

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



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：相場
- 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

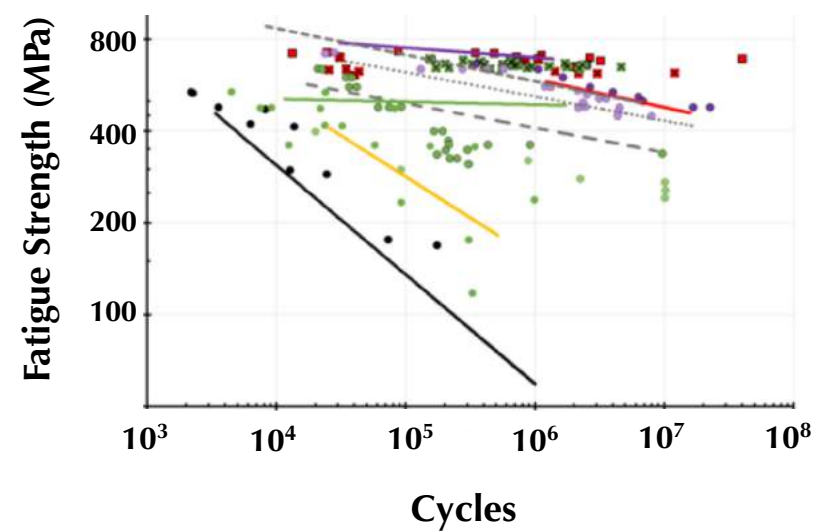
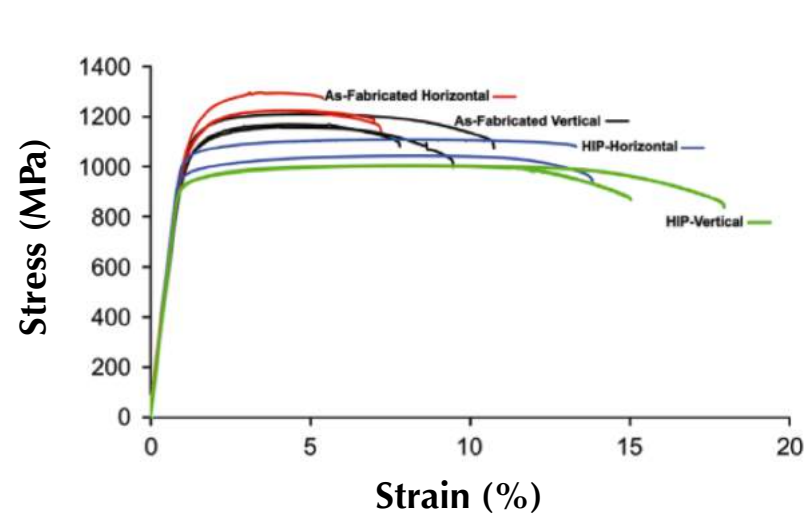
熵，自由能，相互作用

4. 多尺度方法原理

空间多尺度、时间多尺度

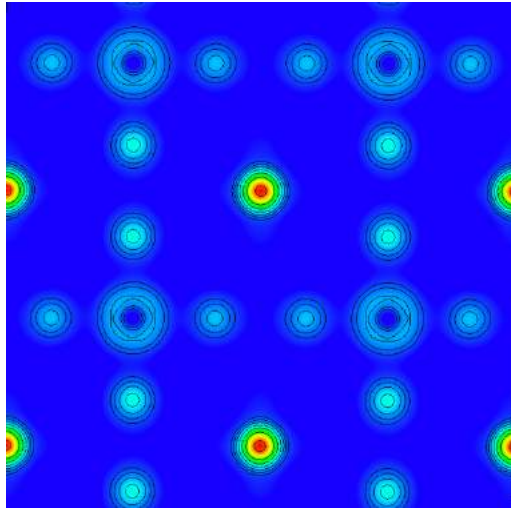
5. 多尺度方法在先进合金、复合材料中的应用

合金材料

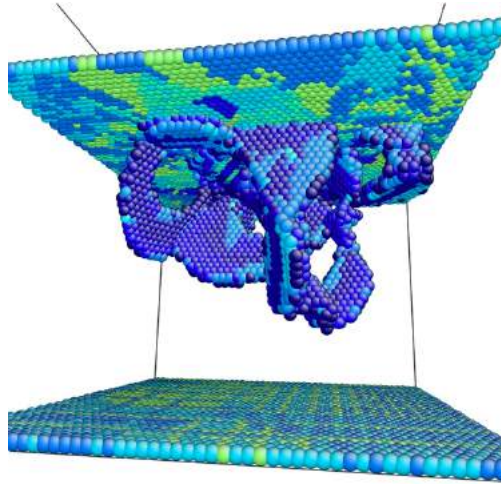


Qiu et al., Mater Sci Engr A, 2013; Li et al., Int J Fatigue 2016

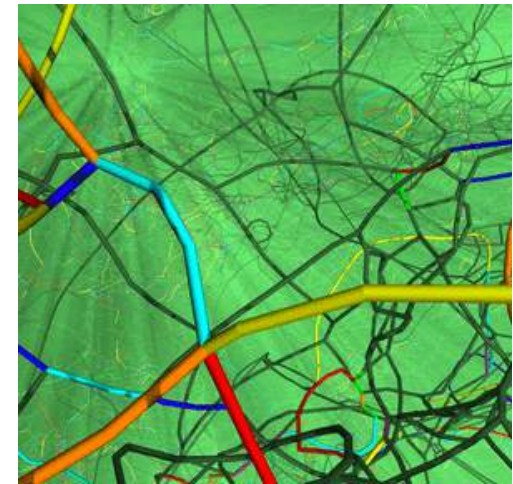
合金材料



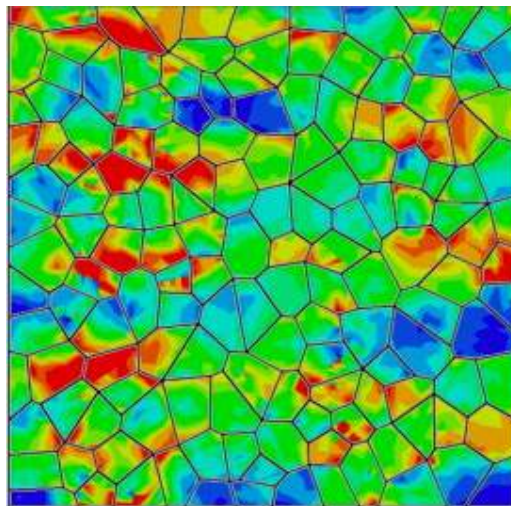
density functional theory
化学成分，原子作用



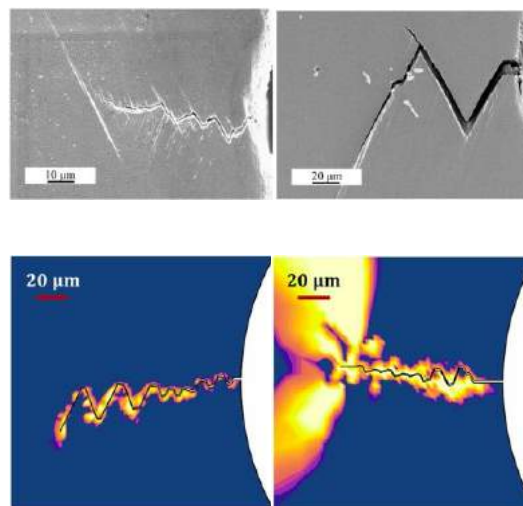
molecular dynamics
晶体结构，位错、缺陷



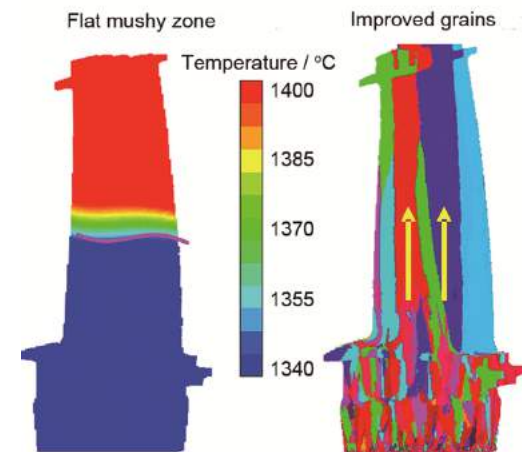
dislocation dynamics
位错动力学



crystal plasticity
晶体塑性

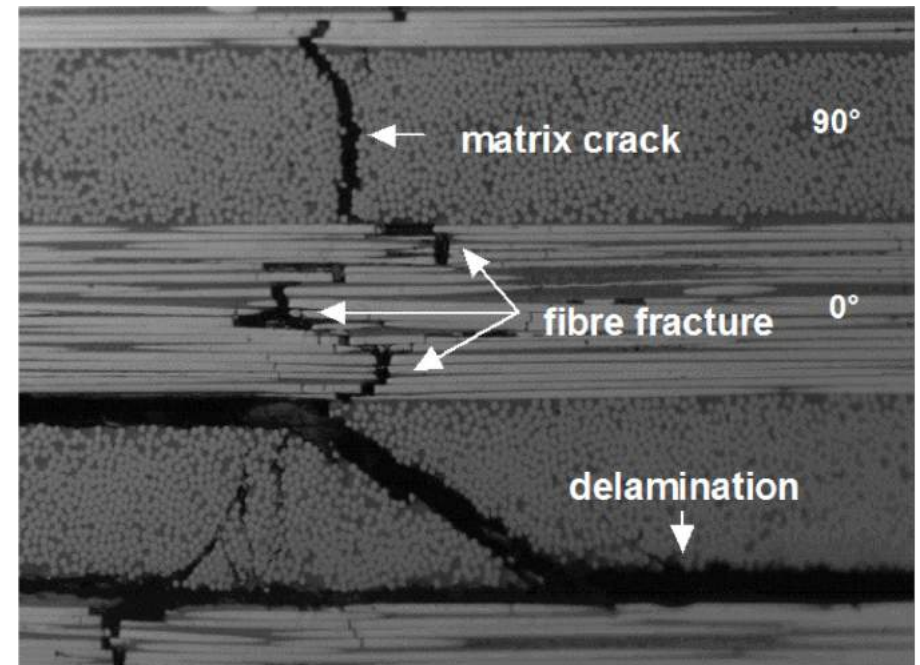
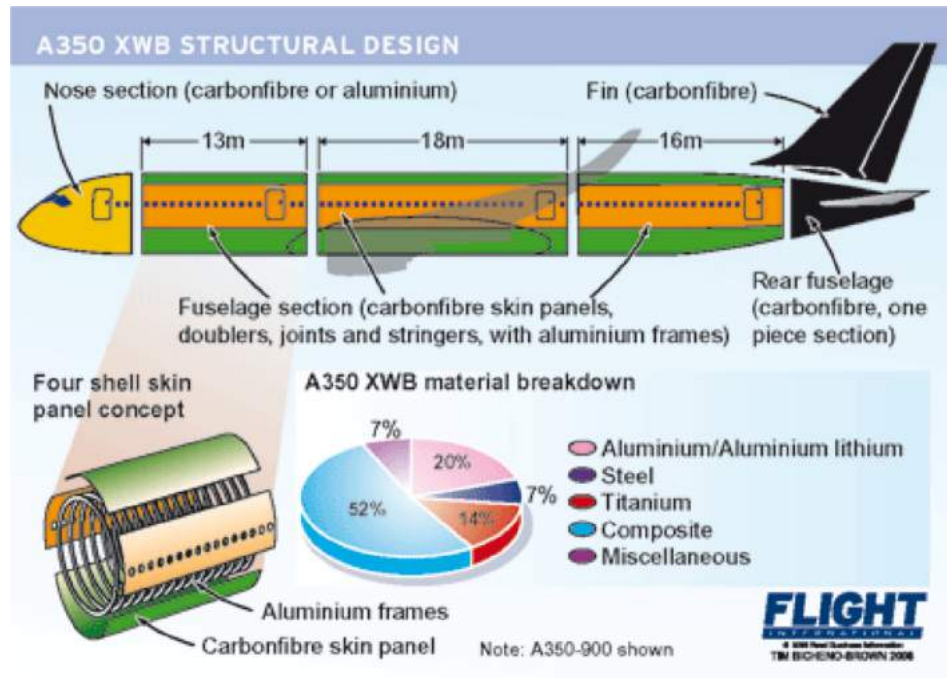


finite element analysis
结构、界面尺度应力分析



industrial design
工业设计

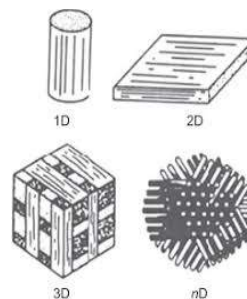
复合材料



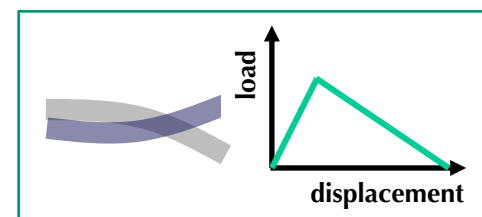
M. Alvarez E. FFA TN 1998-24, Tech Rep 1998



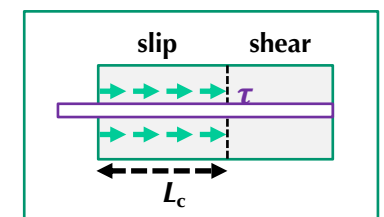
fabrics



composite



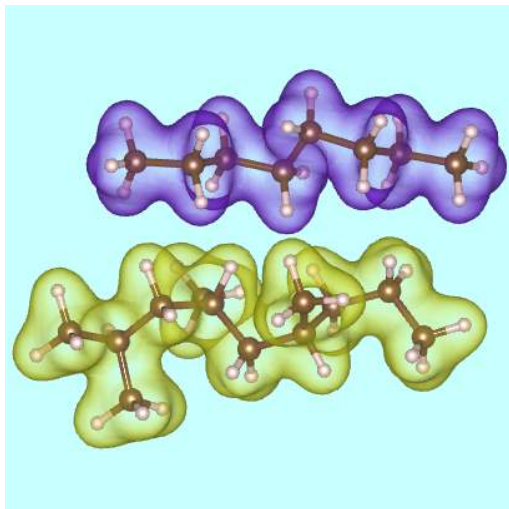
contact



cohesive zone model

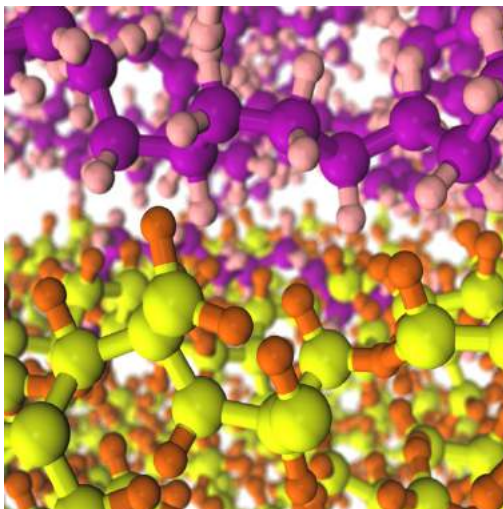
shear-lag model

复合材料



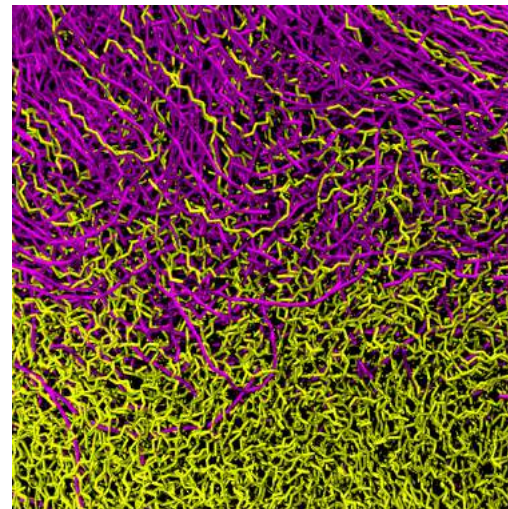
density functional theory

原子作用，光电性质



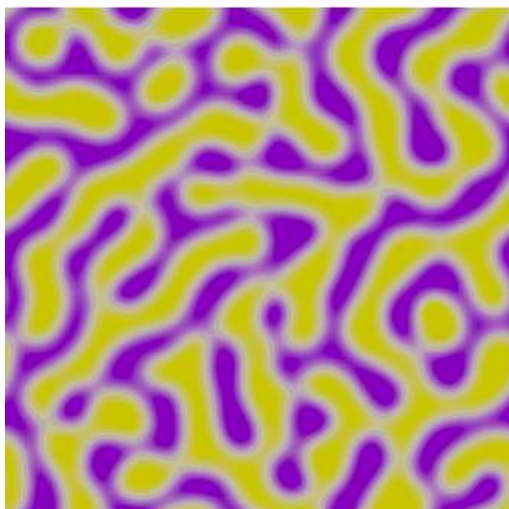
full-atom molecular dynamics

纳米尺度结构、力学、传热



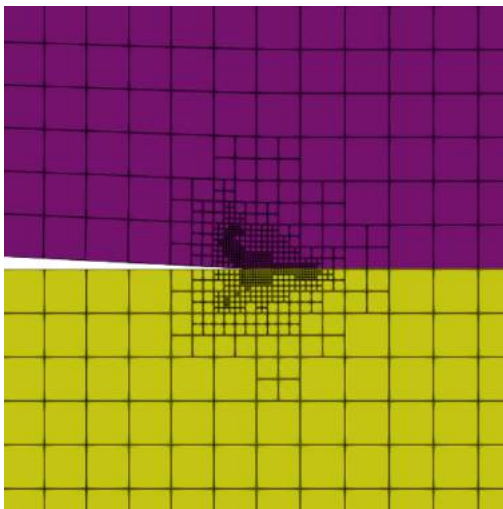
coarse-grained molecular models

微纳米尺度结构、力学



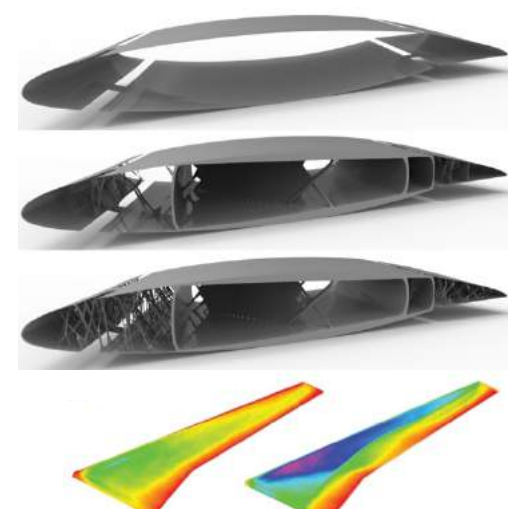
phase-field modeling

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

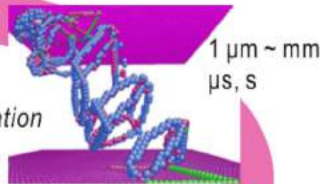
时空尺度与工程问题的复杂度

1 m ~ km **continuum mechanics**
hr, day, yr finite element analysis



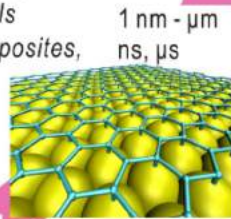
structural engineering,
buckling, failure, optimization

micromechanics
dislocation dynamics
micromechanical model



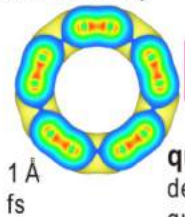
dislocation,
crack propagation

cell, tissue mechanics
bioinspired materials
nanocomposites,
interface



nanomechanics,
protein dynamics,
nanodevices

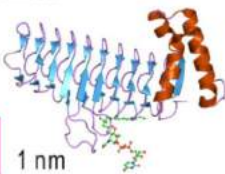
electronic structure,
mechanochemistry



1 Å
fs

quantum mechanics
density functional theory
quantum Monte Carlo

atomistic mechanics
molecular dynamics
Monte Carlo
coarse-grained model

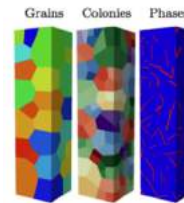


1 nm
ps, ns

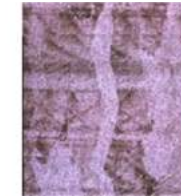
A multiscale and multiphysical simulation paradigm
expanding across both the spatial and temporal scales

- Scanning strategy
 - Pattern
 - Speed
 - Length
 - Hatch distance
- Layer thickness
- Power source
 - Energy density
 - Focus offset
 - Spot size
- Post-processing
 - Stress relief
 - Hot isostatic pressing
 - Polishing

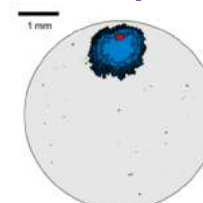
加工参数
(增材制造)



微结构模型
(相场, 晶体塑性)



微结构信息
(SEM, μ -CT)

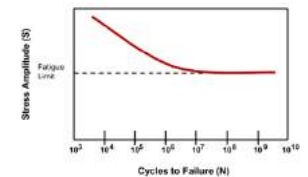


损伤演化
动力学率方程

加工参数 → 力学性能

工艺力学 → 材料力学

微结构及其演化规律



结构设计
寿命预测

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

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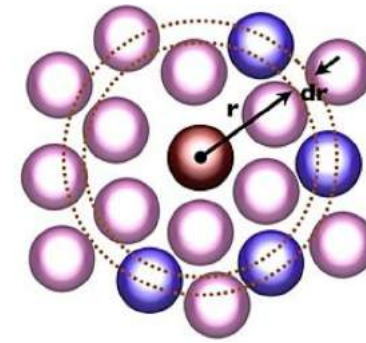
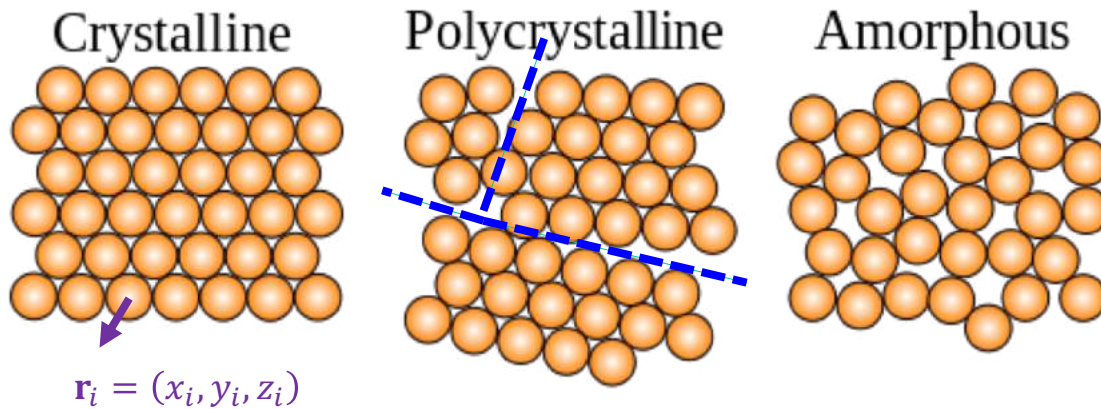
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4. 多尺度方法原理

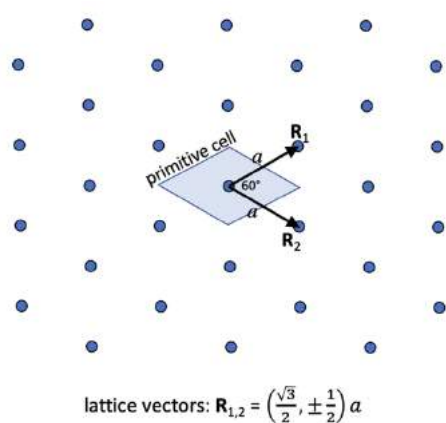
空间多尺度、时间多尺度

5. 多尺度方法在先进合金、复合材料中的应用

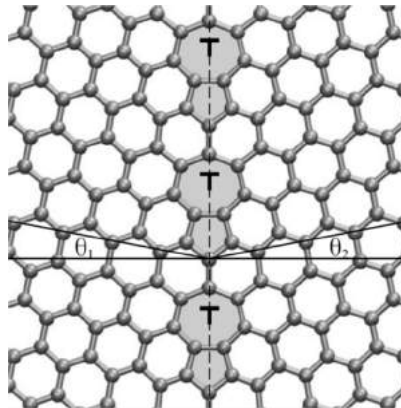
原子结构及其表征 – 粒子



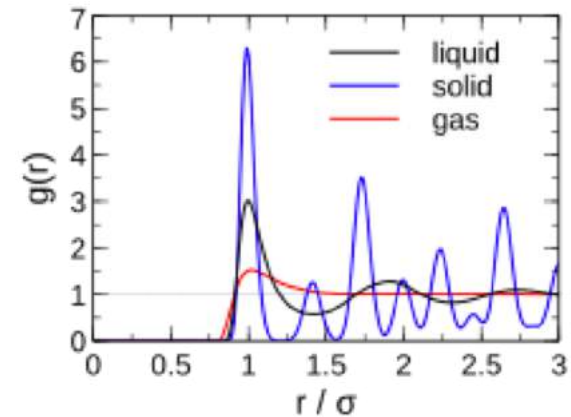
$$g(r) = \frac{1}{\langle n \rangle} \left\langle \sum_i \delta(r - r_i) \right\rangle$$



crystalline **lattice**



lattice **defects (dislocations)**

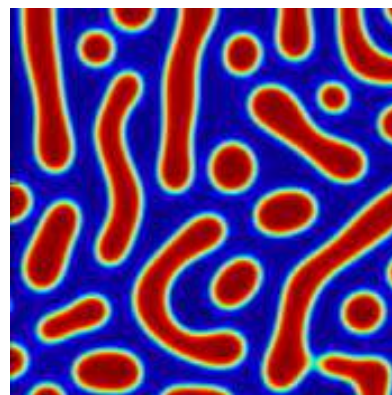
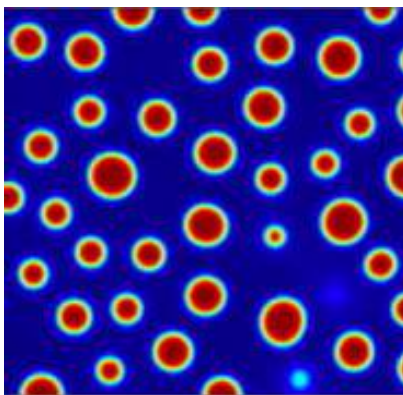
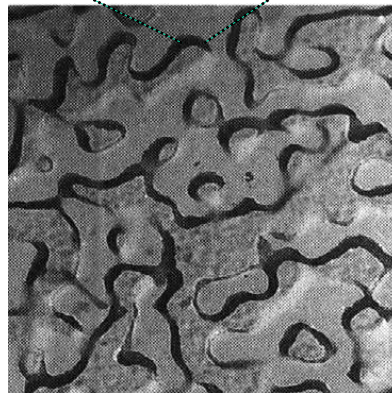
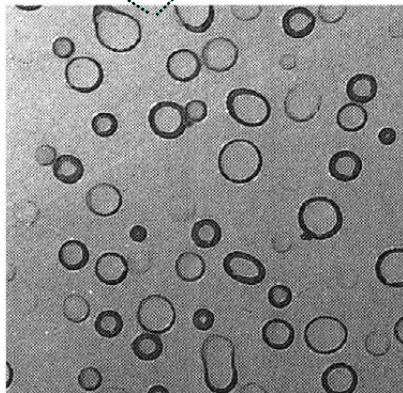
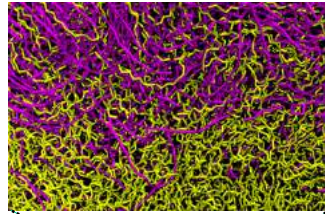
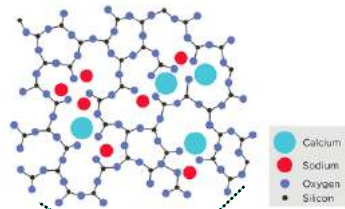


radial distribution function

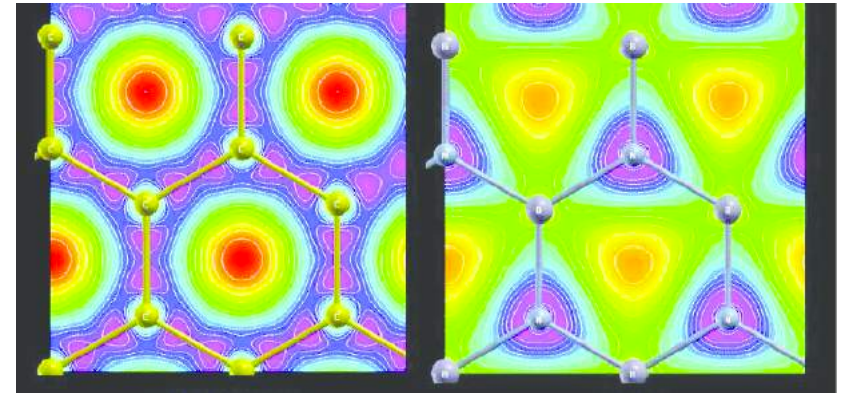
discrete translational/rotational symmetries

continuous rotational symmetry

原子结构及其表征 – 连续



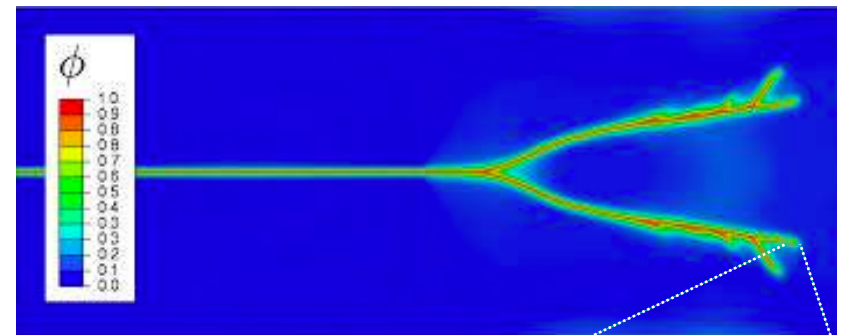
$\rho(\mathbf{r})$: **density** in continuum theories



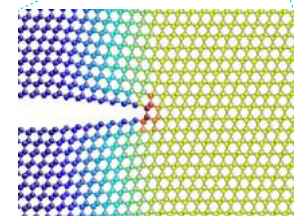
graphene

h-BN

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

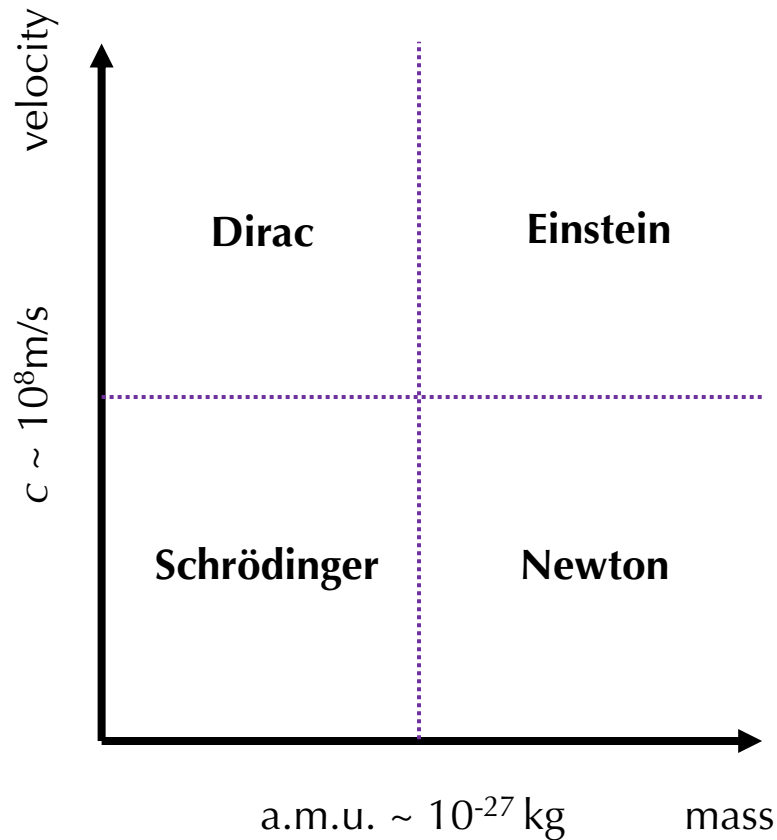


$\phi(\mathbf{r})$: **order parameter**



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

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

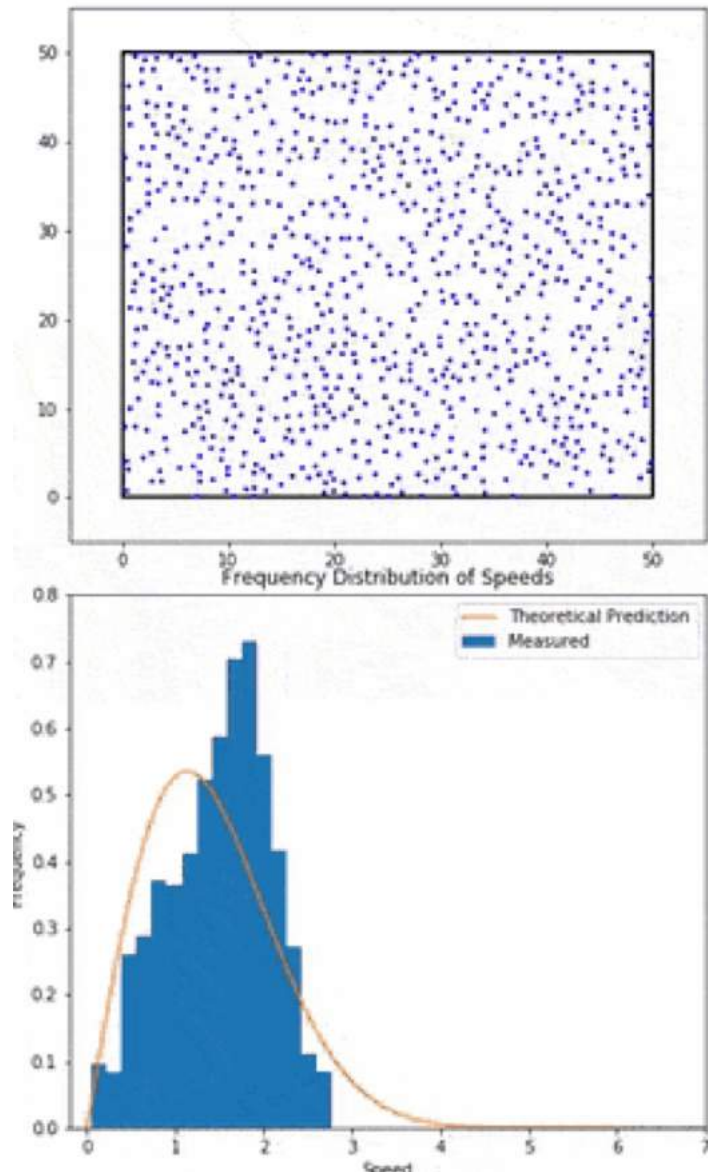
Newtonian equation for quantum particles (e.g. nuclei)

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

E: total (potential) energy

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

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**

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

model reduction

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

phase space of particles \rightarrow thermodynamic variables

the **1st law** of thermodynamics

$$dE = dQ + dW$$

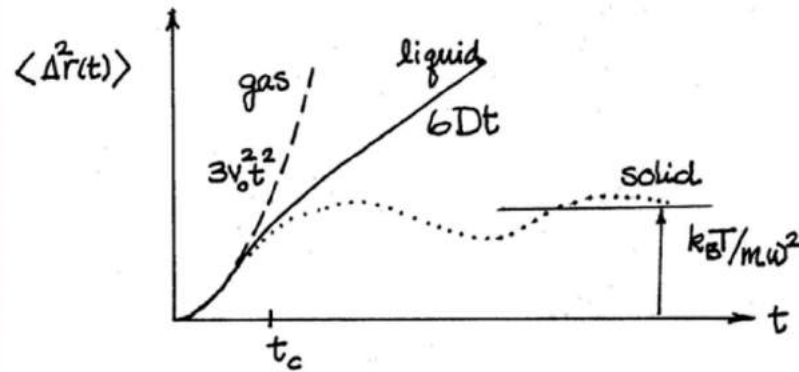
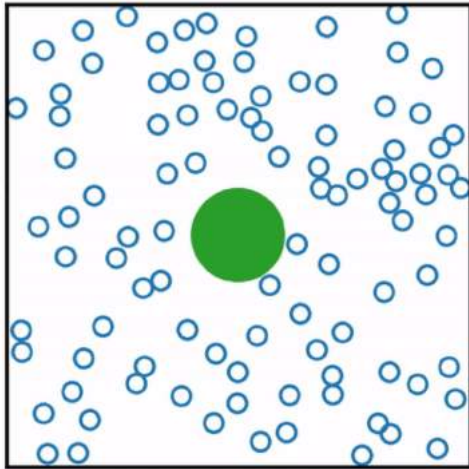
the **2nd law** of thermodynamics

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

fluctuation!

$$dS = \frac{dQ}{T} : \text{change in Clausius entropy}$$

非平衡过程 – 输运



Brownian motion

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

Einstein 1905; Smoluchowski 1906

Stokes-Einstein equation

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

fluctuation-dissipation relations for

diffusion

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

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

shear viscous flow

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

$$\mu = \frac{1}{Vk_B T} \int_0^\infty dt \langle J(0) J(t) \rangle$$

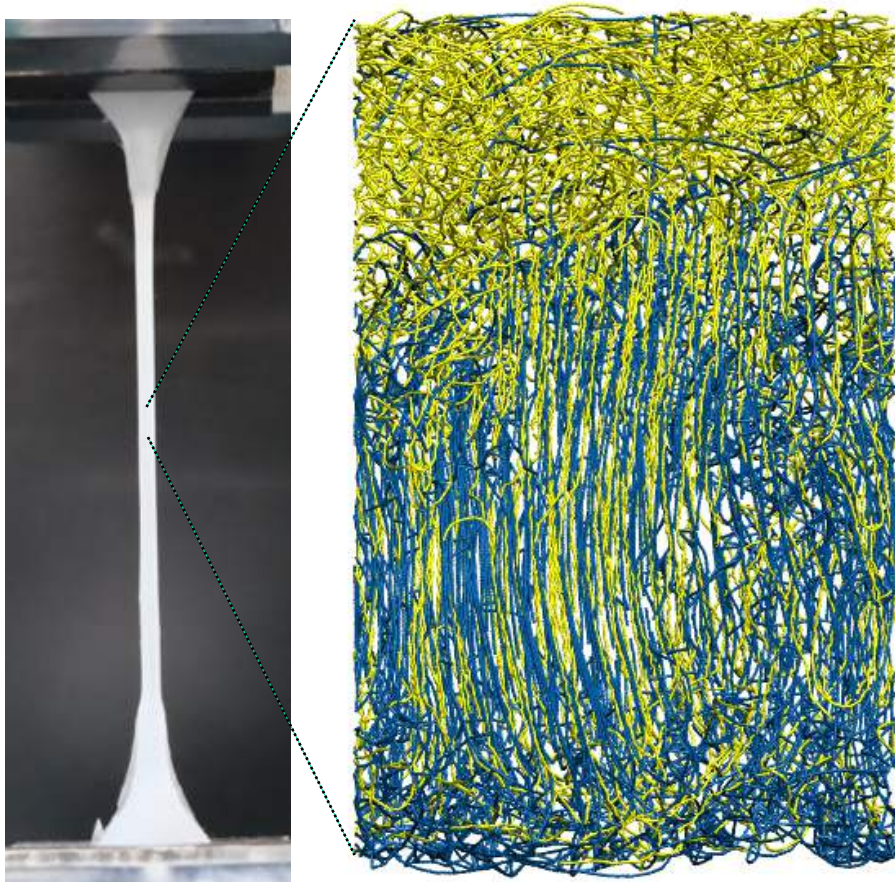
$$J = \sum_{i=1,N} \left(\frac{p_{xi} p_{yi}}{m} + z_i F_{ix} \right) = m \sum_{i=1,N} \dot{x}_i \dot{z}_j + \frac{1}{2} \sum_{j \neq i} z_{ij} F_{ij}^x$$

thermal transfer

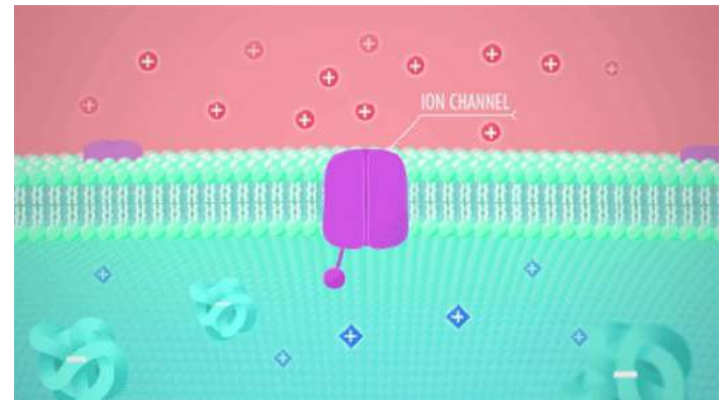
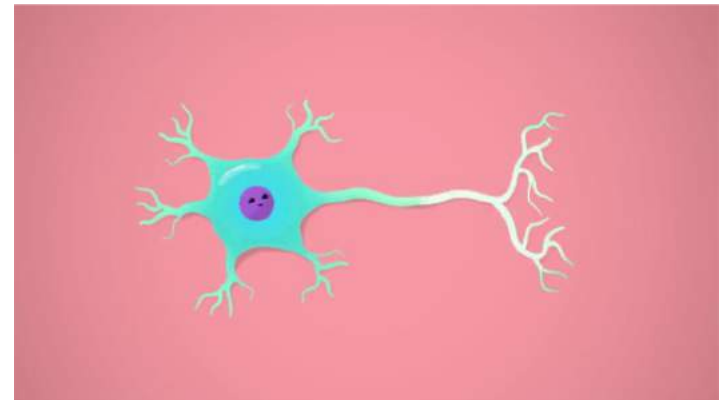
$$\kappa = \frac{1}{2Vk_B T^2 t} \left\langle \sum_{i=1,N} [r_i(t) \tilde{E}_i(t) - r_i(0) \tilde{E}_i(0)]^2 \right\rangle$$

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

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

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熵，自由能，相互作用

4. 多尺度方法原理

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5. 多尺度方法在先进合金、复合材料中的应用

熵



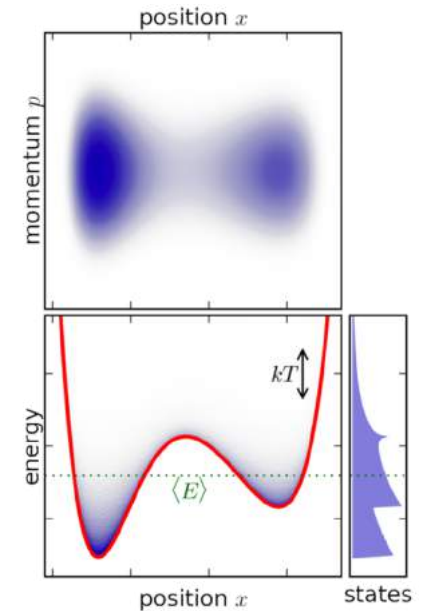
Boltzmann's statistical definition entropy

$$S = k_B \ln W$$

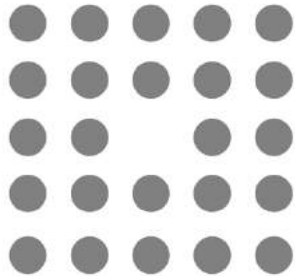
vibrational entropy

$$S = k_B \ln \frac{A}{A_0}$$

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



configurational entropy

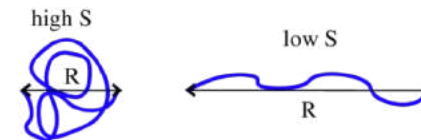


point defects in a N -site lattice

$$S = k_B \ln N$$

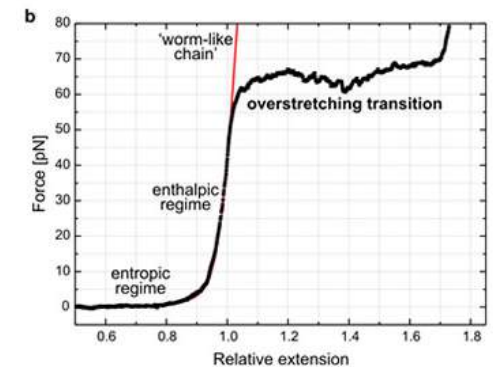
$$F = E - TS$$

raising T promotes formation of the defects



entropic forces

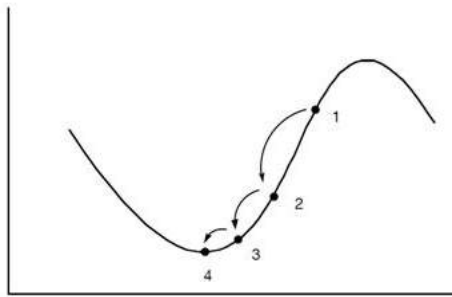
$$f = dF/dR = -TdS/dR$$



Bustamante et al., Science 1994

能量

Time's arrow



E_{pot}

potential energy

$$F = E - TS$$

Helmholtz free energy

$$E = E_{\text{pot}} + E_{\text{kin}}$$

constant N, V, T ; w/ heat exchange

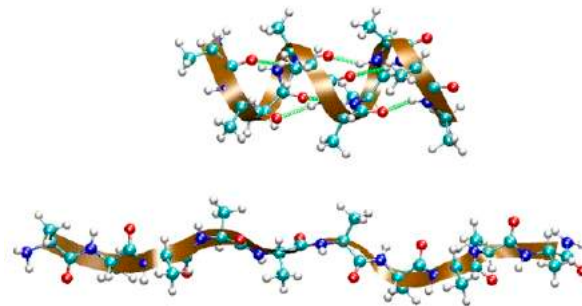
$$G = E - TS + pV$$

Gibbs free energy

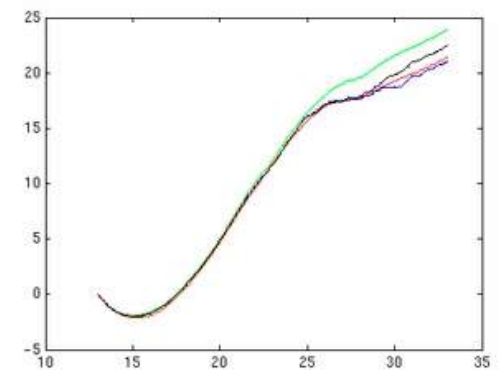
constant N, V, T ; w/ heat exchange

Jarzynsky equality (1996)

$$e^{-\Delta F/k_B T} = \langle e^{-W/k_B T} \rangle$$

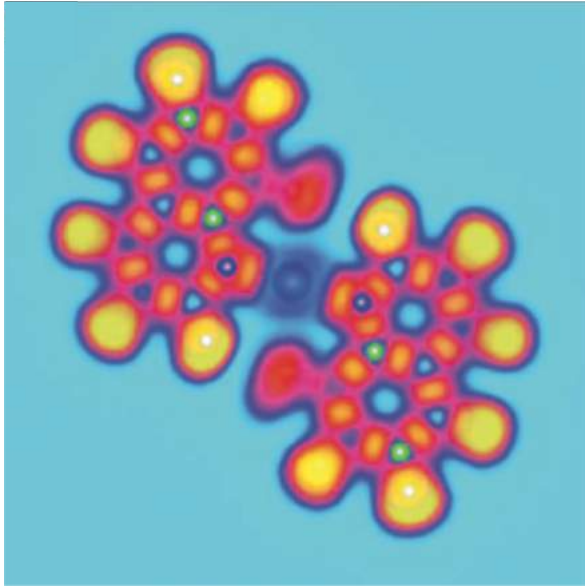


potential of mean force W



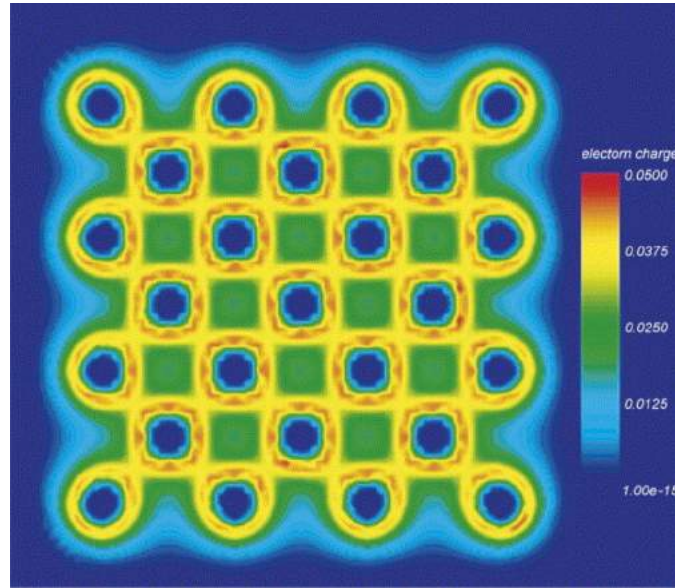
end-to-end distance

相互作用 – 物理图像



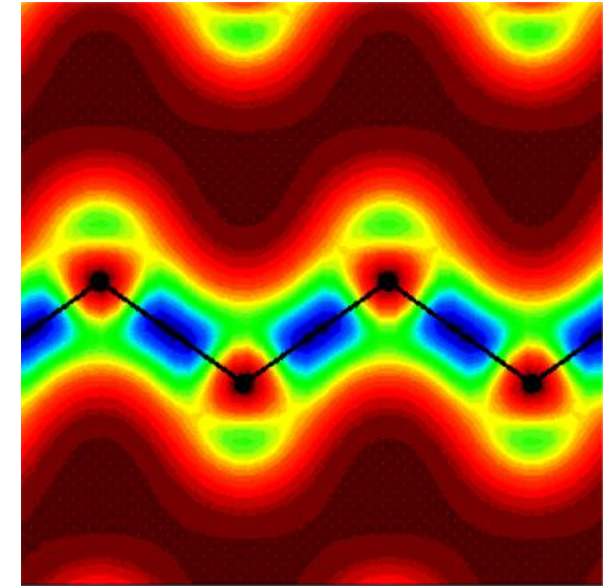
hydrogen bonding

electrostatic + Van der Waals



metallic bonds

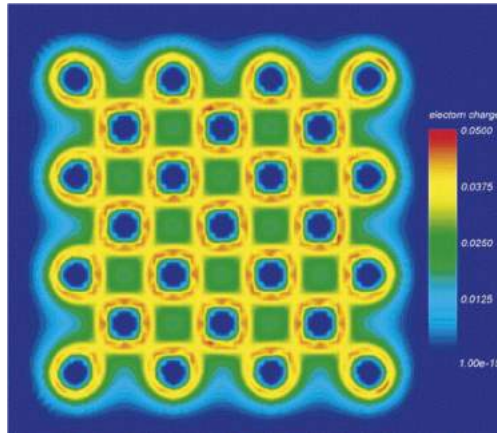
screened ion-ion, ion-electron



covalent bonds

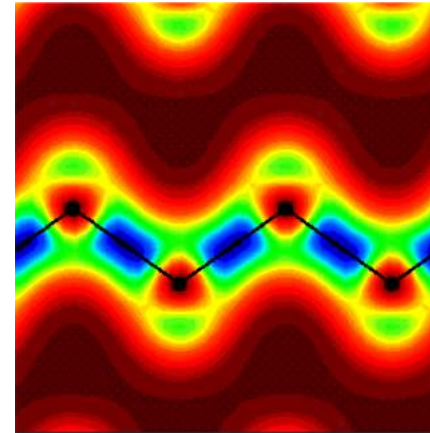
electron-pair sharing

相互作用 – 经验描述



$$V = \sum_i E_i$$

total potential energy
decomposed into
terms associated with
atoms

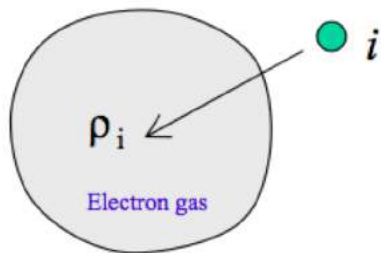


$$V = \frac{1}{2} \sum_{ij} \phi(r_{ij}) \quad \text{two-body}$$

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

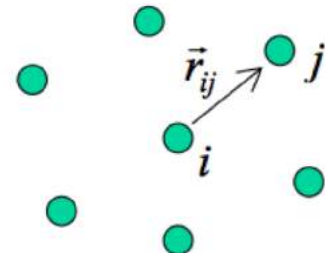
three-body

embedding

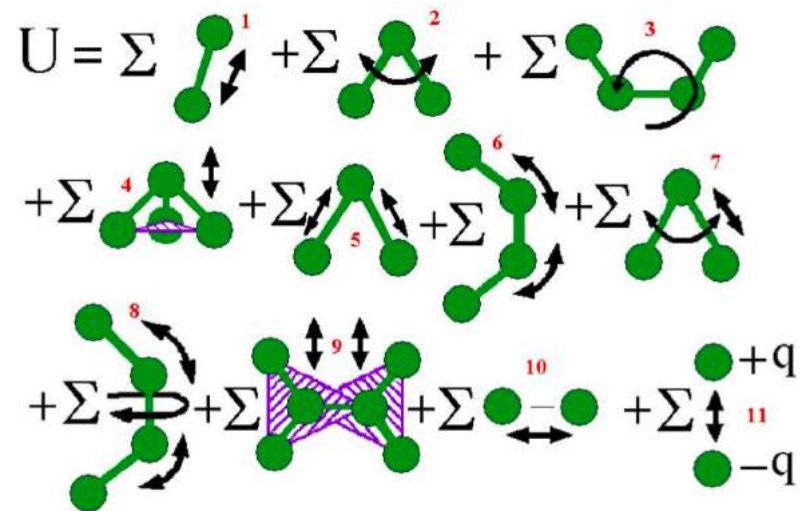


$$E_i = E_i(\bar{\rho}_i) + \frac{1}{2} \sum_{ij} V(r_{ij})$$

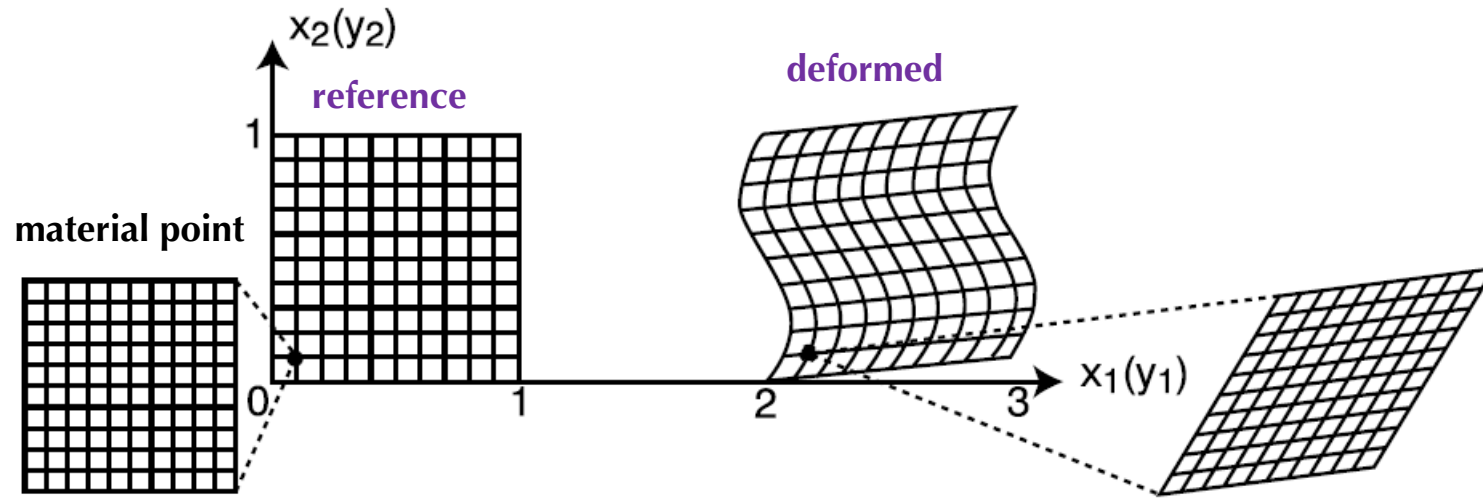
two-body



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



相互作用 – 连续模型



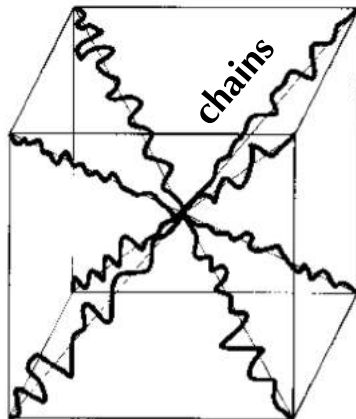
strain energy density

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

deformation gradient

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

entropic elasticity



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

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

extension to non-locality, viscous damping, ...

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

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

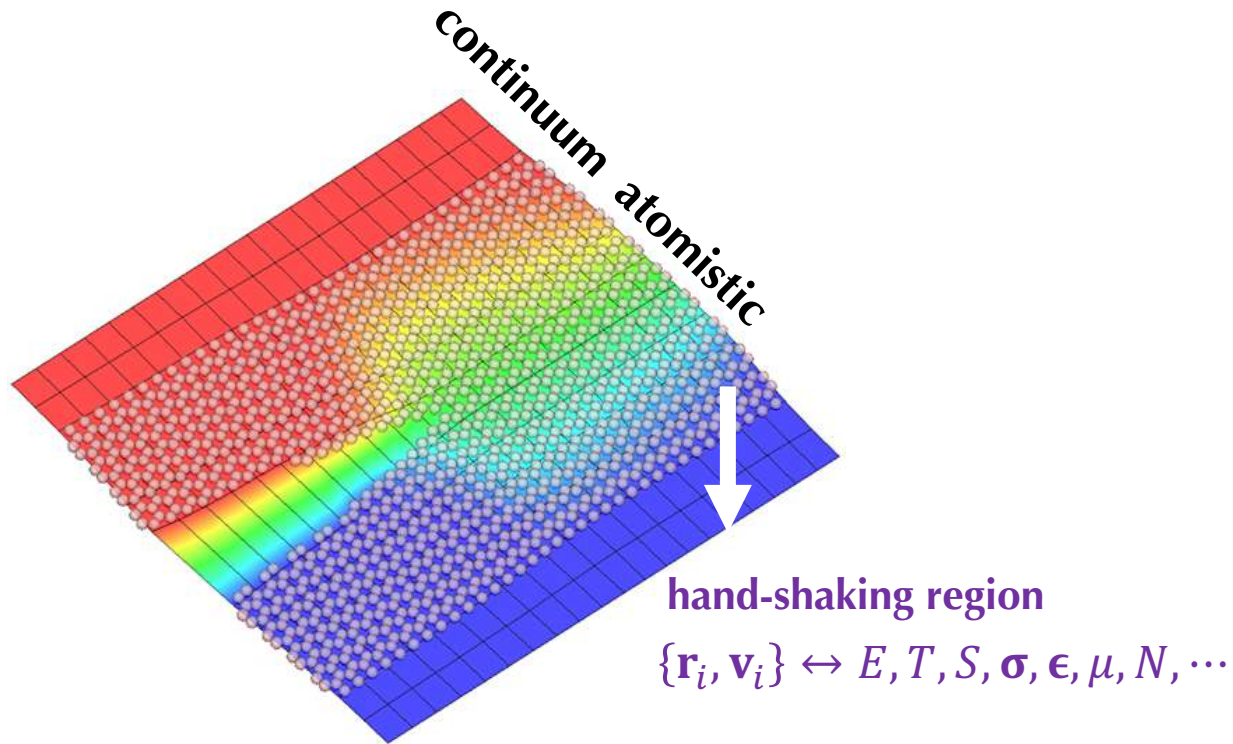
熵，自由能，相互作用

4. 多尺度方法原理

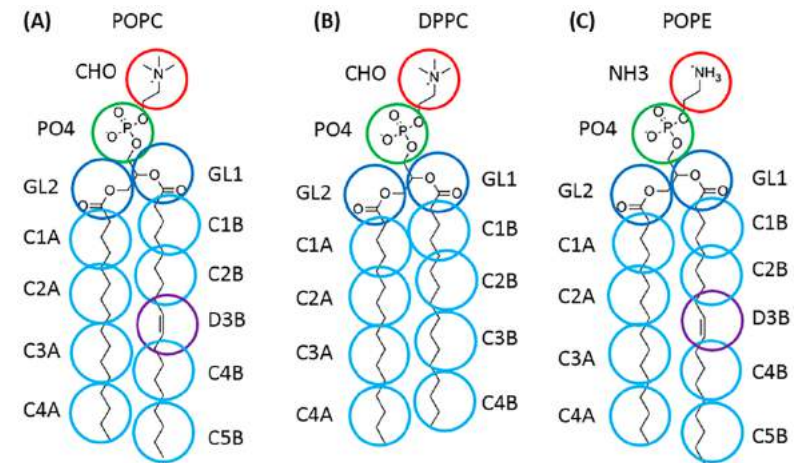
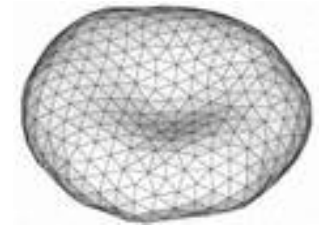
空间多尺度、时间多尺度

5. 多尺度方法在先进合金、复合材料中的应用

空间多尺度

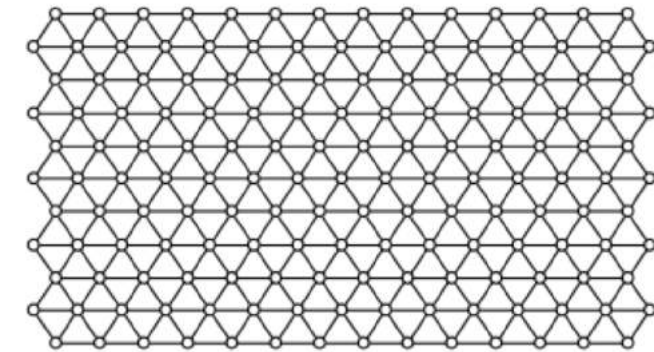


concurrent multiscale methods



shape/topology-based coarse-graining

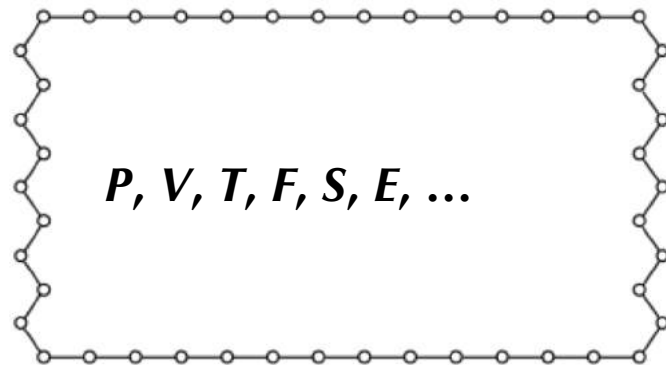
空间多尺度



microscopic dynamics

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

model reduction

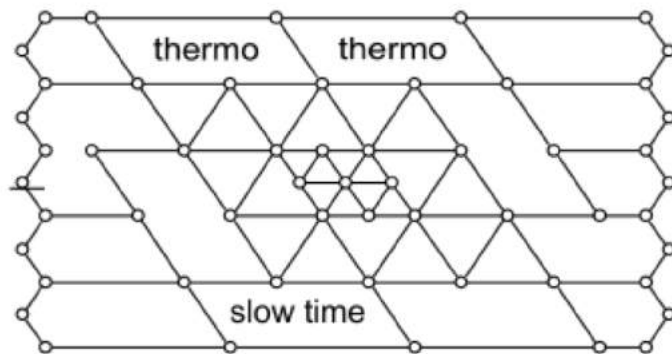


thermodynamics

thermodynamic averages

fluctuation?

entropy?

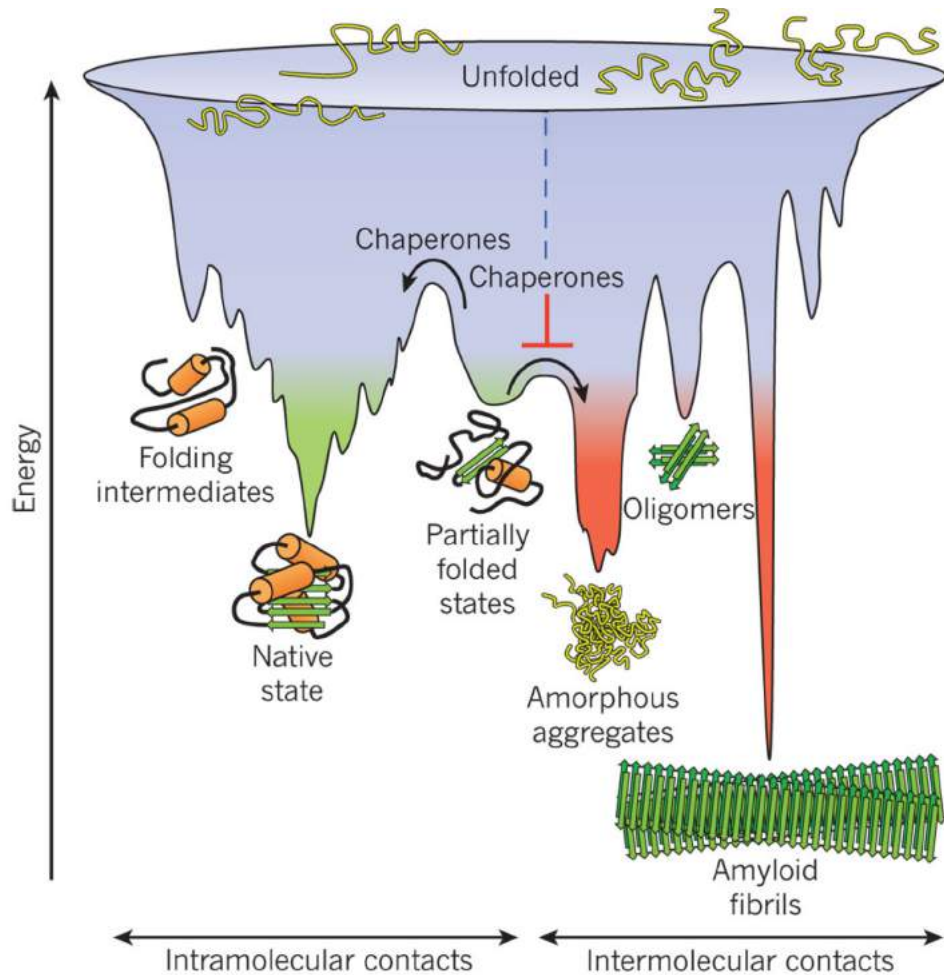


multiscale (coarse-grained) models

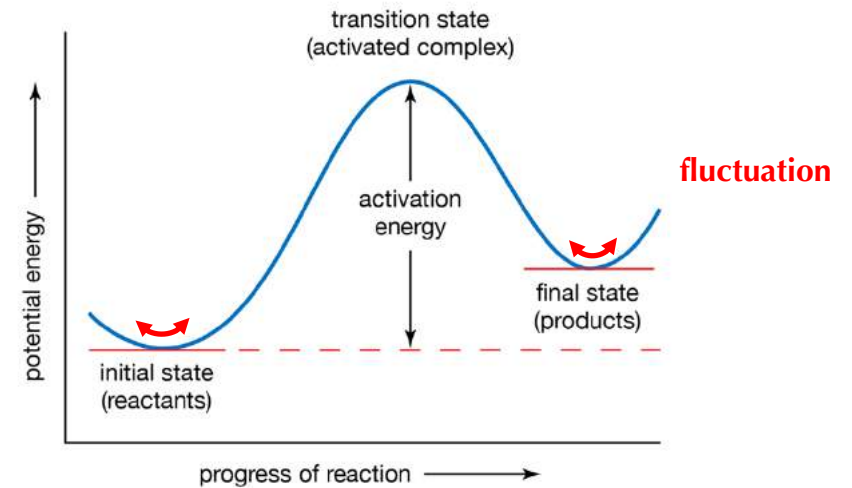
map discrete microscale dynamics to thermodynamics
there are interfaces !

Curtarolo and Ceder PRL 2002

时间多尺度



transition state theory



© Encyclopædia Britannica, Inc.

Arrhenius rate

characteristic timescale

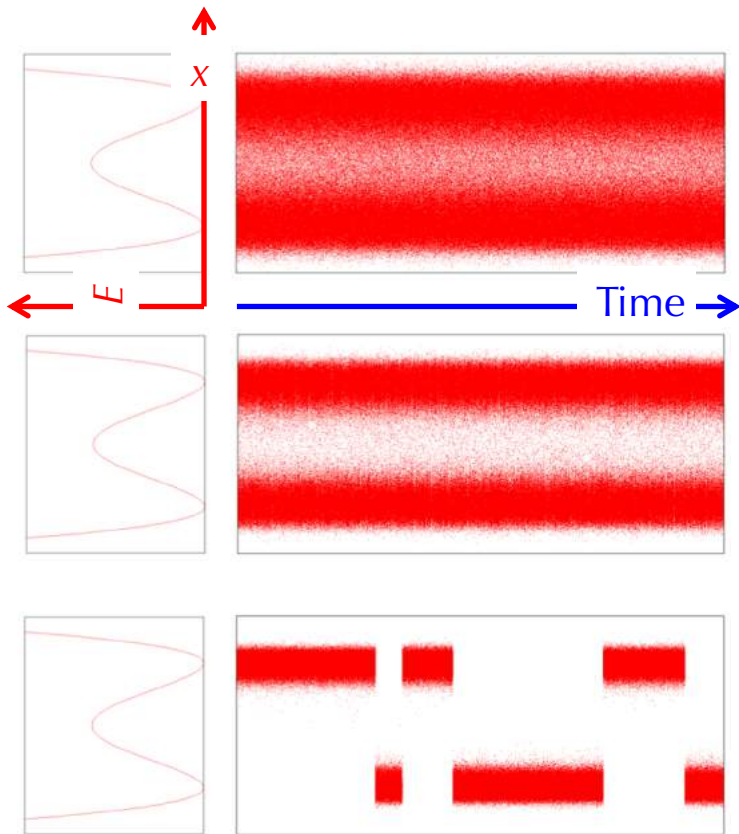
$$k \sim \nu_0 \exp(-E_a/k_B T) \quad \tau \sim \frac{1}{\nu_0} \exp(E_a/k_B T)$$

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

$$E_a \sim 0.75 \text{ eV}, T \sim 300 \text{ K}$$

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

时间多尺度



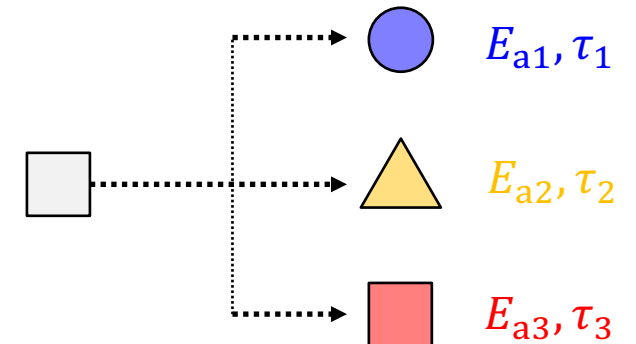
$k_B T = 0.5 E_a$
diffusive behavior

$k_B T = 0.2 E_a$
diffusive behavior

$k_B T = 0.08 E_a$
'instantonic' behavior
 $t_{\text{transition}} \gg t_{\text{corr}}$

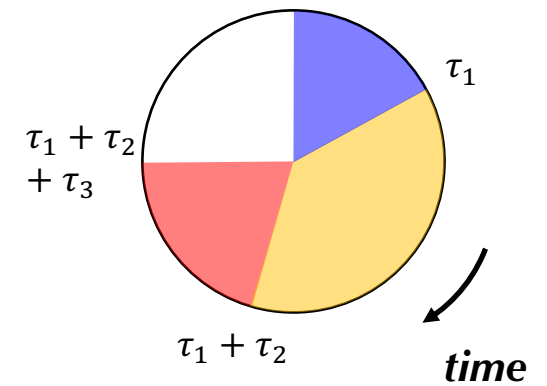
$$\tau \sim \frac{1}{\nu_0} \exp(E_a / k_B T)$$

kinetic Monte Carlo

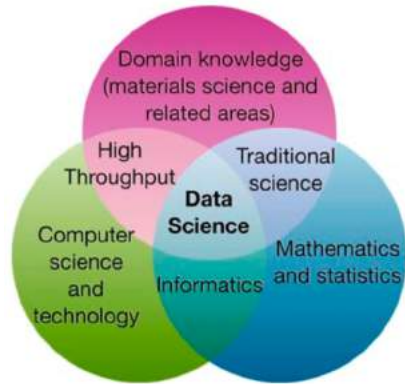


step i

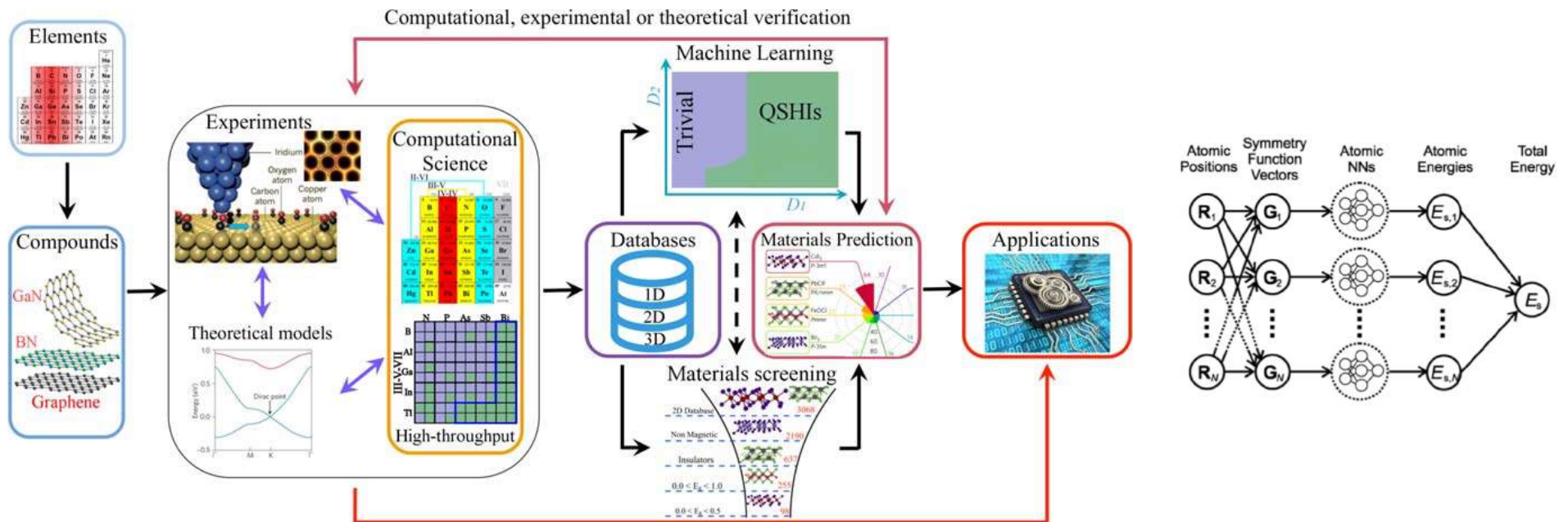
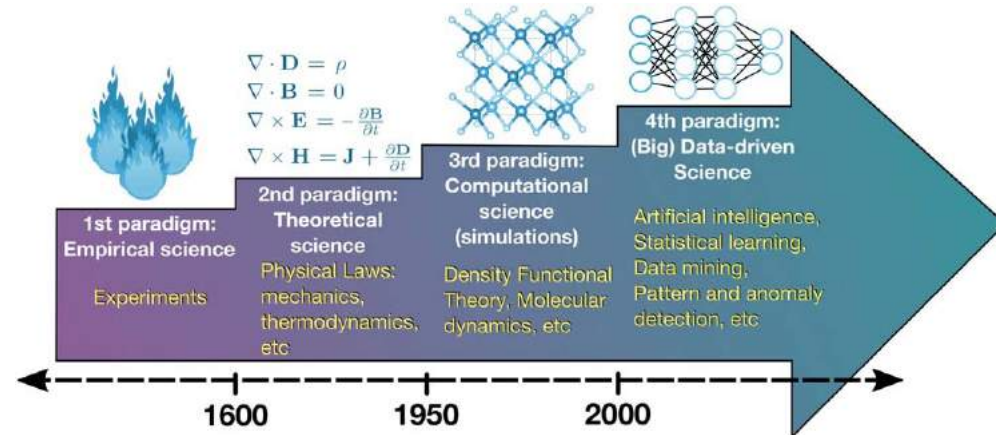
step i+1



数据与机器学习



复杂度 → 数据



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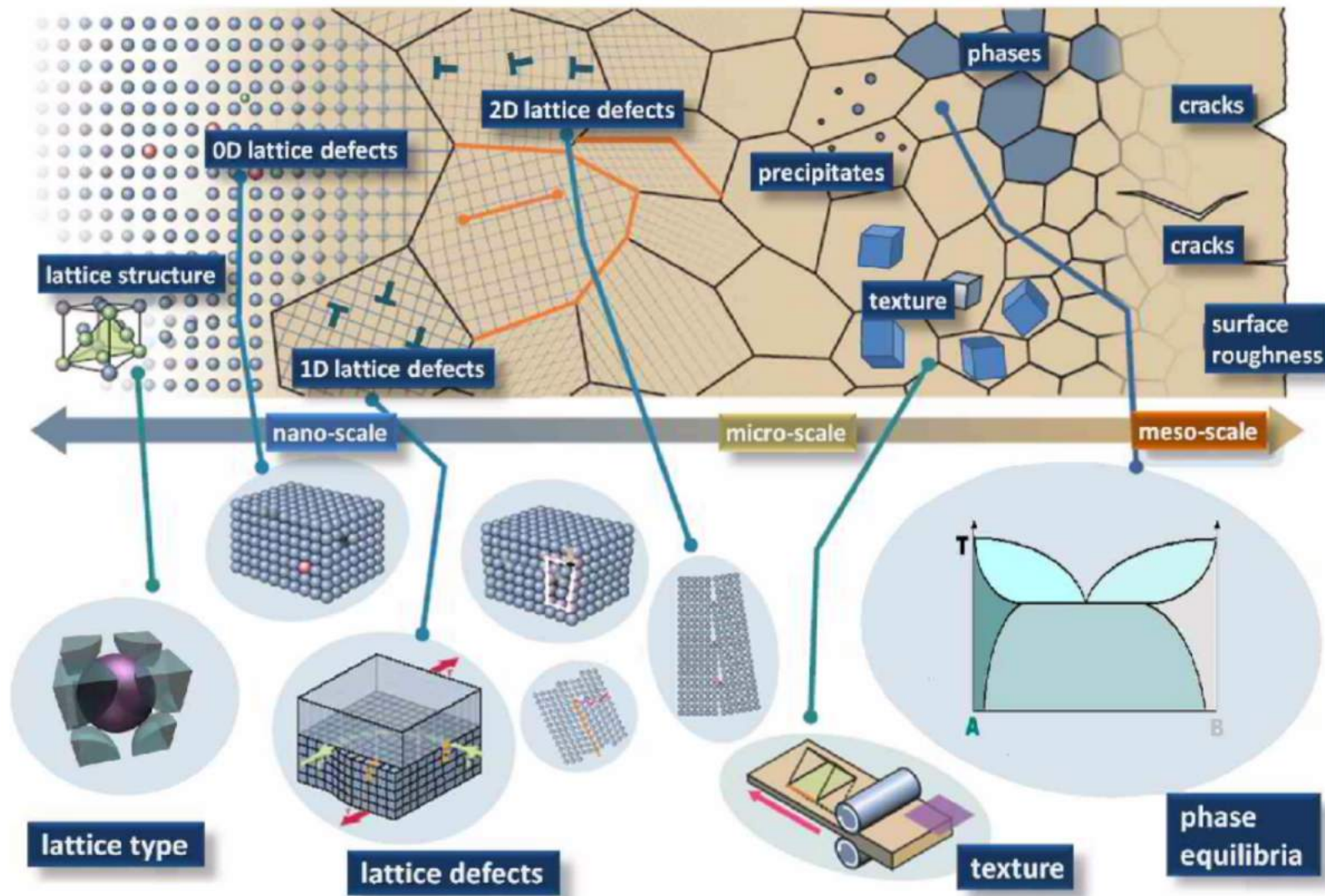
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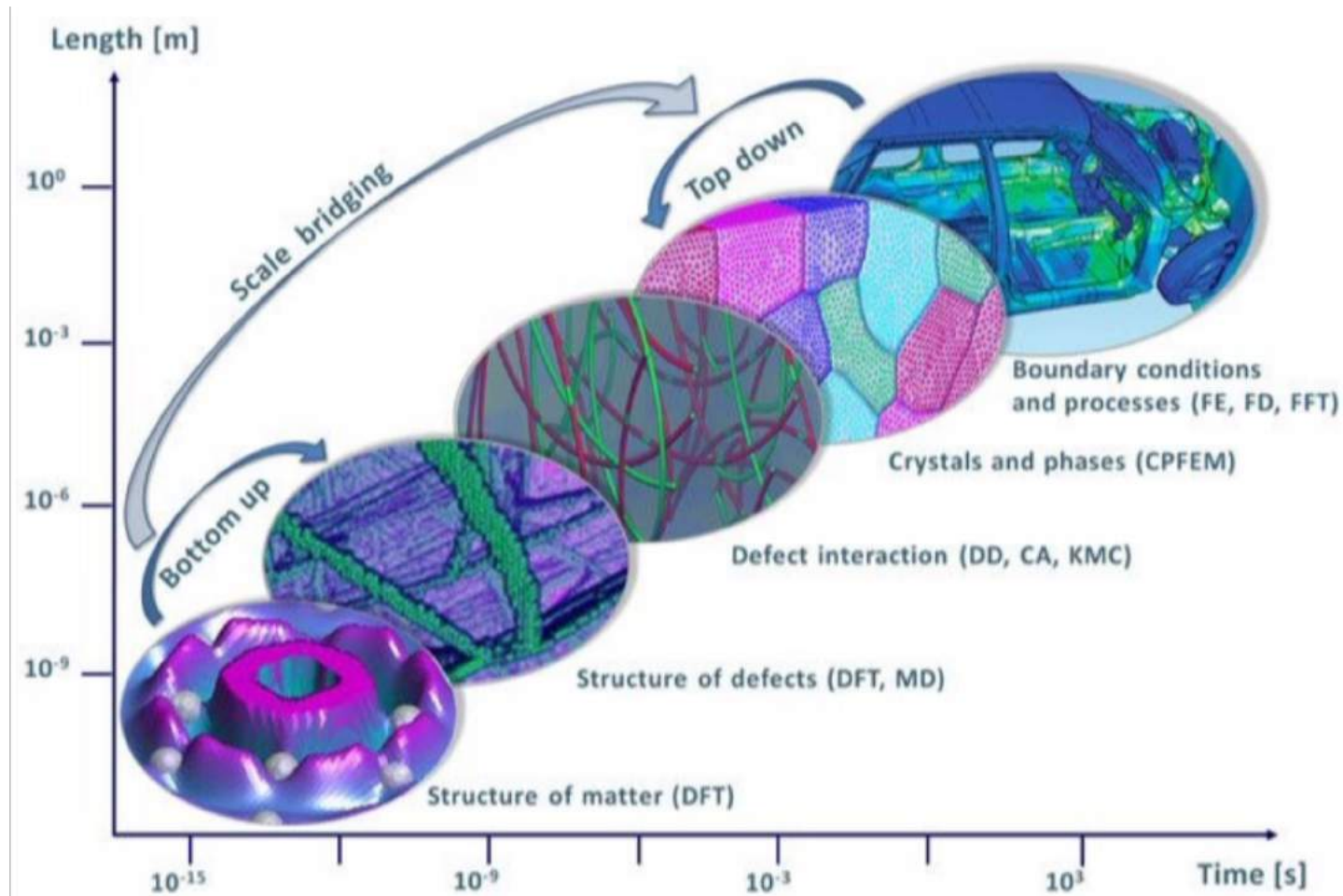
多尺度方法在先进合金中的应用



Multiscale Modeling of Materials in the Max-Planck Society

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

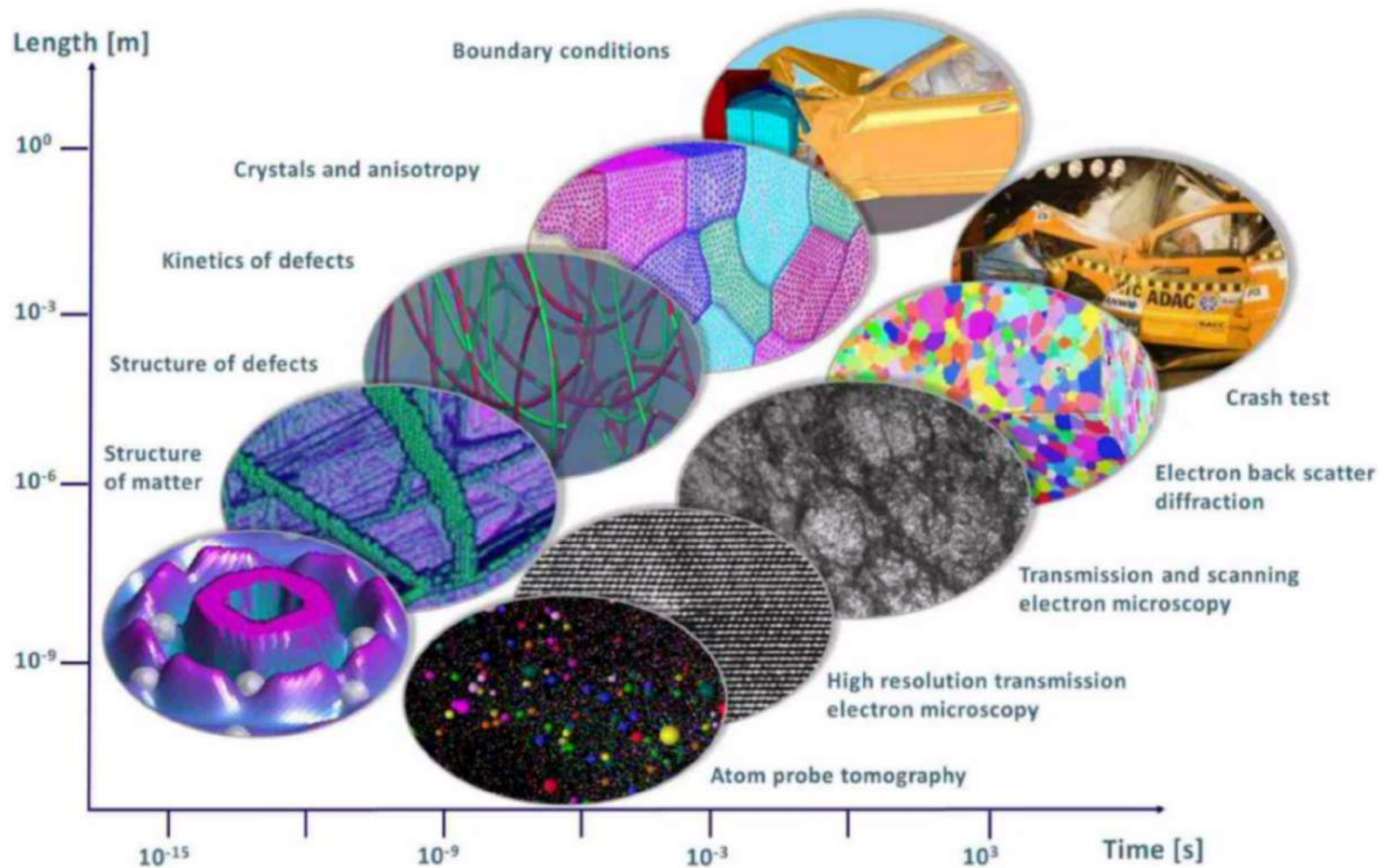
多尺度方法在先进合金中的应用



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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/

Pasquali group @ Rice

多尺度方法在先进复合材料中的应用

Computational

Driving material design through multiscale modeling, topology optimization, and computational tool refinement using high-performance computing.

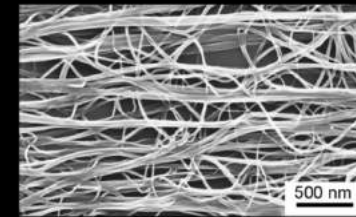
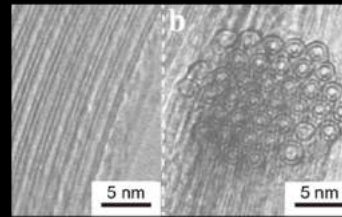
► LAUNCH

- Force field development
- Molecular modeling
- Meso-scale modeling
- Continuum modeling
- Topological optimization



Manufacturing

Scaling-up the manufacturing of highly aligned and concentrated carbon nanotube composite materials.



Material Synthesis

Pioneering precise synthesis techniques and optimizing interphases for carbon nanotube composite performance enhancement.

► LAUNCH

Testing

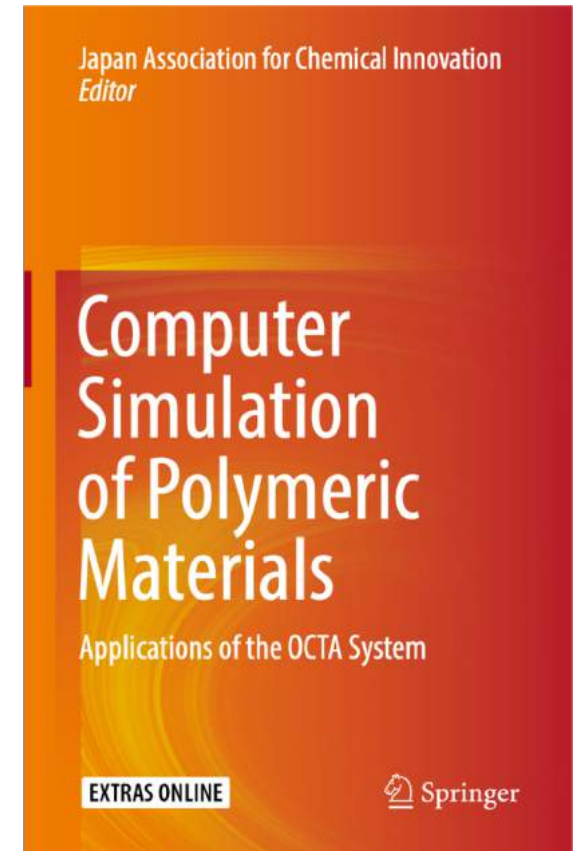
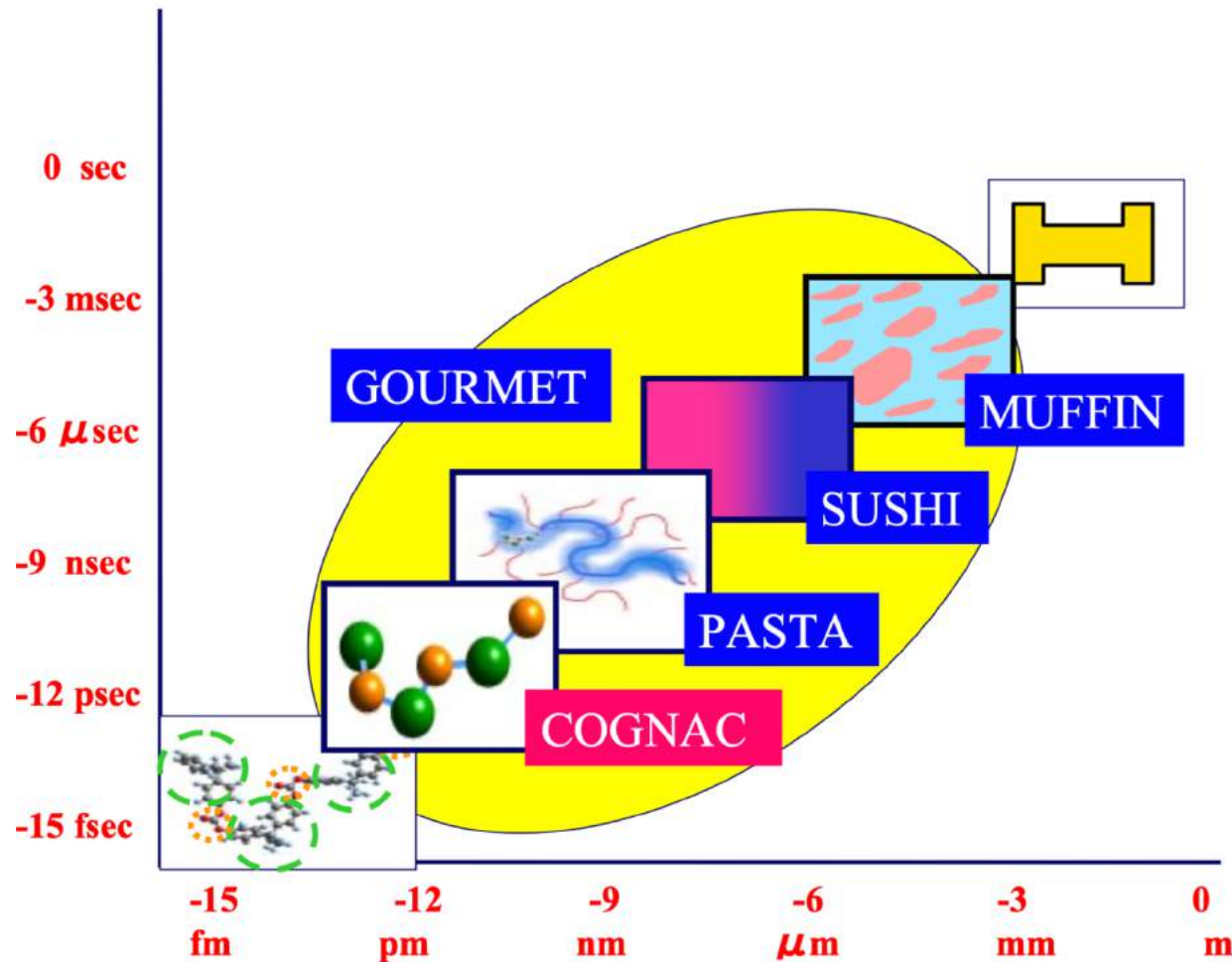
Developing and conducting multiscale characterization of carbon nanotube composite materials.

► LAUNCH

<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.

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>