工业中的多尺度力学方法

2020/01/11 – 01/15

主办单位：国家自然科学基金委员会

承办单位：清华大学应用力学教育部重点实验室

清华大学高性能计算平台

NSFC
National Natural Science
Foundation of China

课程安排

- ❑ 1/1 徐志平：多尺度力学方法介绍
- ❑ 1/2 刘　哲：金属合金中的多尺度力学方法
- ❑ 1/3 曹　鹏：高分子复合材料中的多尺度力学方法
- ❑ 1/4 林　皎：高性能计算技术
- ❑ 2/1 洪家旺：第一性原理
- ❑ 2/2 李晓雁：分子动力学
- ❑ 3/1 崔一南：位错动力学
- ❑ 3/2 张　旭：晶体塑性
- ❑ 4/1 王　涵：机器学习
- ❑ 4/2 施兴华：时空多尺度
- ❑ 5/1 倪　勇：相场
- ❑ 5/2 刘益伦：复合材料跨尺度模拟

多尺度力学方法介绍

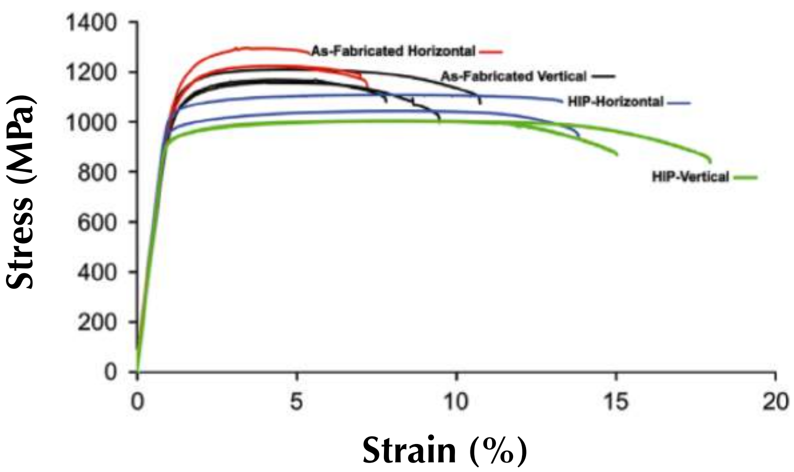
1. 先进合金、复合材料中的多尺度问题
2. 物质科学中的基本概念

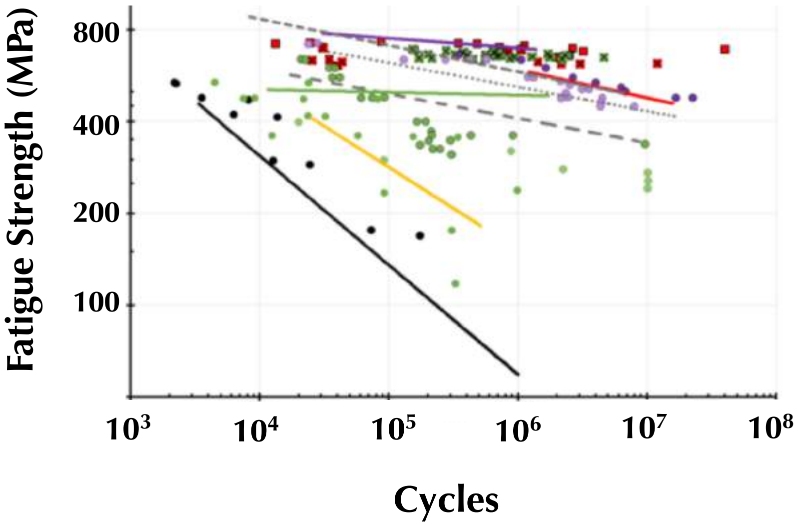
   原子结构，能量，平衡与涨落，非平衡过程
3. 多尺度力学中的基本概念

   熵，自由能，相互作用
4. 多尺度方法原理

   空间多尺度、时间多尺度
5. 多尺度方法在先进合金、复合材料中的应用

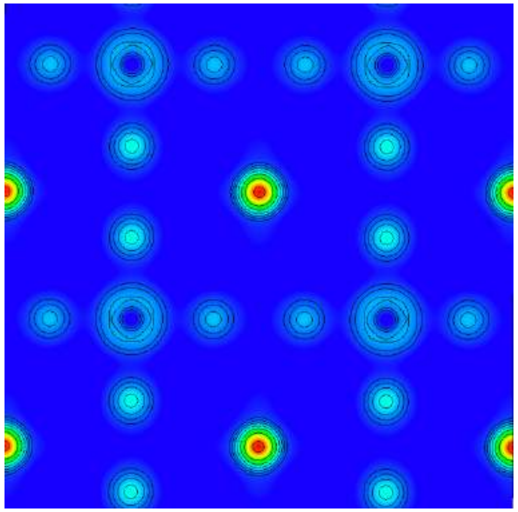
合金材料





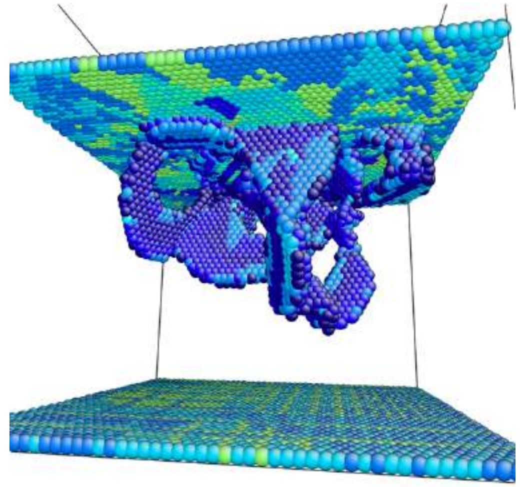
Qiu et al., Mater Sci Engr A, 2013; Li et al., Int J Fatigue 2016

合金材料



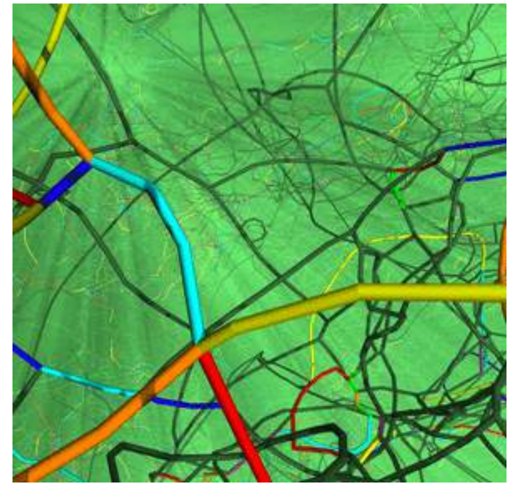
density functional theory

化学成分，原子作用



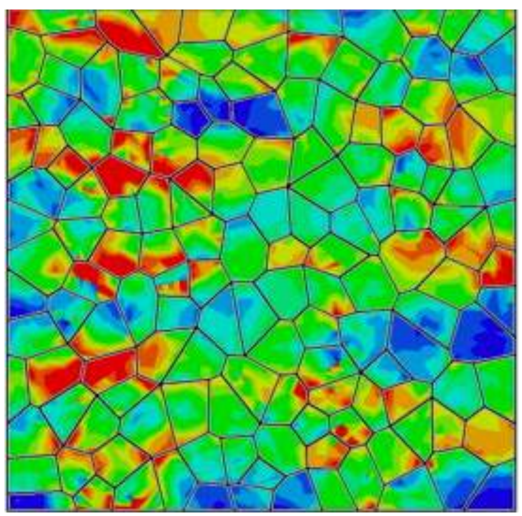
molecular dynamics

晶体结构，位错、缺陷



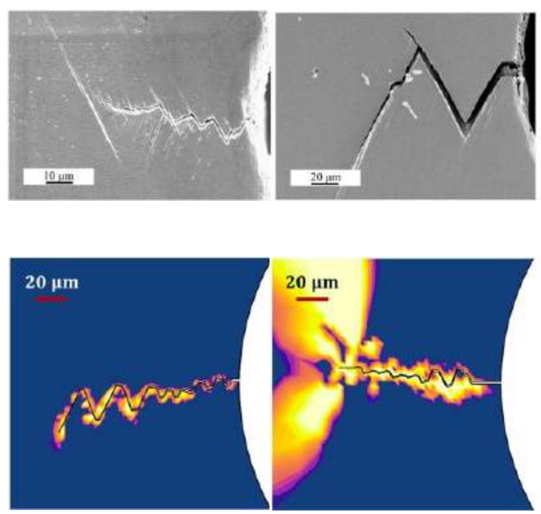
dislocation dynamics

位错动力学



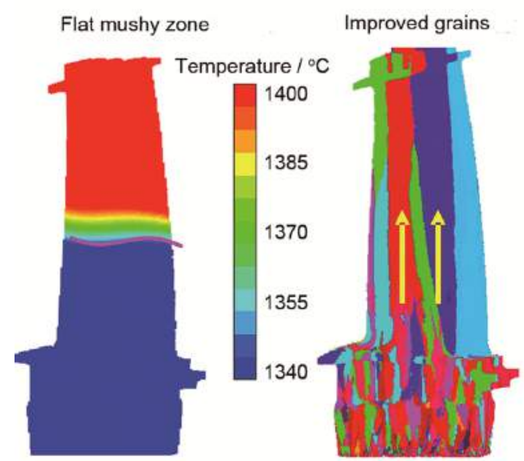
crystal plasticity

晶体塑性



finite element analysis

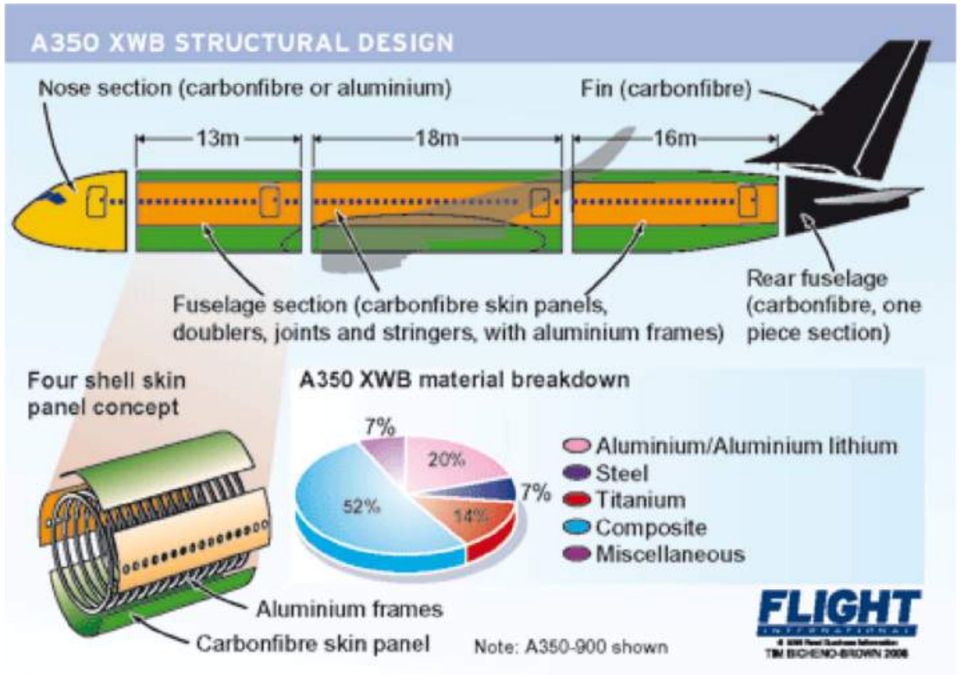
结构、界面尺度应力分析

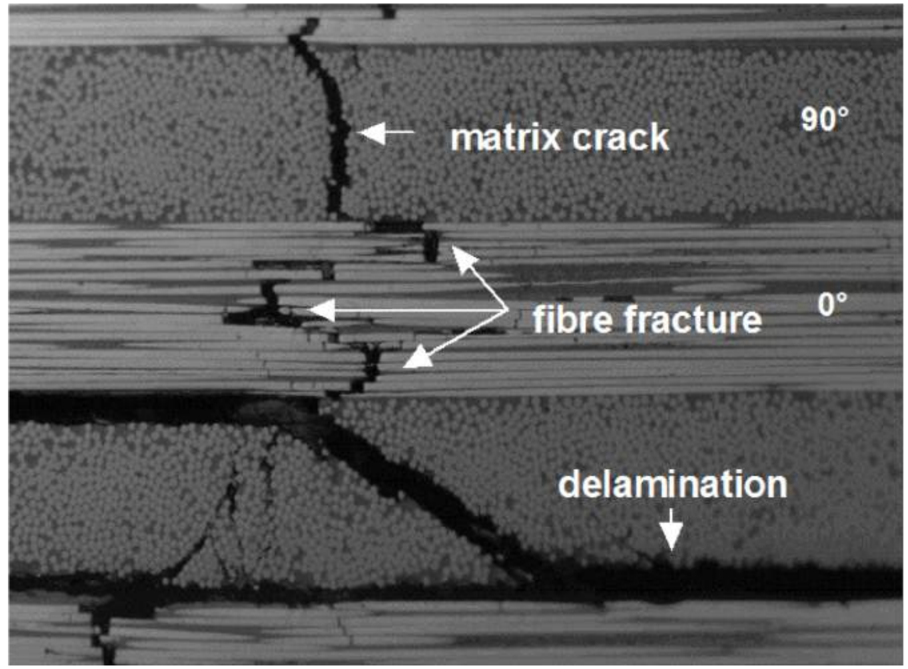


industrial design

工业设计

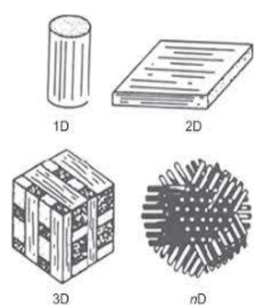
复合材料



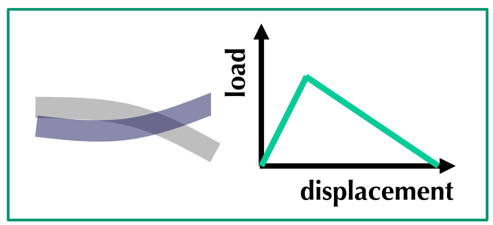


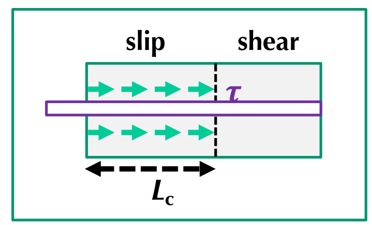
M. Alvarez E. FFA TN 1998-24, Tech Rep 1998

fabrics



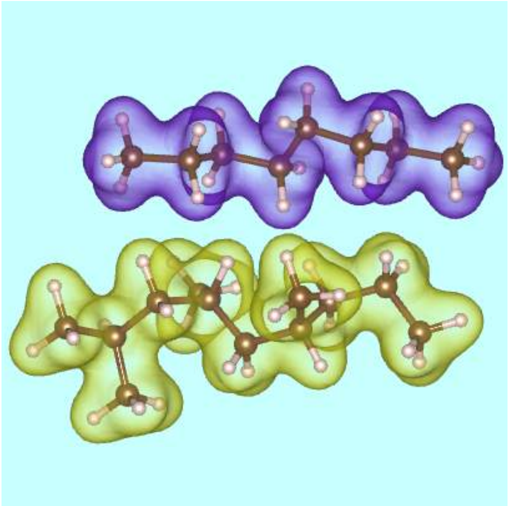
composite



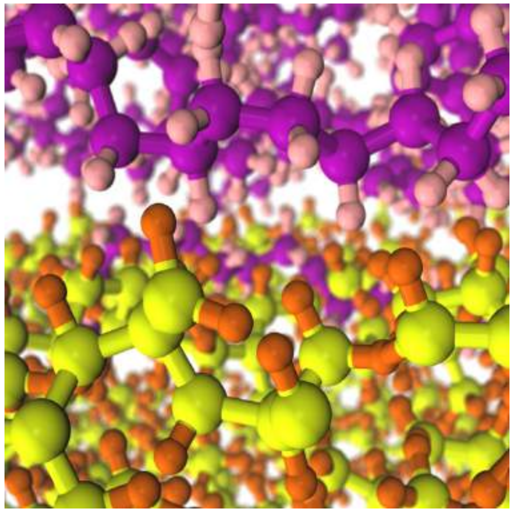


contact　　cohesive zone model　　shear-lag model

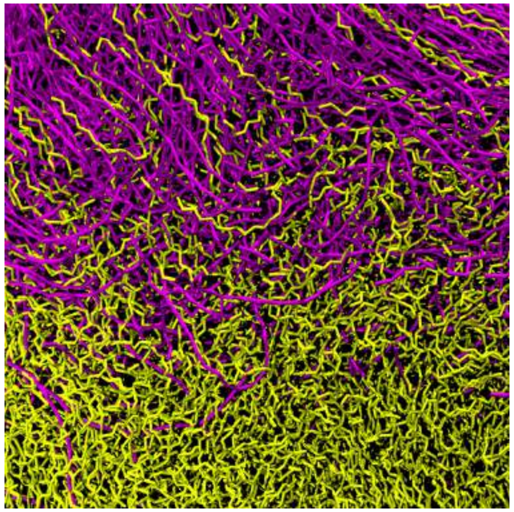
复合材料



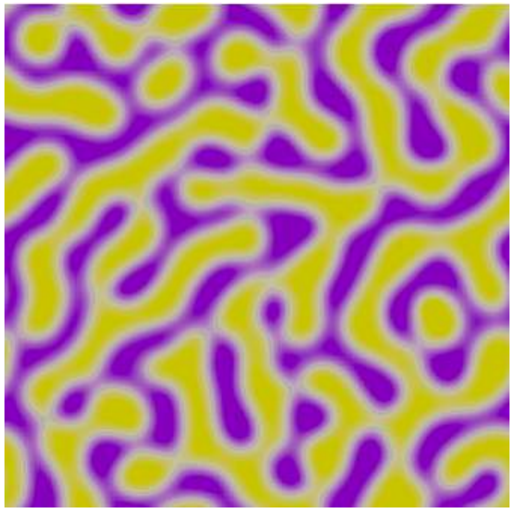
density functional theory
原子作用，光电性质



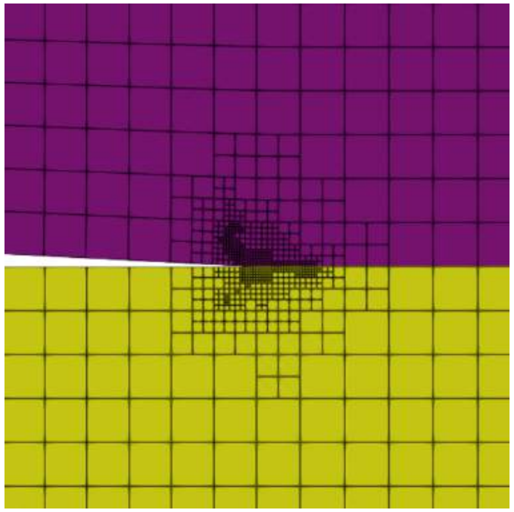
full-atom molecular dynamics
纳米尺度结构、力学、传热



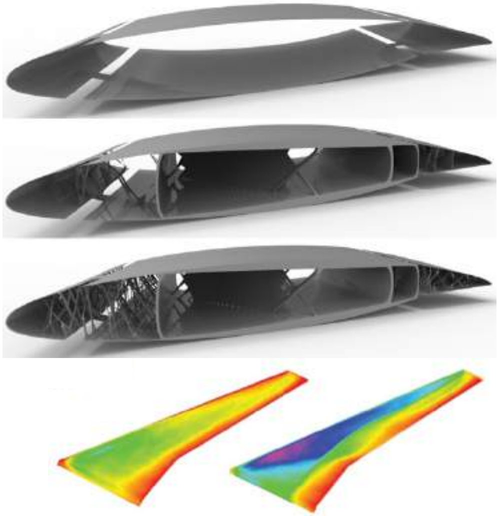
coarse-grained molecular models
微纳米尺度结构、力学



phase-field modeling
介观尺度结构、相变、残余应力

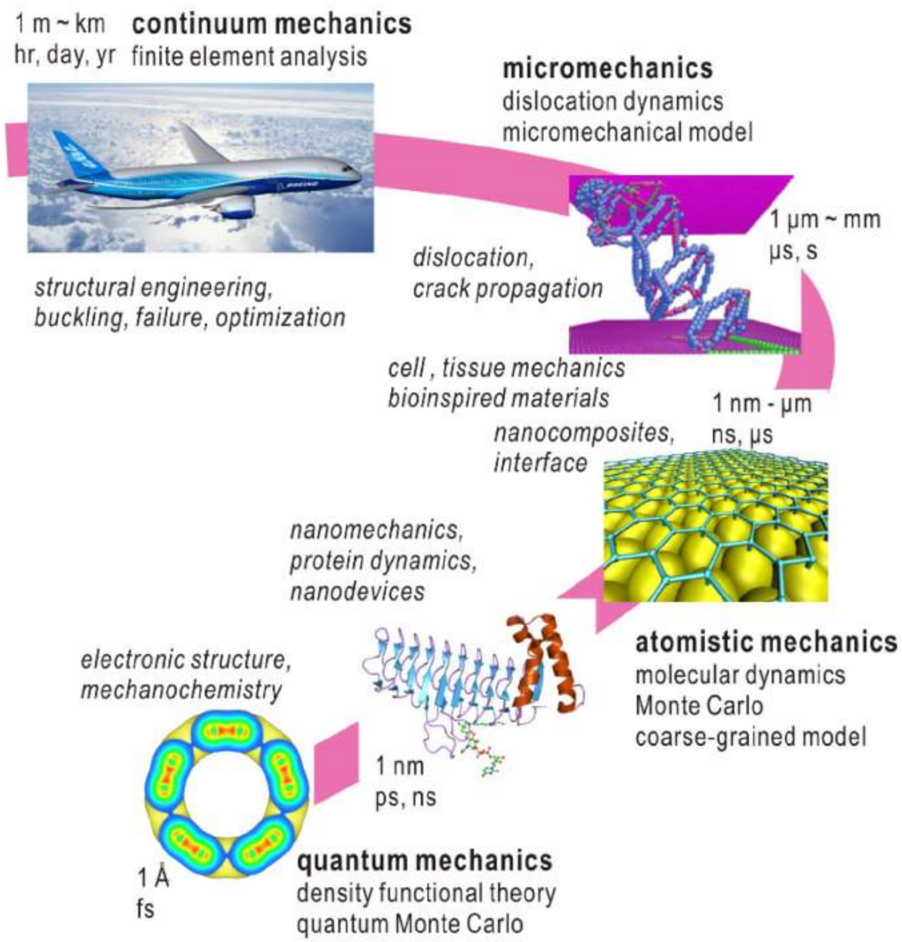


finite element analysis
结构、界面尺度应力分析

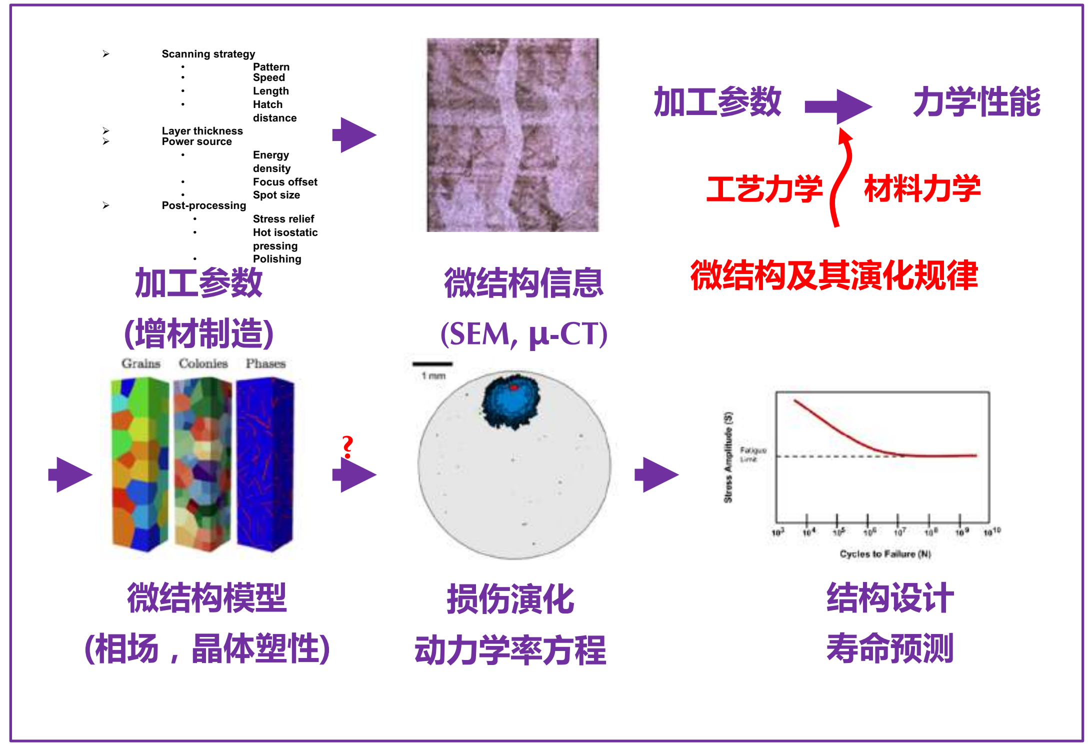


industrial design
工业设计

时空尺度与工程问题的复杂度



A multiscale and multiphysical simulation paradigm expanding across both the spatial and temporal scales



微结构复杂度及其演化规律

模型约化

统计模型、特征参数及其演化规律

多尺度力学方法介绍

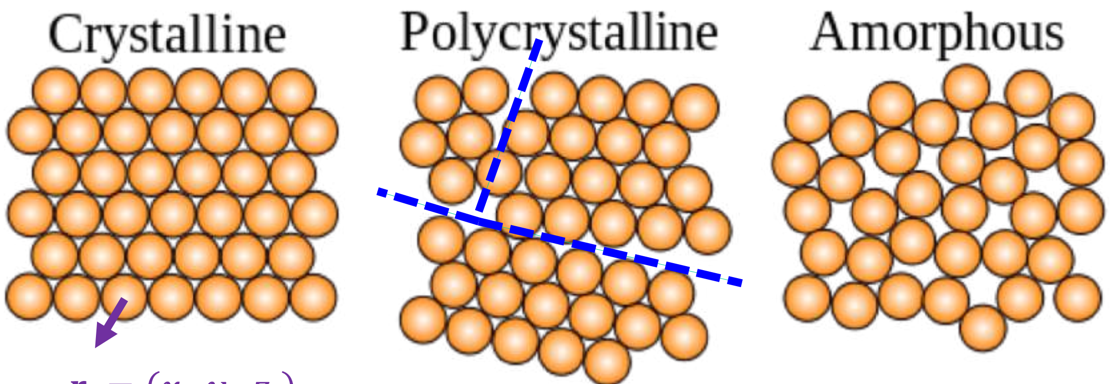
1. 先进合金、复合材料中的多尺度问题
2. **物质科学中的基本概念**

   原子结构，能量，平衡与涨落，非平衡过程
3. 多尺度力学中的基本概念

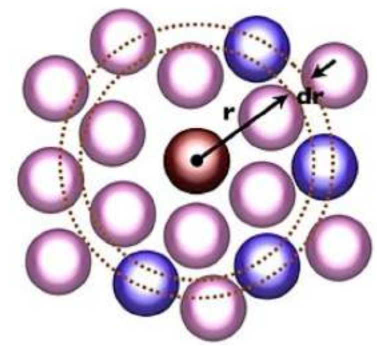
   熵，自由能，相互作用
4. 多尺度方法原理

   空间多尺度、时间多尺度
5. 多尺度方法在先进合金、复合材料中的应用

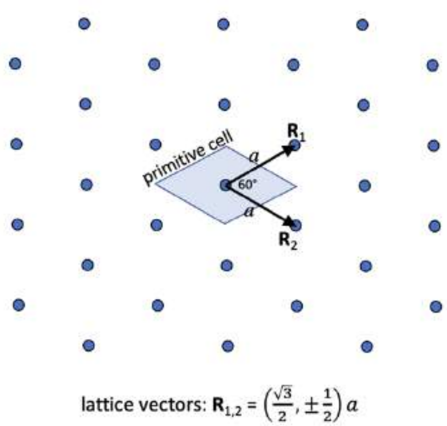
原子结构及其表征 – 粒子



$\mathbf{r}_i = (x_i, y_i, z_i)$

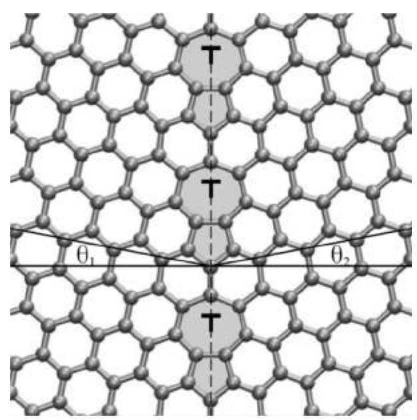


$$g(r) = \frac{1}{\langle n \rangle}\left\langle \sum_i \delta(r - r_i) \right\rangle$$

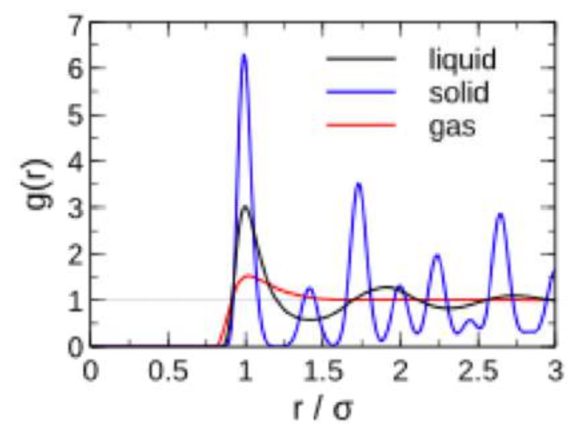


crystalline **lattice**

discrete translational/rotational symmetries



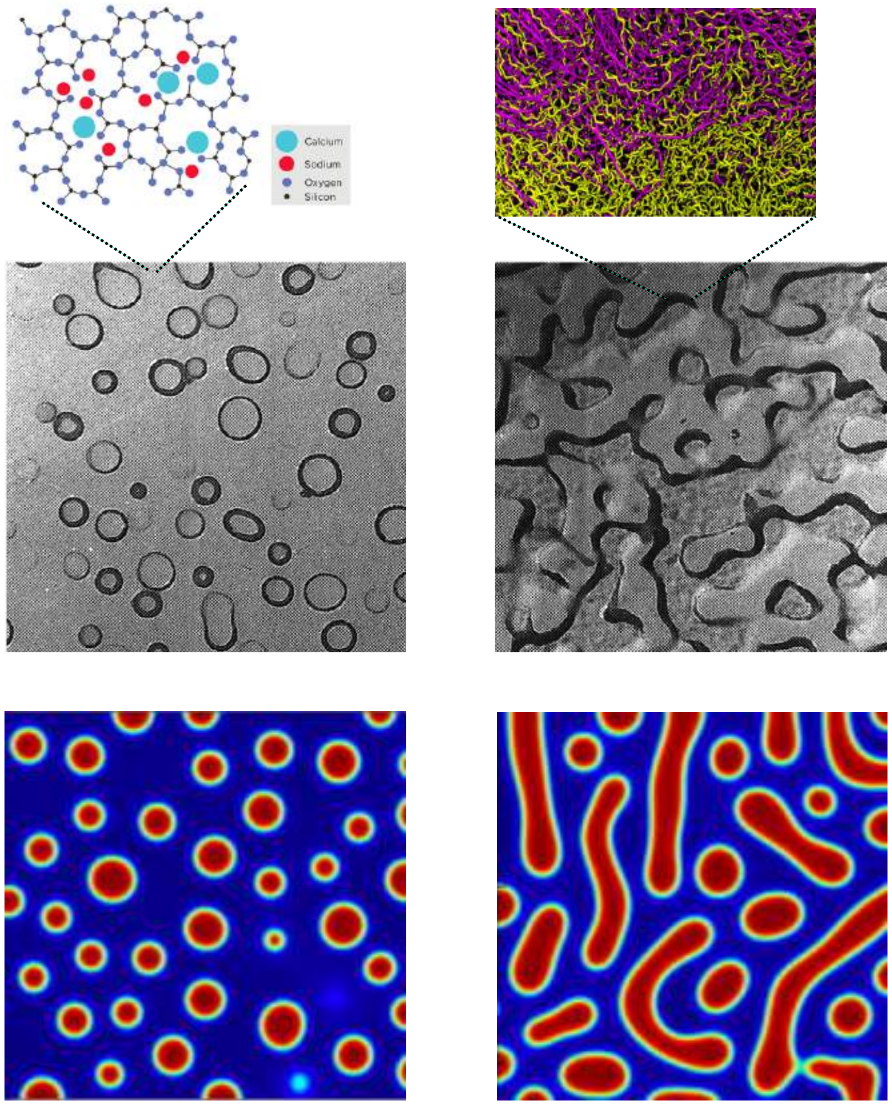
lattice **defects (dislocations)**



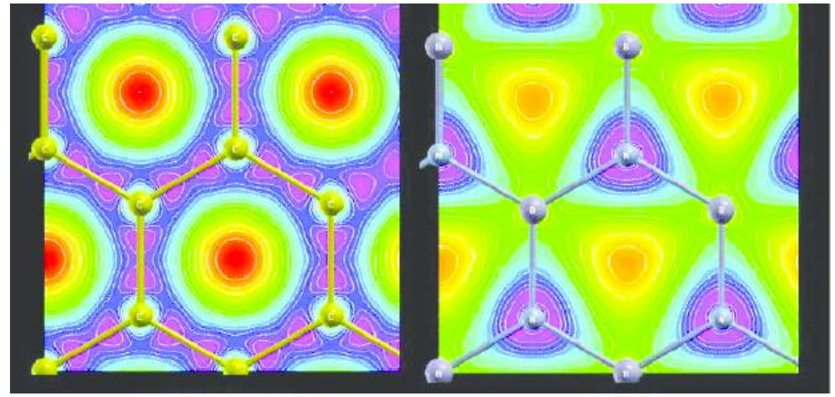
radial distribution function

continuous rotational symmetry

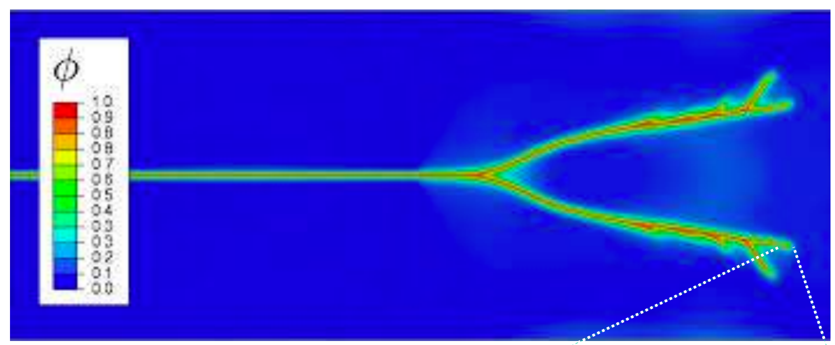
原子结构及其表征 – 连续



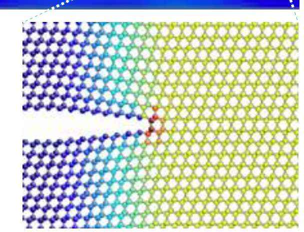
$\rho(\mathbf{r})$: **density** in continuum theories



$n(\mathbf{r}) = \psi^*(\mathbf{r})\psi(\mathbf{r})$: **electron** density



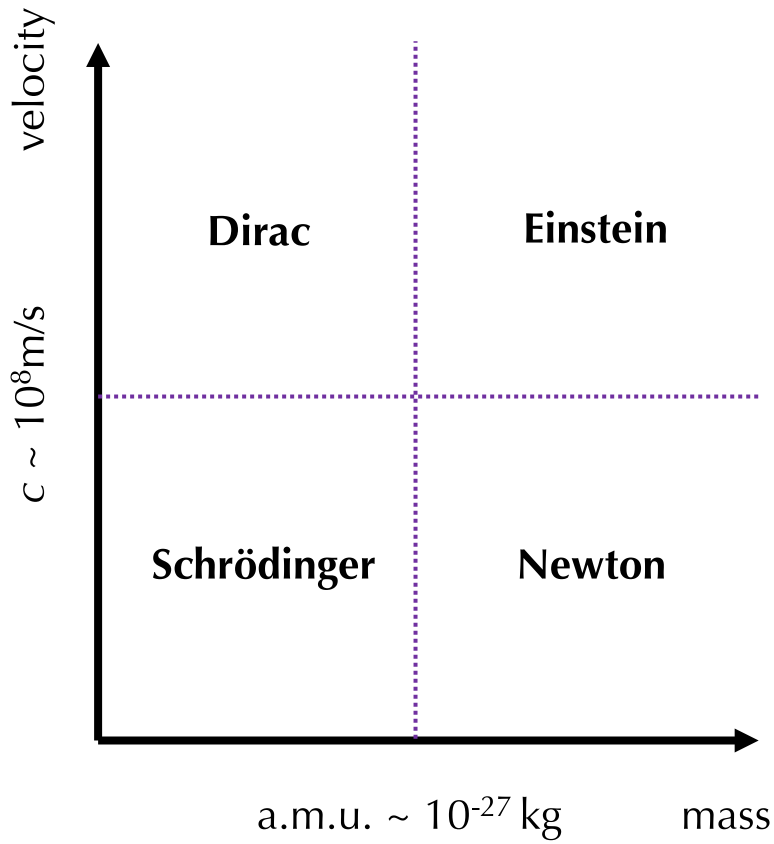
$\phi(\mathbf{r})$: **order** parameter



fields of displacement, strain, stress, crystal orientation, dislocation density, temperature, …

Rawson, Properties & Applications of Glass 1980

能量与运动方程



Schrödinger equation for quantum particles (e.g. electrons)

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = \mathbf{H}\psi(\mathbf{r}, t)$$

H: Hamiltonian

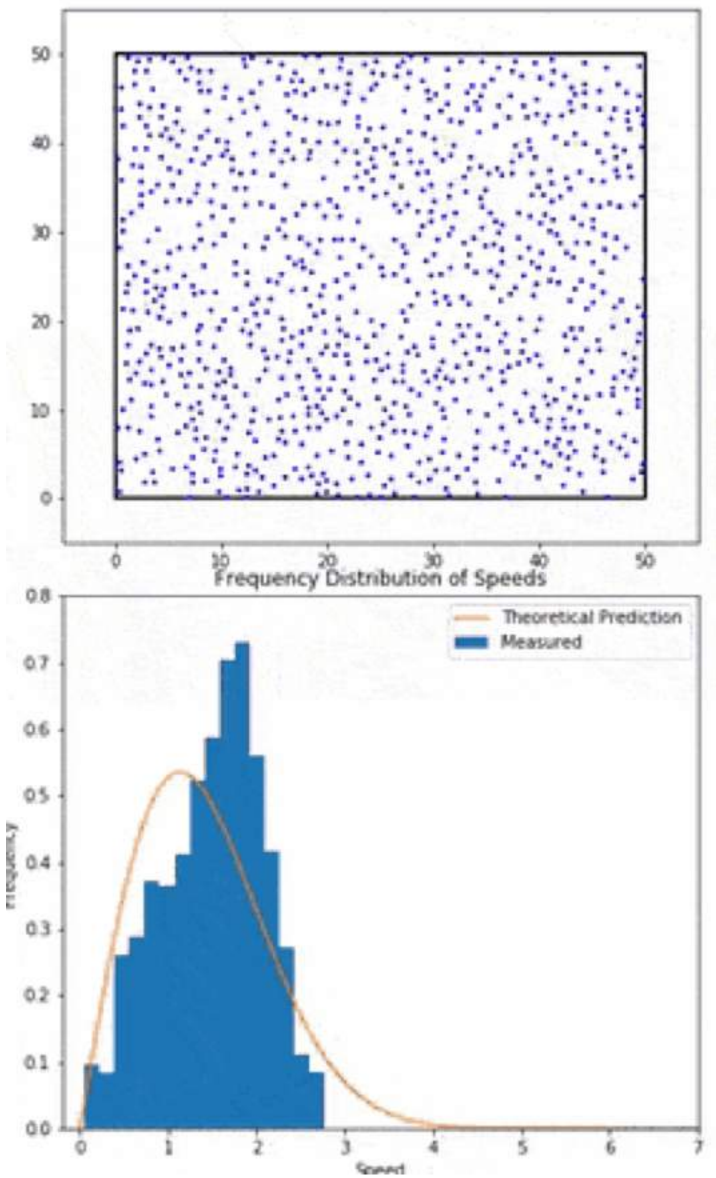
Newtonian equation for quantum particles (e.g. nuclei)

$$m_i \frac{\partial^2 \mathbf{r}_i}{\partial t^2} = \mathbf{f}_i(t) = -\frac{\partial E(\mathbf{r}, t)}{\partial \mathbf{r}_i}$$

***E*: total (potential) energy**

$$1k_\mathrm{B}T \approx 0.025 \text{ eV}, \qquad \frac{1}{2}Y\epsilon^2 a^3 \ll 1 \text{ eV}$$

平衡与涨落 – 热力学



Maxwell-Boltzmann velocity distribution

$$f(v) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-\frac{mv^2}{2k_B T}}$$

kinetic definition of **temperature**

$$E_k = \frac{1}{2} m v_{rms}^2 = \frac{3}{2} k_B T$$

model reduction

$$\{\mathbf{r}_i, \mathbf{v}_i\} \to E, T, S, p, V, \mu, N, \cdots$$

phase space of particles → thermodynamic variables

the **1st law** of thermodynamics

$$\mathrm{d}E = \mathrm{d}Q + \mathrm{d}W$$

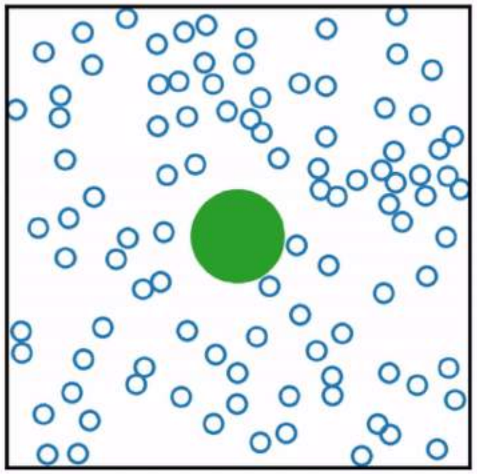
the **2nd law** of thermodynamics

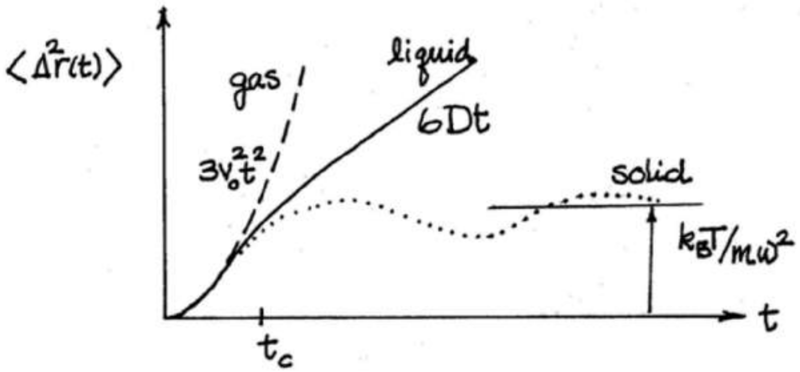
$$\Delta S_{sys} \geq 0$$

fluctuation!

$\mathrm{d}S = \frac{\mathrm{d}Q}{T}$ **: change in Clausius entropy**

非平衡过程 – 输运





Brownian motion

$$\left\langle r^2(t)\right\rangle = \left\langle \left|\mathbf{r}(t)-\mathbf{r}(0)\right|^2\right\rangle = 6Dt$$

Einstein 1905; Smoluchowski 1906

Stokes-Einstein equation

$$D = \frac{k_B T}{6\pi\eta r}$$

fluctuation-dissipation relations for

diffusion

$$D = \frac{1}{6t}\left\langle r^2(t)\right\rangle = \frac{1}{6t}\left\langle \left|\mathbf{r}(t)-\mathbf{r}(0)\right|^2\right\rangle$$

$$D = \frac{1}{3}\int_0^t \left\langle \mathbf{v}(0)\cdot\mathbf{v}(\tau)\right\rangle \mathrm{d}\tau$$

shear viscous flow

$$\mu = \frac{1}{2Vk_B Tt}\left\langle \sum_{i=1,N}\sum_{j=1,N} p_{xi}(t)\,p_{xj}(0)\left[z_i(t)-z_j(0)\right]^2\right\rangle$$

$$= \frac{1}{2Vk_B Tt}\left\langle \sum_{i=1,N}\left[z_i(t)\,p_{xi}(t)-z_i(0)\,p_{xi}(t)\right]^2\right\rangle$$

$$\mu = \frac{1}{Vk_B T}\int_0^\infty \mathrm{d}t\left\langle J(0)\,J(t)\right\rangle$$

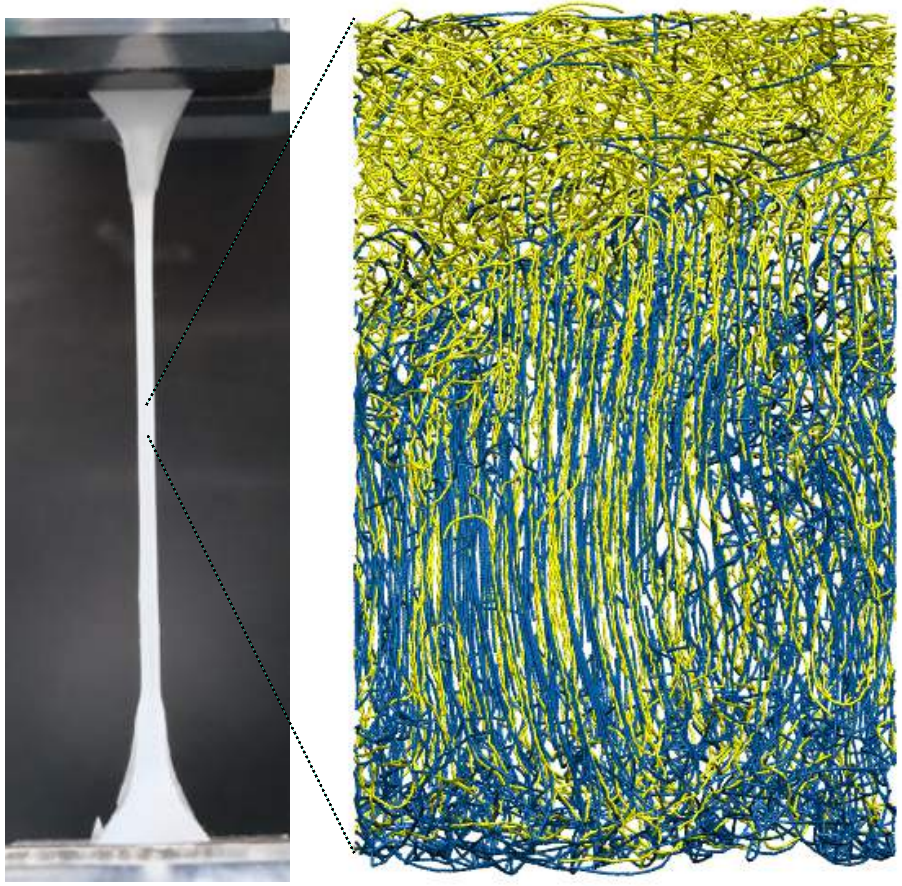
$$J = \sum_{i=1,N}\left(\frac{p_{xi}p_{yi}}{m}+z_iF_{ix}\right) = m\sum_{i=1,N}\dot{x}_i\dot{z}_j + \frac{1}{2}\sum_{j\neq i} z_{ij}F_{ij}^x$$

thermal transfer

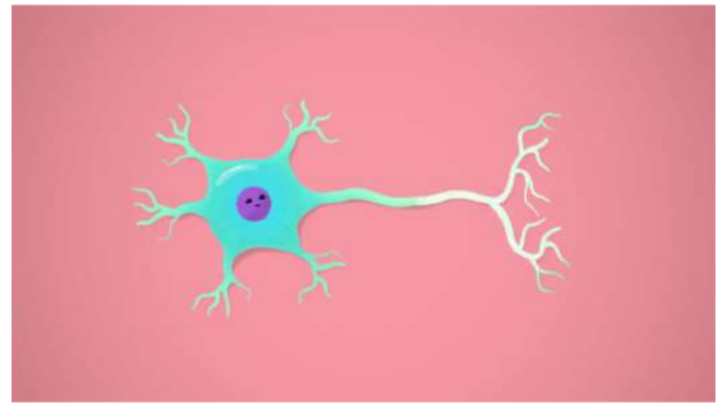
$$\kappa = \frac{1}{2Vk_B T^2 t}\left\langle \sum_{i=1,N}\left[r_i(t)\,\tilde{E}_i(t)-r_i(0)\,\tilde{E}_i(0)\right]^2\right\rangle$$

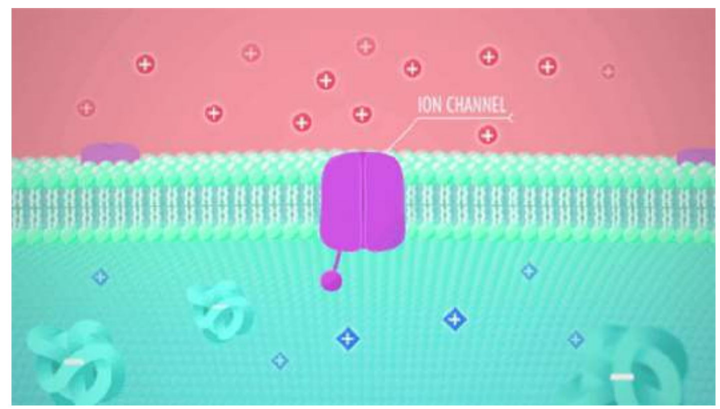
$$\kappa = \frac{1}{Vk_B T^2}\int_0^\infty \left\langle \mathbf{S}(t)\cdot\mathbf{S}(0)\right\rangle \mathrm{d}\tau,\ \ \mathbf{S}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\sum_{i=1,N}\mathbf{r}_i\tilde{E}_i$$

非平衡过程 – 动力学



Far from equilibrium





https://blog.eyewire.org/the-nervous-system-action-potential-crash-course-2/

Active systems

多尺度力学方法介绍

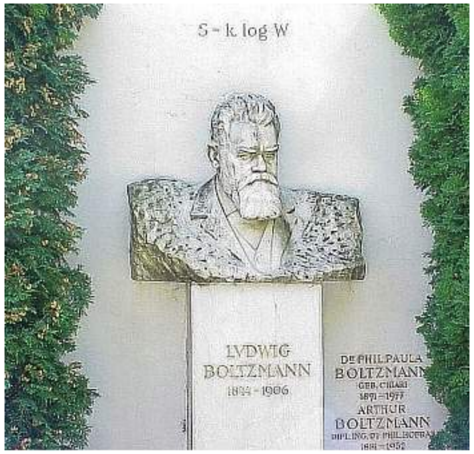
1. 先进合金、复合材料中的多尺度问题
2. 物质科学中的基本概念

   原子结构，能量，平衡与涨落，非平衡过程
3. **多尺度力学中的基本概念**

   熵，自由能，相互作用
4. 多尺度方法原理

   空间多尺度、时间多尺度
5. 多尺度方法在先进合金、复合材料中的应用

熵



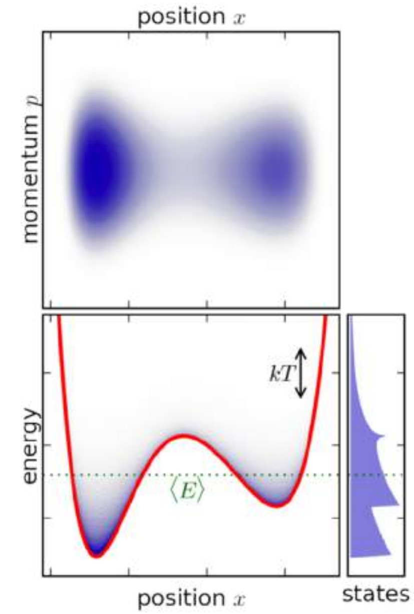
Boltzmann's statistical definition entropy

$$S = k_{\mathrm{B}} \ln W$$

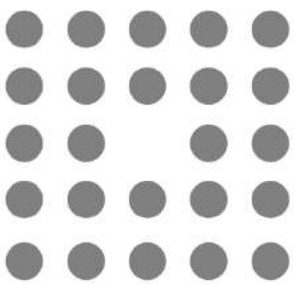
vibrational entropy

$$S = k_{\mathrm{B}} \ln \frac{A}{A_0}$$

the area explored in the phase space of (r, p)



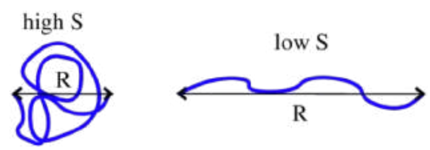
configurational entropy



point defects in a *N*-site lattice

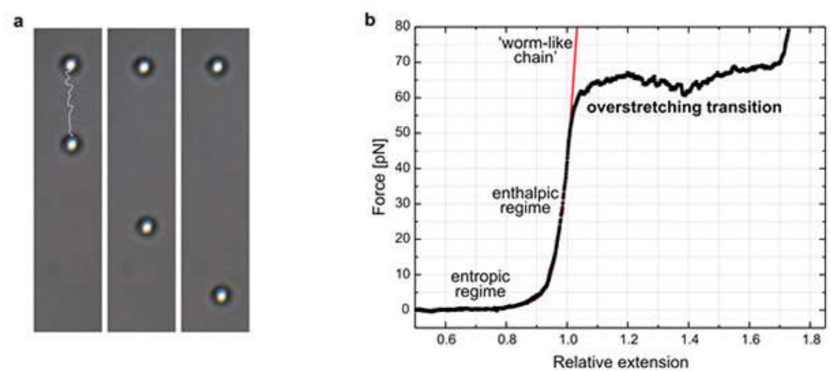
$$S = k_{\mathrm{B}} \ln N$$

F* = *E* – *TS
raising T promotes formation of the defects



entropic forces

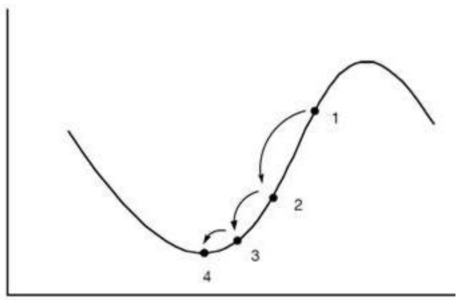
$$f = dF/dR = -T dS/dR$$



Bustamante et al., Science 1994

能量

Time's arrow



E_{pot} — potential energy

$F = E - TS$ — Helmholtz free energy

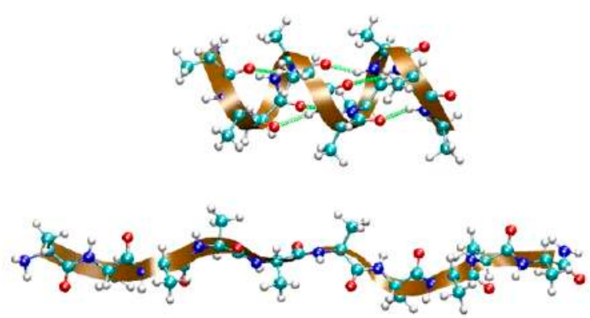
$E = E_{\text{pot}} + E_{\text{pot}}$ — constant N, V, T; w/ heat exchange

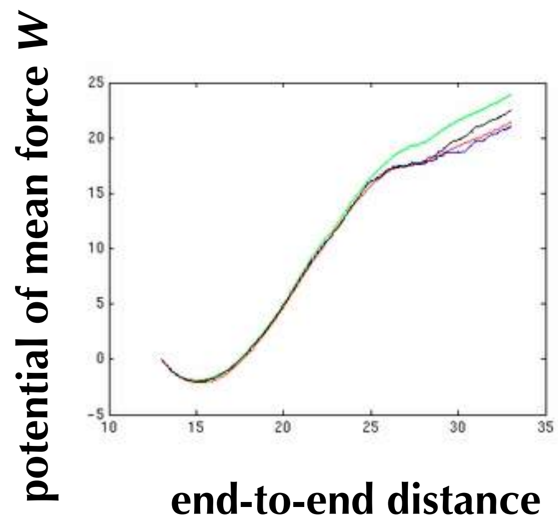
$G = E - TS + pV$ — Gibbs free energy

constant N, V, T; w/ heat exchange

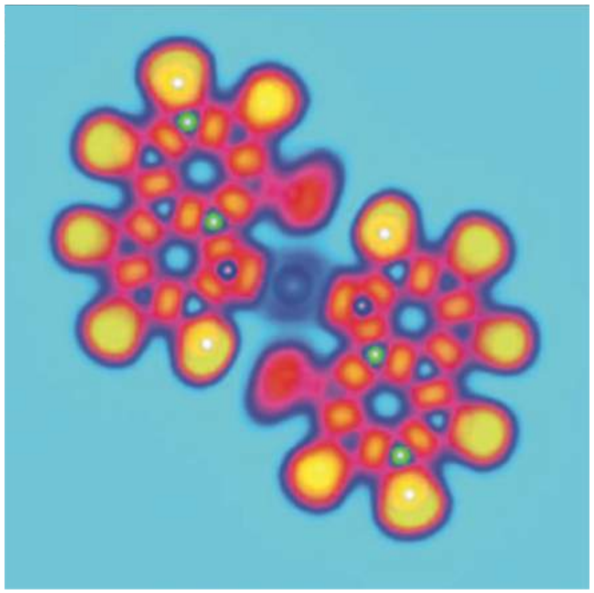
Jarzynsky equality (1996)

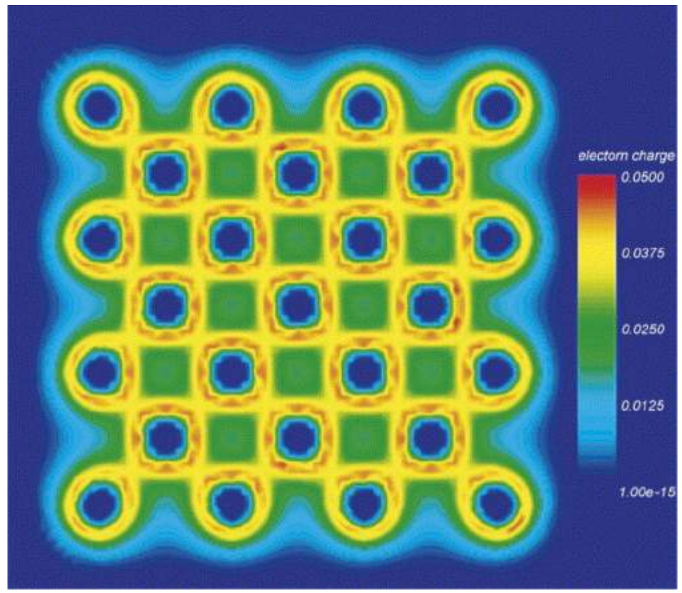
$$e^{-\Delta F/k_{\mathrm{B}}T} = \left\langle e^{-W/k_{\mathrm{B}}T} \right\rangle$$

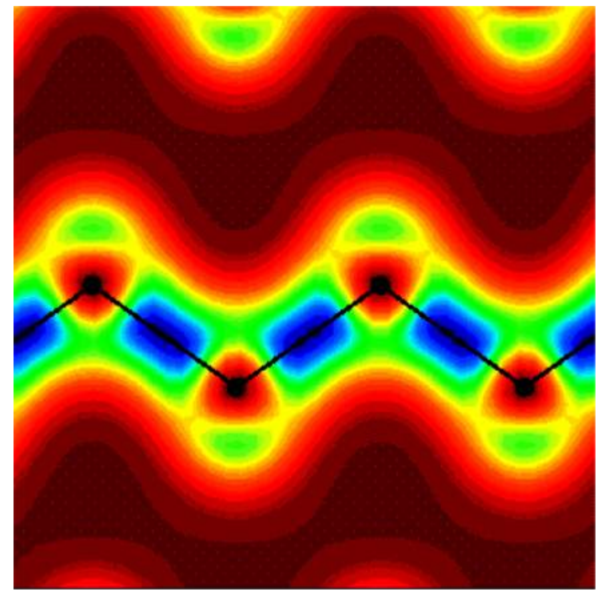




相互作用 – 物理图像







hydrogen bonding

electrostatic + Van der Waals

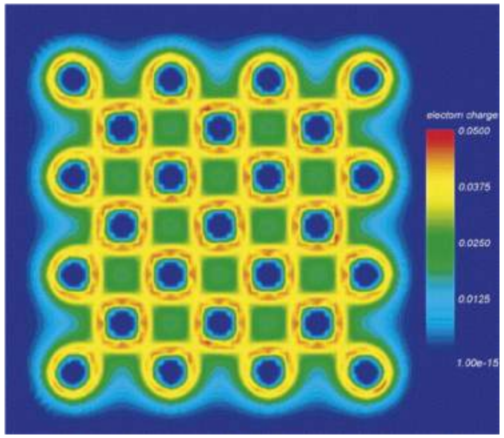
metallic bonds

screened ion-ion, ion-electron

covalent bonds

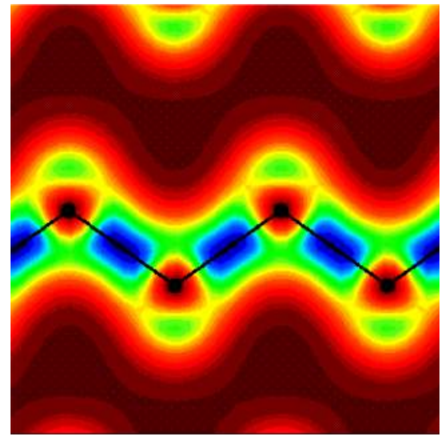
electron-pair sharing

相互作用 – 经验描述



$$V = \sum_i E_i$$

total potential energy decomposed into terms associated with atoms

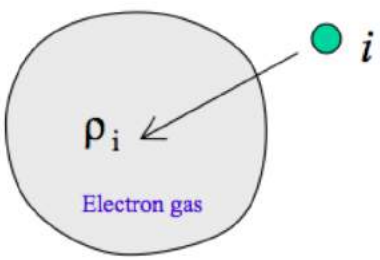


$$V = \frac{1}{2}\sum_{ij}\phi(r_{ij})$$ two-body

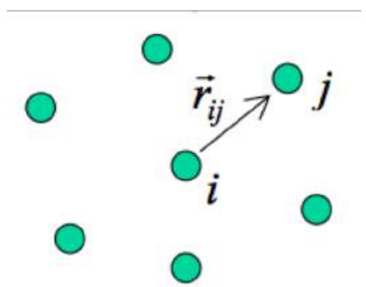
$$+\frac{1}{3}\sum_{ijk} g(r_{ij})g(r_{ij})\left(\cos\theta_{ijk} + \frac{1}{3}\right)^2$$

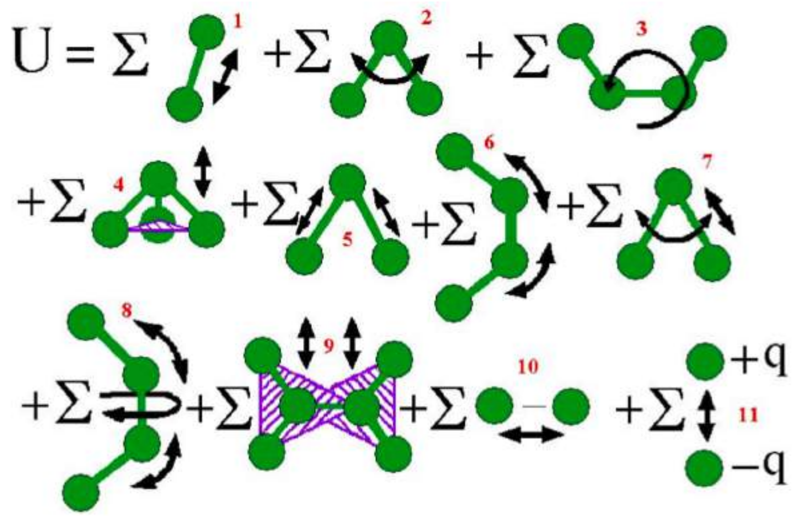
three-body

embedding



two-body

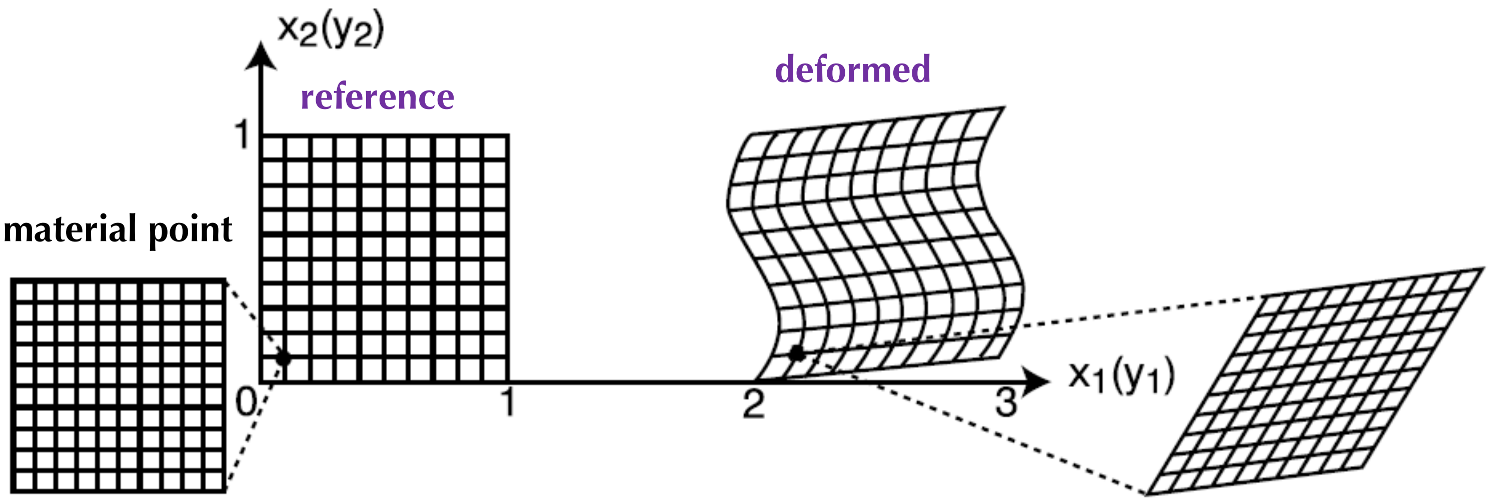




$$E_i = E_i(\bar{\rho}_i) + \frac{1}{2}\sum_{ij} V(r_{ij})$$

$$\bar{\rho}_i = \sum_{ij} \rho_i(r_{ij})$$

相互作用 – 连续模型



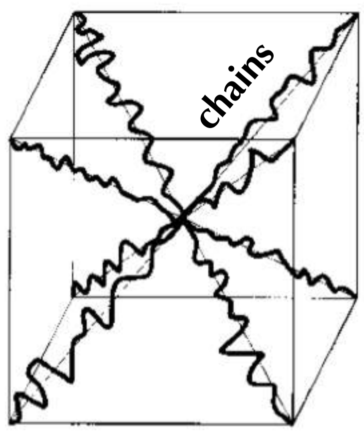
strain energy density

$$W(\{\mathbf{e}_i\}) = \frac{E_{tot}(\{\mathbf{e}_i\}) - E_{tot}(\{\mathbf{E}_i\})}{\Omega}$$

deformation gradient

$$\mathbf{e}_i = \mathbf{F}\mathbf{E}_i$$

entropic elasticity



$$W = Nk_B T\sqrt{n}\left[\beta\lambda_{\text{chain}} - \sqrt{n}\ln\left(\frac{\sinh\beta}{\beta}\right)\right]$$

$$\lambda_{\text{chain}} = \sqrt{\frac{I_1}{3}},\ \beta = L^{-1}\left(\frac{\lambda_{\text{chain}}}{\sqrt{n}}\right)$$

extension to non-locality, viscous damping, …

$$E = E(\rho, \nabla\rho, \cdots)$$

Kuhn and Grun, Kolloid-Z 1942; Arruda and Boyce, JMPS 1993

多尺度力学方法介绍

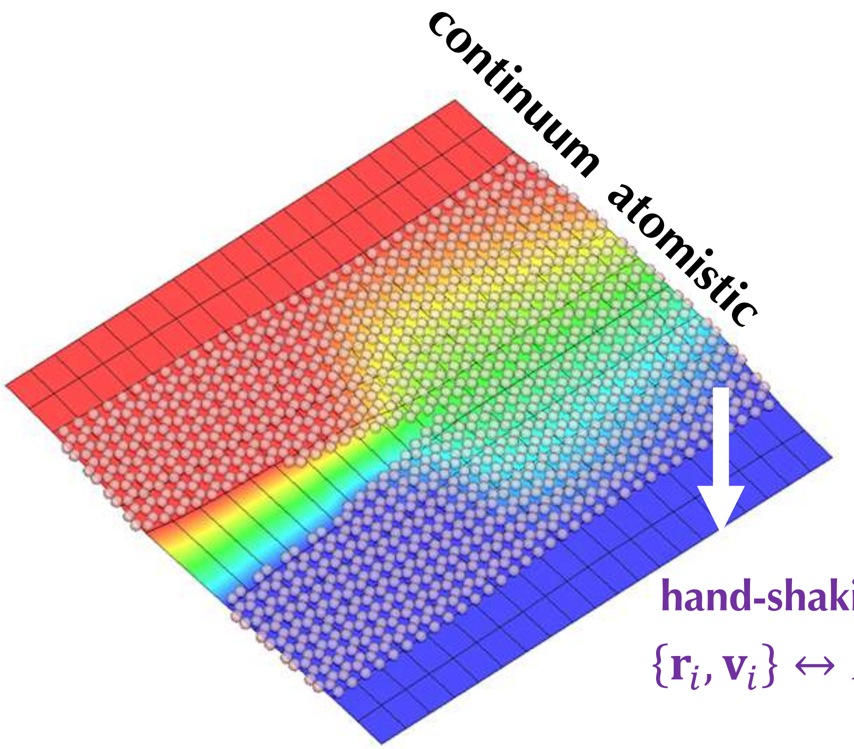
1. 先进合金、复合材料中的多尺度问题
2. 物质科学中的基本概念

   原子结构，能量，平衡与涨落，非平衡过程
3. 多尺度力学中的基本概念

   熵，自由能，相互作用
4. **多尺度方法原理**

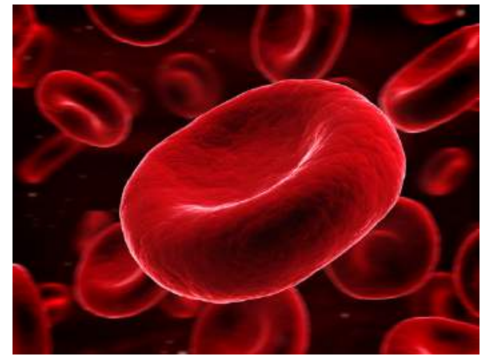
   空间多尺度、时间多尺度
5. 多尺度方法在先进合金、复合材料中的应用

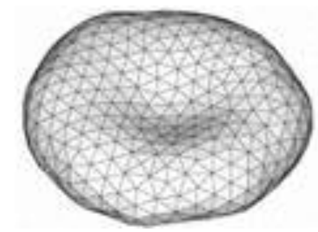
空间多尺度

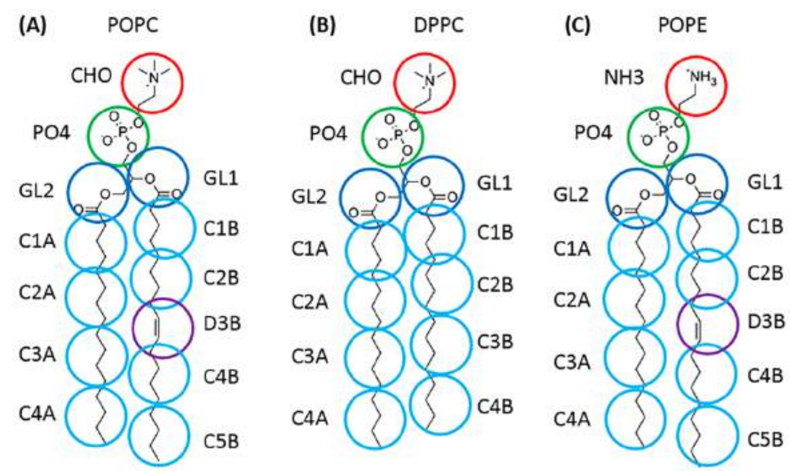


hand-shaking region

$$\{\mathbf{r}_i, \mathbf{v}_i\} \leftrightarrow E, T, S, \boldsymbol{\sigma}, \boldsymbol{\epsilon}, \mu, N, \cdots$$



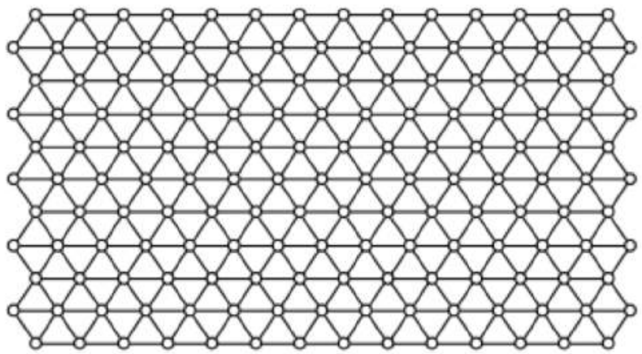




concurrent multiscale methods

shape/topology-based coarse-graining

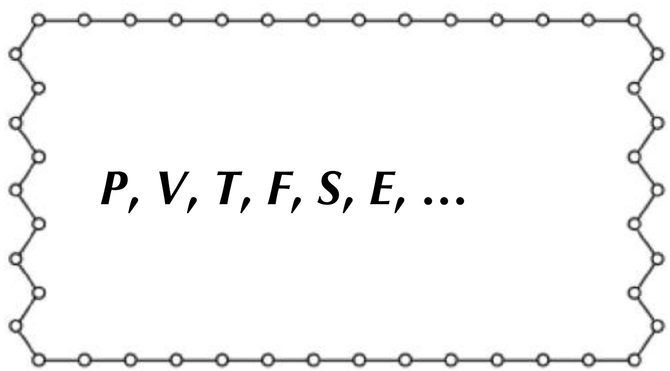
空间多尺度



microscopic dynamics

Hamiltonian description $\{\mathbf{p}_i, \mathbf{q}_i\}$ of particles, time.

model reduction

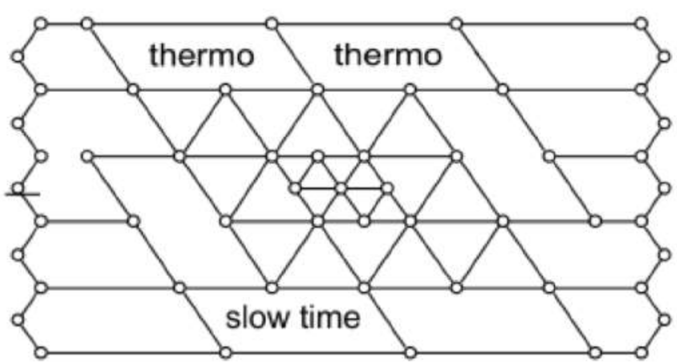


thermodynamics

thermodynamic averages

fluctuation?

entropy?



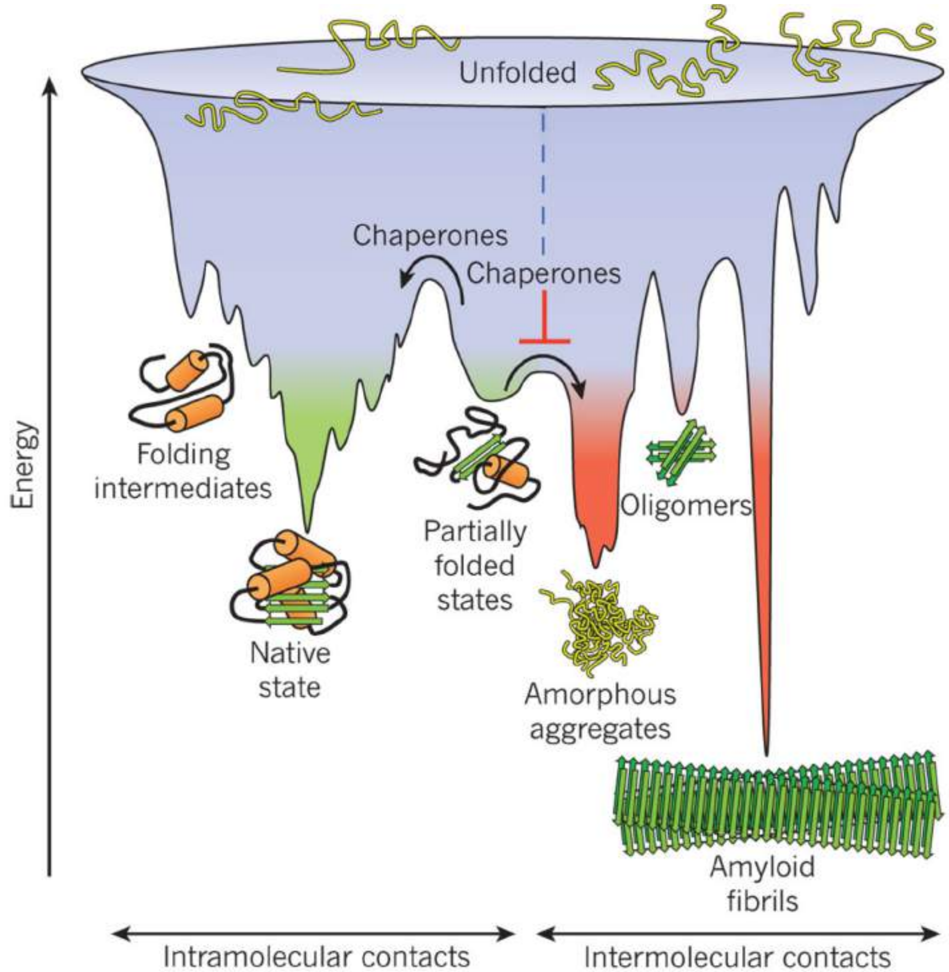
Curtarolo and Ceder PRL 2002

multiscale (coarse-grained) models

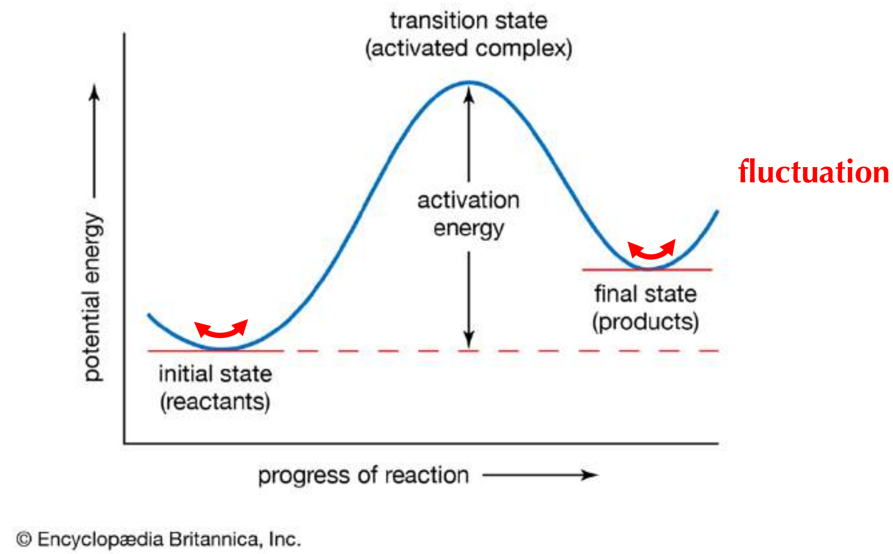
map discrete microscale dynamics to thermodynamics

there are interfaces !

时间多尺度



transition state theory



Arrhenius rate

$$k \sim \nu_0 \exp(-E_a/k_B T)$$

characteristic timescale

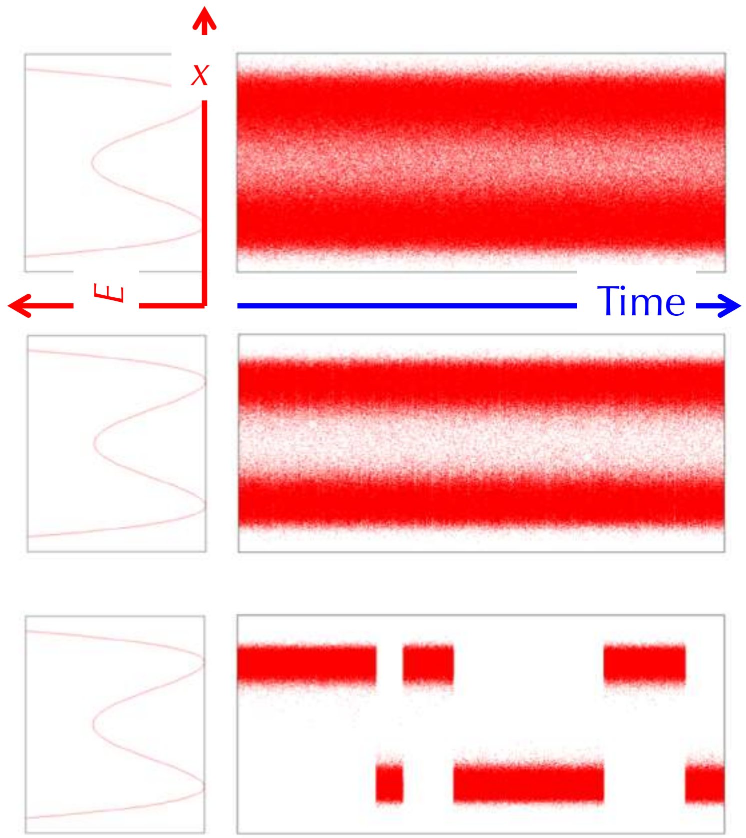
$$\tau \sim \frac{1}{\nu_0} \exp(E_a/k_B T)$$

$\nu_0 \sim 10^{-13}$ s

$E_a \sim 0.75$ eV, $T \sim 300$ K

$\tau \sim 1$ s (10^{15} MD steps!)

时间多尺度

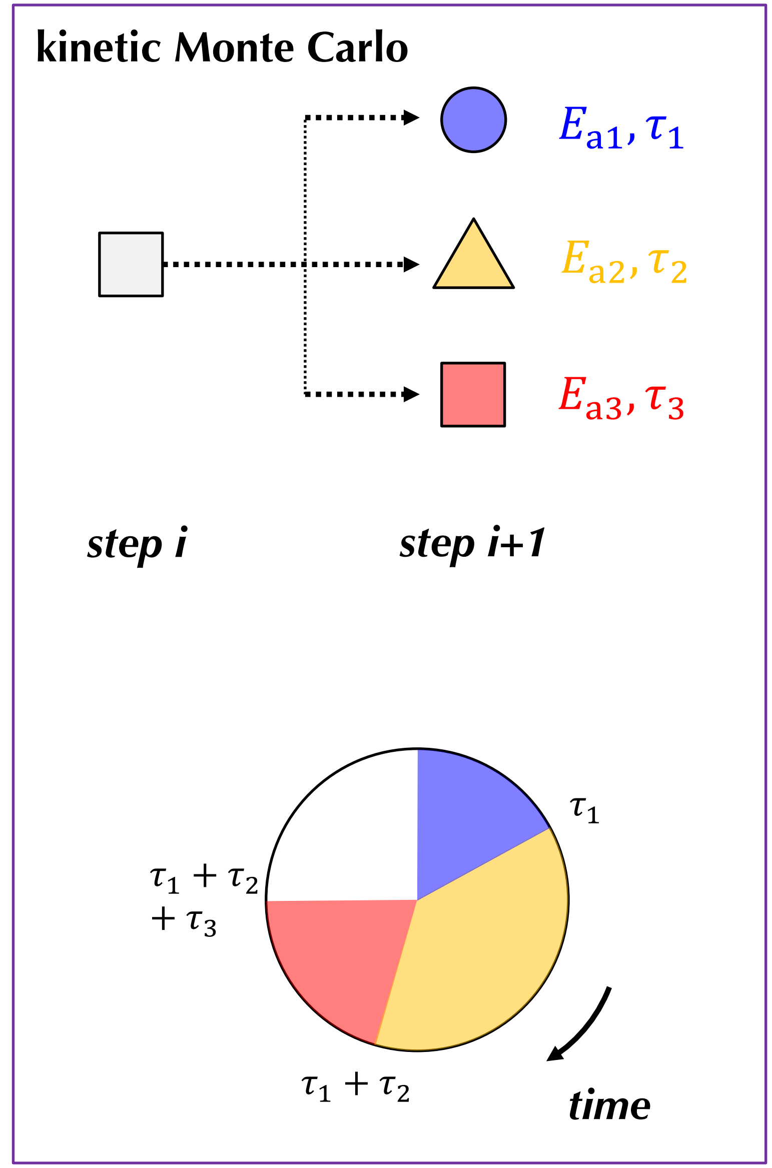


$k_B T = 0.5 E_a$
diffusive behavior

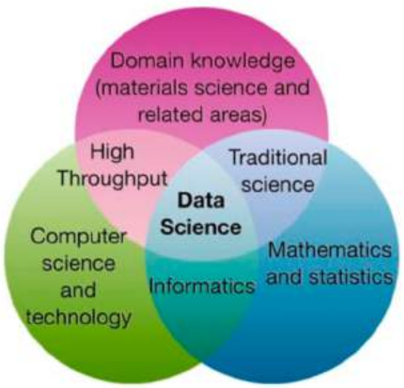
$k_B T = 0.2 E_a$
diffusive behavior

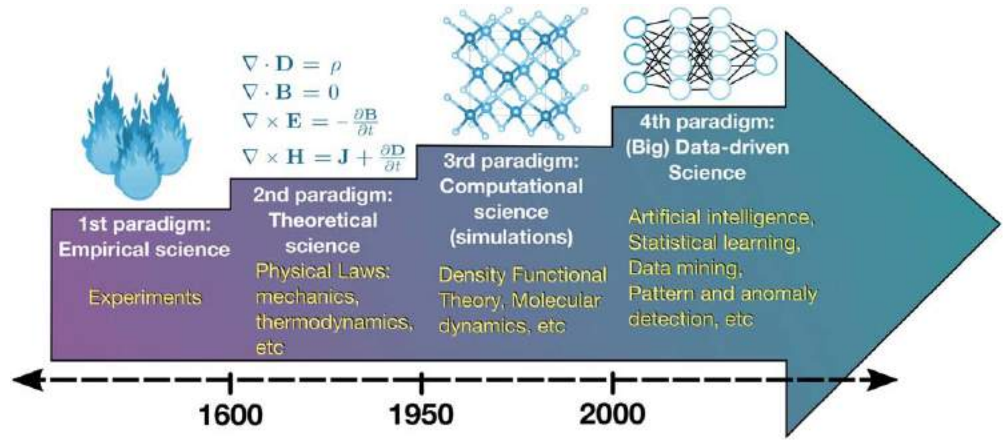
$k_B T = 0.08 E_a$
'instantonic' behavior
$t_{transition} >> t_{corr}$

$$\tau \sim \frac{1}{\nu_0} \exp(E_a / k_B T)$$

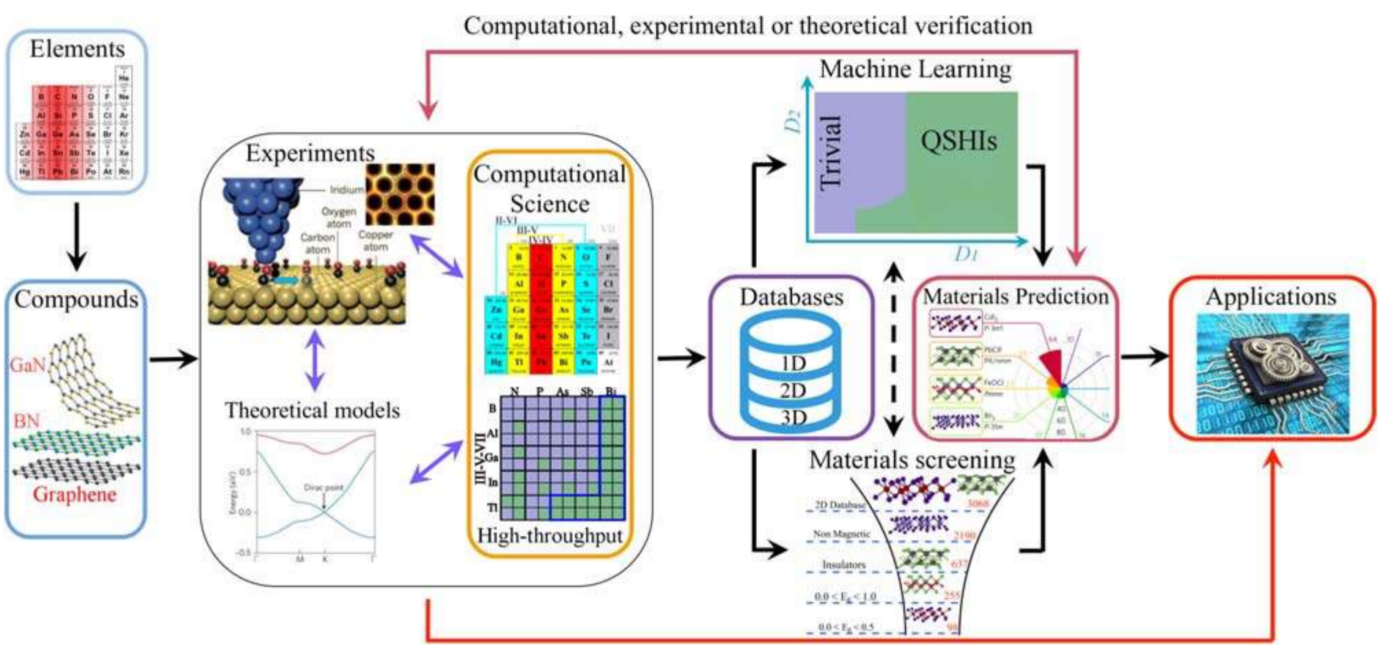


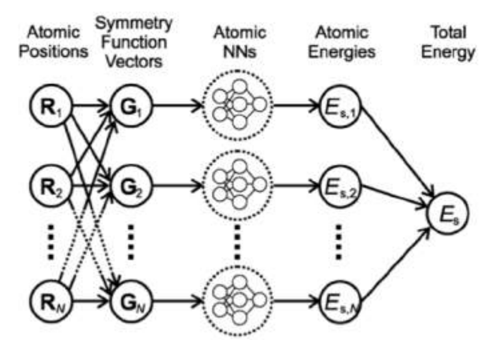
数据与机器学习





复杂度 ➡ 数据





Schleder et al. J Phys Mater 2019

多尺度力学方法介绍

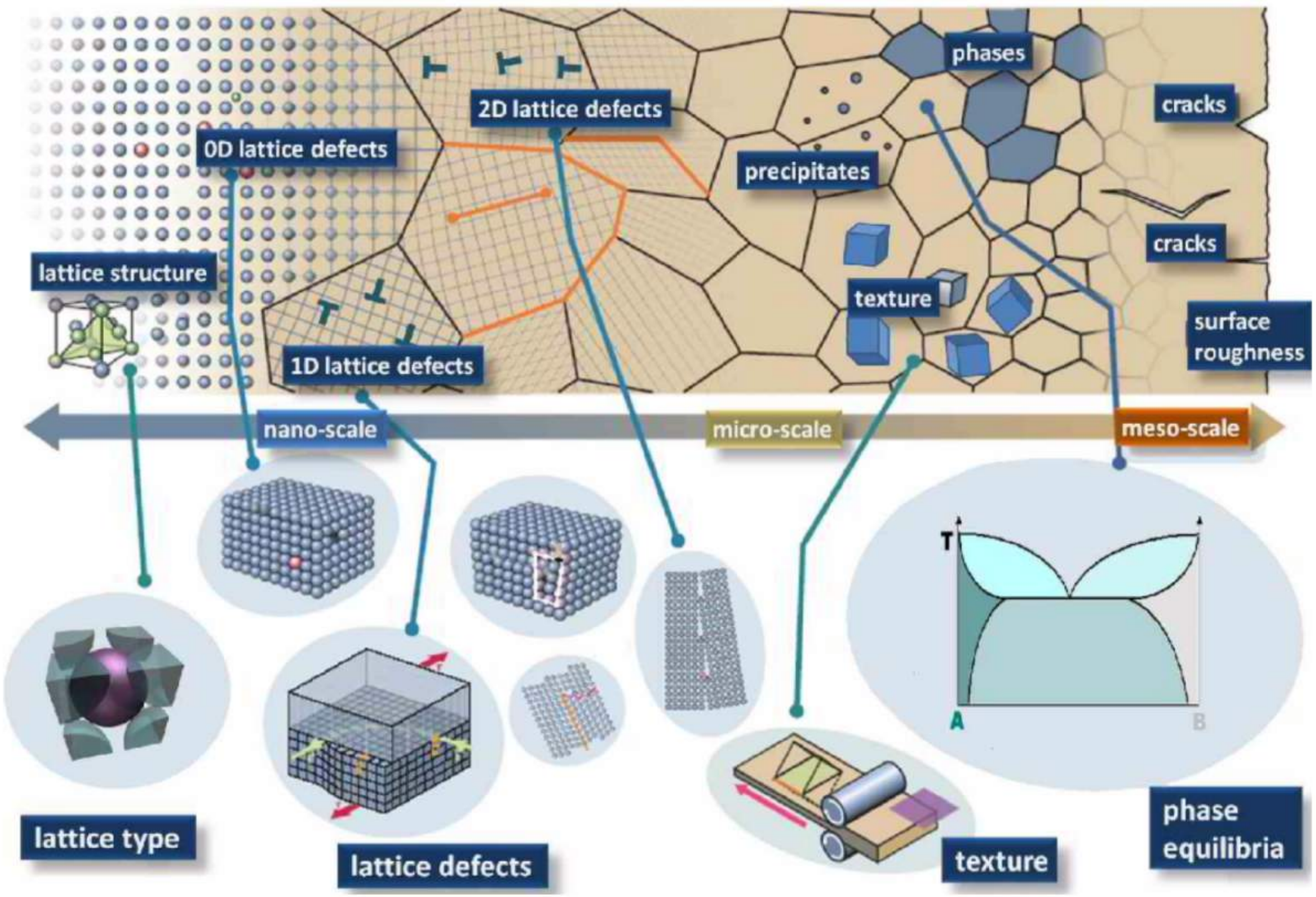
1. 先进合金、复合材料中的多尺度问题
2. 物质科学中的基本概念

   原子结构，能量，平衡与涨落，非平衡过程
3. 多尺度力学中的基本概念

   熵，自由能，相互作用
4. 多尺度方法原理

   空间多尺度、时间多尺度
5. 多尺度方法在先进合金、复合材料中的应用

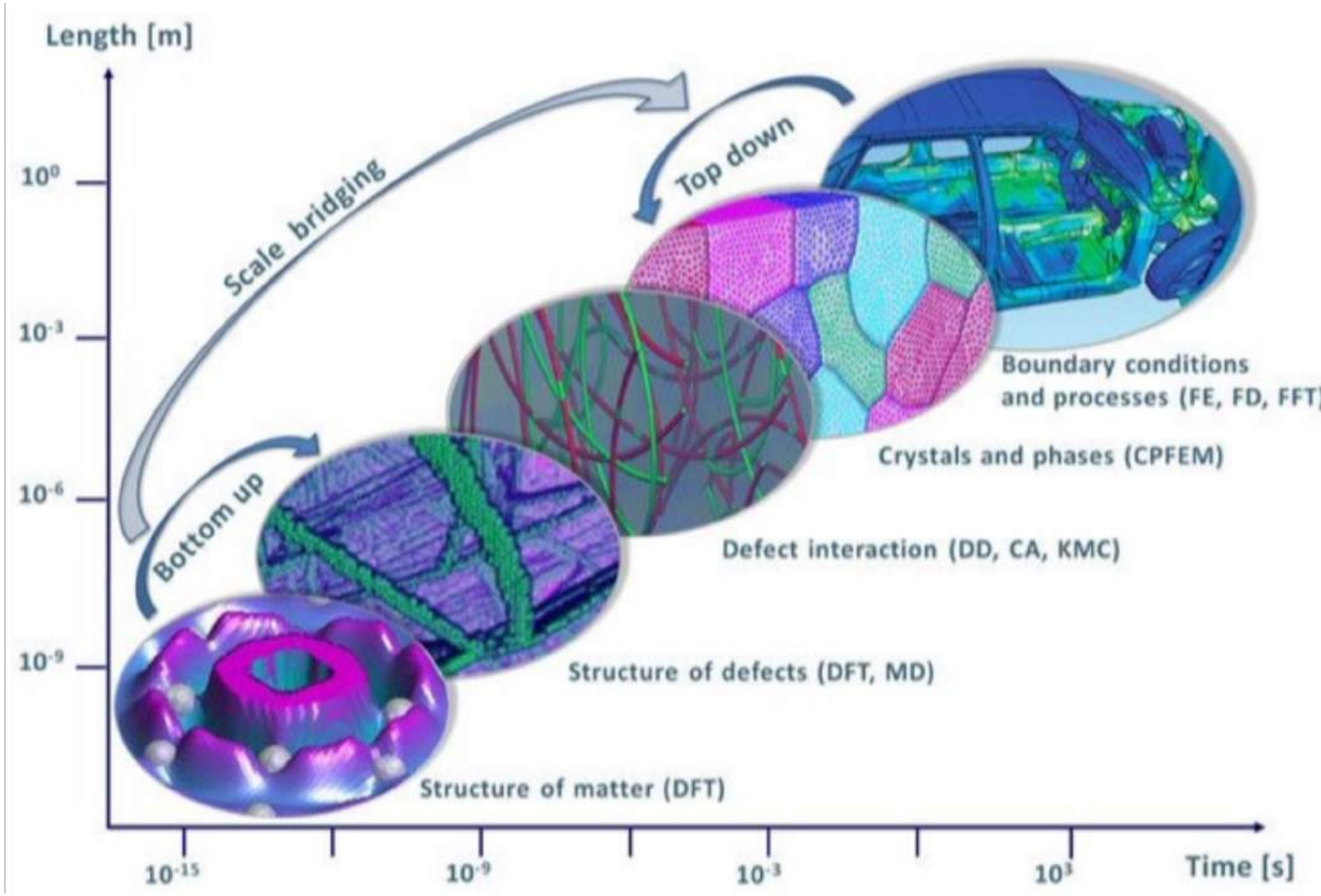
多尺度方法在先进合金中的应用



Multiscale Modeling of Materials in the Max-Planck Society

http://www.dierk-raabe.com/multiscale-modeling

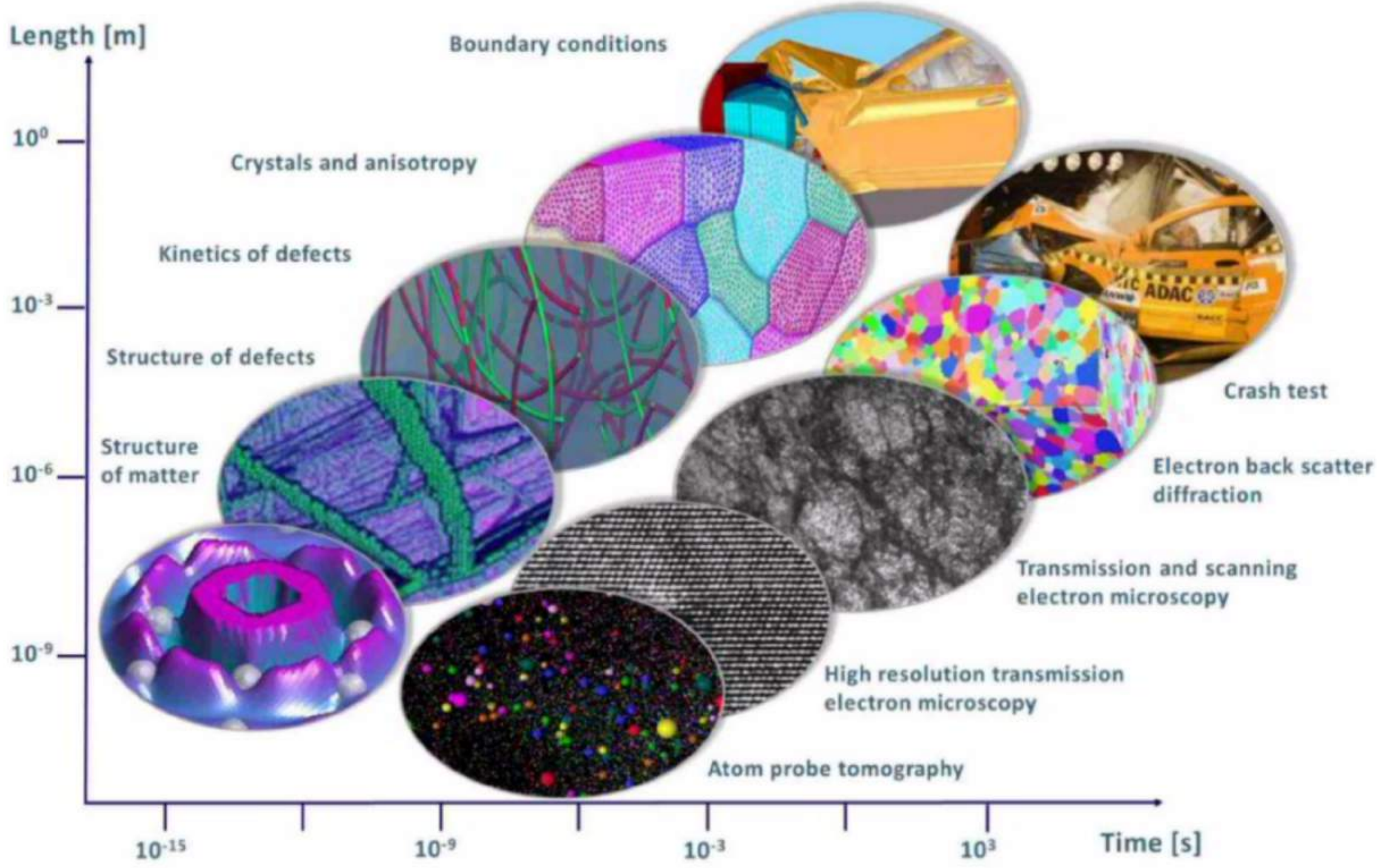
多尺度方法在先进合金中的应用



Multiscale Modeling of Materials in the Max-Planck Society

http://www.dierk-raabe.com/multiscale-modeling

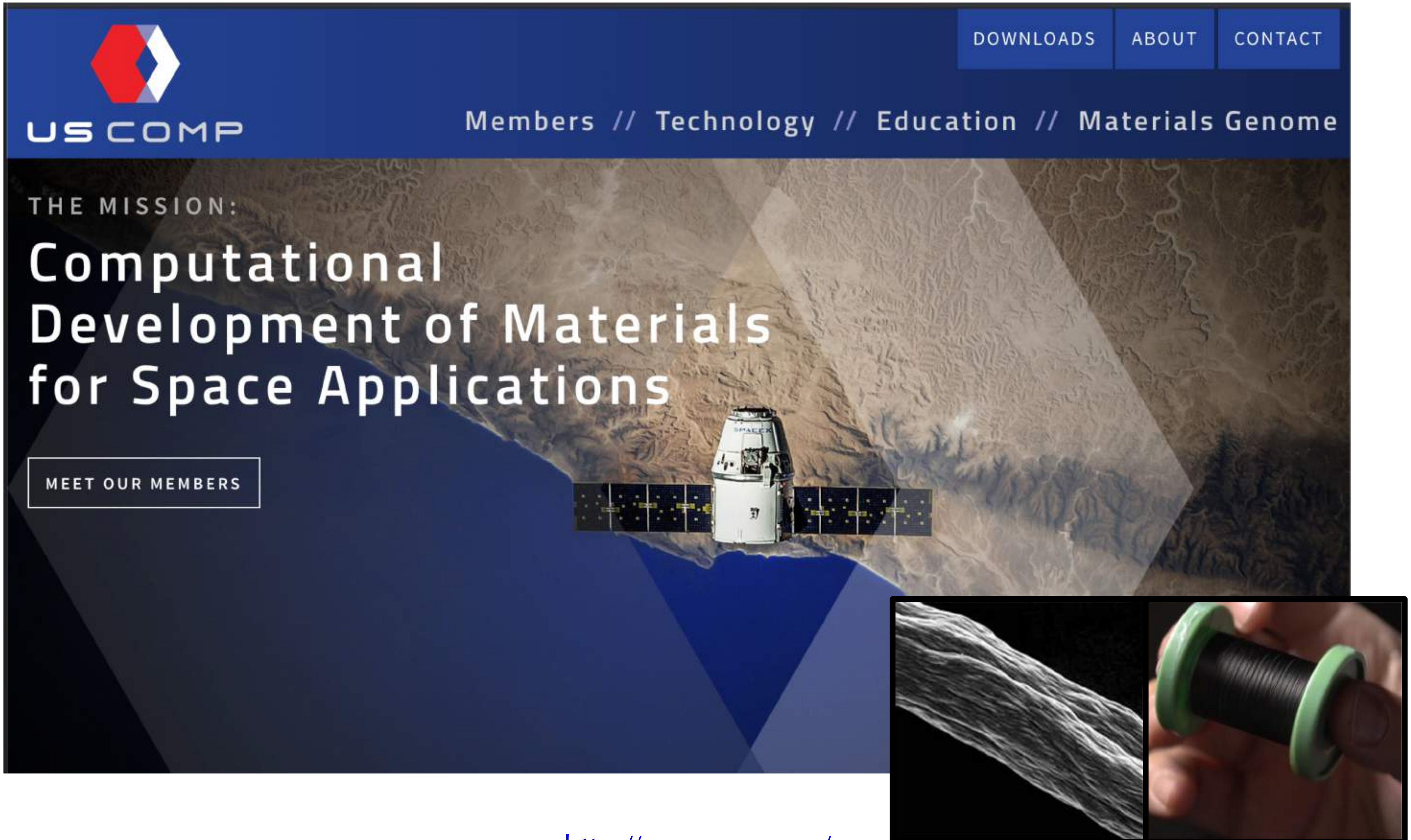
多尺度方法在先进合金中的应用



Multiscale Modeling of Materials in the Max-Planck Society

http://www.dierk-raabe.com/multiscale-modeling

多尺度方法在先进复合材料中的应用

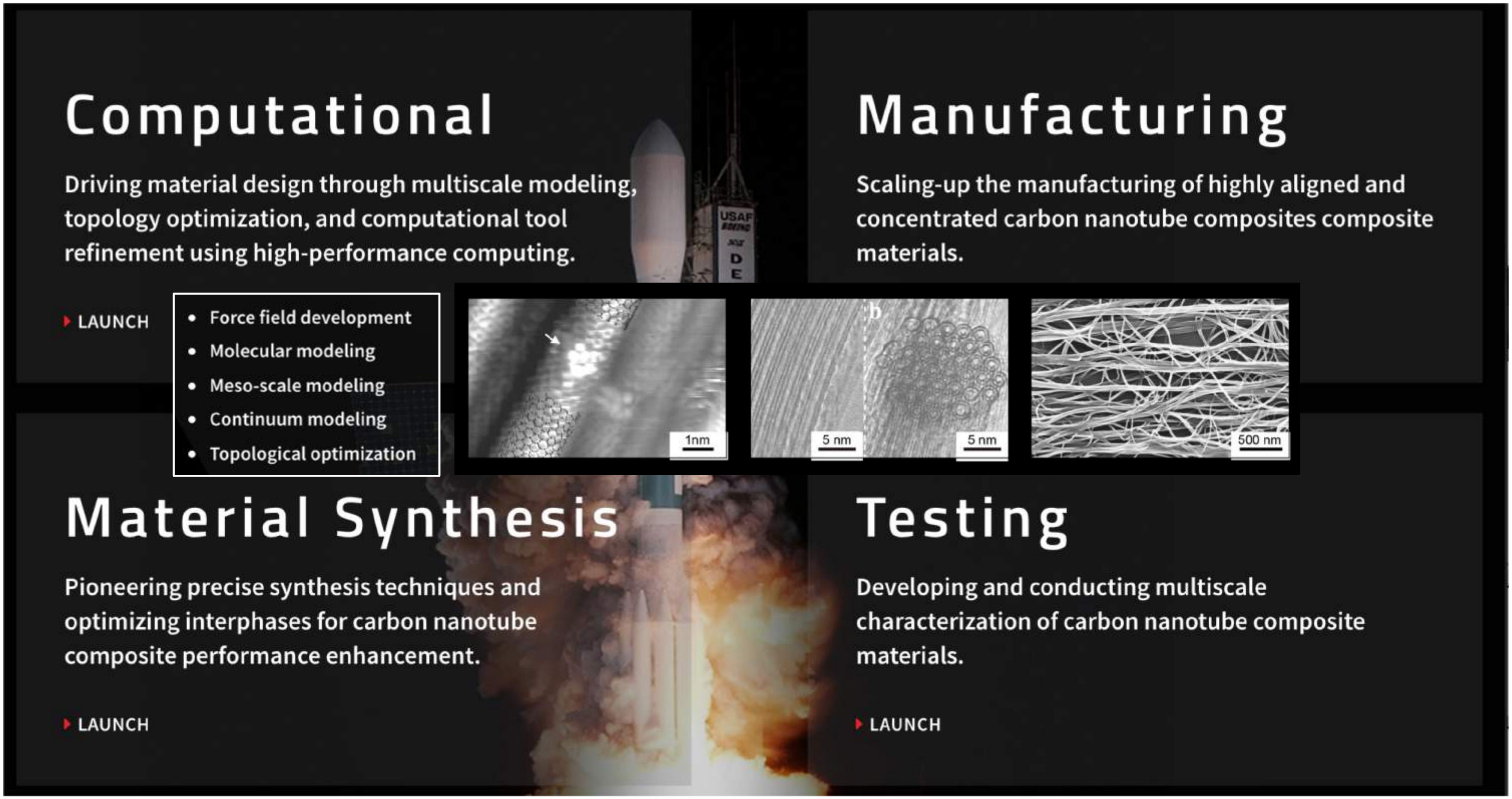


Pasquali group @ Rice

http://us-comp.com/

https://www.nasa.gov/directorates/spacetech/strg/stri/us_comp/

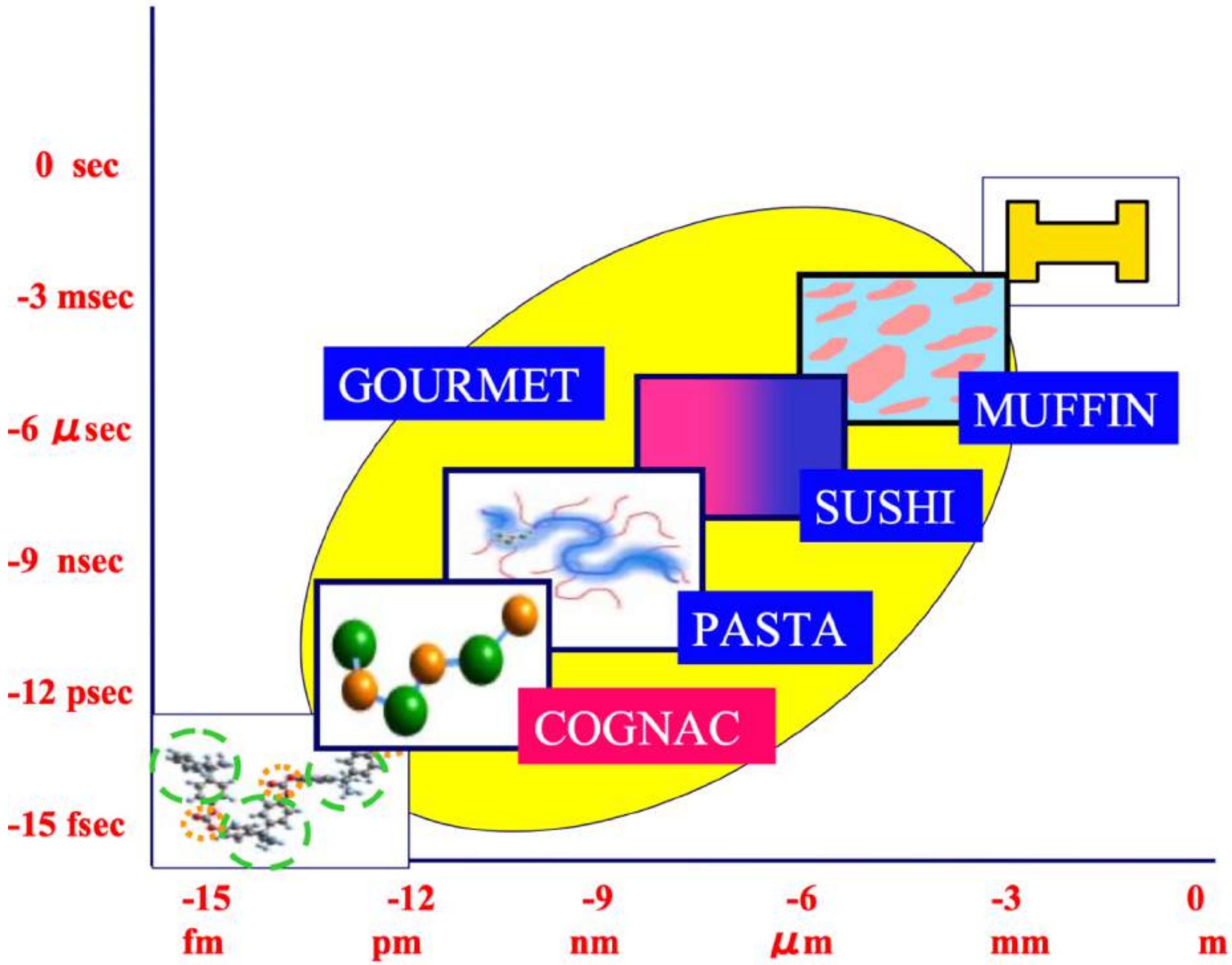
多尺度方法在先进复合材料中的应用

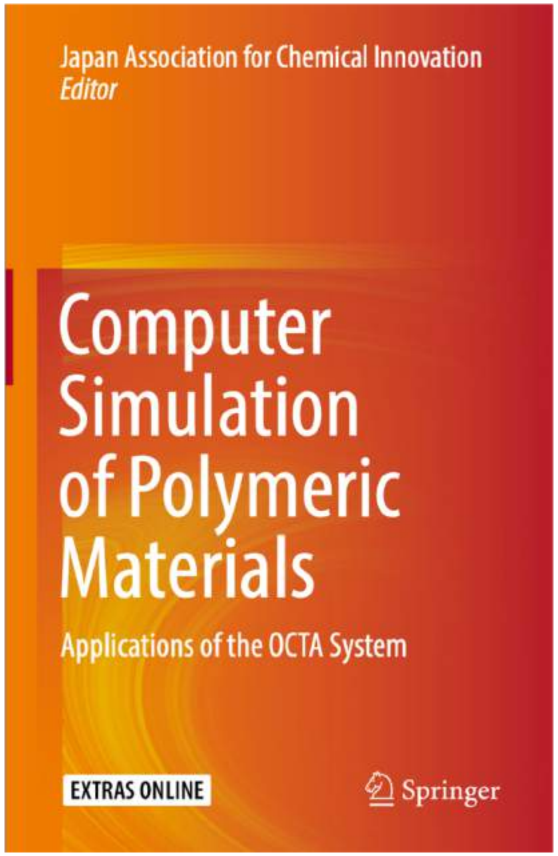


http://us-comp.com/

https://www.nasa.gov/directorates/spacetech/strg/stri/us_comp/

多尺度方法在先进复合材料中的应用





1997, Ministry of International Trade and Industry of Japan

1998-2002, entrusted to NEDO (New Energy and Industrial Technology Development Organization) and conducted at Nagoya University with 11 industries.

http://octa.jp/

小 结

- **复杂度，模型约化，信息传递**

  电子波函数/密度，原子/粒子位置、动量，位错，位移/温度/相场

- **微观结构 (模型)，能量与运动方程 (物理)，数值求解 (方法)**

  合金，复合材料

- **微观粒子描述，连续场描述**

  平衡热力学，熵与涨落

- **多尺度实验方法**

  结构表征、过程与性能测试

Thanks for your attention.

Email: xuzp@tsinghua.edu.cn

Web: http://xuzhiping.gitlab.io