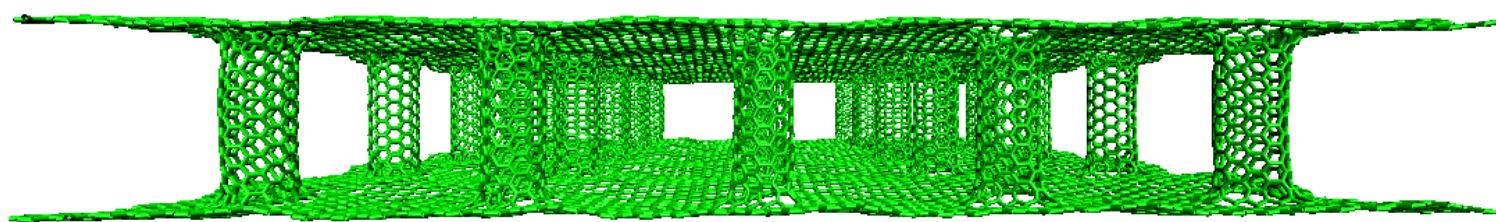


分子动力学模拟集群上机研究背景

碳纳米交链石墨烯力学行为研究

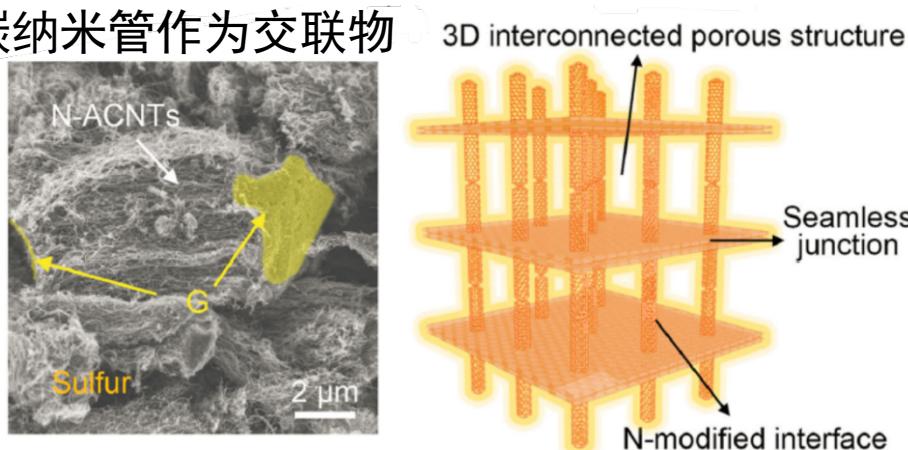
碳纳米管交联



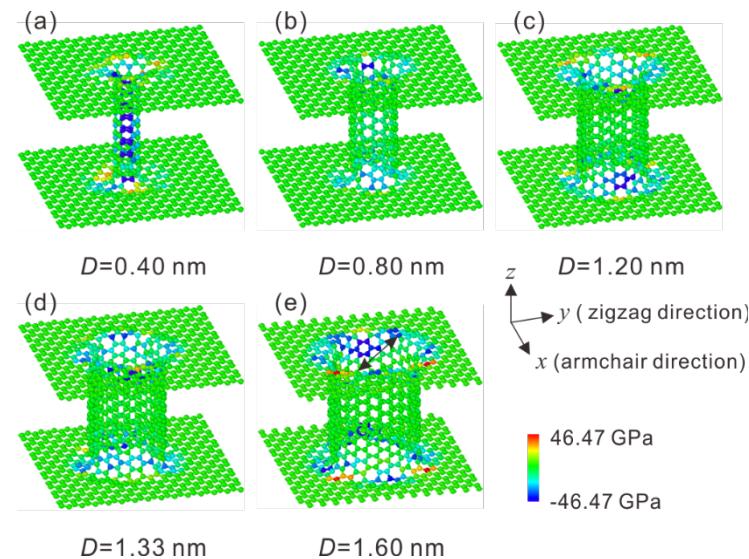
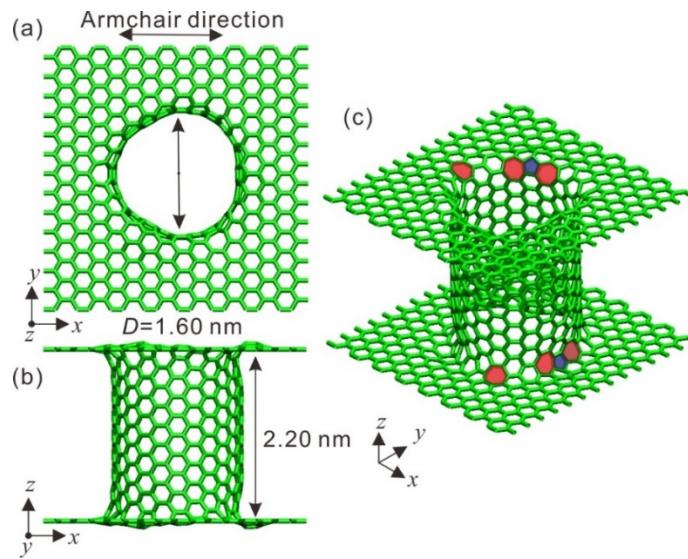
H Qin et al., *Journal of Applied Physics* (2017) **121**: 215104

H Qin et al., *Journal of Applied Physics* (2017) **122**: 125108

碳纳米管作为交联物

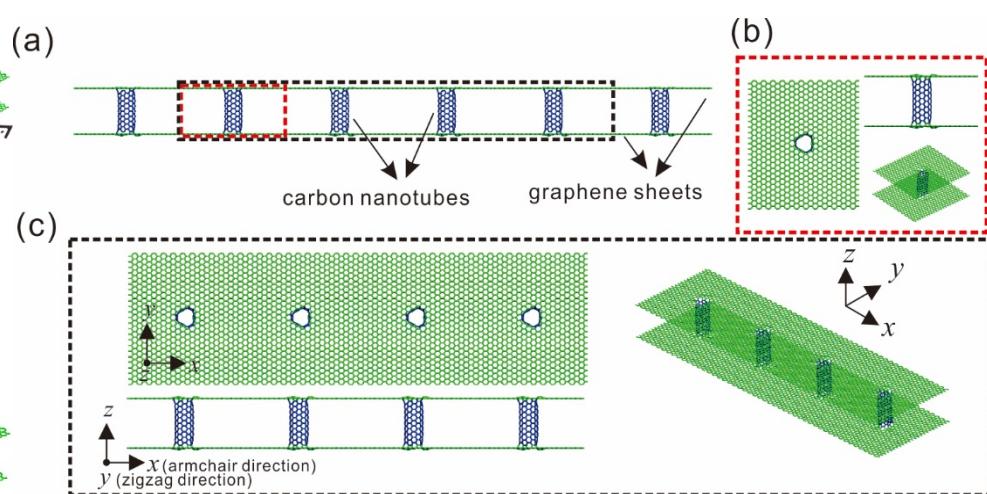
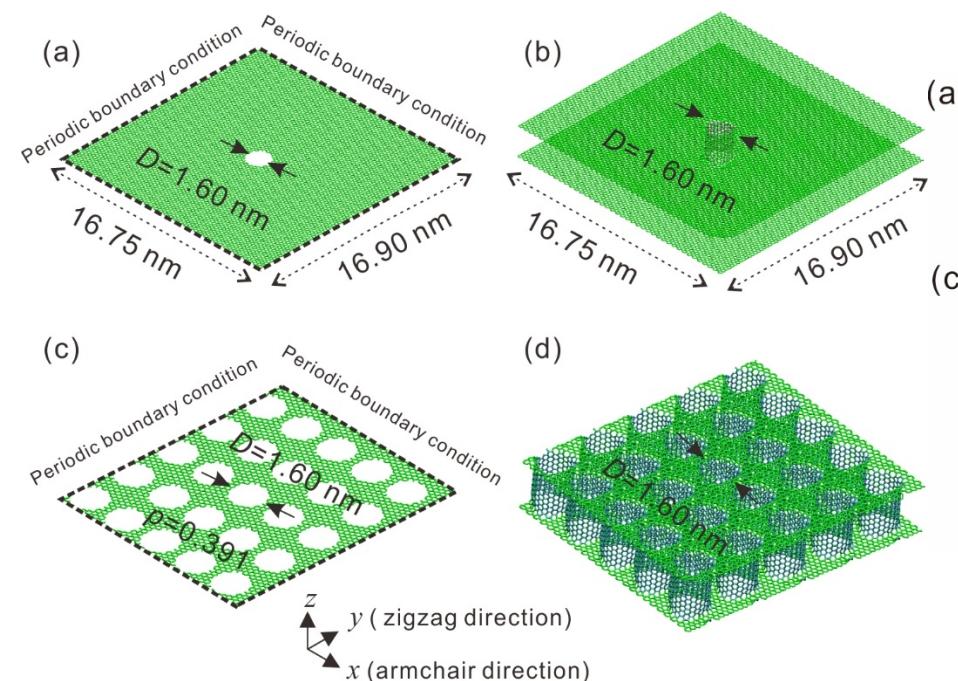


T Cheng et al., *Advanced Materials* (2014)



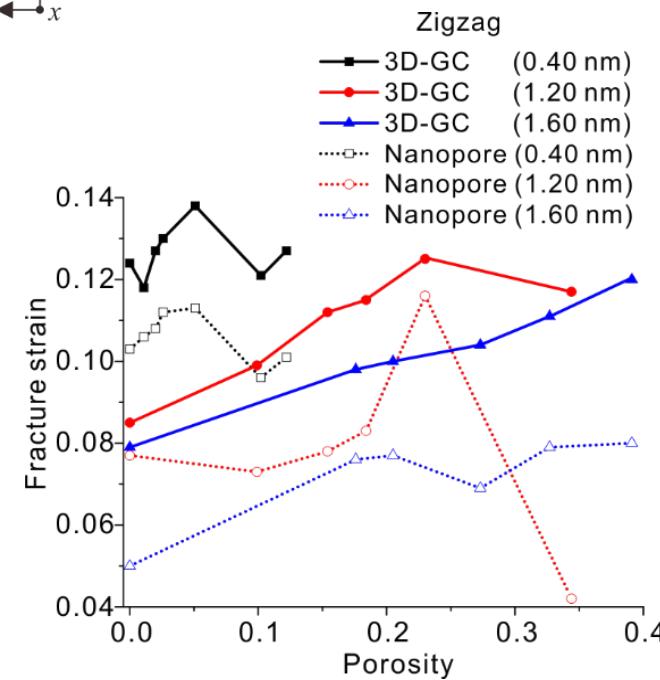
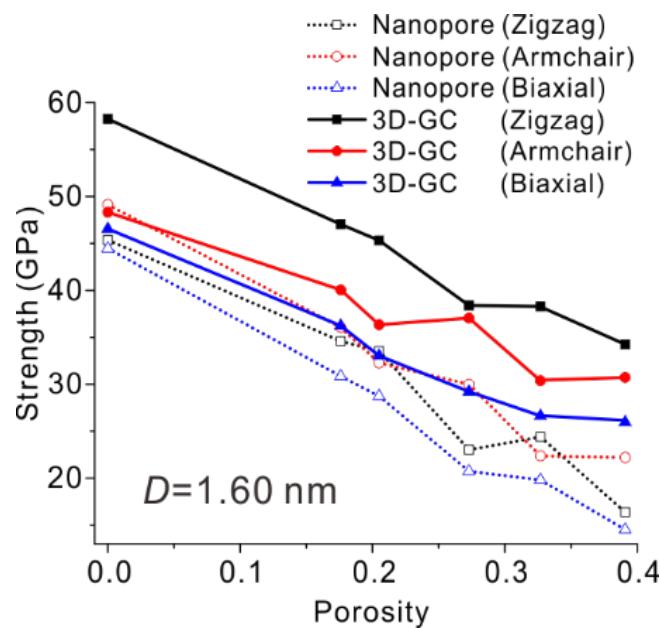
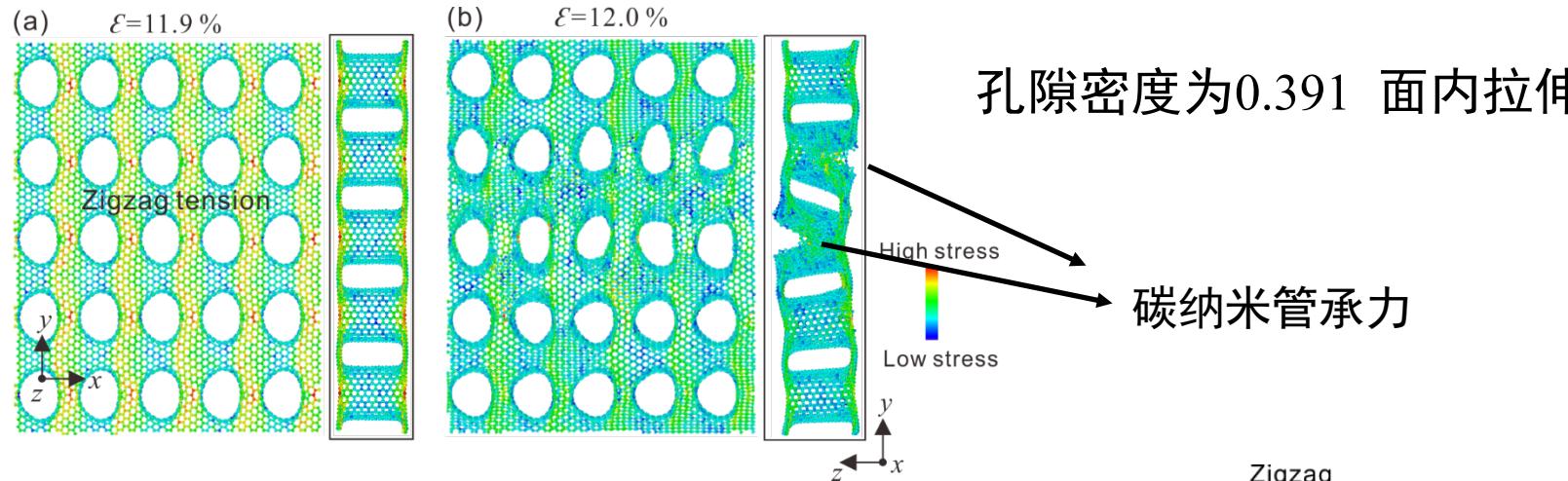
H Qin et al., *Journal of Applied Physics* (2017) **121**: 215104

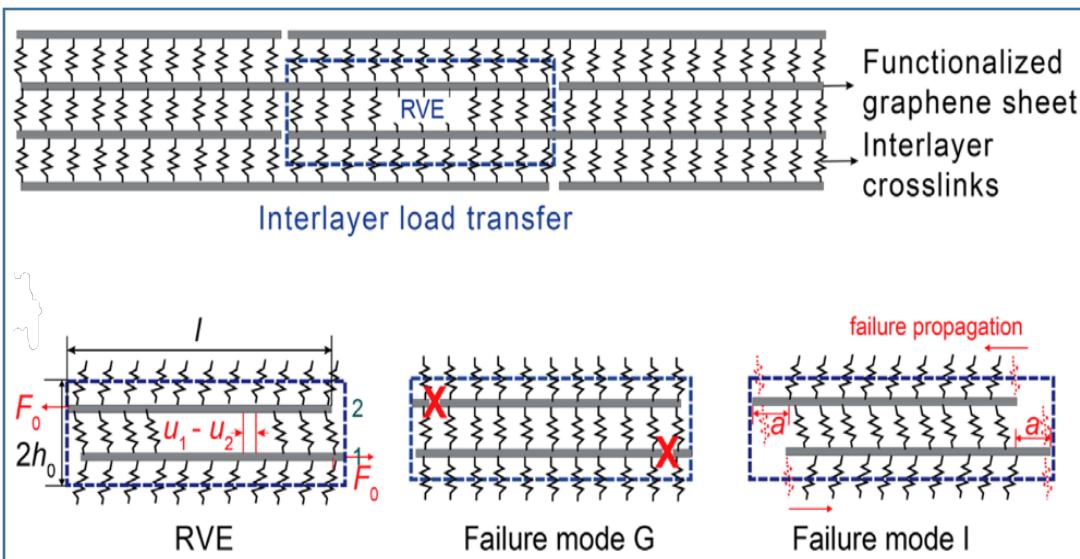
分子动力学模拟模型：



面内拉伸
(断裂强度, 断裂应变, 杨氏模量)

层间剪切

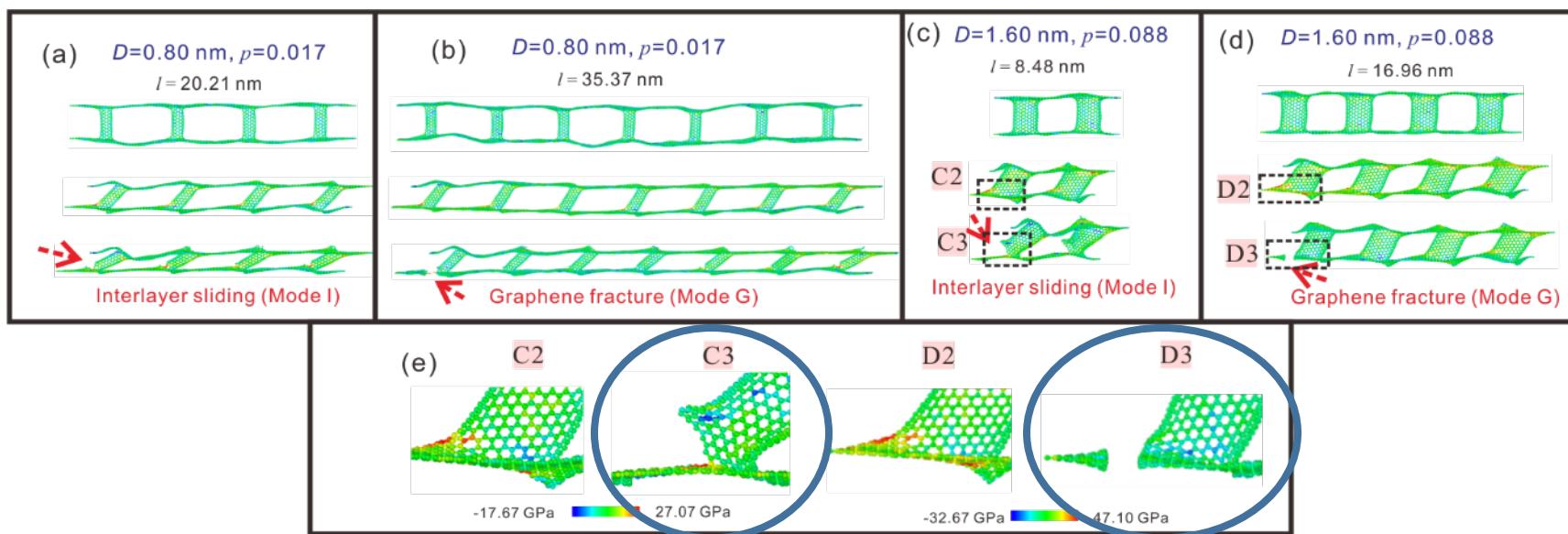




基于可变形拉-剪链模型 石墨烯层状材料失效模式

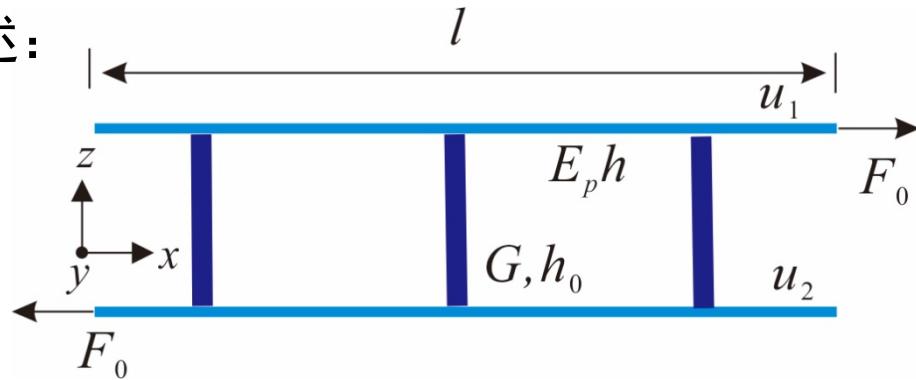
Y Liu et al., 70, *JMPS* (2014) 30-41

3D-GC:



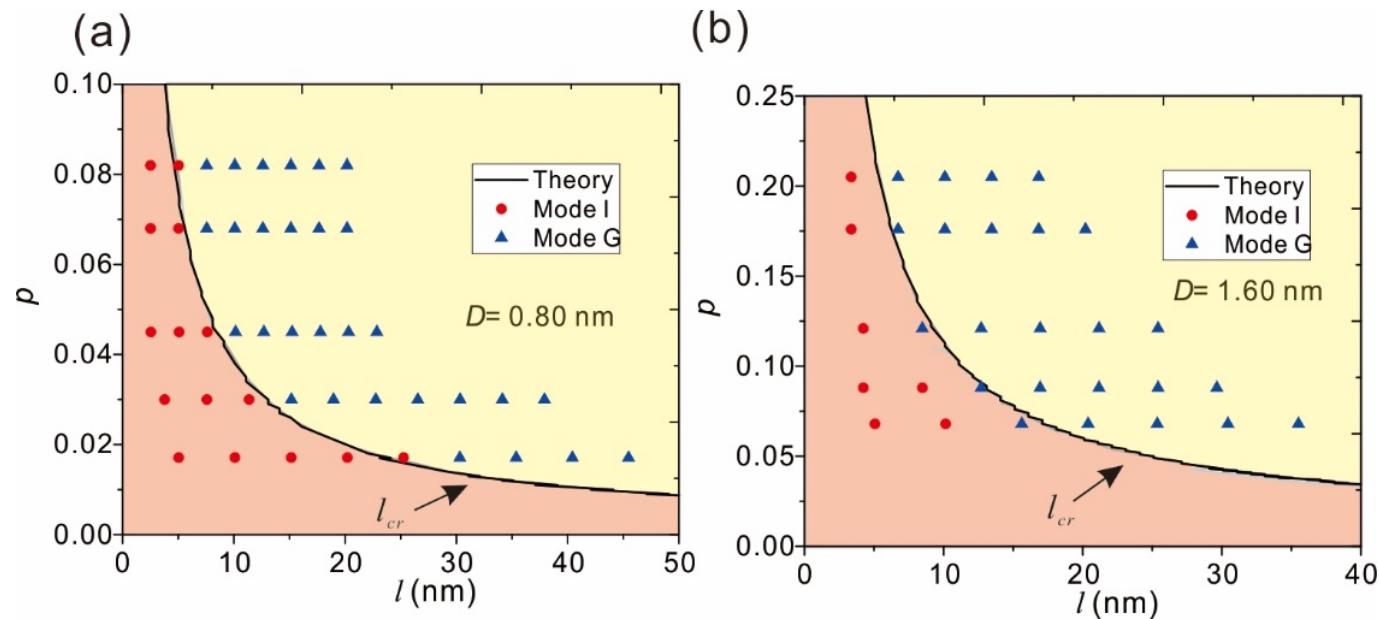
H Qin et al., *Journal of Applied Physics* (2017) 122: 125108

理论模型描述：



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

孔隙密度—长度关系：

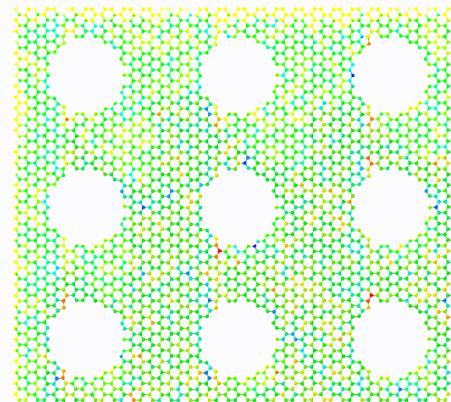
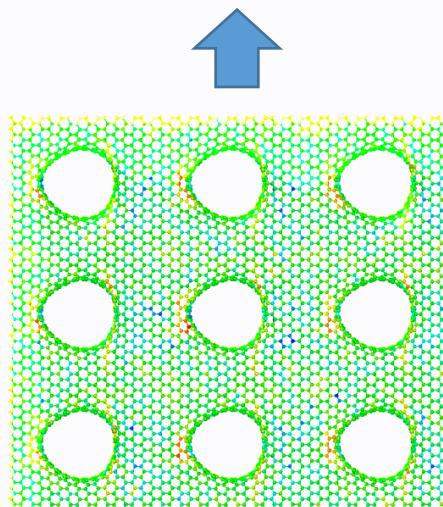


H Qin et al., *Journal of Applied Physics* (2017) **122**: 125108

Example 1

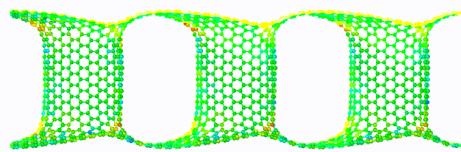
石墨烯复合材料增强增韧分子动力学模拟

拉伸分子动力学模拟



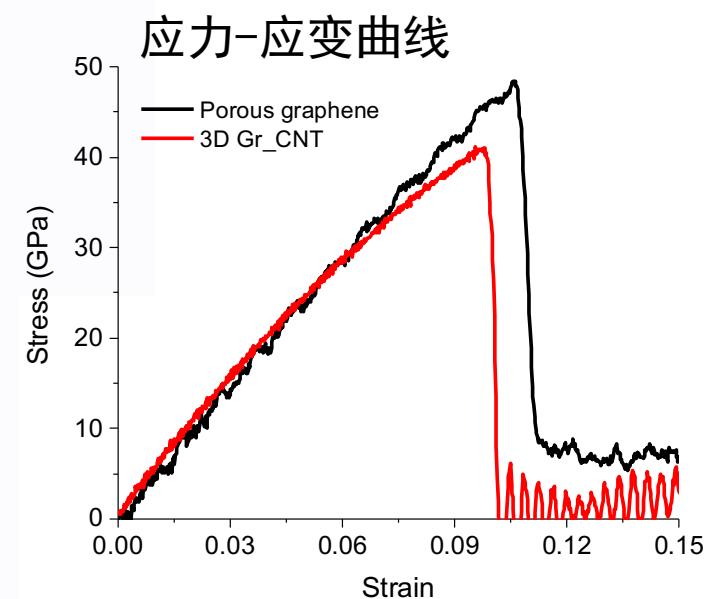
碳纳米管交链石墨烯

纯孔石墨烯



碳纳米管交链石墨烯
gr_cnt.in
gr_cnt.txt

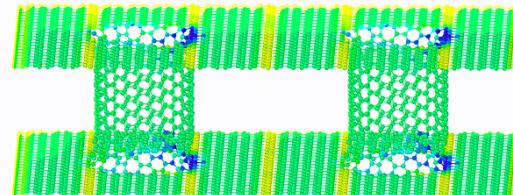
纯孔石墨烯
porous_gr.in
porous_gr.txt



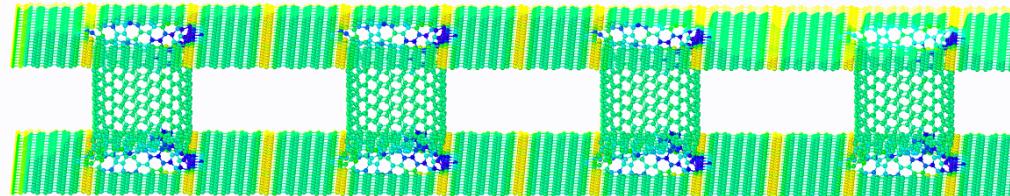
Example 2

碳纳米交链石墨烯拉剪断裂失效模式

碳纳米管撕裂



石墨烯断裂



根据石墨烯层状材料可变形拉-剪链模型，其失效模式可分为层间交链破坏和石墨烯纸断裂

$$\sigma_s = \begin{cases} \frac{D\epsilon_{cr}}{2h_0}, & k_2 \geq \frac{1 + \cosh k_1}{\sinh k_1} \\ \frac{sD\gamma_{cr}}{2L_0(1+c)}, & k_2 < \frac{1 + \cosh k_1}{\sinh k_1} \end{cases}$$

石墨烯断裂
层间交链破坏

Y Liu et al. *J. Mech. Phys. Solids* (2012)