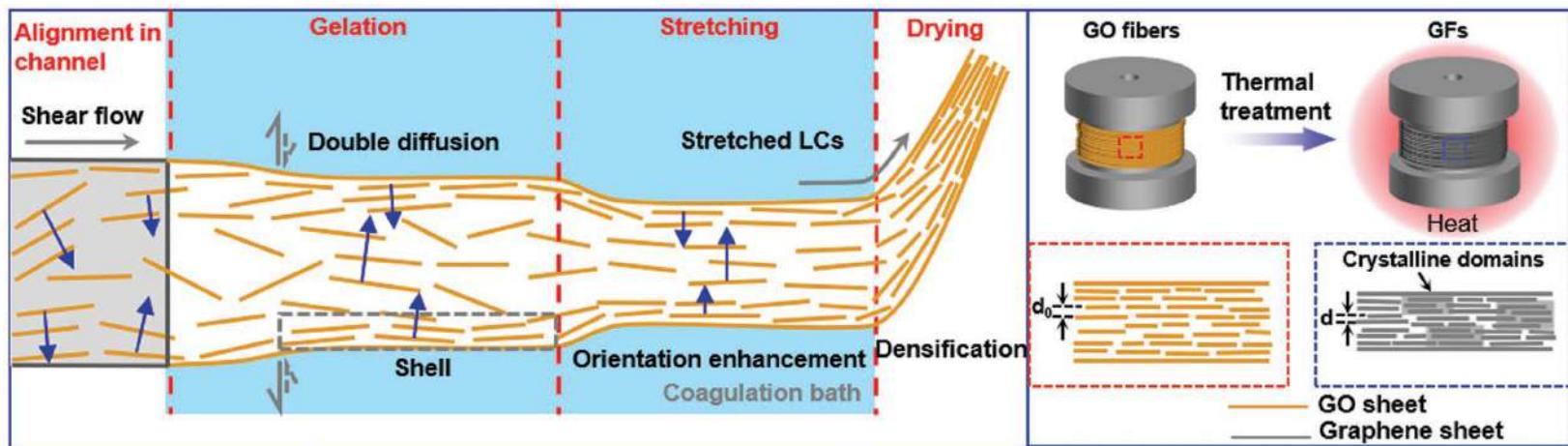
致密化碳纳米管纤维 $\sigma_y \sim 5$ GPa
Wang et al., *Nat. commun.* (2014)



高强度碳纤维 (T1000) $\sigma_y \sim 7$ GPa
Chae et al., *Carbon* (2015)

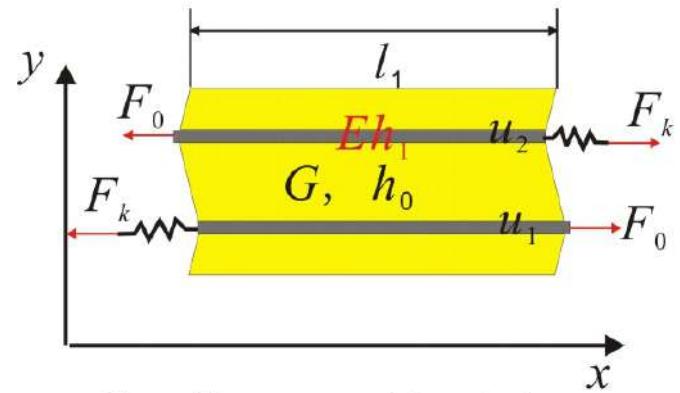
碳纳米材料强度远远低于完美石墨烯强度，缺乏多尺度力学模型和多层次力学设计。

类贝壳结构力学模型



拉剪载荷传递

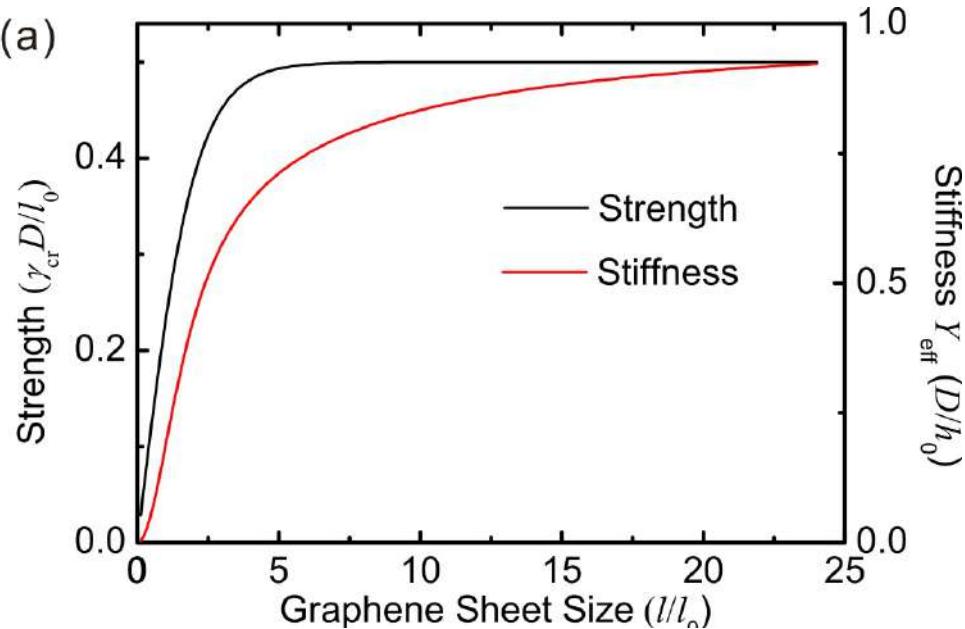
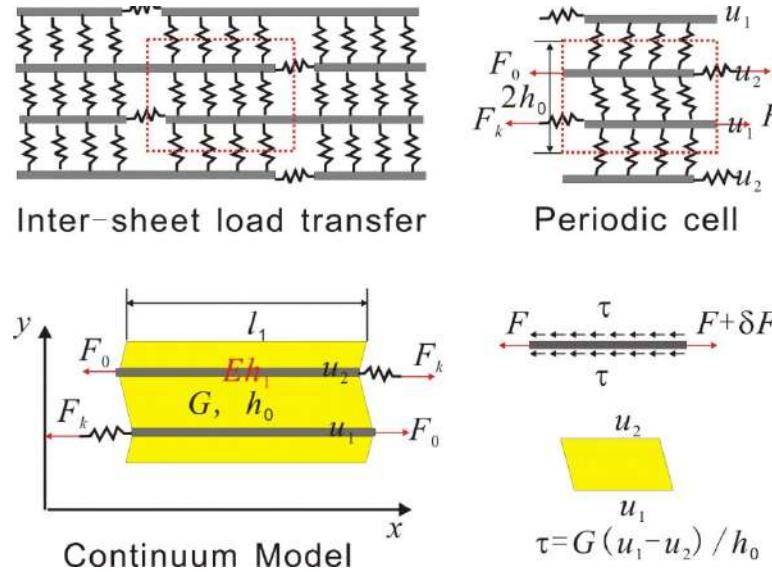
Fang et al., *Adv. Mater.* (2019)



Continuum Model

JMPS (2012)

可变形拉剪链模型

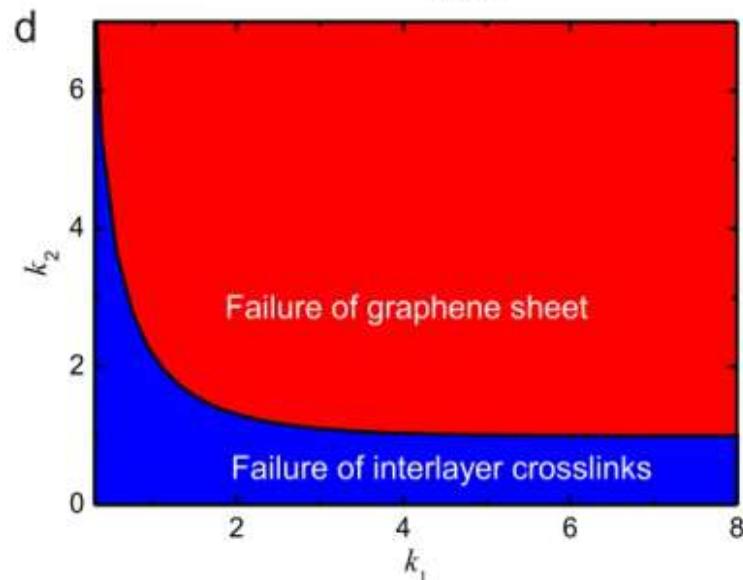
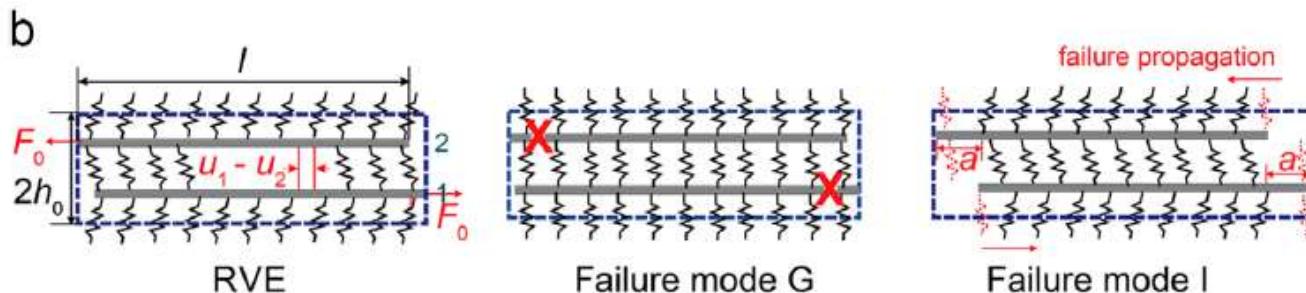
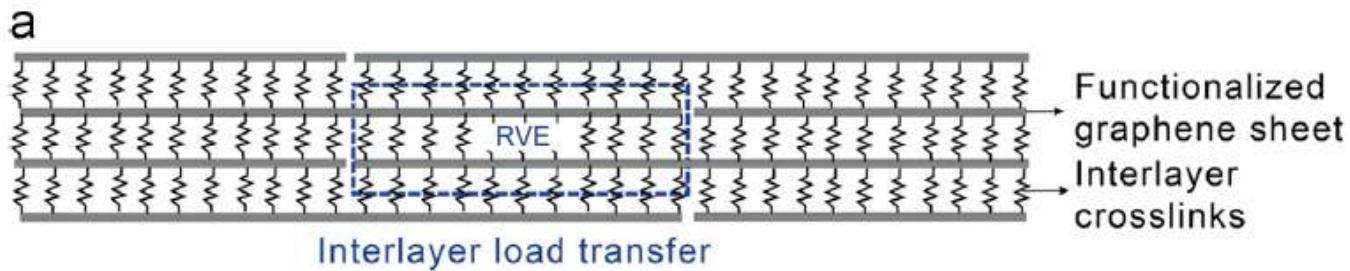


- 1、片层中心对称排布
- 2、层间剪切线弹性

剪切载荷传递尺寸

$$l_0 = 2\pi \sqrt{D_t h / C_{44}}$$

失效模式



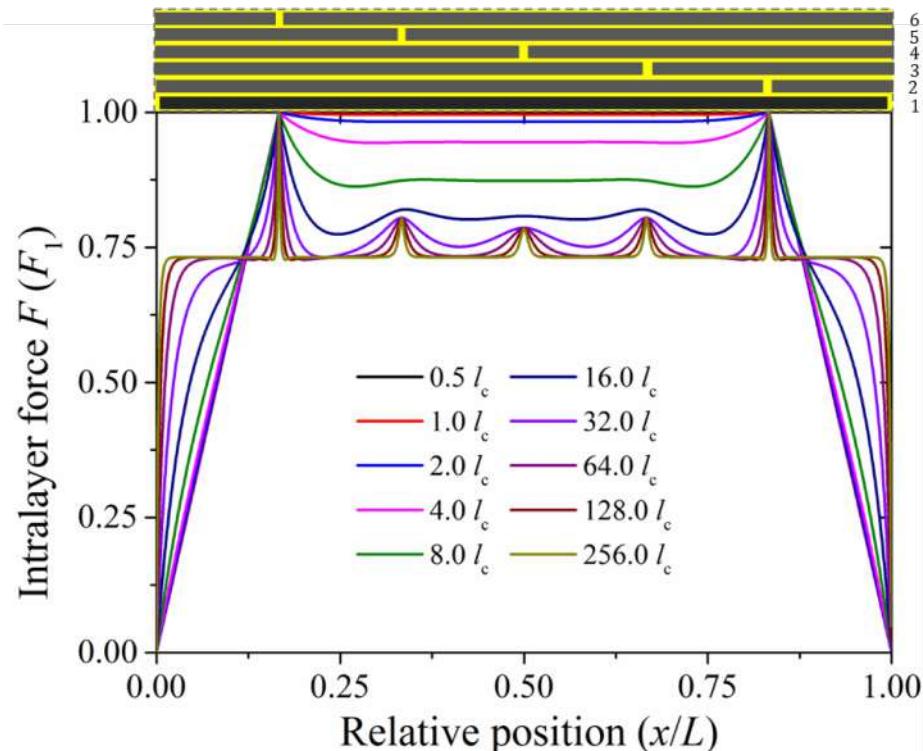
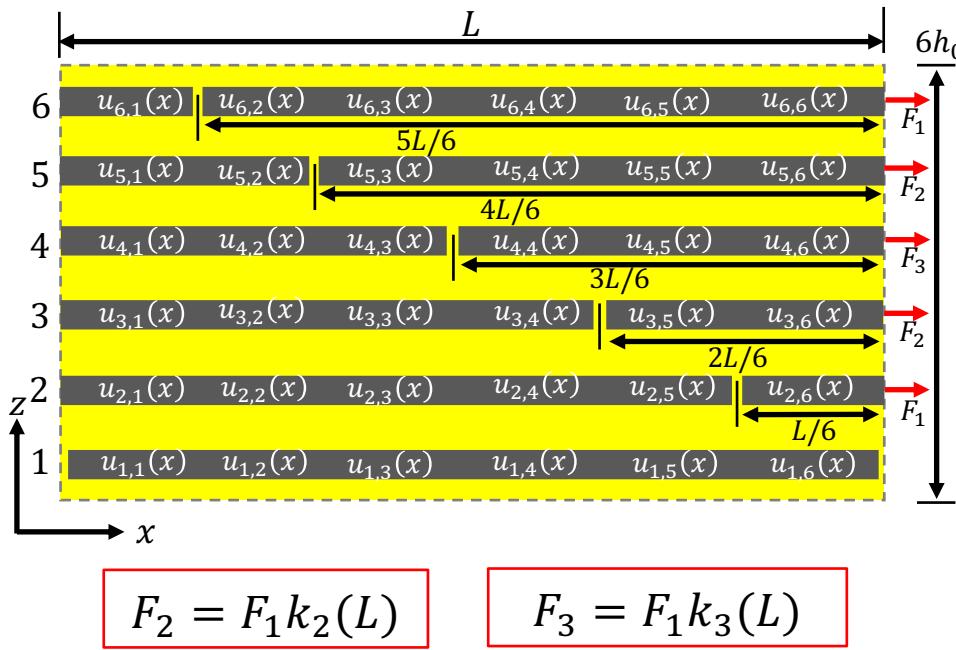
Two parameters:

$$k_1 = l/l_0 \quad k_2 = \gamma_{\text{cr}}(4Gh_0/D)^{1/2}/\varepsilon_{\text{cr}}$$

$$\varepsilon(l) = \frac{F_0}{D} \leq \varepsilon_{\text{cr}} \Rightarrow k_2 \geq \frac{1 + \cosh k_1}{\sinh k_1} \quad \text{Mode G}$$

$$\gamma(l) = \frac{F_0 l_0}{h_0 D} \frac{1 + c}{s} \leq \gamma_{\text{cr}} \Rightarrow k_2 < \frac{1 + \cosh k_1}{\sinh k_1} \quad \text{Mode I}$$

片层排布影响



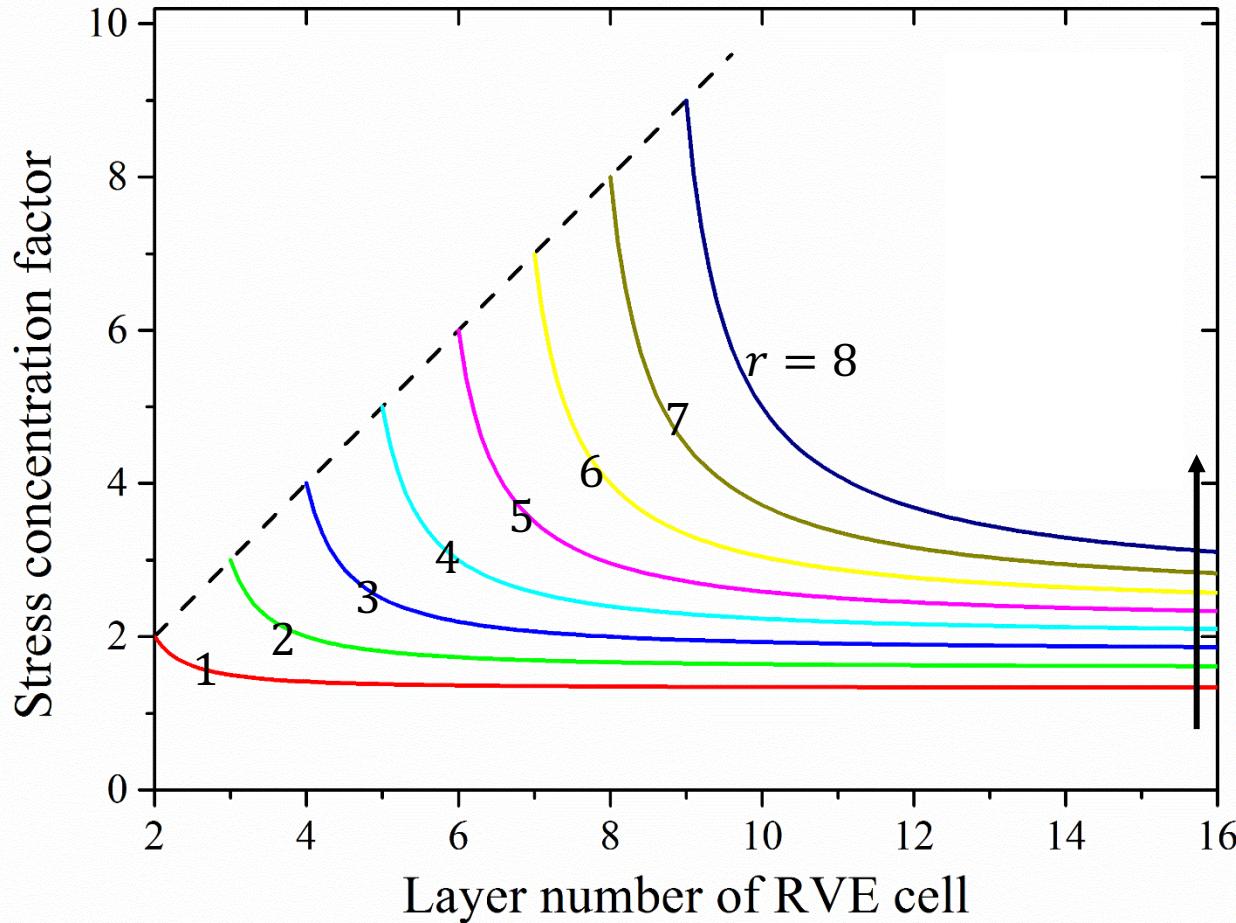
For graphene platelet 1:

$$F_{1,j}(x) = D \frac{\partial u_{1,j}(x)}{\partial x} \quad (j = 1, 2, 3, 4, 5, 6)$$

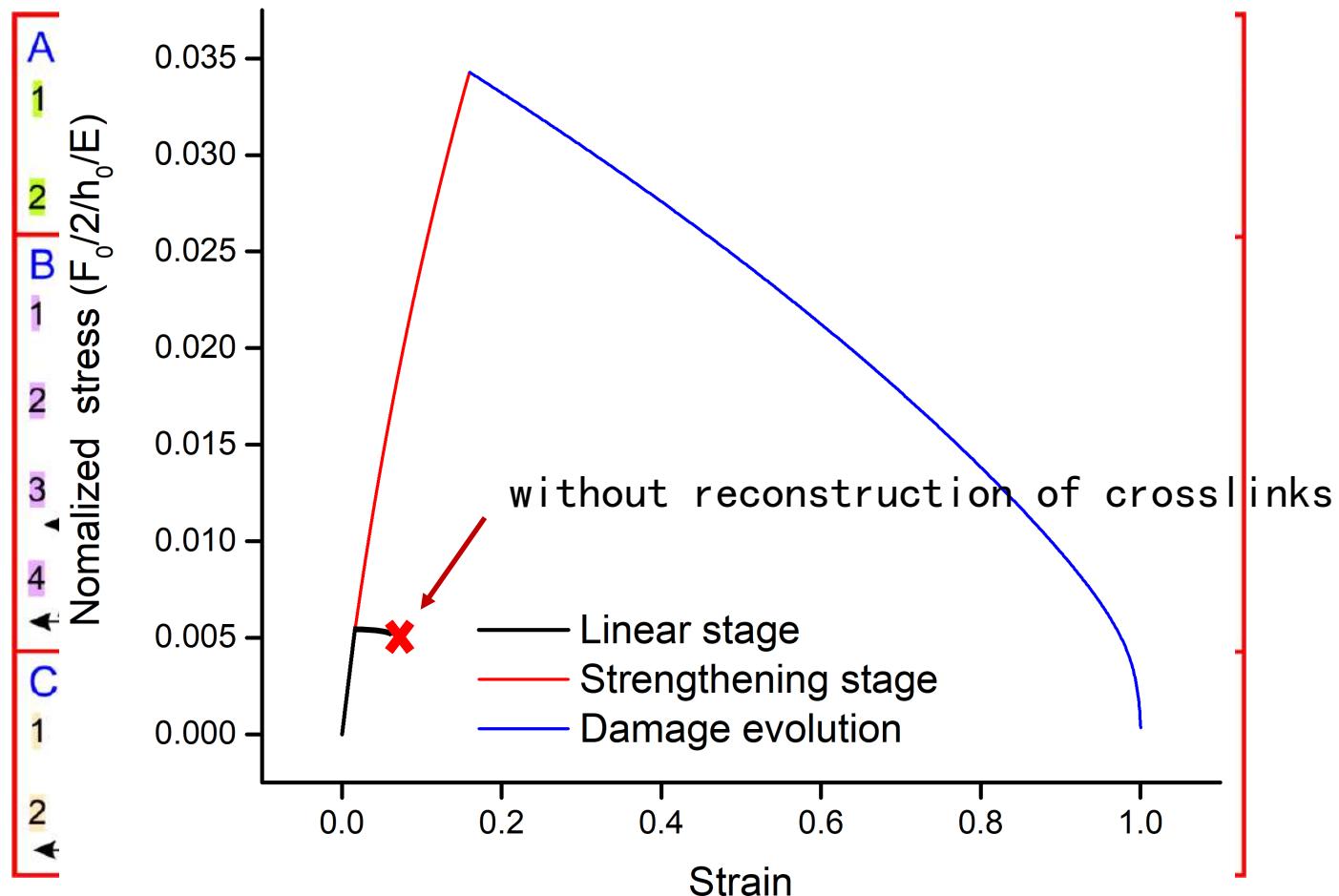
- For graphene with small length, the distribution of intralayer force is straight line, behaving like a rigid platelet. While for big one, small peaks appear.
- The effect of a break on intralayer force will decrease with the increase of the distance from the graphene platelet

Characteristic length: $l_c = \sqrt{\frac{Dh_0}{G}}$

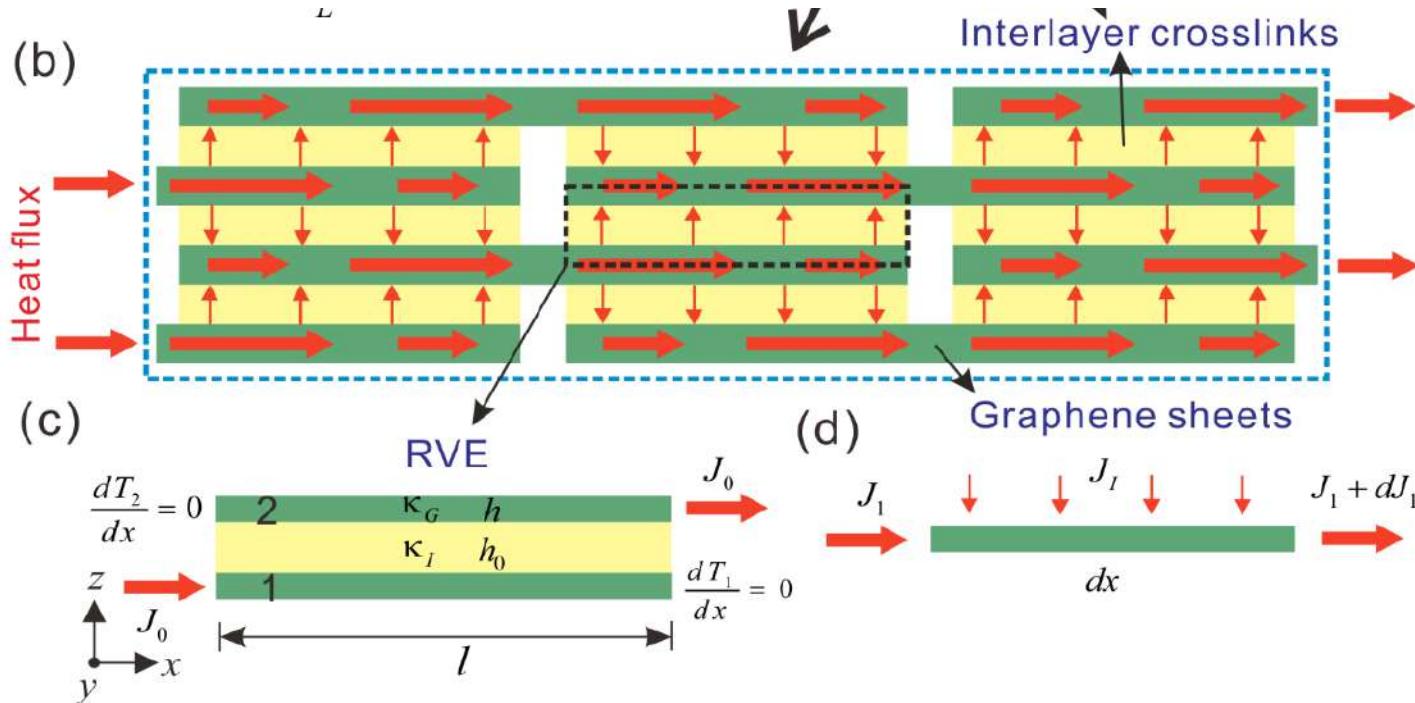
层状材料应力集中



自修复交链模型



面内热导模型



控制方程

$$-\kappa_G \frac{d^2 T_1}{dx^2} = \kappa_I (T_1 - T_2)$$

$$-\kappa_G \frac{d^2 T_2}{dx^2} = \kappa_I (T_2 - T_1)$$

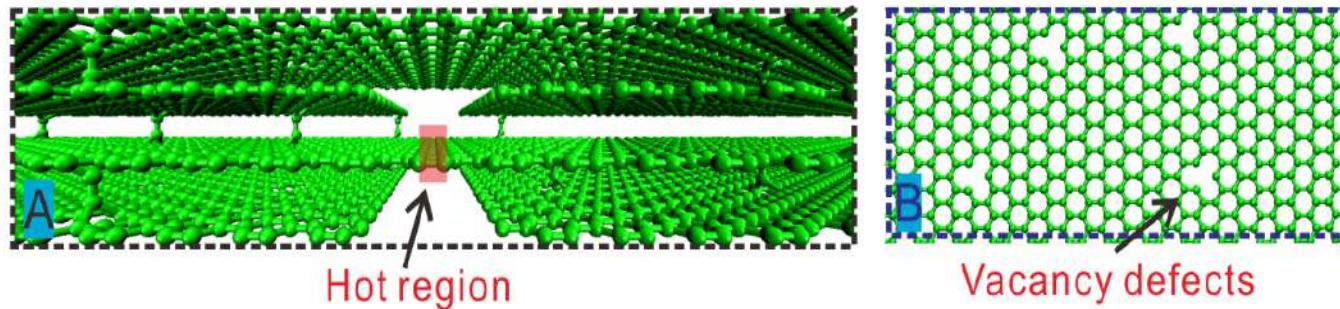
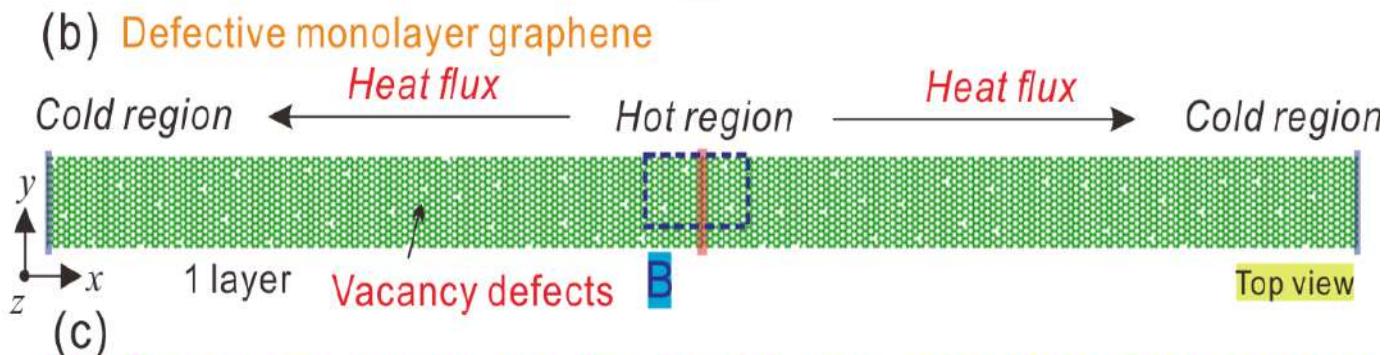
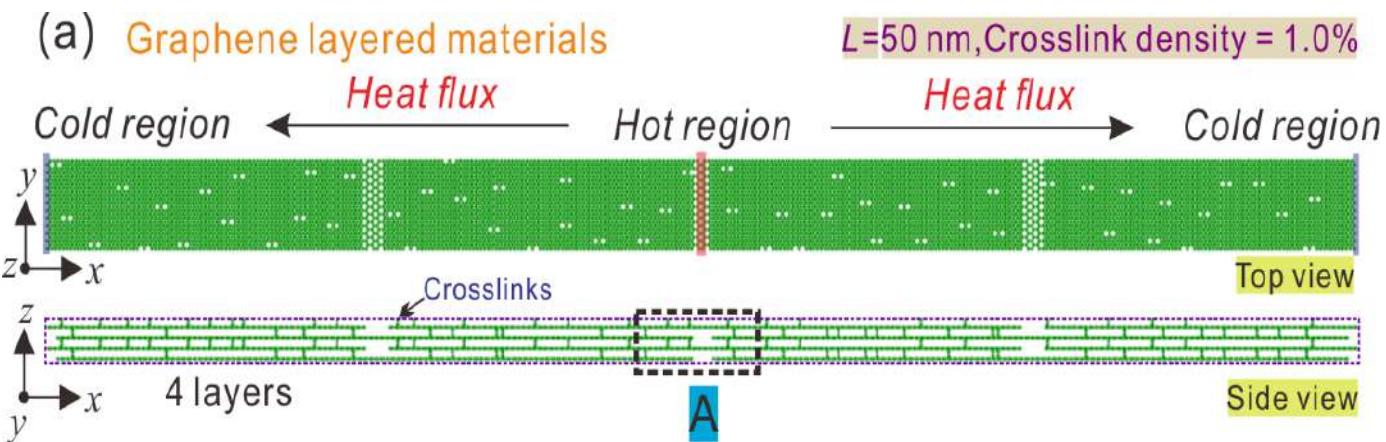
等效热导

$$K = \frac{\kappa_G}{h_0 \left(\frac{1}{2} + \frac{1}{\lambda l} \frac{2 + e^{\lambda l} + e^{-\lambda l}}{e^{\lambda l} - e^{-\lambda l}} \right)}$$

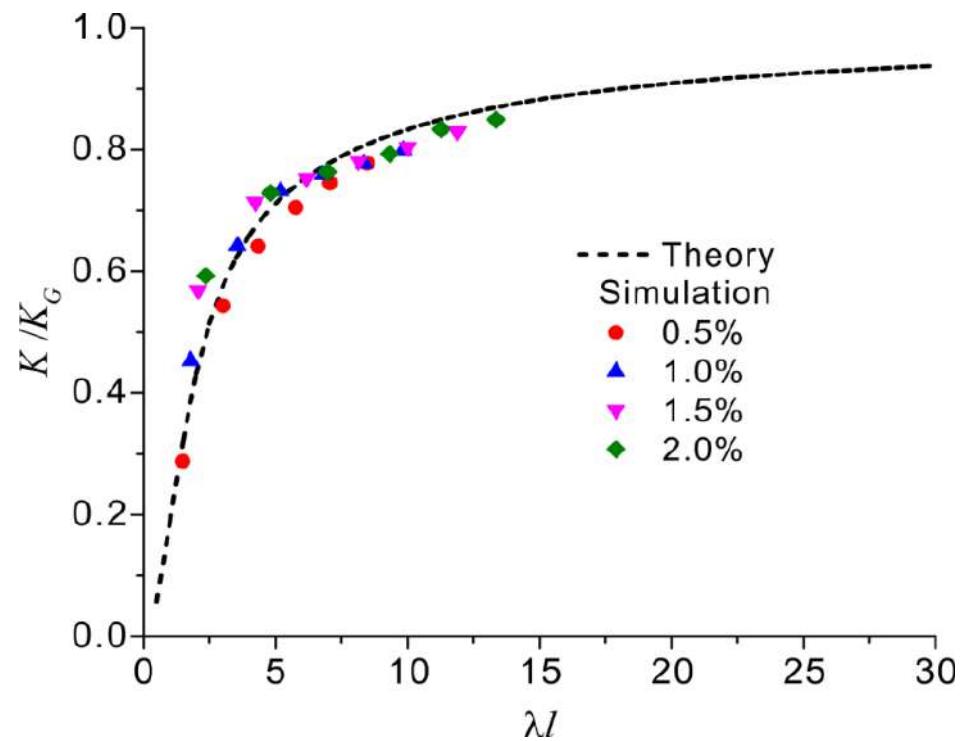
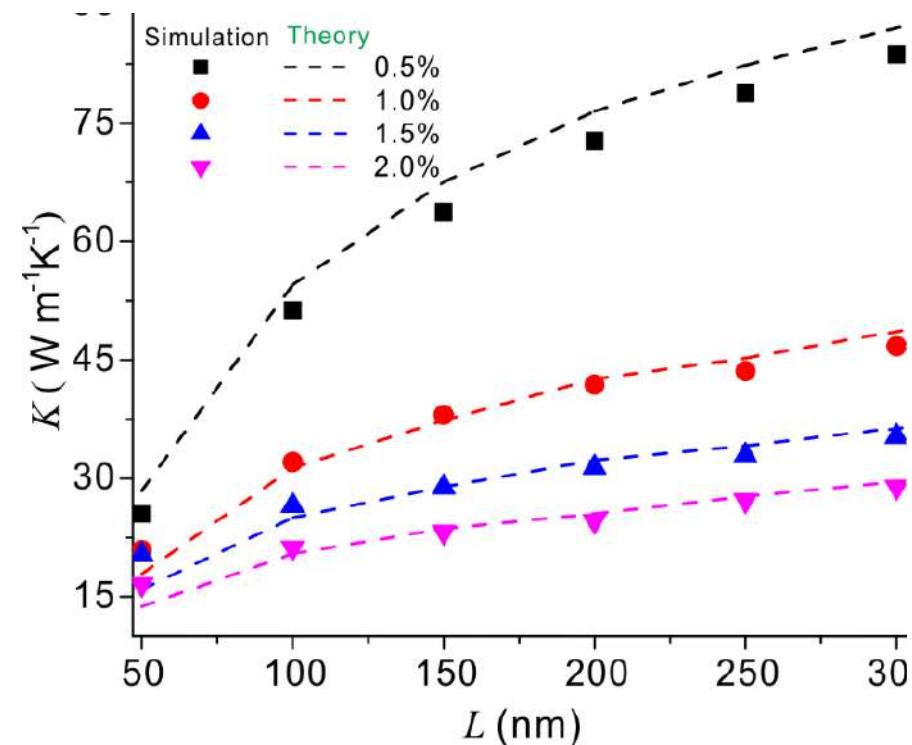
特征参数

$$\lambda l = \sqrt{2 \frac{\kappa_I}{\kappa_G h h_0} l}$$

分子动力学模拟



等效热导



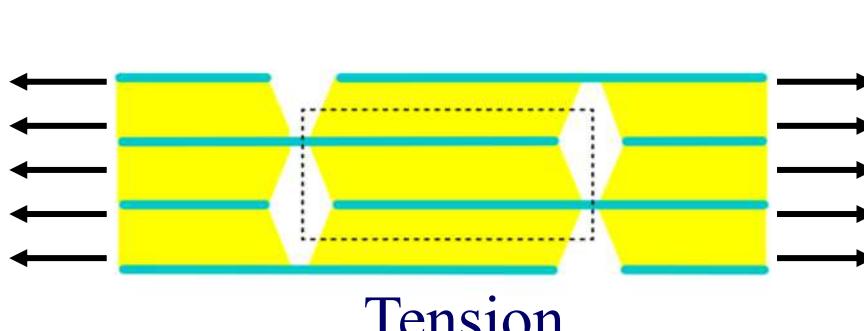
目录

2.3 界面力学性能增强



面内和层间载荷传递竞争机制

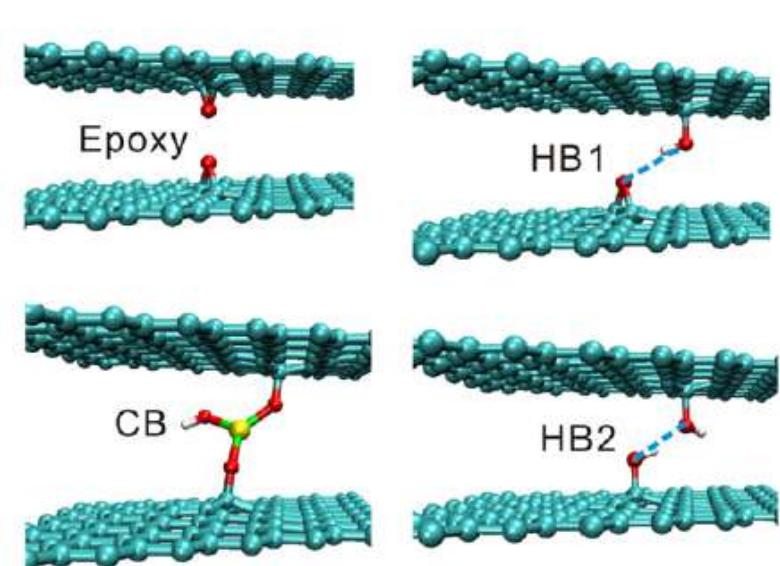
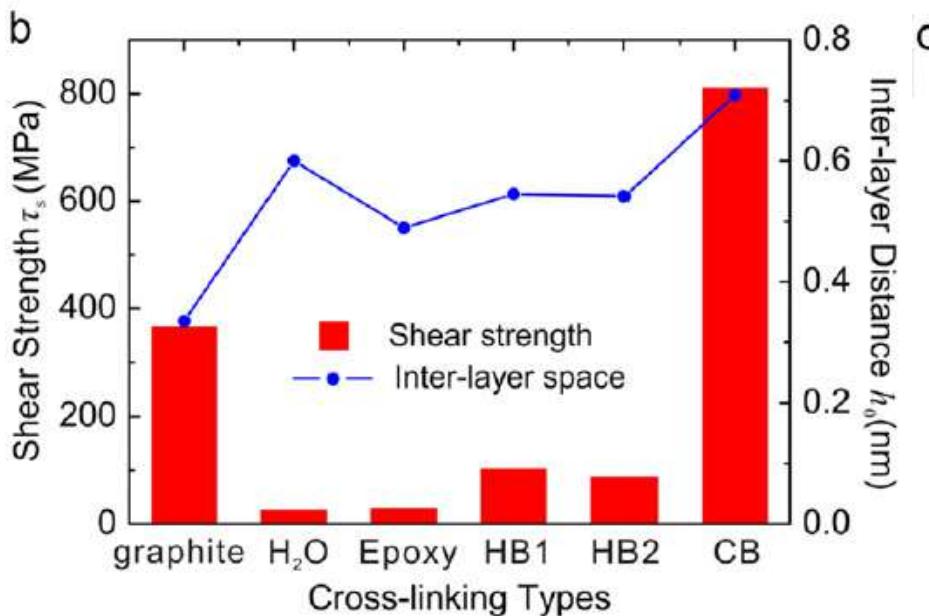
- 为了提高石墨烯层状材料力学性质，必须提高其面内载荷传递能力；
- 增加石墨烯层间交链密度，往往降低其面力学性质；
- 石墨烯层状材料力学性质优化需要考虑面内和层间载荷传递的平衡。



The diagram illustrates a layered material under tension. A central vertical column of layers is shown with horizontal arrows pointing to the right, labeled "Tension". To the left, a series of horizontal arrows point to the left, indicating the direction of stress transfer. A dashed rectangular box highlights a specific region where the layers are shown to be slipping relative to each other, representing shear stress.

$$\sigma_s = \min \begin{cases} \sigma_{cr} \frac{h}{2h_0} & (\text{mode G}) \\ \gamma_{cr} \sqrt{\frac{GEh}{h_0}} \frac{\sinh(l/l_0)}{1 + \cosh(l/l_0)} & (\text{mode I}) \end{cases}$$

石墨烯层间交链

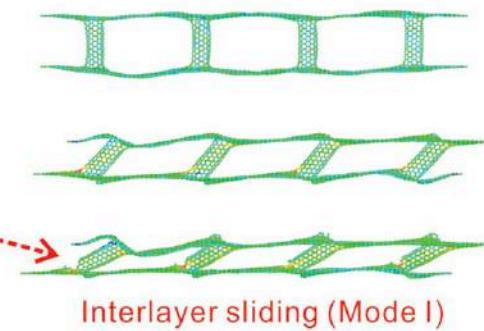


Pristine graphene	$h_0 = 0.335 \text{ nm}$	$G = 2.548 \text{ GPa}$	$\gamma_{\text{cr}} = 0.144$
Hydrogen bond	0.545 nm	763 MPa	0.135
Coordinative bond	0.71 nm	970 MPa	0.76

石墨烯碳纳米管交链

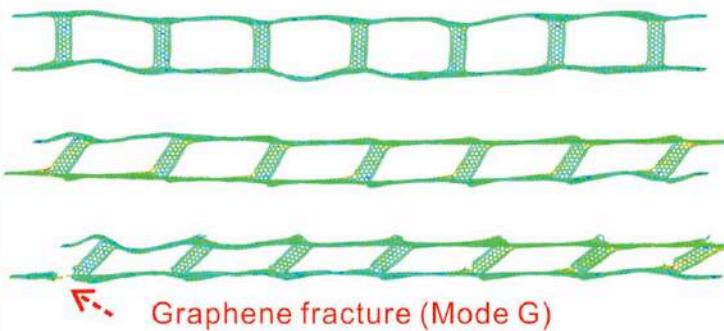
(a) $D=0.80 \text{ nm}, p=0.017$

$l = 20.21 \text{ nm}$



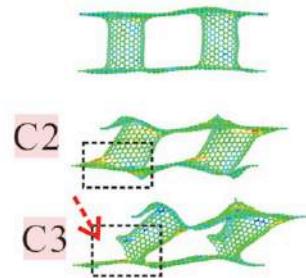
(b) $D=0.80 \text{ nm}, p=0.017$

$l = 35.37 \text{ nm}$



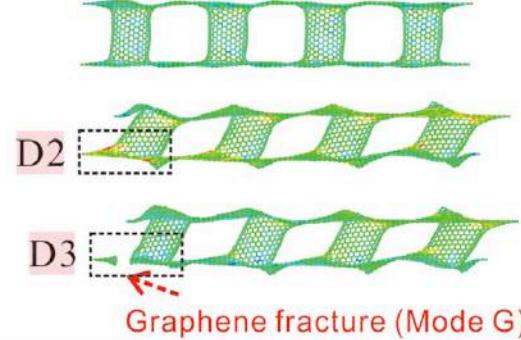
(c) $D=1.60 \text{ nm}, p=0.088$

$l = 8.48 \text{ nm}$

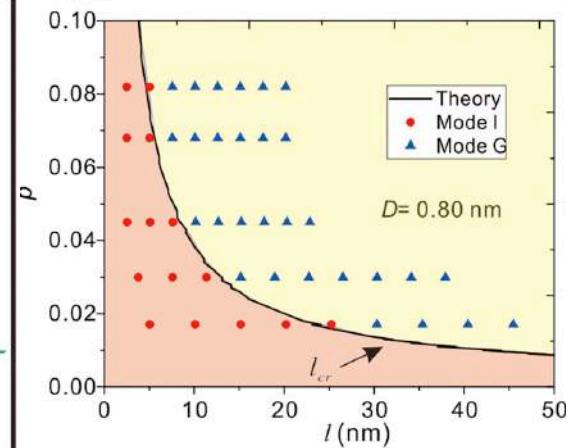


(d) $D=1.60 \text{ nm}, p=0.088$

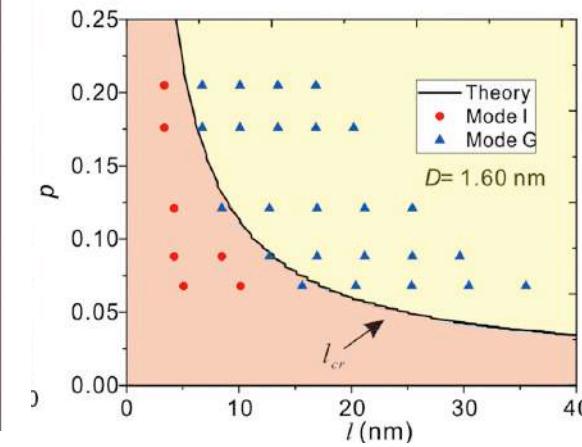
$l = 16.96 \text{ nm}$



(a)

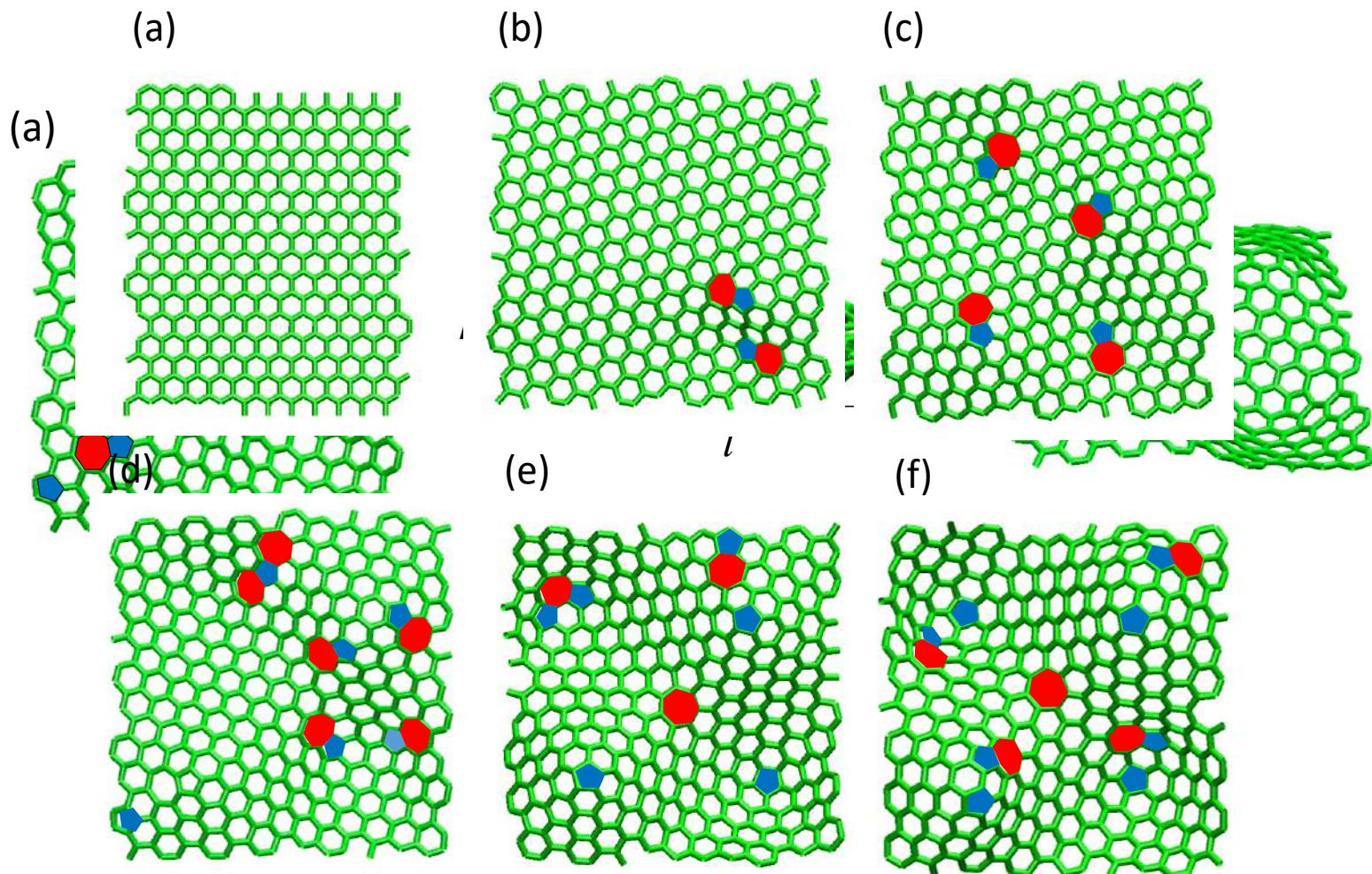


(b)

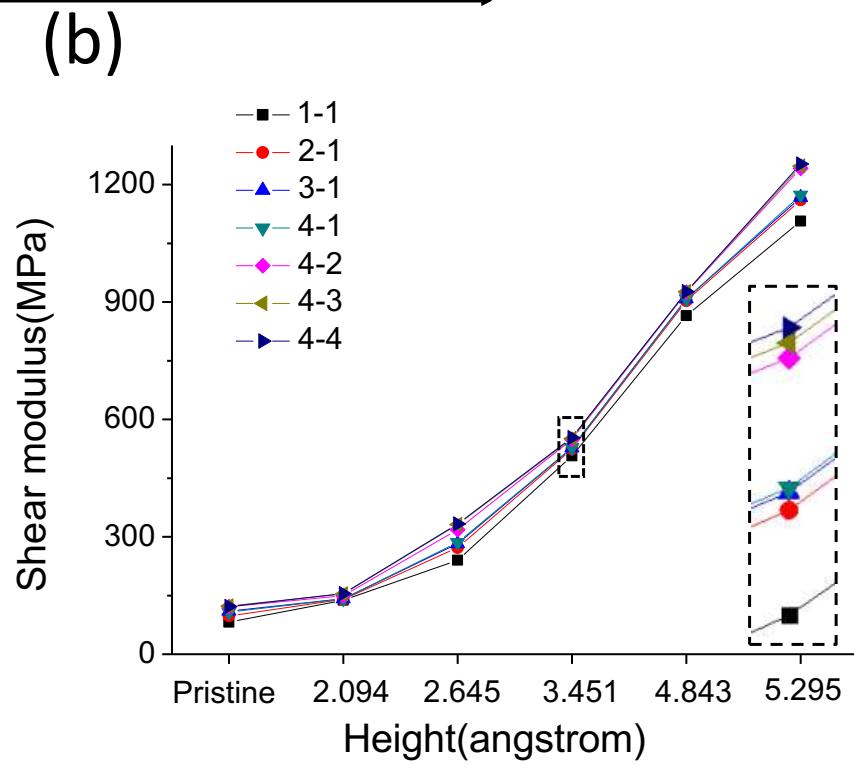
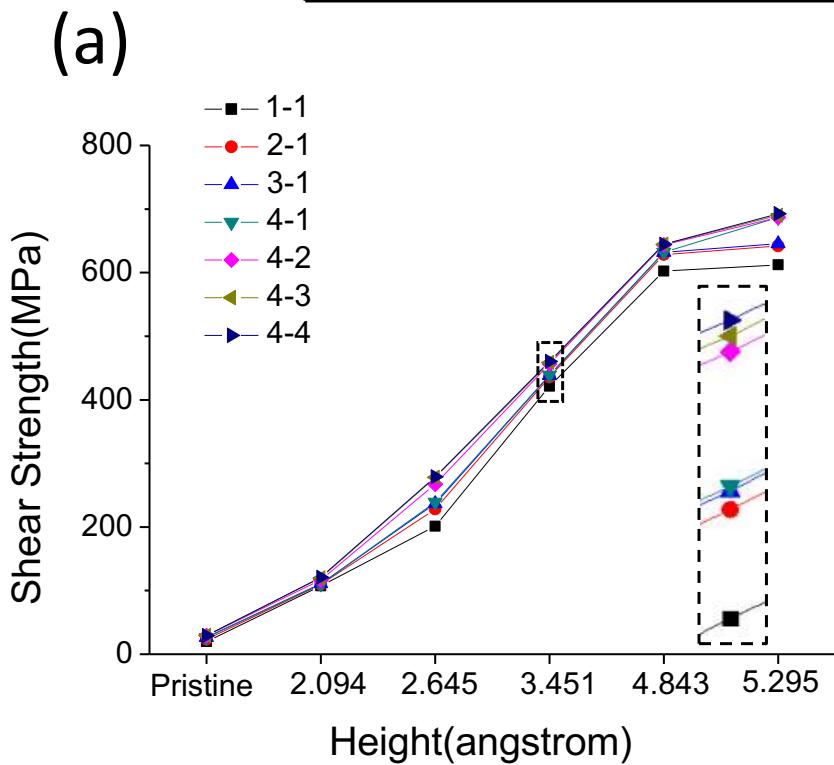
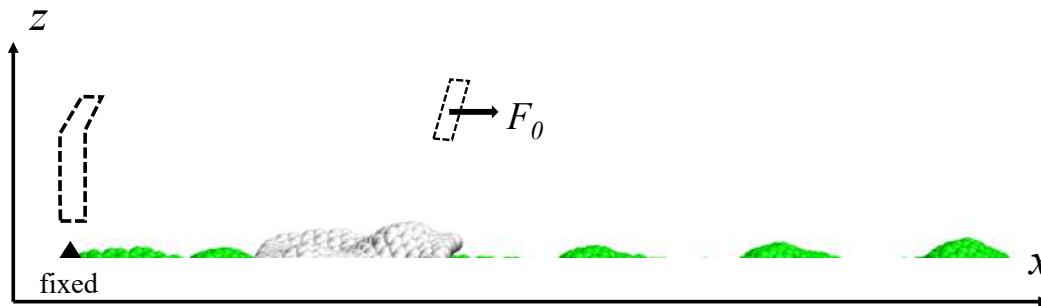


$$\frac{\sigma_p l_0}{E_p h_0 \gamma_{cr}} = \frac{\sinh(l_{cr}/l_0)}{1 + \cosh(l_{cr}/l_0)}$$

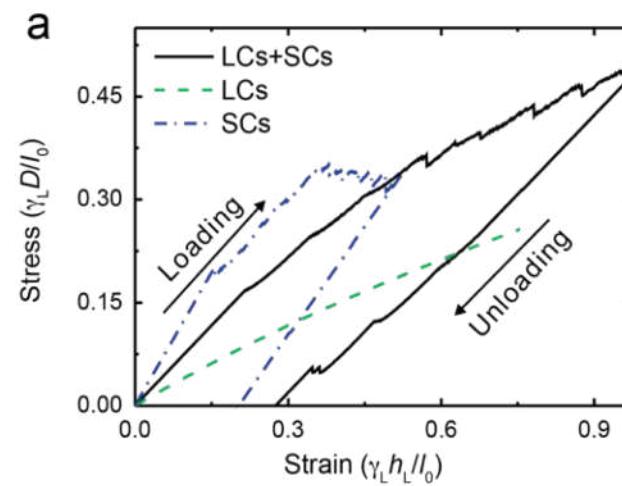
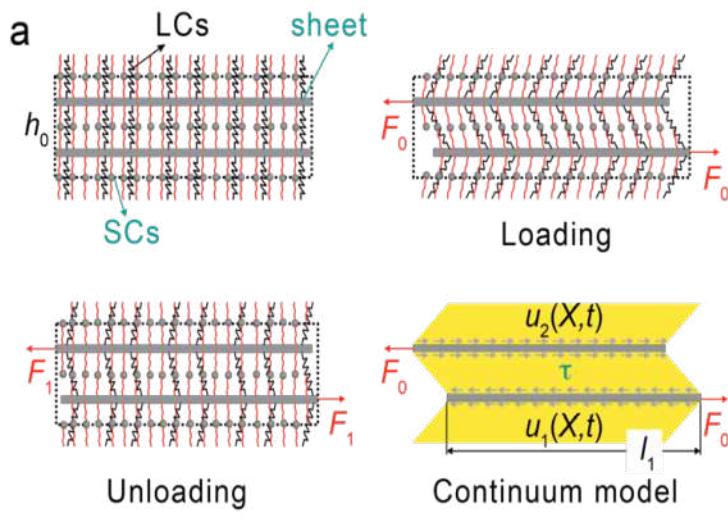
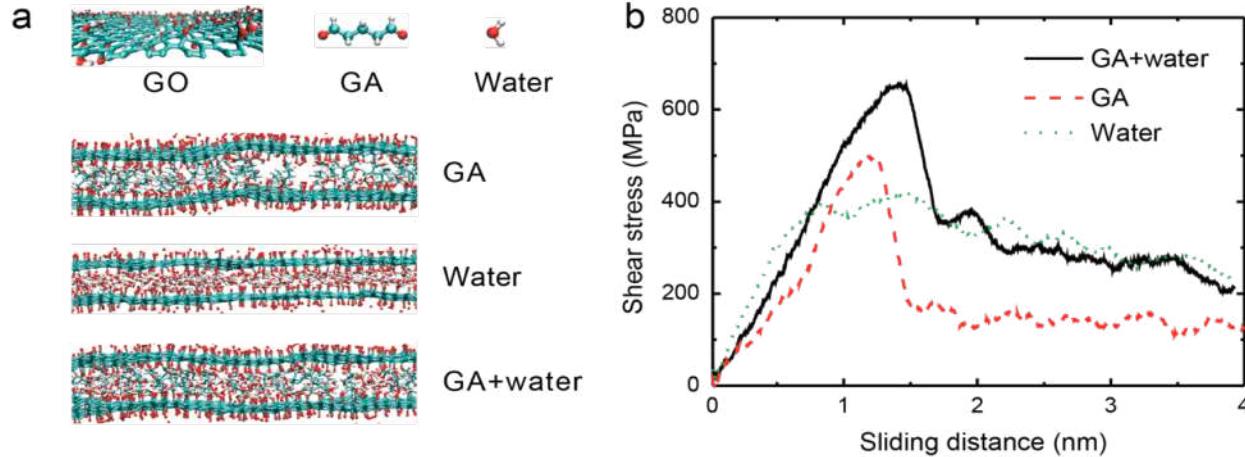
起皱石墨烯



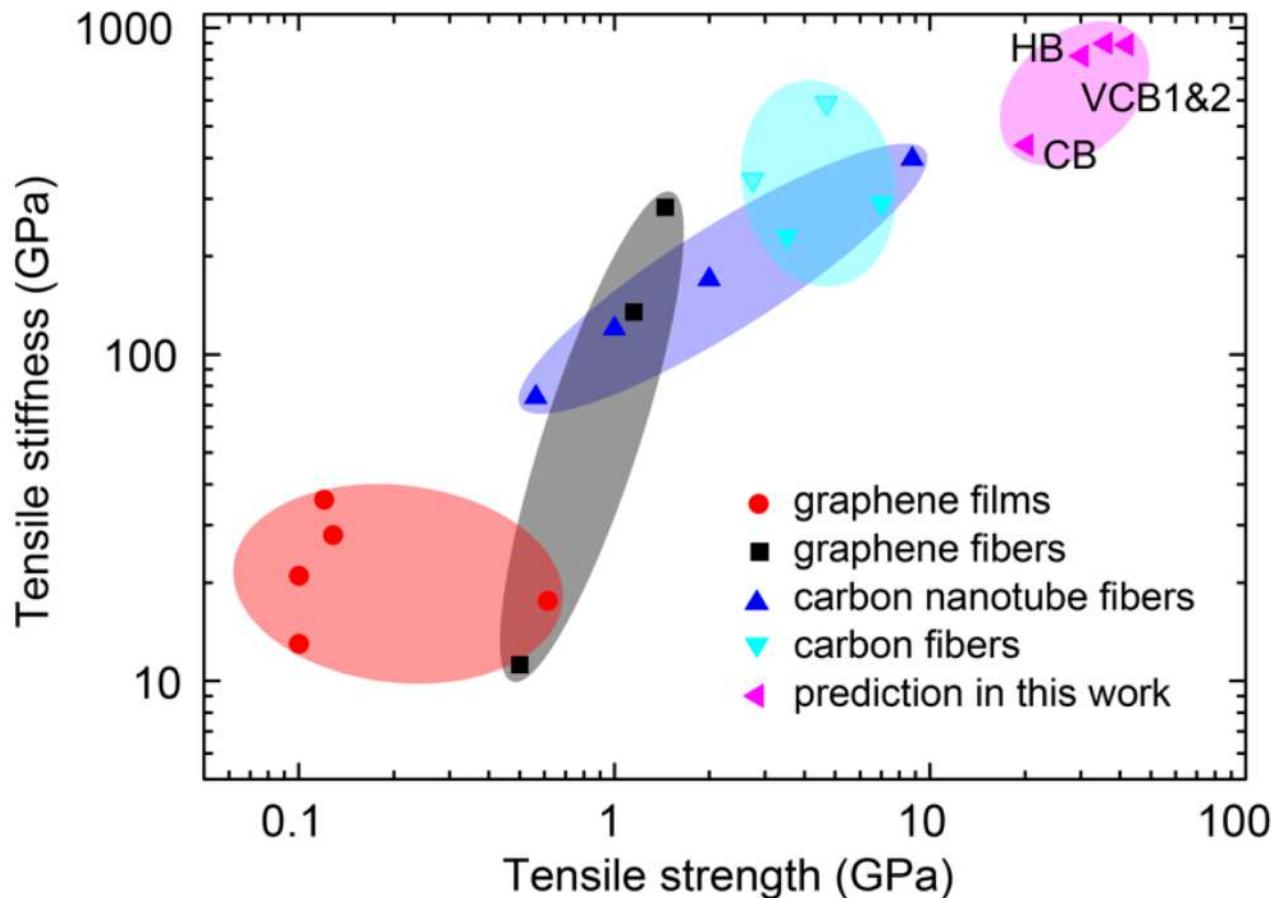
起皱石墨烯层间剪切



双链模型



石墨烯层状材料力学性质优化设计



目录

1. 碳纤维增强复合材料多尺度力学行为
2. 碳纳米材料纳米尺度力学行为
3. 碳纤维增强复合材料宏观力学行为

目录

3.1 纤维增强复合材料细观有限元分析

3.2 纤维增强复合材料宏观有限元分析

3.1 纤维增强复合材料细观有限元分析

真实的复合材料

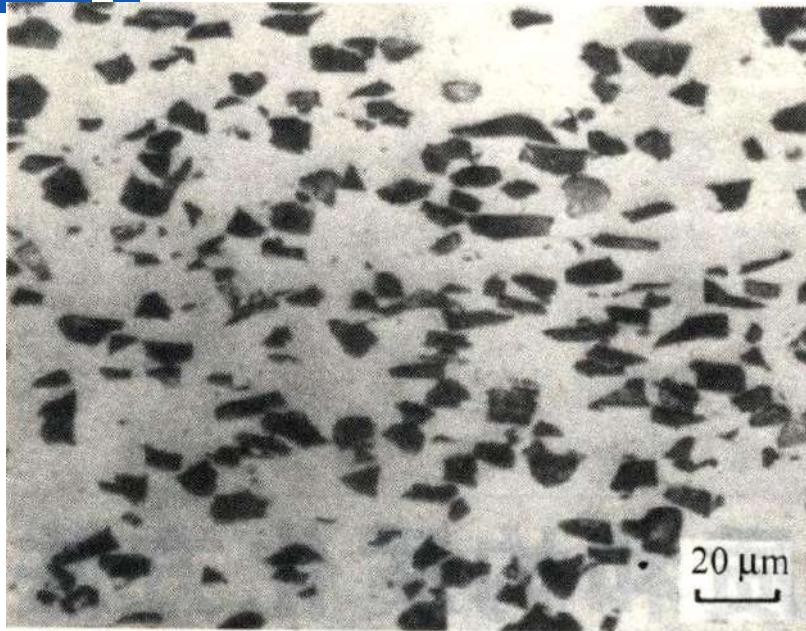


图 10-1 SiCp/Al 复合材料

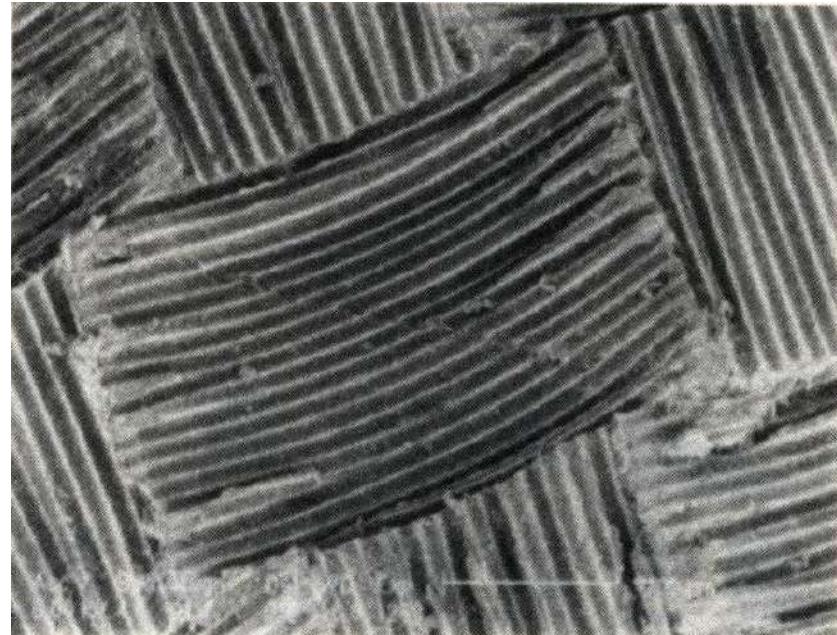


图 10-2 玻璃纤维编织复合材料

- ◆ 从某种意义上复合材料是相当复杂的结构, 如何研究其性能?
- ◆ 精确的理论解(如弹性力学解), 不可能!!
- ◆ 数值求解(如有限元), 计算规模受限于计算机技术发展水平

但科学和工程问题不会等着完美的解决问题的方法, 它们需要立刻给出答案

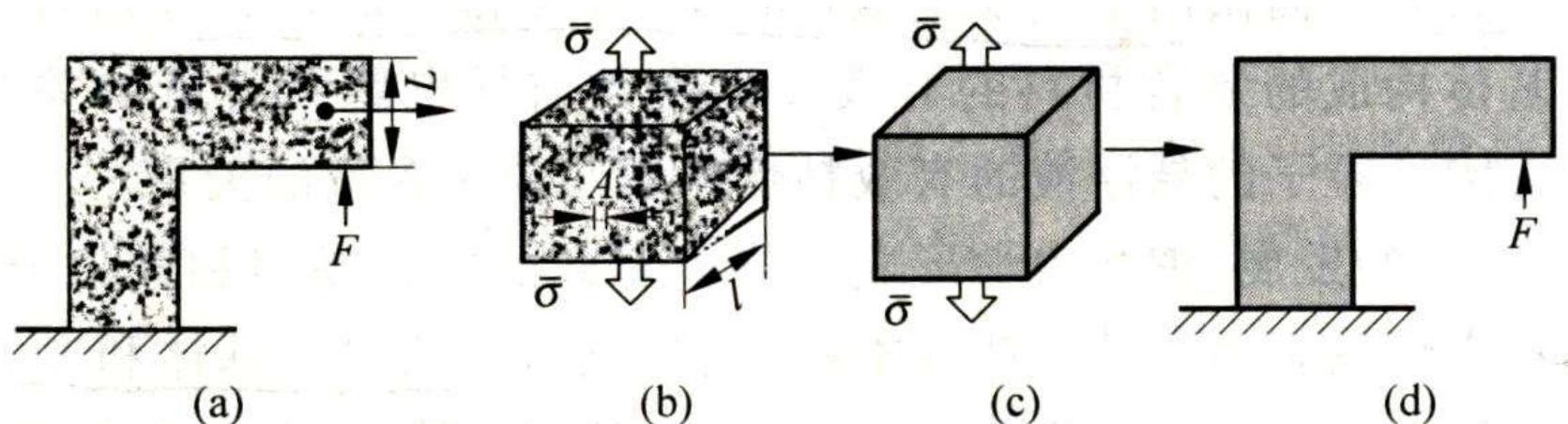
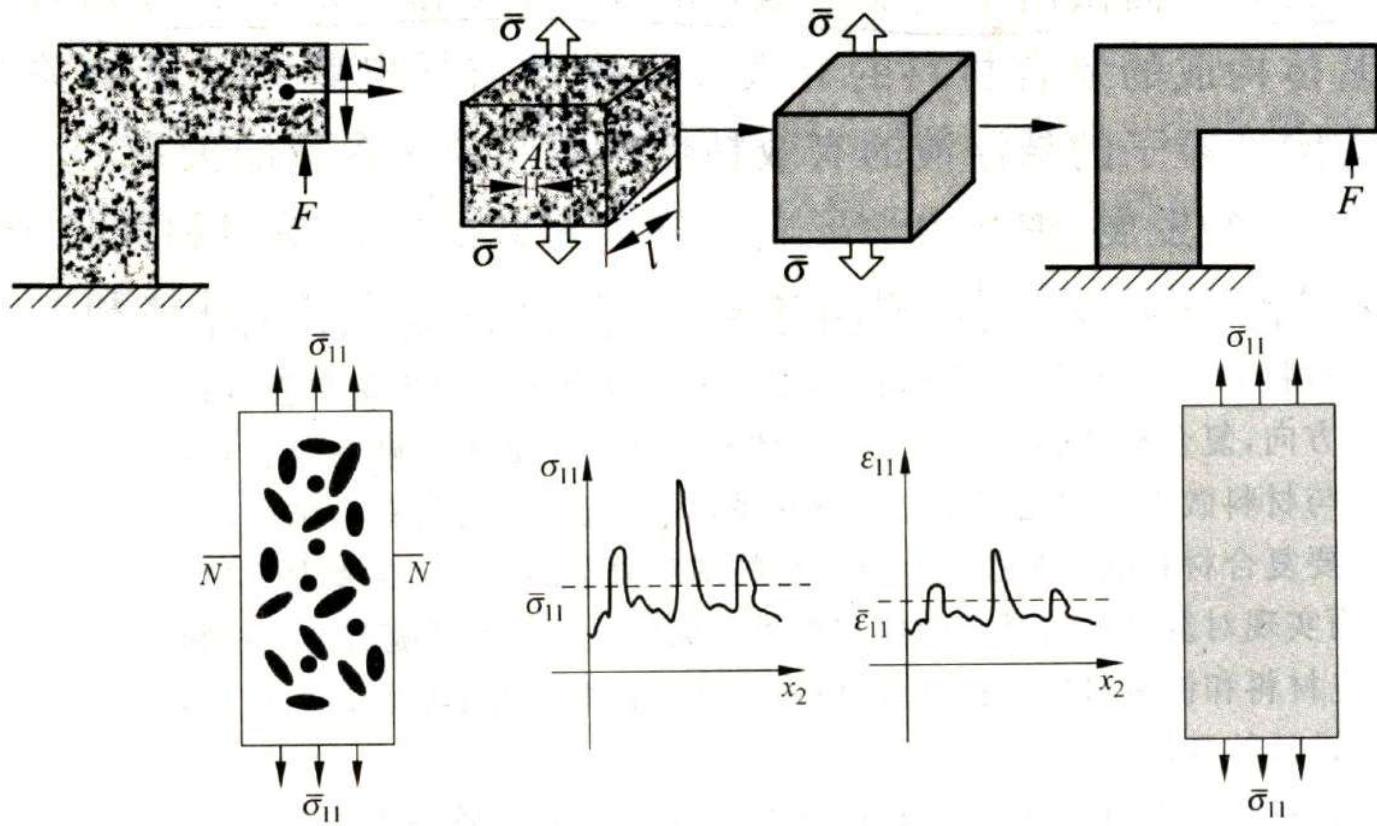


图 10-4 复合材料结构、代表单元和等效结构的概念

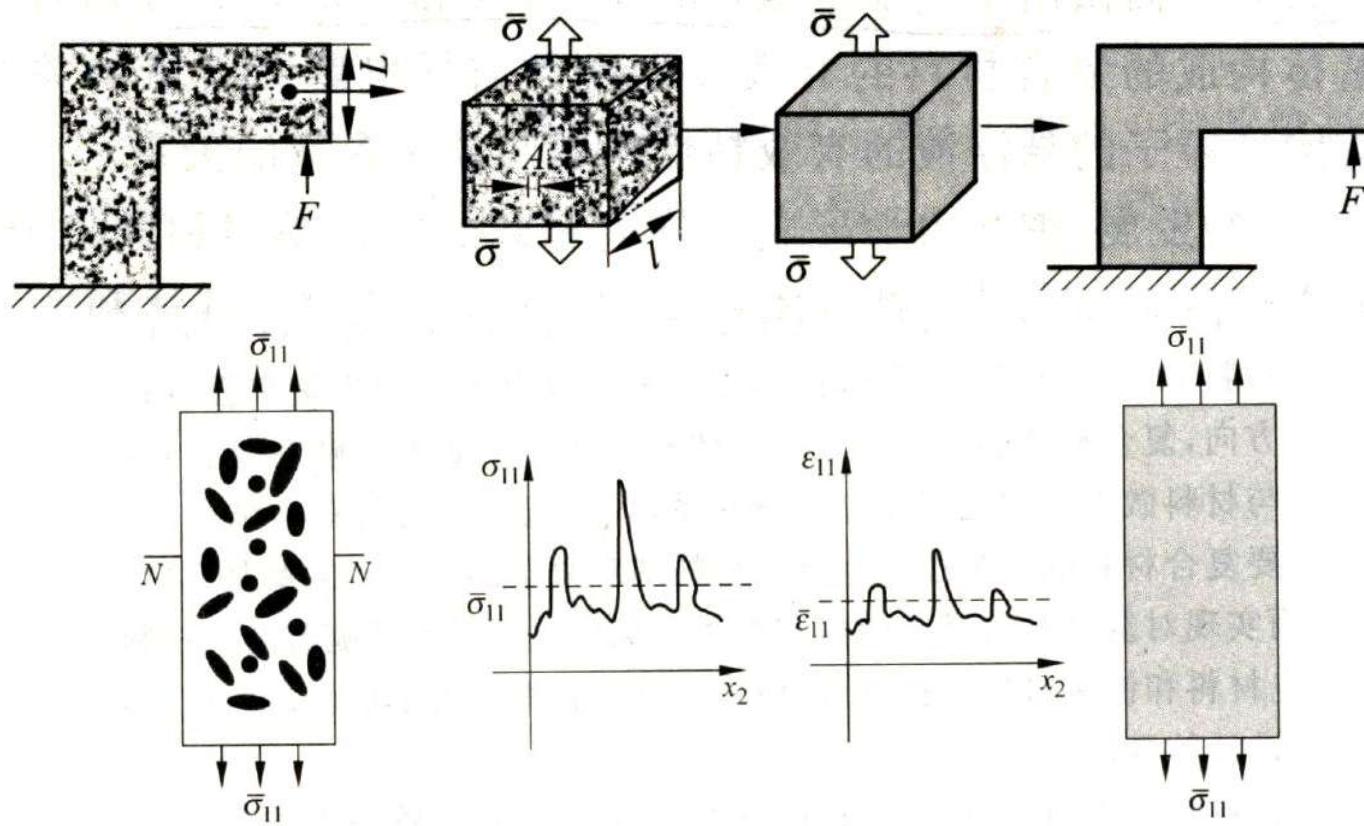
- ◆ 我们力学工作者所具有的能力, 就是利用现有的研究能力和水平, 通过对真实问题进行简化、近似、均质化来平衡准确性、效率及成本之间的关系, 来达到一个对问题的最佳解决方案。
- ◆ 求解并不是越准确越好, 很多的随机因素会使材料行为是个统计过程

尺度 - 空间分辨率的体现



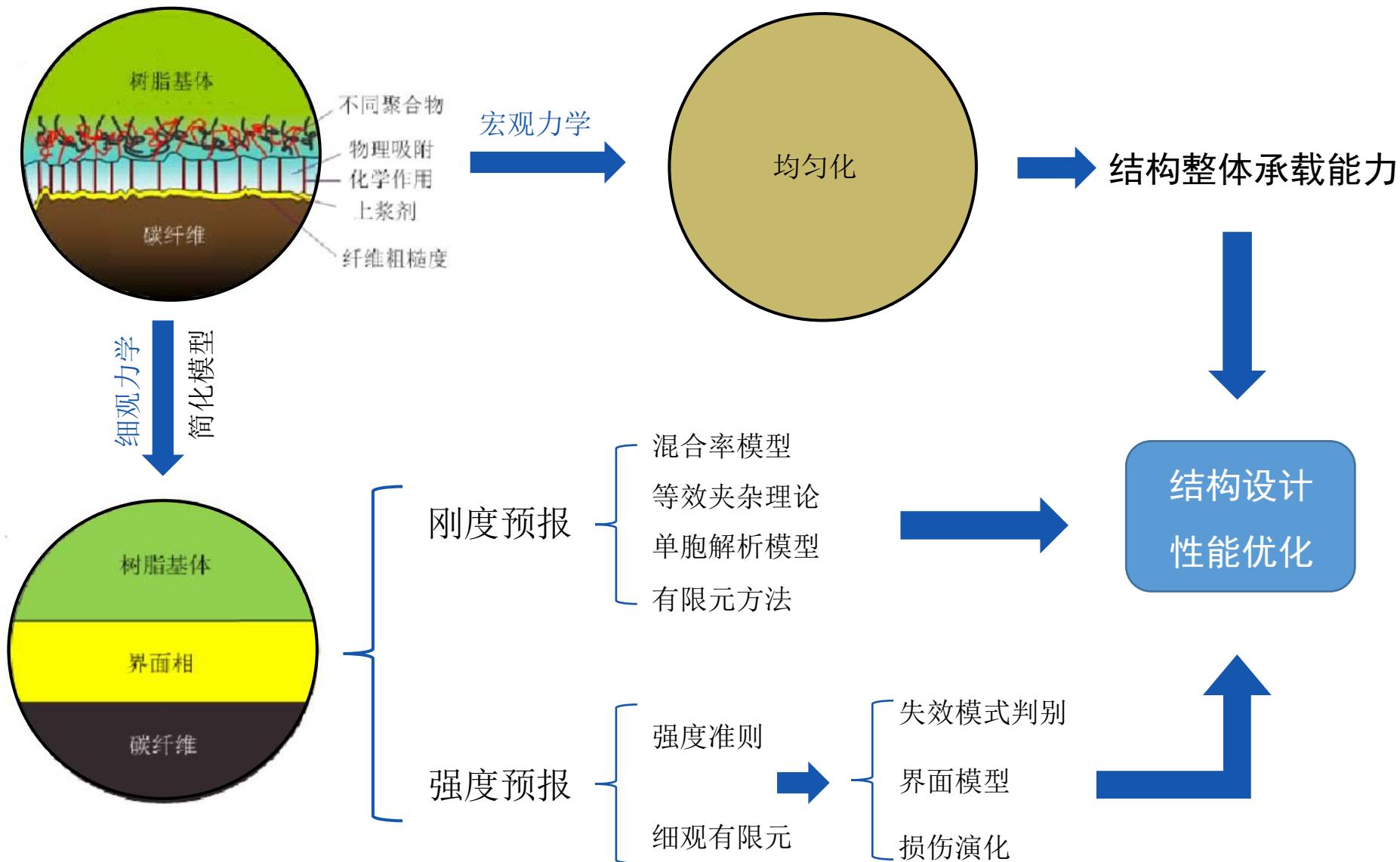
- ◆ 结构的特征尺度 L
- ◆ 材料非均质化的尺度/夹杂尺度 A
- ◆ 均匀化是一个统计平均的处理，要求统计样本足够多，所以在 $L \gg A$ 时才可以做均匀化处理

还存在一个尺度



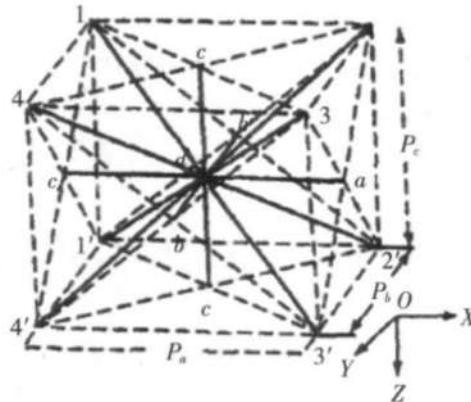
- ◆ 所关心载荷或变形的特征尺度 L_f , 如压痕实验, 所以均匀化亦要求 $L_f \gg A$ 才可以进行
- ◆ 材料非均质化的尺度/夹杂尺度 A

多尺度研究方法



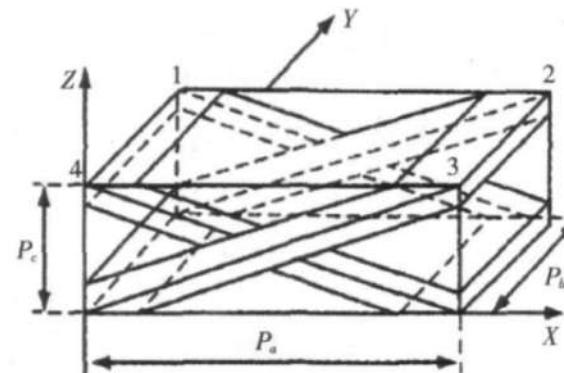
理论分析

“米”字型单胞模型



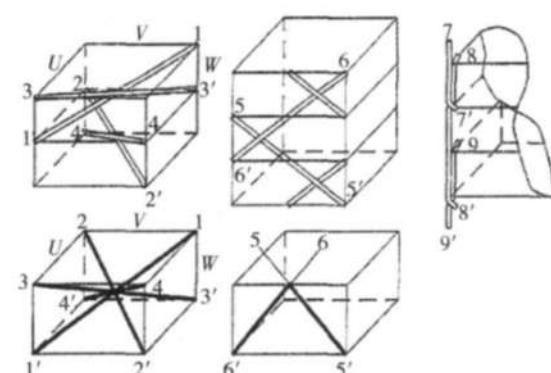
Ma et al., *J. Astm Special Technical Publication.* (1986).

纤维倾斜模型



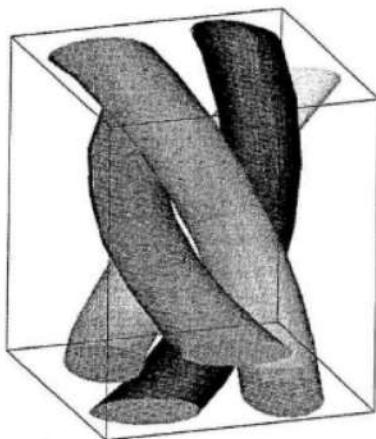
Yang et al., *J. Compos.* (1986)

三胞模型

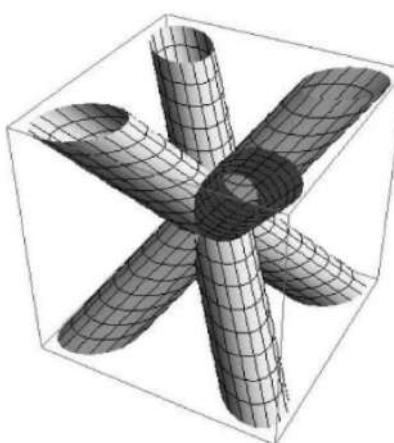


Wu et al., *Compos. Sci. Technol.* (1996)

螺旋纤维模型



Kalidindi et al., *Compos. Sci. Technol.* (1997)



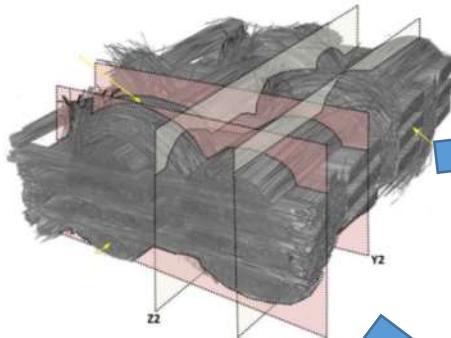
Zeng et al. *Compos. Sci. Technol.* (2004)

宏观性能预报，获取平均性能参数

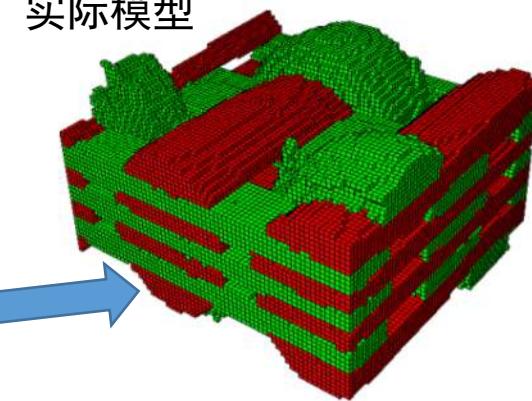
- 优点：建模快，效率高
- 缺点：无法获得材料细观应力分布

数值模拟

μ CT扫描图像（基体隐含）

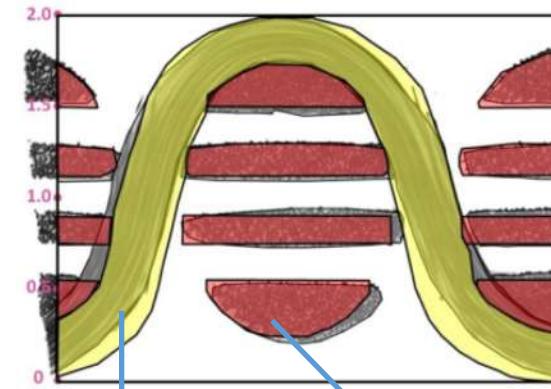


实际模型

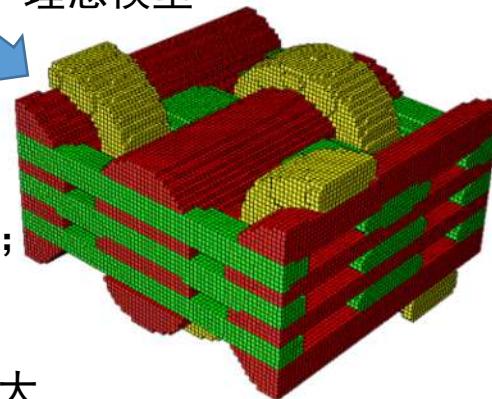


模型细节对比
→

灰色为实
际模型

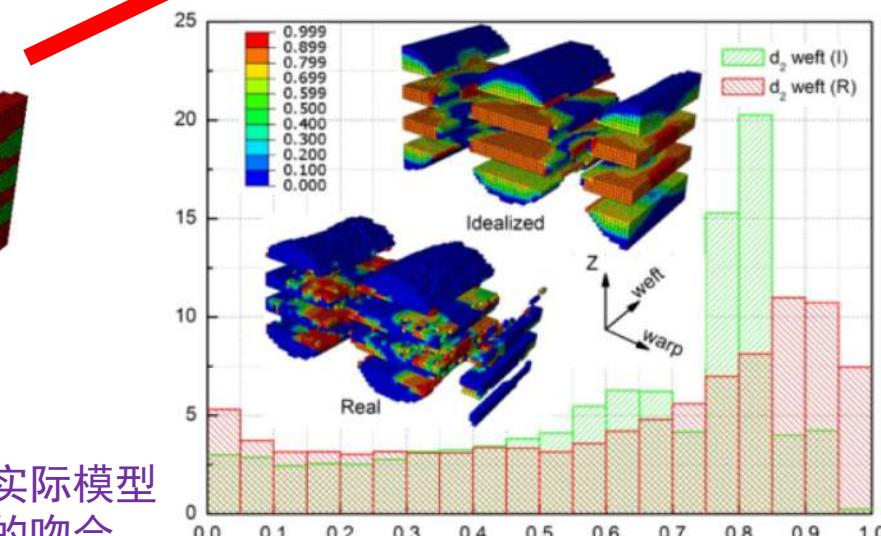


理想模型



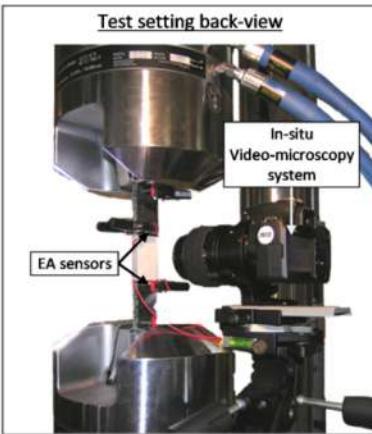
- 用途：性能和强度分析
- 优点：能够获得细观响应；
求解结果精确
- 缺点：建模复杂，计算量大

在渐进损伤分析中，实际模型
与实验数据能够很好的吻合



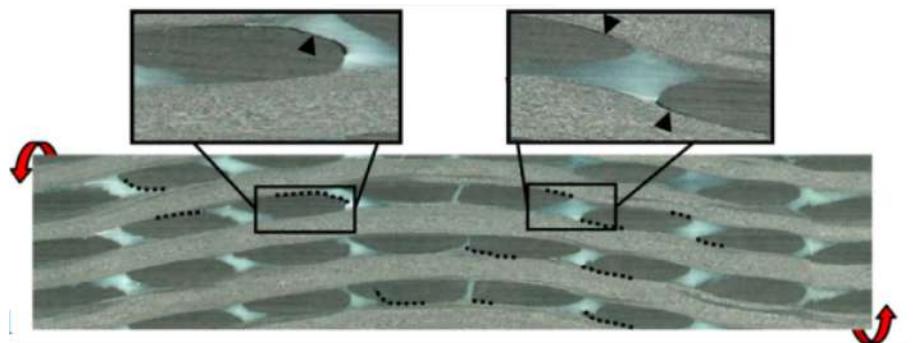
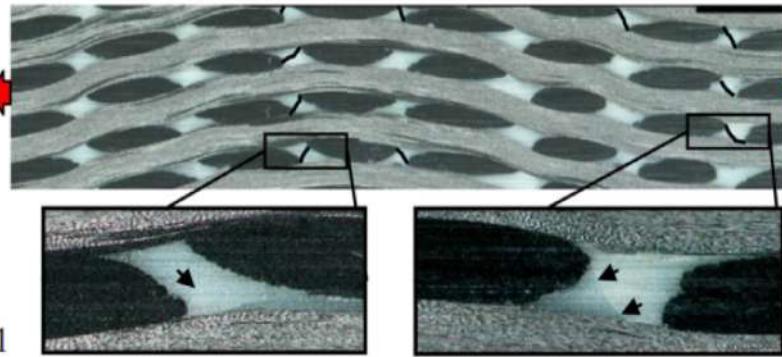
Bahei-El-Din et al., *Int. J. Solids Struct.*(2004) Sun et al. *Compos. Struct.*(2004) Liu et al. *Compos Struct.*(2017)

实验分析

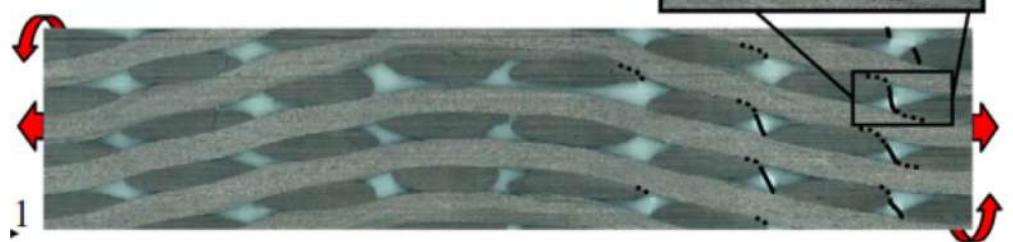


比例拉伸扭转实验

显微观察技术
波发射技术
数字图像技术



..... : Debondings
— : Matrix cracks



确定了与多轴荷载相关的损伤机制

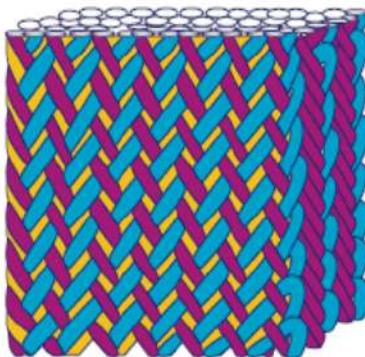
Brandt et al., Compos. Sci. Technol.(1996)

Bogdanovich et al., Compos. Struct.(2013)

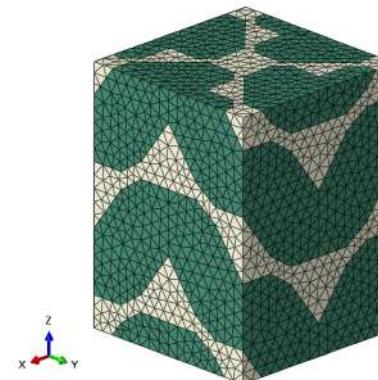
Tableau et al., Compos Struct.(2019)

细观建模

宏观编织复合材料可以看成是由细观胞元周期性排列组成，如图所示。直接分析胞元模型即可获得材料宏观上的各种力学性能。



三维四向

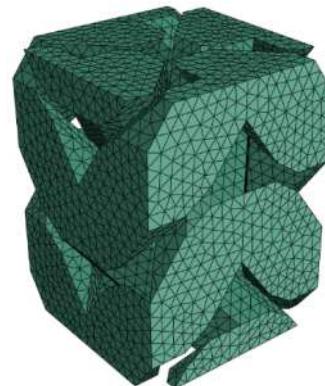


细观单胞模型

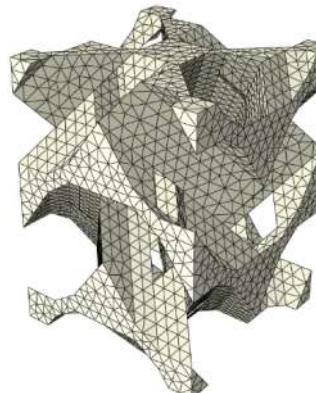
基于实验观察，单胞模型中的纱线走向近似为直线，纱线截面近似为八边形。



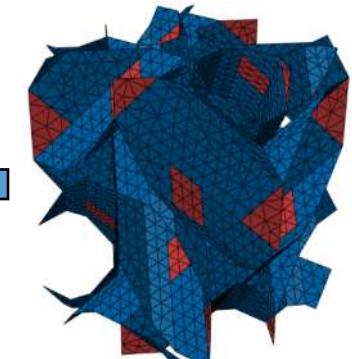
单胞



编织纱线



基体

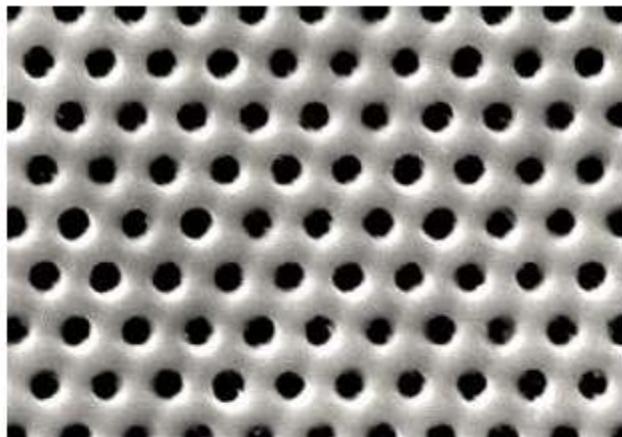


界面

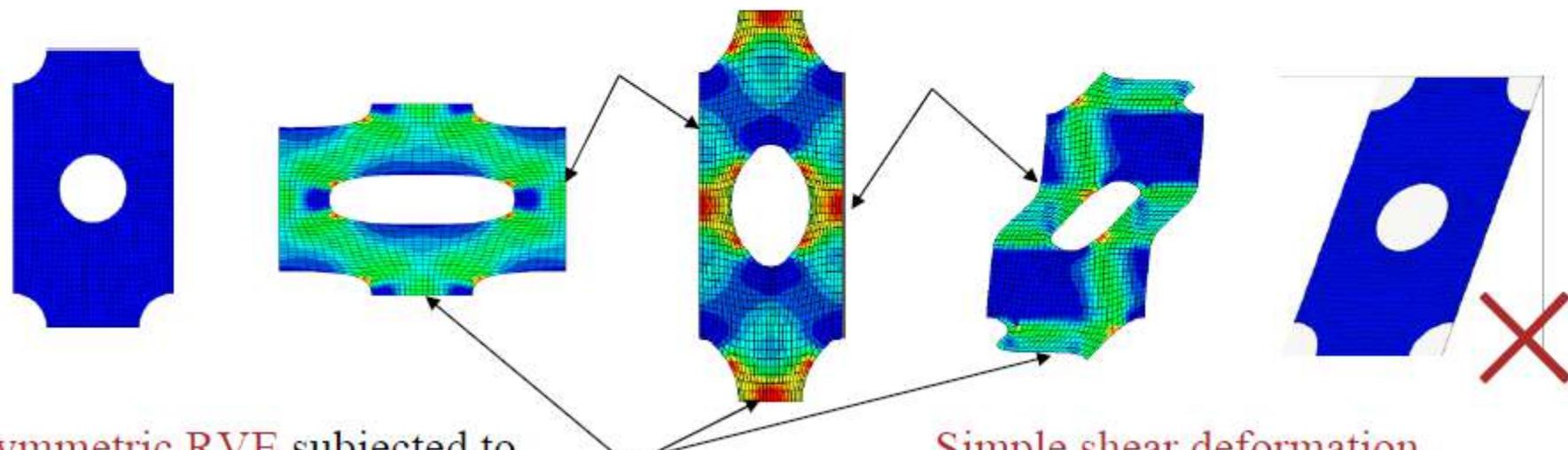




周期边界



- Periodic boundary conditions (PBC) must be applied to the surface of RVE.



symmetric RVE subjected to
normal tractions

Simple shear deformation
flexual surface

周期性边界条件

为了保证在单胞模型的相对面中的应力和位移连续，需要在分析中对单胞模型施加周期性边界条件。

周期性结构中的位移场表示为：

$$u_i = \bar{\varepsilon}_{ik} x_k + u_i^*$$

其中， $\bar{\varepsilon}_{ik}$ 为单胞模型的平均应变， x_k 为节点坐标， u_i^* 为周期性位移修正量。在相对位置处，两节点之间的位移就可以分别表示为：

$$u_i^{j+} = \bar{\varepsilon}_{ik} x_k^{j+} + u_i^*$$

$$u_i^{j-} = \bar{\varepsilon}_{ik} x_k^{j-} + u_i^*$$

$j+$ 和 $j-$ 分别对应两相对面（正面/从面）上的对应节点。以上两式相减就可以得到相对面之间的位移差，即

$$u_i^{j+} - u_i^{j-} = \bar{\varepsilon}_{ik} (x_k^{j+} - x_k^{j-}) = \bar{\varepsilon}_{ik} \Delta x_x^j$$

Δx_x^j 为两节点之间的坐标差，因此当 $\bar{\varepsilon}_{ik}$ 给定后，等式的右边为常数。

在有限元分析中，通过建立对立面、对立边和对立角点之间的**约束方程**实现周期性边界条件的施加，而约束方程是通过参考点建立的，当给定参考点的位移 $\bar{\varepsilon}_{ik}$ 后，对应节点之间就实现了位移差，也就实现了位移荷载的施加。

下面以六面体模型为例，说明周期性边界条件的施加方法。

周期性边界条件的施加举例

以六面体单胞模型尺寸为 $W_x \times W_y \times h$ ，原点为 D ，在三种典型荷载 $(\varepsilon_x^0, \varepsilon_y^0, \gamma_{xy}^0)$ 的作用下，周期性边界条件可以表示为（仅举例说明）：

- 垂直于x轴的两对立面上节点的约束方程为：

$$(ABFE-DCGH) \quad \begin{cases} u|_{x=W_x} - u|_{x=0} = W_x \varepsilon_x^0 \\ v|_{x=W_x} - v|_{x=0} = 0 \\ w|_{x=W_x} - w|_{x=0} = 0 \end{cases}$$

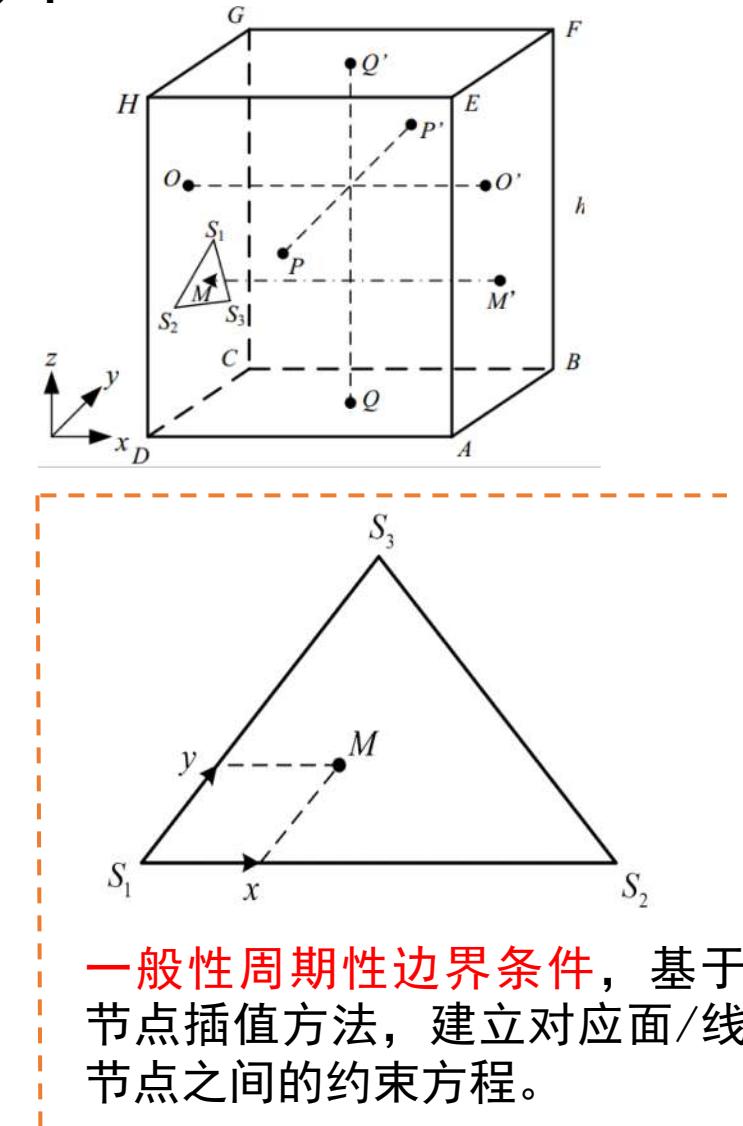
- 平行x轴的边BC，以AD为参考边：

$$(BC-AD) \quad \begin{cases} u_{BC} - u_{AD} = W_y \gamma_{xy}^0 \\ v_{BC} - v_{AD} = W_y \varepsilon_y^0 \\ w_{BC} - w_{AD} = 0 \end{cases}$$

- 角节点A，以节点D为参考点：

$$(A-D) \quad \begin{cases} u_A - u_D = W_x \varepsilon_x^0 \\ v_A - v_D = 0 \\ w_A - w_D = 0 \end{cases}$$

要求节点一一对应，即网格周期性，对于复杂模型
网格划分难度很大。



一般性周期性边界条件，基于
节点插值方法，建立对应面/线
节点之间的约束方程。

纱线和基体的强度准则（以Hashin强度准则为例）

Hashin强度准则：（判断纱线的初始损伤，区分了损伤模式）

➤ 横向压缩：

$$\phi_{T(Z)^c} = \frac{1}{F_T^c} \left[\left(\frac{F_T^c}{2F_{TZ}^S} \right)^2 - 1 \right] (\sigma_T + \sigma_Z) + \left(\frac{\sigma_T + \sigma_Z}{2F_{TZ}^S} \right)^2 + \frac{(\sigma_{TZ}^2 - \sigma_T \sigma_Z)}{(F_{TZ}^S)^2} + \left(\frac{\sigma_{LT}}{F_{LT}^S} \right)^2 + \left(\frac{\sigma_{ZL}}{F_{ZL}^S} \right)^2 \geq 1$$

➤ 纵向拉伸：

$$\phi_{Lt} = \left(\frac{\sigma_L}{F_L^t} \right)^2 + \alpha \left(\frac{\sigma_{LT}}{F_{LT}^s} \right)^2 + \alpha \left(\frac{\sigma_{ZL}}{F_{ZL}^s} \right)^2 \geq 1$$

➤ 横向拉伸：

$$\phi_{T(Z)^t} = \left(\frac{\sigma_T + \sigma_Z}{F_T^t} \right)^2 + \frac{(\sigma_{TZ}^2 - \sigma_T \sigma_Z)}{(F_{TZ}^S)^2} + \left(\frac{\sigma_{LT}}{F_{LT}^S} \right)^2 + \left(\frac{\sigma_{ZL}}{F_{ZL}^S} \right)^2 \geq 1$$

➤ 纵向压缩：

$$\phi_{Lc} = \left(\frac{\sigma_L}{F_L^c} \right)^2 \geq 1$$

最大应力准则：（判断基体的初始损伤）

拉伸： $\phi_{M,t} = \frac{|\sigma_1^t|}{F_m^t} \geq 1$

压缩： $\phi_{M,c} = \frac{|\sigma_3^c|}{F_m^c} \geq 1$

在以上判据中，如果 $\phi_I \geq 1$ ，则当前应力状态下，材料发生了损伤。

损伤起始后，材料的刚度会发生退化， d 表示损伤因子，则损伤后的本构关系表示为：

$$\sigma = C(d)\varepsilon$$

损伤因子 d 的表达式为：

$$d_I = 1 - \frac{X_{eq}^{Ii} (X_{eq}^{If} - X_{eq}^I)}{X_{eq}^I (X_{eq}^{If} - X_{eq}^{Ii})}, \quad (I = Lt, Tt, Zt, Lc, Tc, Zc, Mt, Mc)$$

其中， X_{eq}^I 是等价位移， X_{eq}^{Ii} 是损伤初始时刻的等价位移， X_{eq}^{If} 是完全损伤时的等价位移：

$$X_{eq}^{Ii} = \frac{X_{eq}^I}{\sqrt{\phi_I}}, \quad X_{eq}^{If} = \frac{2G_I}{\sigma_{eq}^{Ii}}$$

其中， ϕ_I 是由强度准则计算得到的 I 损伤模式下的值， G_I 和 σ_{eq}^{Ii} 分别为组分材料破坏模式 I 下的断裂能密度和初始破坏等价应力，求解公式为：

$$\sigma_{eq}^{Ii} = \frac{\sigma_{eq}^I}{\sqrt{\phi_I}}$$

不同破坏模式下的等价应力和等价位移可通过查表得到。(Fang et al. Comp. Struct. 2009)

将求解得到的 d_I 带入到损伤后的本构方程，即可实现损伤的演化。

- 1. Wang et al. Compos. Sci. Technol. (2001)
- 2. Hashin Z. J. Appl. Mech. (1980)
- 3. Lapczyk et al. Compos. Part A. (2007)
- 4. Maimí et al. Mech. Mater. (2007)

界面的强度准则

本构方程：(traction-separation law)

$$\sigma_n = K\delta_n, \quad \sigma_{s1} = K\delta_{s1}, \quad \sigma_{s2} = K\delta_{s2}$$

其中，下标 n ， $s1$ 和 $s2$ 分别代表法向和两个切线方向。 K 为界面的弹性刚度。
初始损伤判据为：

$$\left\{\frac{\langle\sigma_n\rangle}{N}\right\}^2 + \left\{\frac{\sigma_{s1}}{S}\right\}^2 + \left\{\frac{\sigma_{s2}}{S}\right\}^2 \geq 1, \quad \text{其中 } \langle\sigma_n\rangle = \frac{(\sigma_n + |\sigma_n|)}{2}$$

其中 $\langle\sigma_n\rangle$ 为消除正压应力对界面初始损伤的影响， N 和 S 分别为法相和切向的强度。
界面损伤演化为：

$$\begin{aligned} \sigma_n &= K(1 - d_i)\delta_n, \quad (\sigma_n \geq 0) & \sigma_n &= K_n, \quad (\sigma_n < 0) \\ \sigma_{s1} &= K(1 - d_i)\delta_{s1} & \sigma_{s2} &= K(1 - d_i)\delta_{s2} \end{aligned}$$

其中， d_i 为损伤因子，可通过等效位移表示为：

$$d_i = \frac{\bar{\delta}_f(\bar{\delta} - \bar{\delta}_0)}{\bar{\delta}(\bar{\delta}_f - \bar{\delta}_0)}$$

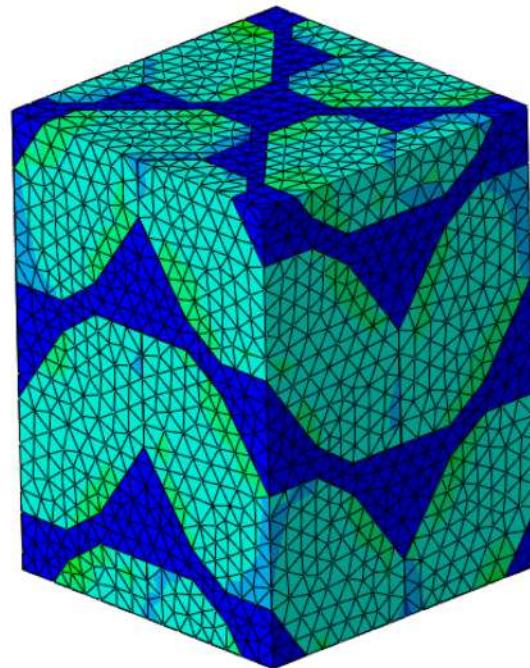
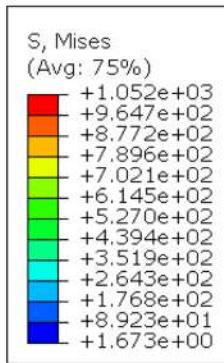
$\bar{\delta}$ 、 $\bar{\delta}_0$ 和 $\bar{\delta}_f$ 分别表示当前等效位移、初始损伤时的等效位移和完全损伤损伤时的等效位移。其中

$$\bar{\delta} = \sqrt{\langle\delta_n\rangle^2 + \delta_{s1}^2 + \delta_{s2}^2}$$

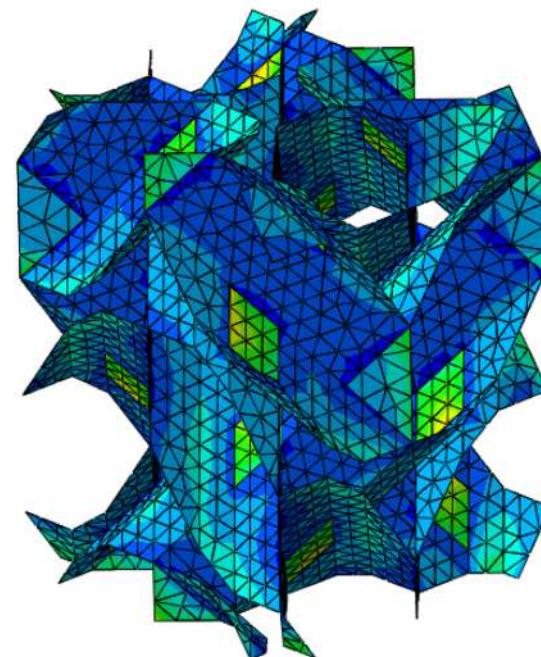
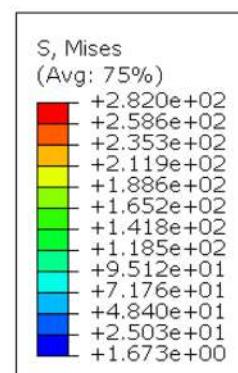
界面参数的选取对模量的计算结果影响很小，但是对强度的计算影响很大

刚度分析-弹性常数的获取

在施加周期性边界条件时，通过给参考点分别施加轴向位移荷载或切向位移荷载，可实现轴向的拉压和剪切。在计算完成后，通过输出参考点的支反力 F_R ，以及对应荷载方向的面积 A 和施加的平均应变 $\bar{\varepsilon}$ ，可求解得到模型的弹性模量、剪切模量和泊松比。



(a) 单胞应力云图

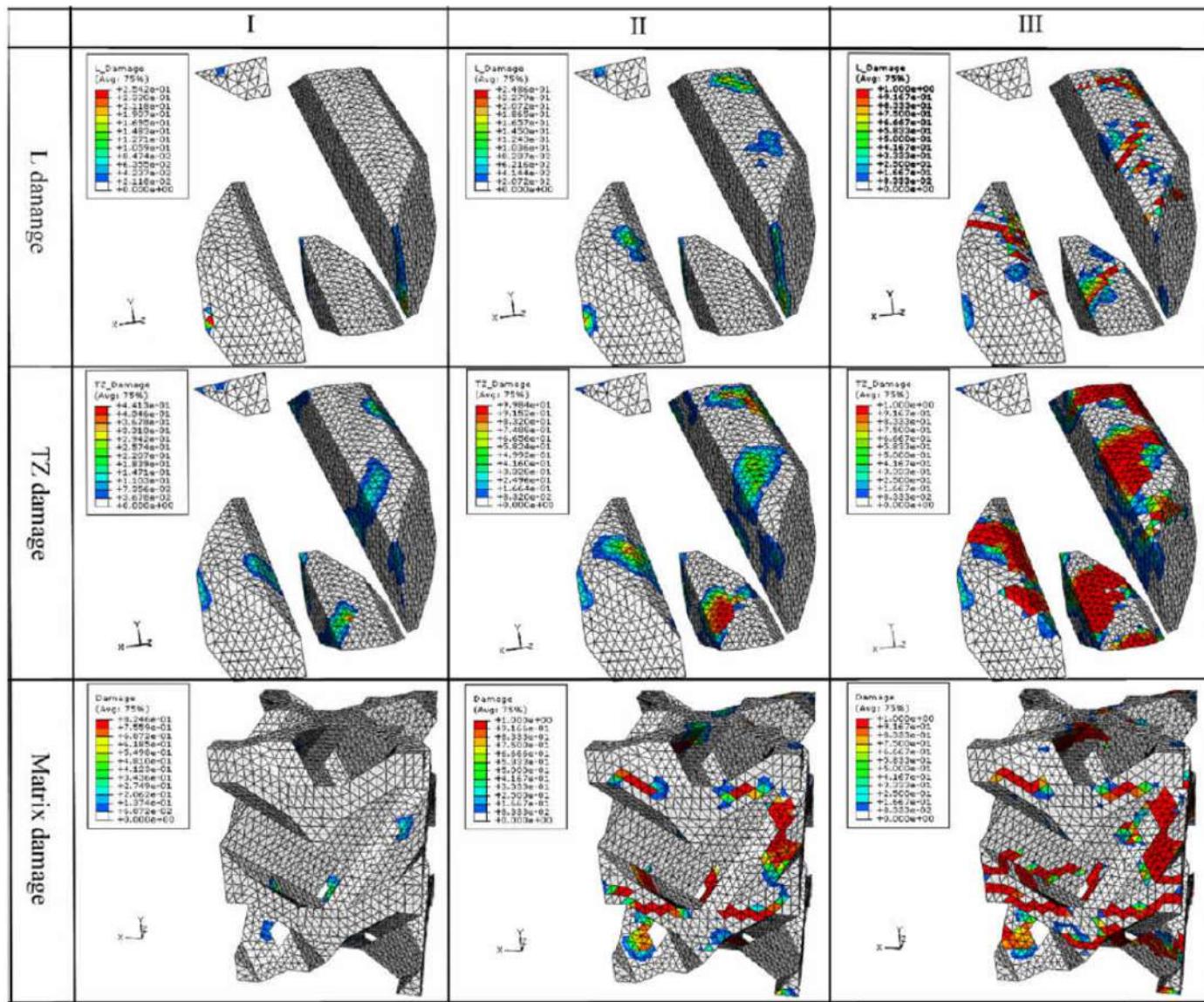


(b) 界面应力云图

荷载 $\bar{\varepsilon}_z = 1\%$ 时的应力云图

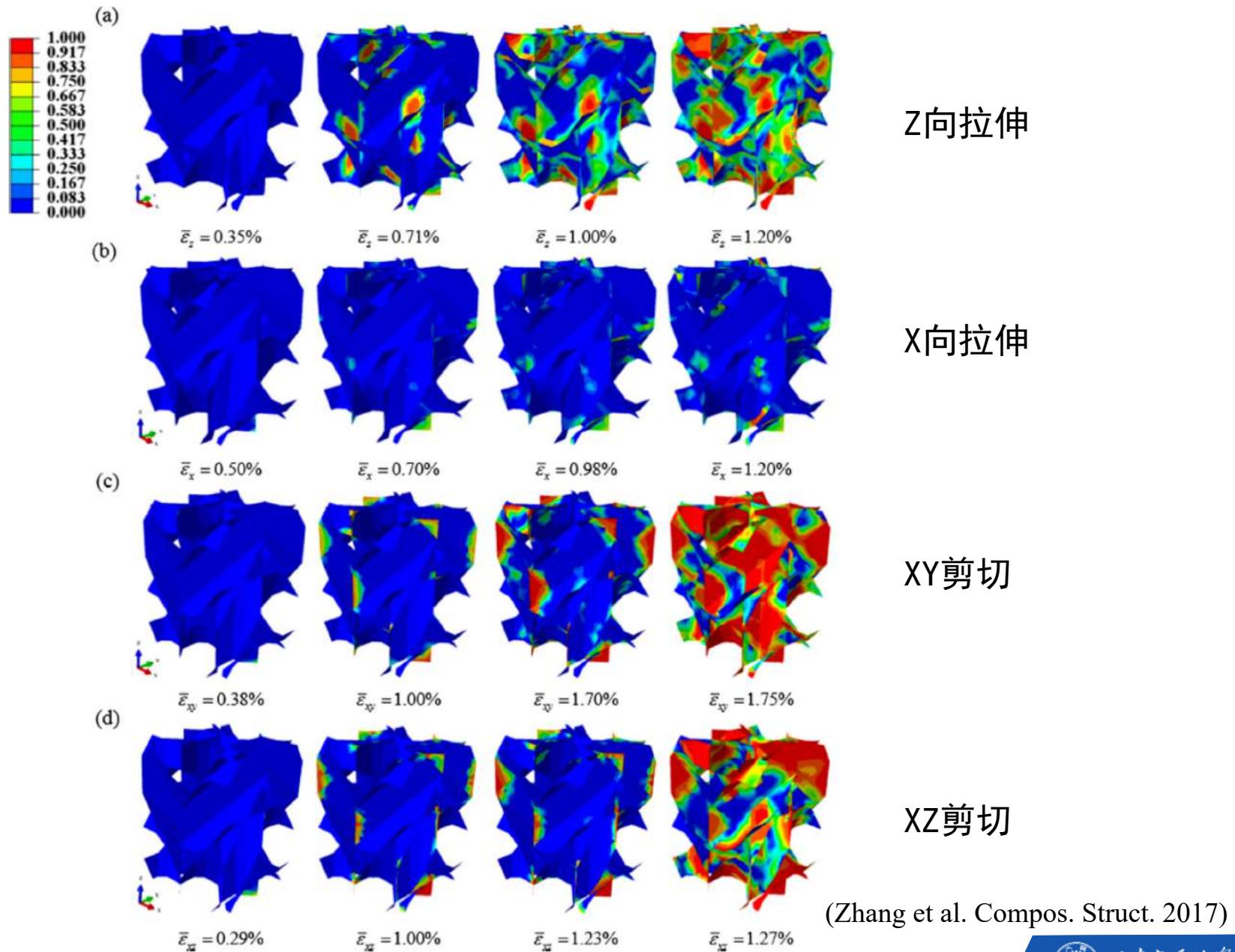
强度分析-纱线和基体

沿编织方向拉伸荷载作用下，纱线和基体的损伤演化过程



(Fang et al. Compos. Struct. 2009)

强度分析-界面

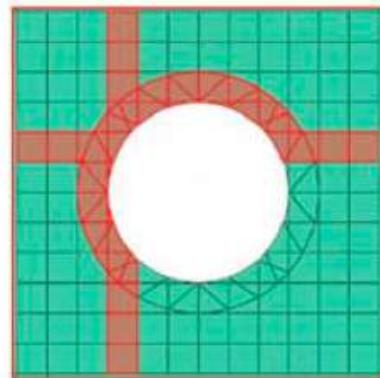
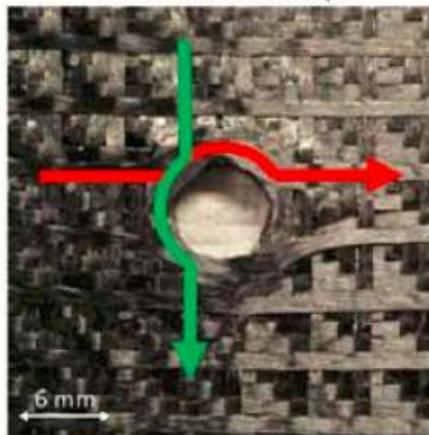


3.2 纤维增强复合材料宏观有限元分析

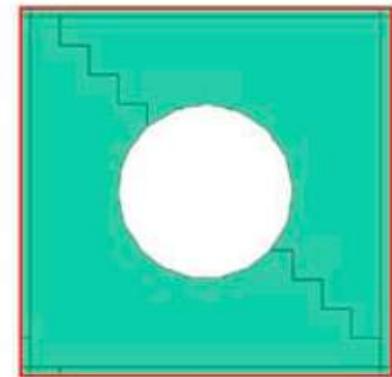
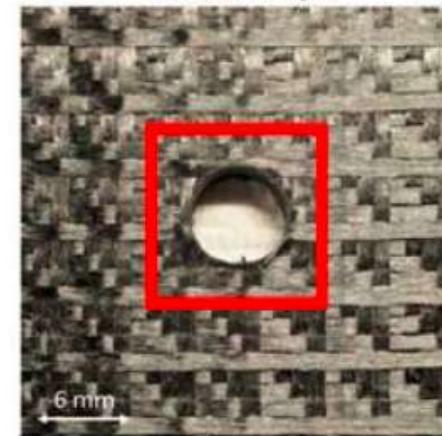


均匀化模型

Tailor Woven Sample



Drilled Sample



$$F_f^t = \left(\frac{\sigma_{11}}{X^T} \right)^2 + \alpha \left(\frac{\tau_{12}}{S^L} \right)^2$$

$$F_f^c = \left(\frac{\sigma_{11}}{X^C} \right)^2$$

$$F_m^t = \left(\frac{\sigma_{22}}{Y^T} \right)^2 + \left(\frac{\tau_{12}}{S^L} \right)^2$$

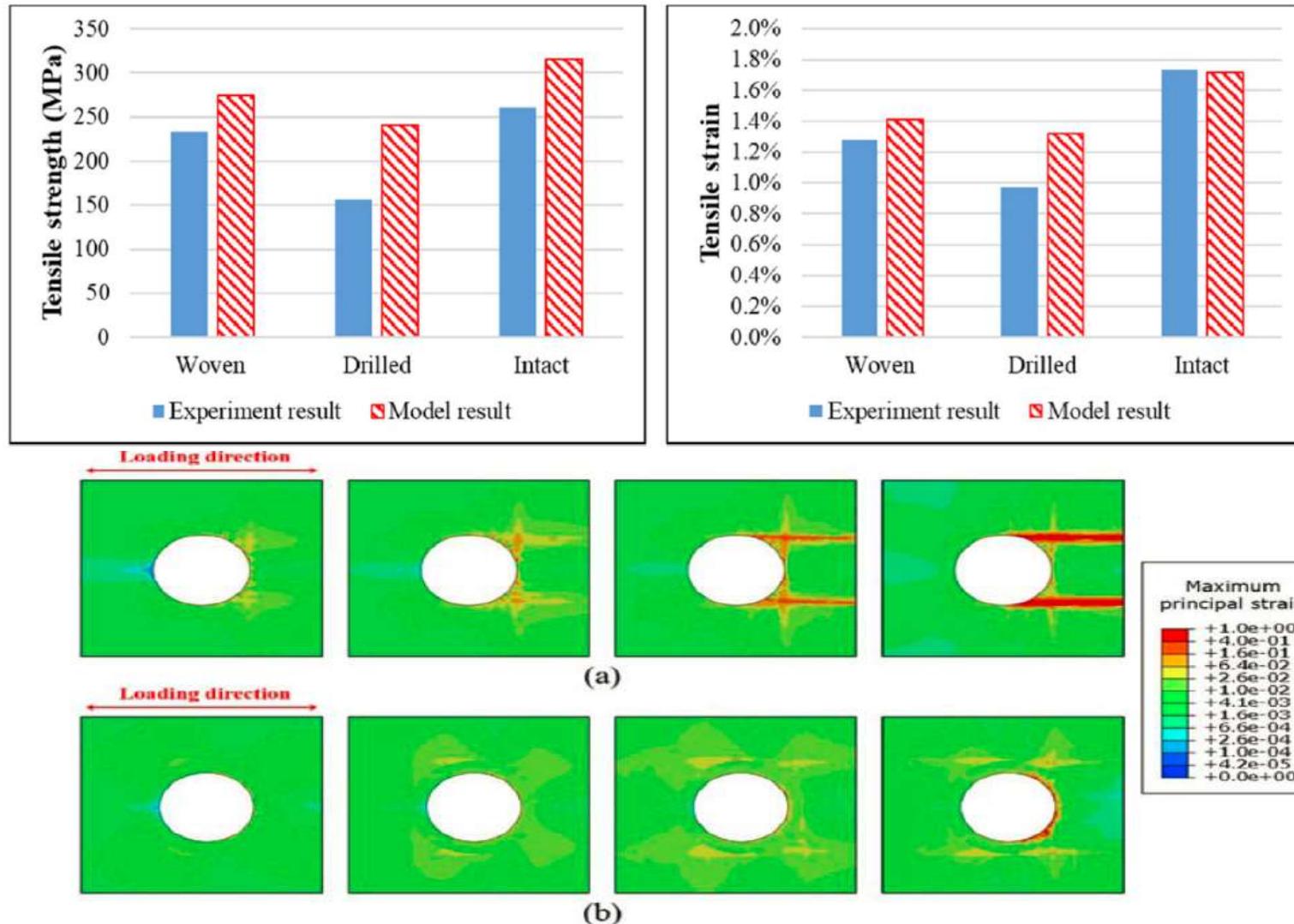
$$F_m^c = \left(\frac{\sigma_{22}}{2S^T} \right)^2 + \left[\left(\frac{Y^C}{2S^T} \right)^2 - 1 \right] \frac{\sigma_{22}}{Y^C} + \left(\frac{\tau_{12}}{S^L} \right)^2$$

$$C_d = \frac{1}{D} \begin{bmatrix} (1-d_f)E_1 & (1-d_f)(1-d_m)v_{21}E_1 & 0 \\ (1-d_f)(1-d_m)v_{12}E_2 & (1-d_m)E_2 & 0 \\ 0 & 0 & (1-d_s)GD \end{bmatrix}$$

$$D = 1 - (1-d_f)(1-d_m)v_{12}v_{21}$$

打孔复合材料板-拉伸力学分析

切割孔会导致纤维的断裂以及孔边缺陷的产生，因此会大大降低材料的强度。可以把纤维在开孔处绕行，以降低材料性能的退化。



(Zhang et al. COMPOS PART B-ENG, 2020)

谢 谢。