相场方法

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HUAWEI

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提纲

1. 相场方法基本思想与发展历史

1.1材料微结构演化现象：相变与动边界问题

1.2相场模拟基础：相场变量的选择，总自由能、动力学方程的构建，动力学方程的数值求解格式

1.3相场模型的分类：粗粒化相场、晶体相场和生物膜泡相场

1.4相场方法的发展趋势

2. 相场方法的应用举例

2.1相分离

2.2膜泡形状

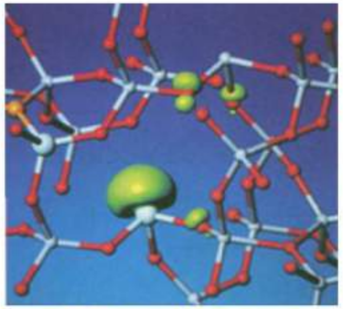
2.3结构相变

2.4位错

2.5裂纹

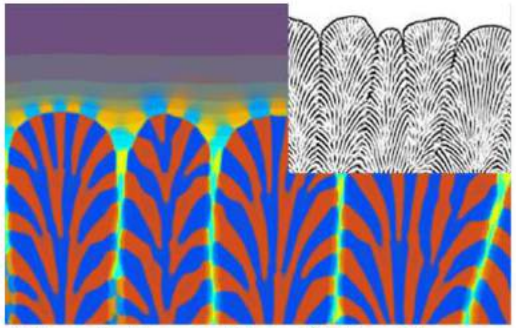
3. 相场方法的上机实践

多尺度固体力学发展趋势



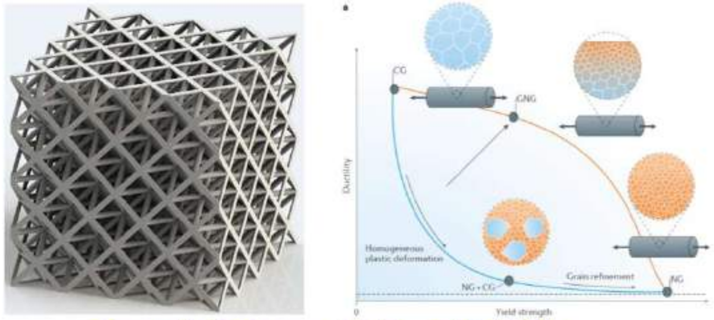
Wimmer*, *Science* 1995, 269,1397

第一性原理计算材料设计



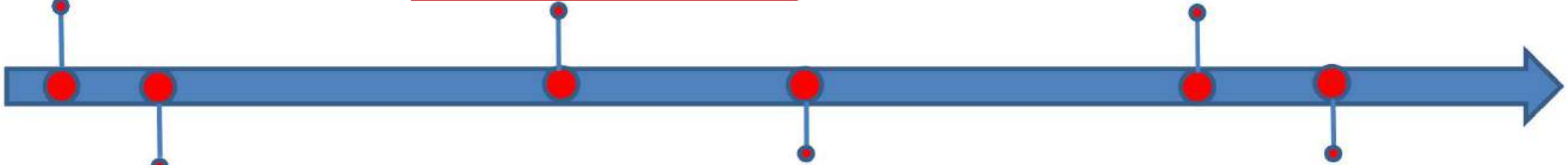
Chen*, *Annu. Rev. Mater. Res.* 2002, 32, 113

相场模拟材料微结构演化

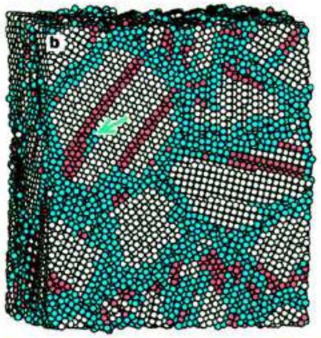


Greer*, *Science* 2014, 345,1322;
Lu*, *Nat. Rev. Mater.* 2016,1,1

微结构调控实现高性能轻质强韧化设计

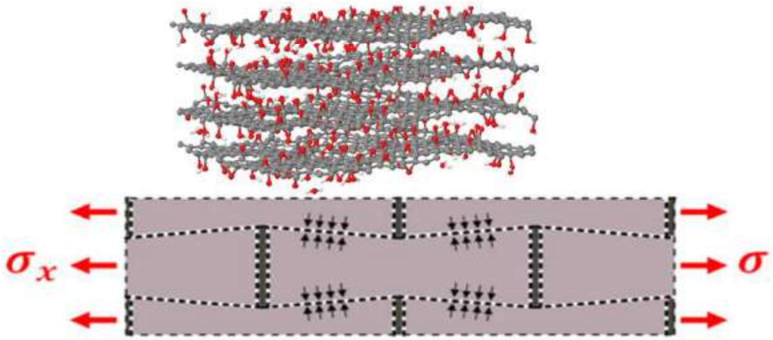


分子动力学模拟



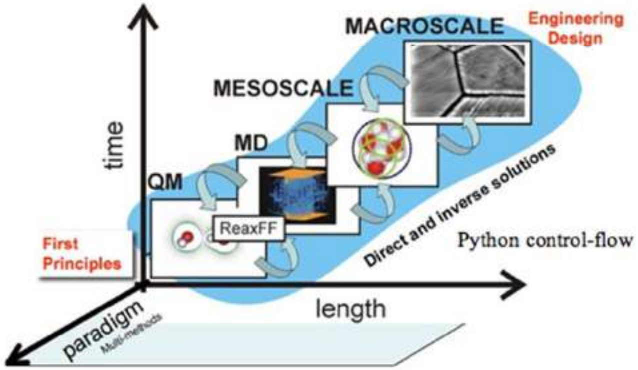
Schiøtz*, *Nature* 1998, 391, 561

仿贝壳纳米单元优化设计

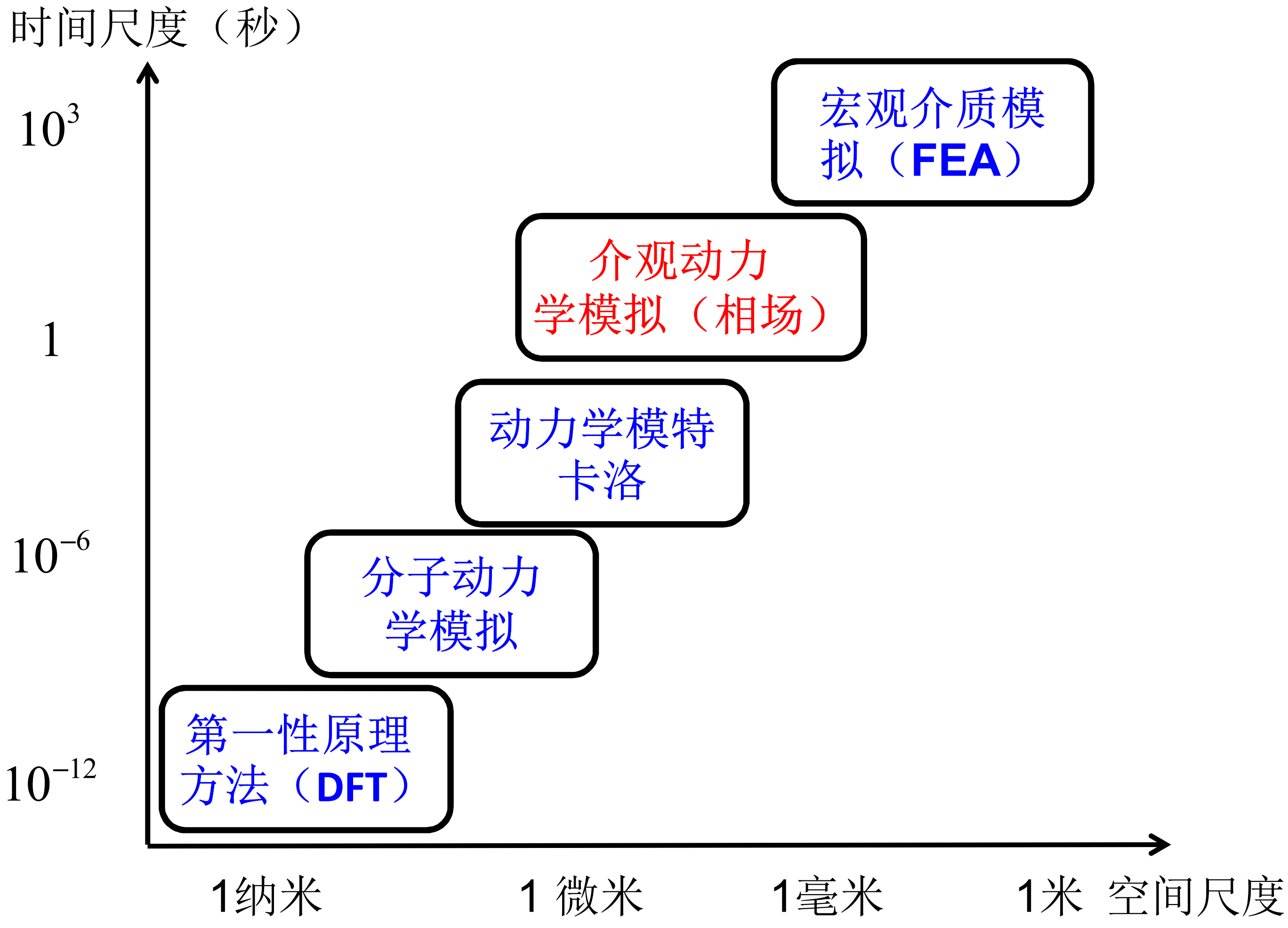


Espinosa*, *Nat. Commun.* 2011, 2,173

多尺度集成计算设计+实验合作



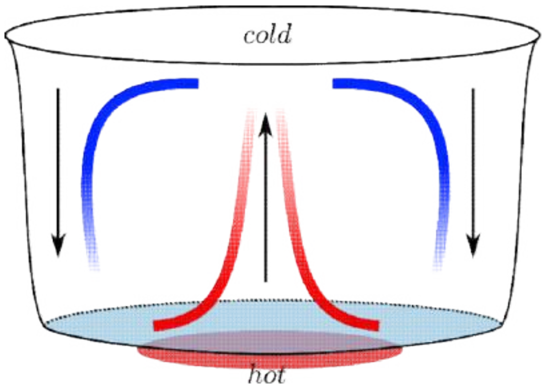
多尺度材料模拟



时间尺度（秒）
10^3
1
10^{-6}
10^{-12}
宏观介质模拟（FEA）
介观动力学模拟（相场）
动力学模特卡洛
分子动力学模拟
第一性原理方法（DFT）
1纳米
1 微米
1毫米
1米 空间尺度

开放系统中的不稳定性与斑图

instability



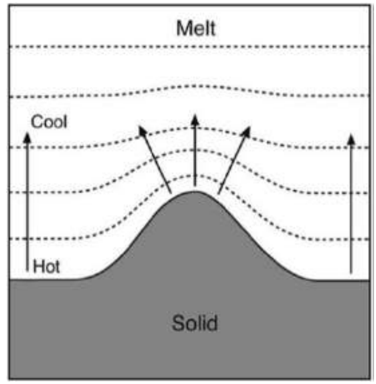
$$\begin{cases}\frac{\partial u}{\partial t}=\nabla^2 u+uv-u-\alpha\\ \frac{\partial v}{\partial t}=d\nabla^2 v+\beta-uv\end{cases}$$

$$u_{ss}=\beta-\alpha;$$

$$v_{ss}=\frac{\beta}{\beta-\alpha}$$

$$\alpha_c=\beta-\sqrt{\beta d}+\frac{d}{2}\left(\sqrt{1+\frac{4\beta}{\sqrt{\beta d}}}-1\right)$$

$$k^2=\frac{(\alpha-\beta)^2-\alpha d}{2d(\alpha-\beta)}$$

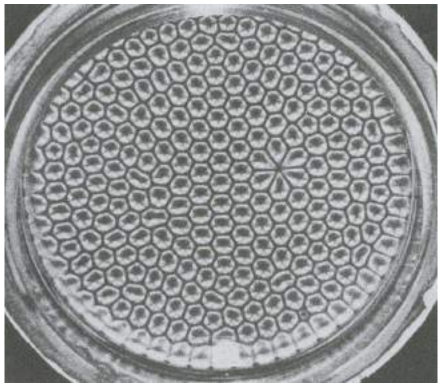


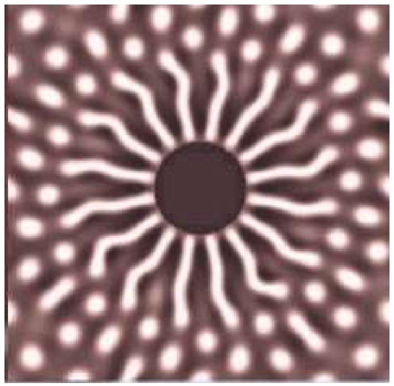
Rayleigh-Benard Instability(1900)

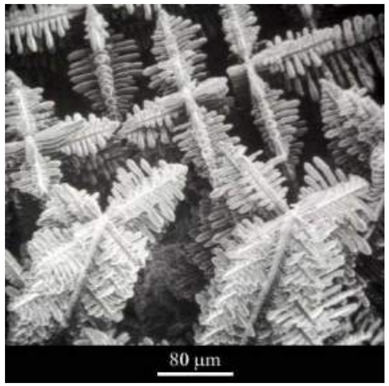
Turing instability (1952)

MS Instability (1963)

Pattern

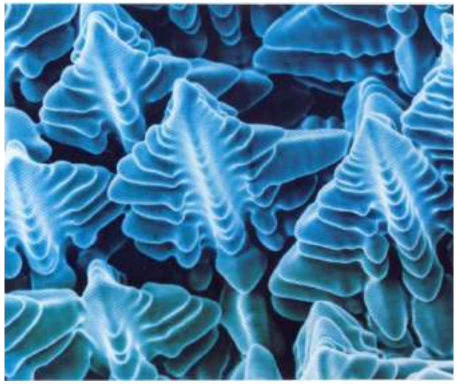




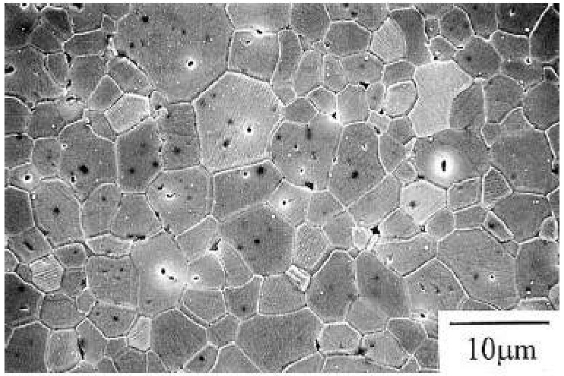


From google images

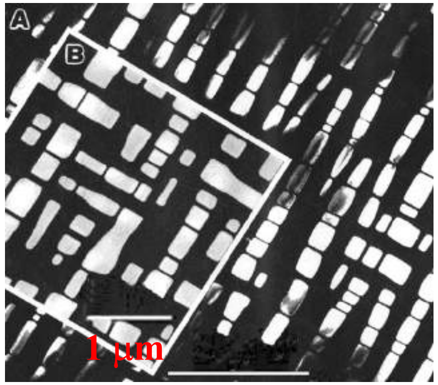
材料微结构演化：各种运动界面



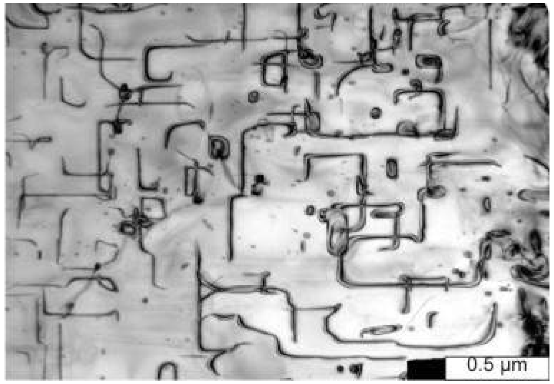
Solidification



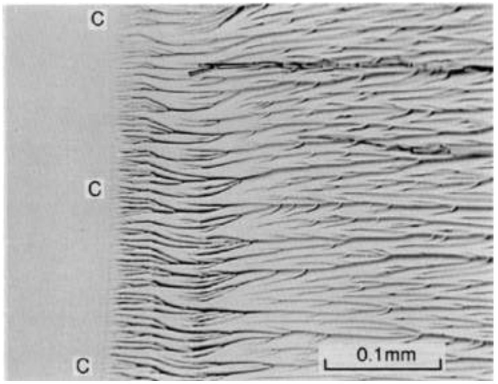
Grain growth



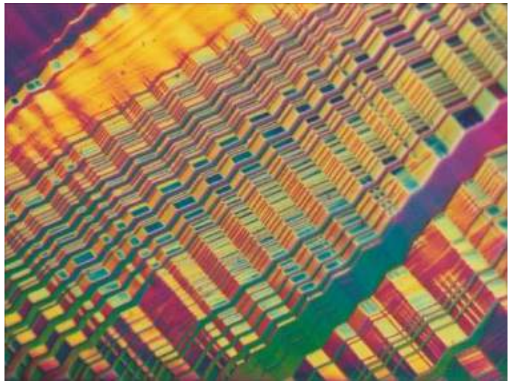
Precipitation



Dislocation network



Crack pattern

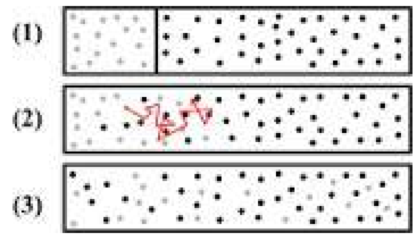


Structural domain

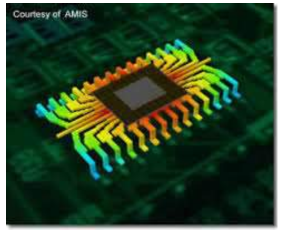
From the google images

微结构演化伴随的各种输运现象

- 扩散 $J_c = -D\nabla C$

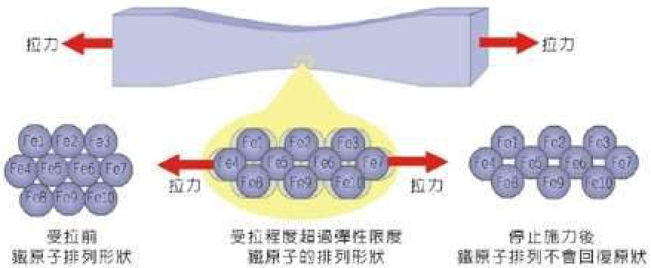


- 热传导 $J_q = -k\nabla T$



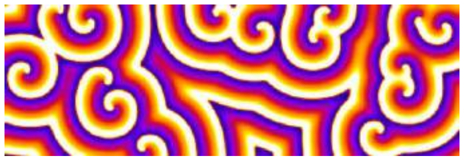
- 电流 $I = \dfrac{-\nabla\Phi}{R}$

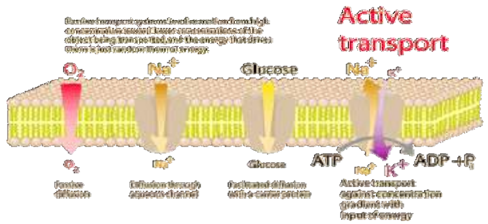
- 粘性，塑性 $\dot{\varepsilon} = \dfrac{\sigma}{\eta}$



- 化学反应 $J_i = L_{ij} A_j$

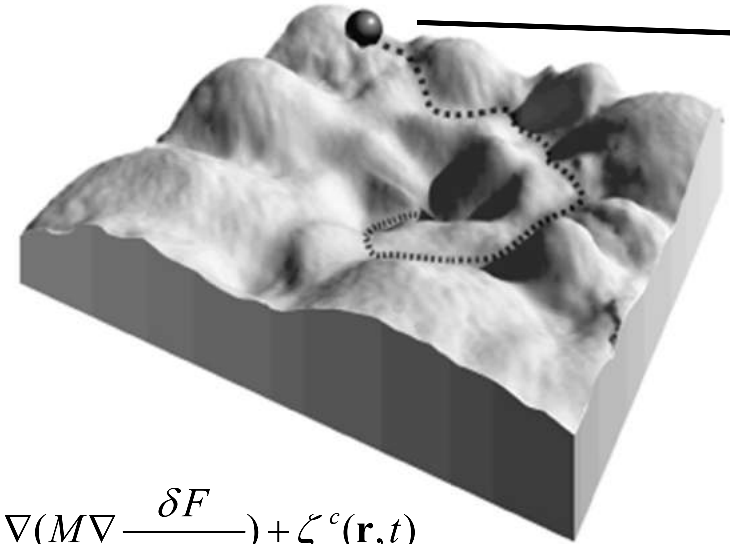
- 开放系统，耗散结构





相场方法的基本原理

$$F\left(c,\eta_i,\varepsilon,\nabla c,\nabla\eta_i,\ldots\right)$$



系统在构形空间中演化

➢ 系统描述:

相场变量选择，扩散界面

➢系统演化:

系统不可逆熵产生大于0

➢热力学: 多重热力学力做功

➢动力学: 多重热力学流耗散

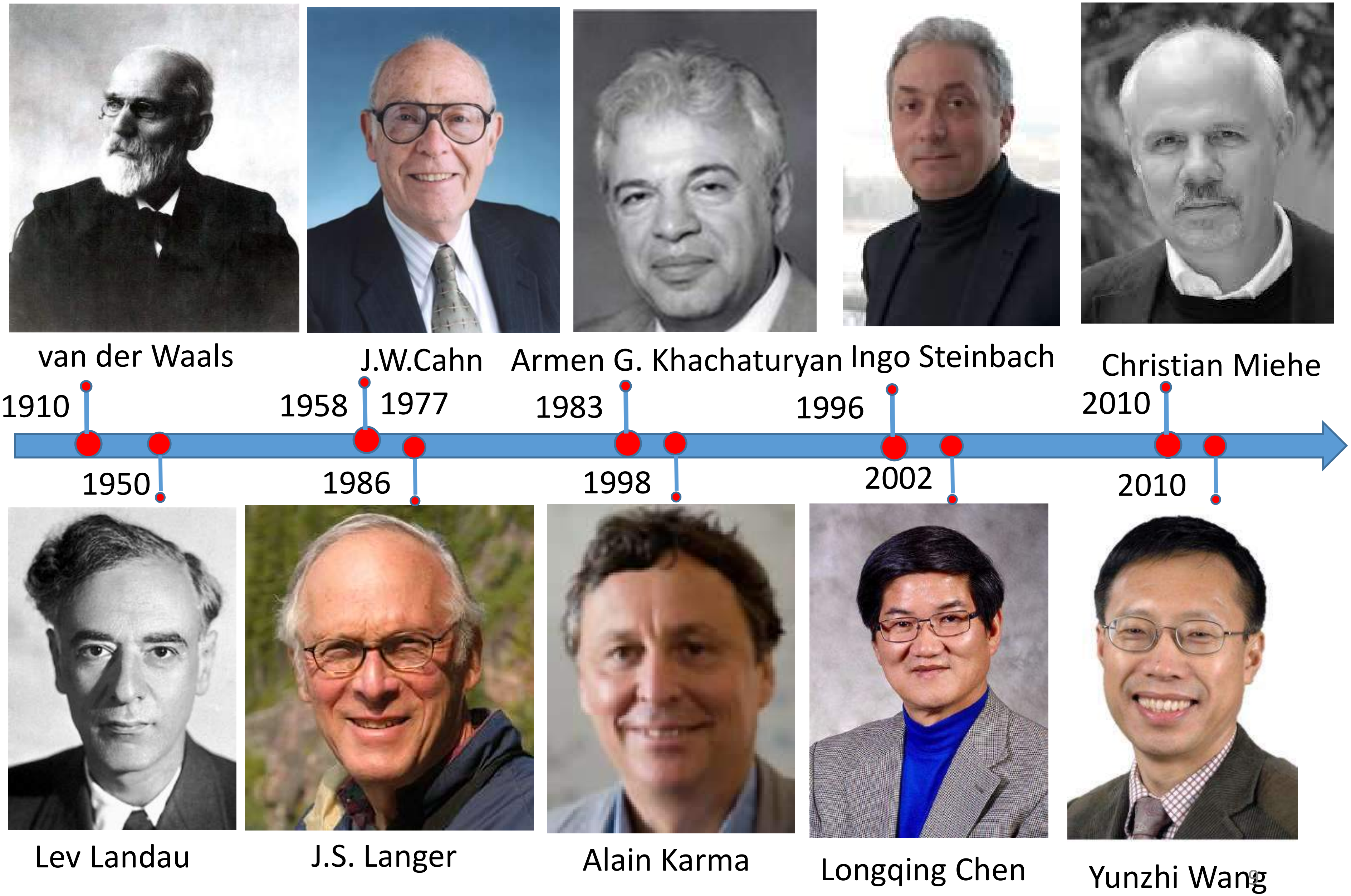
$$\frac{\partial c(\mathbf{r},t)}{\partial t}=\nabla(M\nabla\frac{\delta F}{\delta c(\mathbf{r},t)})+\zeta^{c}(\mathbf{r},t)$$

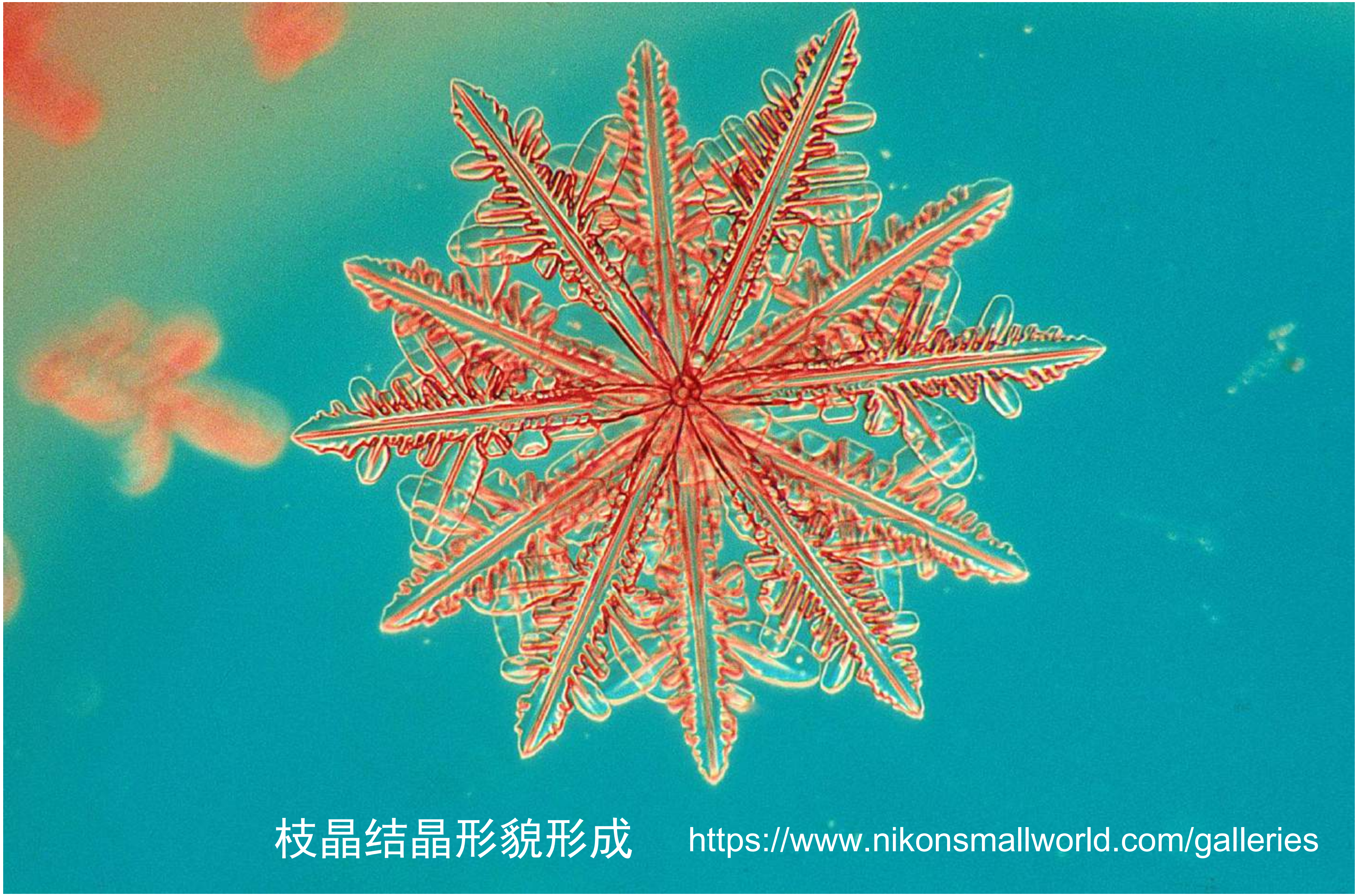
$$\frac{\partial \eta_p(\mathbf{r},t)}{\partial t}=-L\frac{\delta F}{\delta \eta_p(\mathbf{r},t)}+\zeta_p^{\eta}(\mathbf{r},t)$$

GL-like kinetic equations

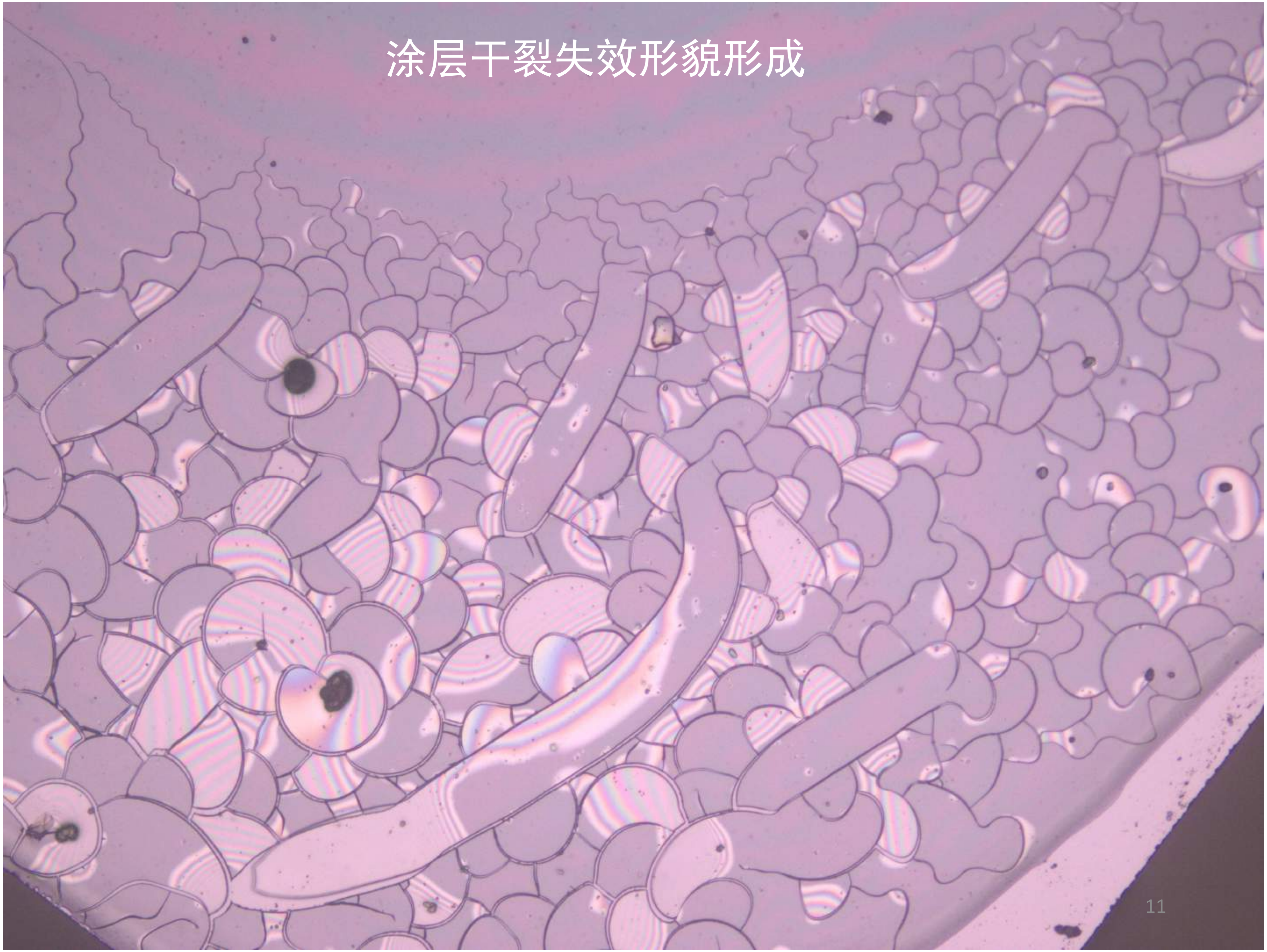
相场法基于密度泛函理论，采用连续变量来模拟不连续现象。 通过引入场变量梯度描述界面，求解基于非平衡热力学建立的场变量时空演化的系列偏微分方程，从而获得瞬时微观结构演化信息。

相场模拟历史

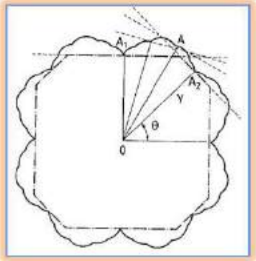

van der Waals
1910
J.W.Cahn
1958
1977
Armen G. Khachaturyan
1983
Ingo Steinbach
1996
Christian Miehe
2010
1950
1986
1998
2002
2010
Lev Landau
J.S. Langer
Alain Karma
Longqing Chen
Yunzhi Wang


枝晶结晶形貌形成
https://www.nikonsmallworld.com/galleries

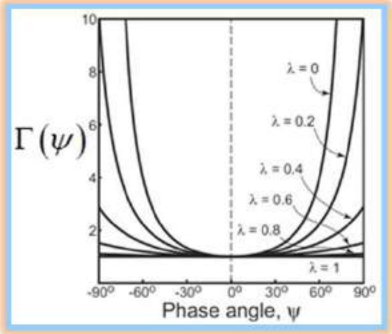
涂层干裂失效形貌形成

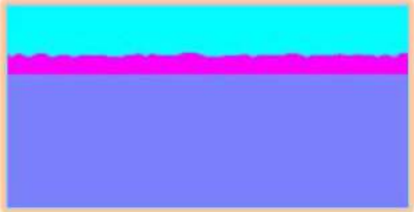


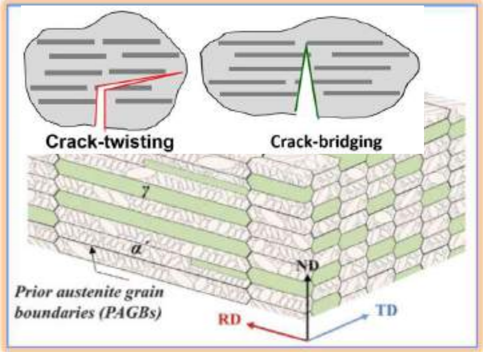
界面演化力学



$$\mathrm{d}G = \gamma(\mathbf{n})\,dA$$







界面热力学-
界面能

C. Herring Phys. Rev. 82 (1951) 87

J. Dundurs (1990)

界面的力学边界条件

界面断裂
与强度

Hutchinson (1992)

P.Sharma(2003)

表界面效应-
尺寸效应

应力驱动
表界面不稳定性

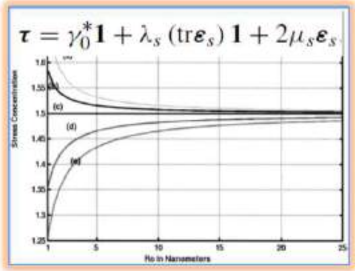
A. Karma et al., Nature (2010)

应力驱动
失效界面演化

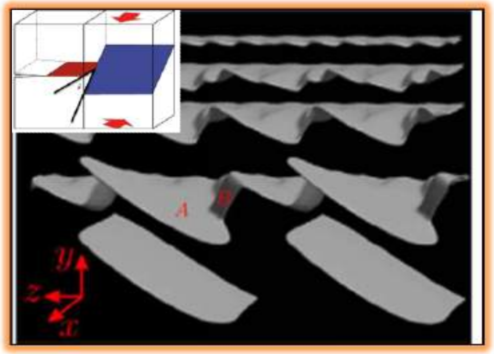
复杂界面结构调控
与力学行为设计

R.O. Ritchie et al., Science (2020)

➢ 理想界面：
面力，位移连续
➢ 非理想界面：
异质界面、表面、分离面、接触面···



$$[\boldsymbol{\sigma}]\cdot\mathbf{n} = -\nabla_s \cdot \boldsymbol{\tau}$$

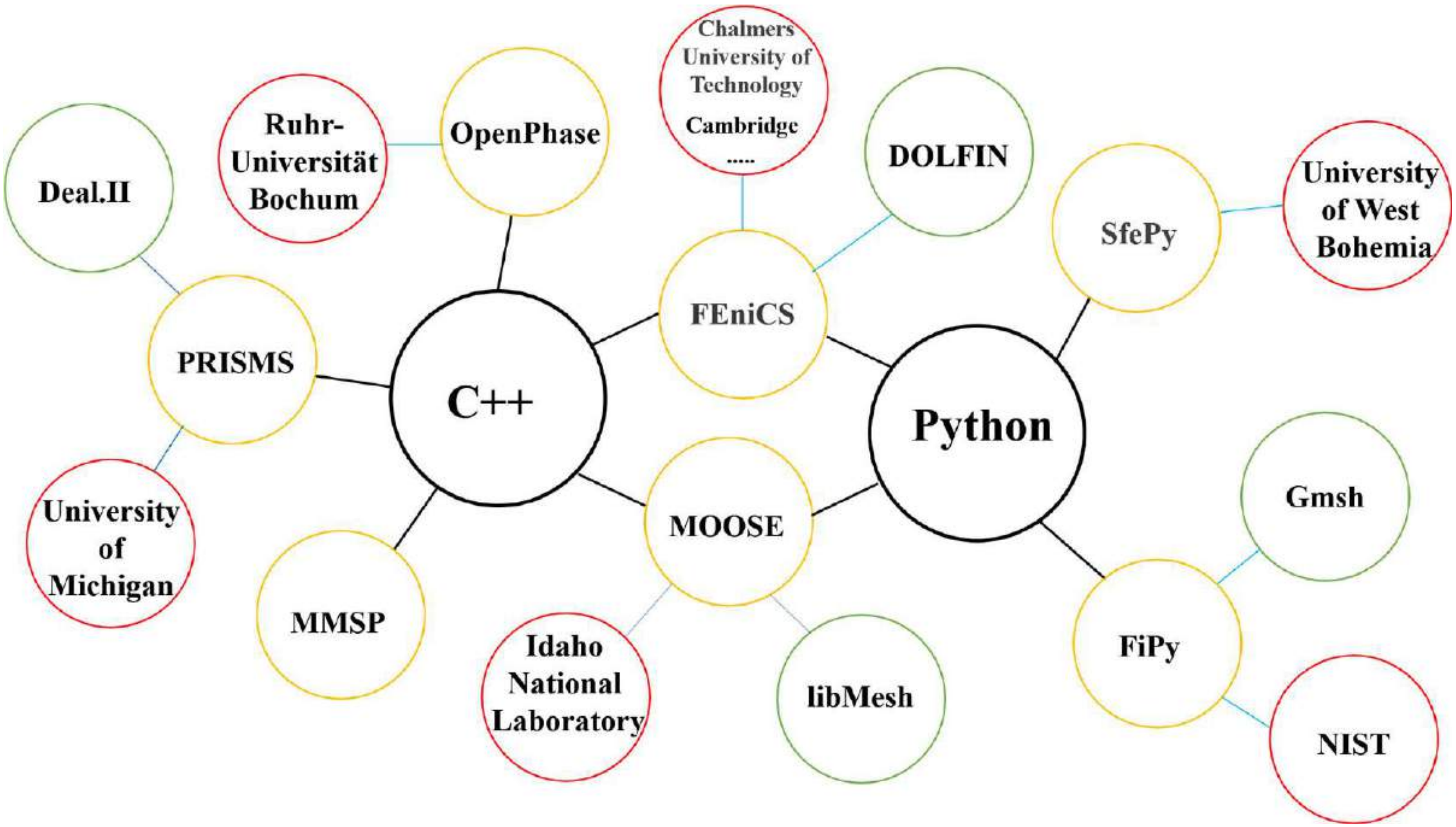


静态、简单几何界面 ➡ 时空演化、复杂拓扑界面

相场模拟软件

软件名称	团队	网址	国别
MOOSE	INL 国家实验室	https://mooseframework.org	美国
μ-PRO@	PSU Long-Qing Chen group	http://mupro.co	美国
OpenPhase Software	Ruhr-University Bochum Ingo Steinbach group	https://openphase-solutions.com	德国
PRISMS-PF	(PRISMS) Center at University of Michigan	http://prisms-center.github.io/phaseField	美国
FEniCS	Chalmers University of Technology	https://fenicsproject.org/	瑞典
FiPy	NIST	https://www.ctcms.nist.gov/fipy/	美国
SfePy	University of West Bohemia	http://sfepy.org/doc-devel/index.html	捷克
COMSOL 多物理场仿真软件		https://cn.comsol.com/	瑞典

相场模拟软件：开源趋势



开发高效的偏微分方程求解器

ACS Energy Lett. 2020, 5, 3254–3259

提纲

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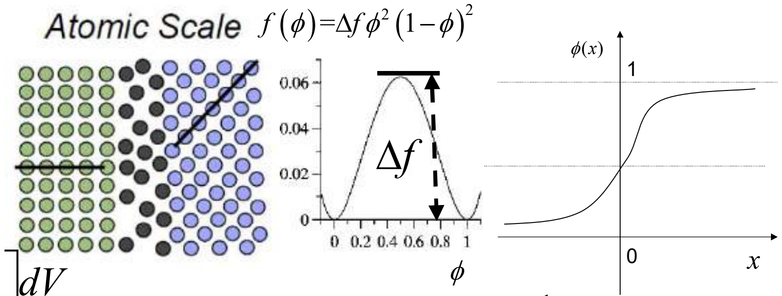
3. 相场方法的上机实践

相场方法的三步曲

相描述

- 相场变量与朗道自由能的选取

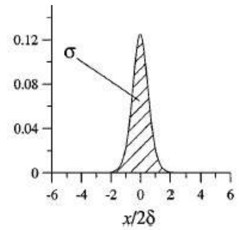
$$F=\int\left[f(\phi)+\beta(\nabla\phi)^2+f_{long}\right]dV$$



$$\delta F=0 \Rightarrow \phi(x)=\frac{1}{2}[1+\tanh(\frac{x}{2\delta})]$$

界面

- 相场变量的高阶梯度描述 $\beta(\nabla\phi)^2$



$$\sigma=\frac{1}{3}\sqrt{\beta\Delta f}$$

$$\delta=\sqrt{\beta/\Delta f}$$

动力学方程

- 非平衡热力学与多物理场多过程耦合

$$\frac{d\phi}{dt}=-L_\phi\left(\frac{\partial F}{\partial\phi}\right)$$

梯度界面模型参数确定方程

$$\beta=3\sigma\delta \qquad \Delta f=3\sigma/\delta$$

等温过程相场模型的非平衡热力学

非守恒序参量 $\boxed{\dfrac{\partial \eta_i}{\partial t} = -L_{ij}\dfrac{\delta F}{\delta \eta_j} + \xi\,(\mathbf{r},t)}$

$\boxed{\mathrm{d}F = -TdS_i \le 0}$

自由能最小化

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{\delta F}{\delta \eta}\frac{\partial \eta}{\partial t}$$

$$= \frac{\delta F}{\delta \eta}\left(-L\frac{\delta F}{\delta \eta}\right)$$

$$= -L\left(\frac{\delta F}{\delta \eta}\right)^2 \le 0$$

Langevin 噪声项： $\langle \xi(\mathbf{r},t)\xi(\mathbf{r}',t')\rangle = 2LK_BT\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$

等温过程相场模型的非平衡热力学

守恒序参量 $\boxed{\frac{\partial \phi_i}{\partial t} + \nabla \cdot J_{\phi_i} = 0}$ $\boxed{J_{\phi_i} = -M \cdot \nabla \frac{\delta F}{\delta \phi_i}}$

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{\delta F}{\delta \phi_i}\frac{\partial \phi_i}{\partial t}$$

$$= \frac{\delta F}{\delta \phi_i}\left(-\nabla \cdot J_{\phi_i}\right)$$

$$= \frac{\delta F}{\delta \phi_i}\left(\nabla_n \cdot M_{nm} \nabla_m \frac{\delta F}{\delta \phi_i}\right)$$

$$= \left(\frac{\delta F}{\delta \phi_i} M_{ij} \nabla \frac{\delta F}{\delta \phi_j}\right)_{\partial S} - M_{mn} \nabla_m \frac{\delta F}{\delta \phi_i} \nabla_n \frac{\delta F}{\delta \phi_i}$$

$$= -M_{mn} \nabla_m \frac{\delta F}{\delta \phi_i} \nabla_n \frac{\delta F}{\delta \phi_i} \le 0$$

等温过程相场模型的非平衡热力学

耦合序参量

$$\frac{\partial \eta_i}{\partial t} = -L_{ij}\frac{\delta F}{\delta \eta_j}$$

$$\frac{\partial \phi_i}{\partial t} = \nabla \cdot M\nabla \frac{\delta F}{\delta \phi_i}$$

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{\delta F}{\delta \phi_i}\frac{\partial \phi_i}{\partial t} + \frac{\delta F}{\delta \eta_i}\frac{\partial \eta_i}{\partial t}$$

$$= -M_{mn}\nabla_m \frac{\delta F}{\delta \phi_i}\nabla_n \frac{\delta F}{\delta \phi_i} - L_{ij}\left(\frac{\delta F}{\delta \eta_i}\right)\left(\frac{\delta F}{\delta \eta_j}\right)$$

$$\leq 0$$

非等温单组分固化相场模型的非平衡热力学

$$\frac{ds}{dt} = -\nabla\cdot J_s + \dot{\sigma}$$

$$ds = \left(\frac{\partial s}{\partial u}\right)_\phi du + \left(\frac{\partial s}{\partial \phi}\right)_u d\phi \qquad \frac{du}{\partial t} = -\nabla\cdot \mathbf{j}_u$$

$$\frac{ds}{dt} = \left(\frac{\partial s}{\partial u}\right)_\phi (-\nabla\cdot \mathbf{j}_u) + \boxed{\frac{-1}{T}\left(\frac{\partial f}{\partial \phi}\right)_T} \frac{d\phi}{dt} \qquad \left(\frac{\partial s}{\partial u}\right)_\phi = \frac{1}{T}$$

$$ds = \frac{du}{T} - \frac{1}{T}\left(\frac{\partial u}{\partial \phi}\right)_s d\phi \qquad du = 0 \qquad \left(\frac{\partial s}{\partial \phi}\right)_u = -\frac{1}{T}\left(\frac{\partial u}{\partial \phi}\right)_s$$

$$f = u - Ts \qquad df = -sdT + \left(\frac{\partial u}{\partial \phi}\right)_s d\phi \qquad \left(\frac{\partial s}{\partial \phi}\right)_u = \frac{-1}{T}\left(\frac{\partial f}{\partial \phi}\right)_T$$

非等温单组分固化相场模型的非平衡热力学

$$\mathbf{J}_s = \frac{\mathbf{j}_u}{T}$$

$$\boxed{\dot{\sigma} = \mathbf{j}_u \cdot \nabla \frac{1}{T} + \frac{-1}{T}\left(\frac{\partial f}{\partial \phi}\right)\frac{d\phi}{dt} \geq 0}$$

等温过程： $\nabla \frac{1}{T} = 0$ $\quad \frac{d\phi}{dt} = -L\left(\frac{\partial f}{\partial \phi}\right)$

非等温过程： $\nabla \frac{1}{T} \neq 0$ $\quad \mathbf{j}_u = M\nabla \frac{1}{T}$ $\quad \boxed{\frac{d\phi}{dt} = -L\left(\frac{\partial f}{\partial \phi}\right)}$

$$\frac{du}{dt} = -\nabla \cdot \left(M\nabla \frac{1}{T}\right)$$

$$u = p(\phi)u_s(T) + \left[1 - p(\phi)\right]u_L(T) \qquad p(\phi) = \begin{matrix} 1 & \text{solid phase} \\ 0 & \text{liquid phase} \end{matrix}$$

$$f = p(\phi)f_s\left[u_s(T)\right] + \left[1 - p(\phi)\right]f_L\left[u_L(T)\right] + wg(\phi)$$

非等温单组分固化相场模型的非平衡热力学

$$u = p(\phi)u_s(T) + \left[1 - p(\phi)\right]u_L(T) \qquad L(T) = u_L(T) - u_s(T)$$

$$= u_L(T) - p(\phi)L(T)$$

$$f = u - Ts + wg(\phi) \qquad \frac{\partial(f/T)}{\partial T} = -\frac{u}{T^2}$$

$$f(T,\phi) = T\left(-\int_T^{T_M} \frac{u}{\xi^2} d\xi\right) + wg(\phi)$$

$$= T\left(-\int_T^{T_M} \frac{u_L}{\xi^2} d\xi - p(\phi)\int_T^{T_M} \frac{L(\xi)}{\xi^2} d\xi\right) + wg(\phi)$$

$$\frac{du}{dt} = \dot{u}_L - \dot{p}(\phi)L(T) - p(\phi)\dot{L}(T) \qquad \frac{du}{dt} = -\nabla \cdot \left(M\nabla\frac{1}{T}\right)$$

$$u_L(T) = u_L(T_M) + c_v(T - T_M)$$

非等温单组分固化相场模型的非平衡热力学

$$k\nabla^2 T = c_v\dot{T} - p'(\phi)L(T)\dot{\phi} - p(\phi)L'(T)\dot{T} \qquad M = kT^2$$

$$\frac{d\phi}{dt} = -L_\phi \frac{\delta F}{\delta \phi} \qquad \dot{\phi} = -L_\phi\left(-p'(\phi)\int_T^{T_M}\frac{L(\xi)}{\xi^2}d\xi + wg'(\phi) - \varepsilon_\phi\nabla^2\phi\right)$$

$L(T)$ 为常数

$$\dot{T} = \frac{1}{c_v}\nabla\cdot(k\nabla T) + \frac{L(T)}{c_v}p'(\phi)\dot{\phi}$$

非等温多组分固化过程相场模型的非平衡热力学

$$\frac{ds}{dt} = -\nabla \cdot \mathbf{J}_s + \dot{\sigma}$$

$$ds = \left(\frac{\partial s}{\partial u}\right)_{\phi,c} du + \left(\frac{\partial s}{\partial \phi}\right)_{u,c} d\phi + \left(\frac{\partial s}{\partial c}\right)_{u,\phi} dc$$

$$\frac{du}{\partial t} = -\nabla \cdot \mathbf{j}_u \qquad \frac{dc}{\partial t} = -\nabla \cdot \mathbf{j}_c \qquad \mathbf{J}_s = \frac{\mathbf{j}_u - \mu \mathbf{j}_c}{T}$$

$$\frac{ds}{dt} = \frac{1}{T}(-\nabla \cdot \mathbf{j}_u) \boxed{-\frac{1}{T}\left(\frac{\partial f}{\partial c}\right)_{\phi,T}} (-\nabla \cdot \mathbf{j}_c) \boxed{-\frac{1}{T}\left(\frac{\partial f}{\partial \phi}\right)_{c,T}} \frac{d\phi}{dt}$$

$$\dot{\sigma} = \mathbf{j}_s \cdot \nabla \frac{1}{T} - \mathbf{j}_c \cdot \frac{1}{T} \nabla \left[\left(\frac{\partial f}{\partial c}\right)_{\phi,T}\right] - \frac{1}{T}\left(\frac{\partial f}{\partial \phi}\right)_{c,T} \frac{d\phi}{dt} \geq 0$$

等温过程： $\nabla \frac{1}{T} = 0$ $$\frac{d\phi}{dt} = -L\left(\frac{\partial f}{\partial \phi}\right)$$

$$\frac{dc}{dt} = -\nabla \cdot \left[\frac{-M_c}{T} \nabla \left(\frac{\partial f}{\partial c}\right)\right]$$

非等温过程： $\nabla \frac{1}{T} \neq 0$ $\mathbf{j}_s = M \nabla \frac{1}{T}$ $$\boxed{\frac{d\phi}{dt} = -L\left(\frac{\partial f}{\partial \phi}\right)}$$

$$\frac{du}{dt} = -\nabla \cdot \left(M \nabla \frac{1}{T}\right) \qquad \boxed{\frac{dc}{dt} = -\nabla \cdot \left[\frac{-M_c}{T} \nabla \left(\frac{\partial f}{\partial c}\right)\right]}$$

$$u = p(\phi) u_s(T,c) + [1 - p(\phi)] u_L(T,c) \quad p(\phi) = \begin{cases} 1 & \text{solid phase} \\ 0 & \text{liquid phase} \end{cases}$$

$$f = p(\phi) f_s[u_s(T,c)] + [1 - p(\phi)] f_L[u_L(T,c)] + wg(\phi)$$

$$\boxed{\frac{du}{dt} = \dot{u}_L - \dot{p}(\phi) L(T) - p(\phi) \dot{L}(T) = -\nabla \cdot \left(M \nabla \frac{1}{T}\right)}$$

相场方程的数值计算方法

$$\frac{\partial C}{\partial t}=\nabla\cdot\left(\frac{D}{N_v k_B T}\nabla\frac{\delta F^{tot}}{\delta C}\right)$$

$$F^{tot}=\int_V N_V\left[\Omega C\left(1-C\right)+k_B T\left(C\ln C+\left(1-C\right)\ln\left(1-C\right)\right)+\frac{\kappa}{2}\left|\nabla C\right|^2\right]dV,$$

$$\Omega^*=\frac{\Omega}{k_B T}\qquad t^*=\frac{Dt}{l^2}\qquad \nabla^*=\nabla l\qquad \kappa^*=\frac{\kappa}{k_B T l^2}$$

$$f^*=\Omega^* C\left(1-C\right)+\left(C\ln C+\left(1-C\right)\ln\left(1-C\right)\right)$$

$$\frac{\partial C}{\partial t^*}=\left(\nabla^*\right)^2\left[\frac{\partial f^*}{\partial C}-2\kappa^*\left(\nabla^*\right)^2 C\right]$$

•有限差分法: 多重网格

•时间显式差分，空间采用半隐式傅里叶谱方法

•有限元法：自适应网格

王杰等，材料微结构演化的相场模拟，固体力学学报，37, 1-33(2016)

半隐式傅里叶谱方法

$$\frac{\partial \tilde{C}(\xi,t)}{\partial t} = -\xi^2 \tilde{f}^*(C(\xi,t)) - k^* \xi^4 \tilde{C}(\xi,t)$$

$$\tilde{C}^{n+1} = \frac{\tilde{C}^n - \xi^2 \tilde{f}^*(C^n)\Delta t}{1 + k^* \xi^4 \Delta t}$$

$$\xi = \frac{\pi}{\mathrm{N}}\left[0,\ldots\frac{N}{2}-1,-\frac{N}{2},\ldots-1\right]$$

优点：

•微分方程变为了代数方程

•利用快速Fourier变换，大大提高计算效率

缺点：

•周期边界条件

•高阶振荡

Chen, L. Q., & Shen, J. Applications of semi-implicit Fourier-spectral method to phase field equations. Computer Physics Communications, 108, 147-158 (1998).

提纲

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1.3相场模型的分类：粗粒化相场、晶体相场和生物膜泡相场。

1.4相场方法的发展趋势。

2. 相场方法的应用举例

2.1相分离

2.2膜泡形状

2.3结构相变

2.4位错

2.5裂纹

3. 相场方法的上机实践

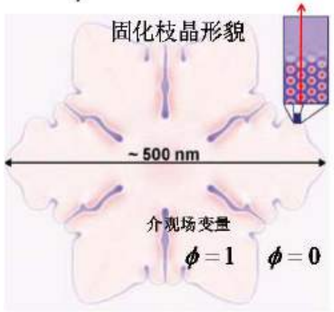
➢ 微观相场模型

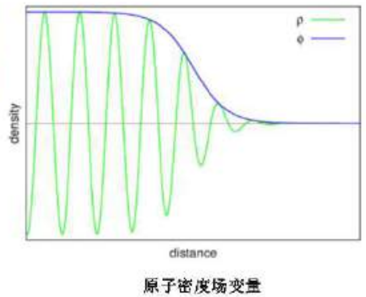
$$\frac{\mathrm{d}P(\boldsymbol{r},t)}{\mathrm{d}t}=\sum_{\boldsymbol{r}'}L(\boldsymbol{r}-\boldsymbol{r}')\left[\frac{\delta F}{\delta P(\boldsymbol{r}',t)}\right]$$

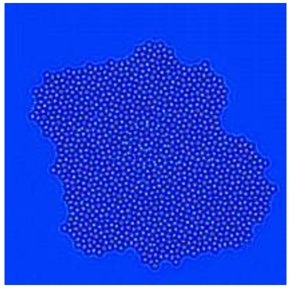
Khachaturyan, A. G. (2013). Theory of structural transformations in solids. Courier Corporation.

$$F_{\text{chem}}=\frac{1}{2}\sum_{\boldsymbol{r},\boldsymbol{r}'}W(\boldsymbol{r}-\boldsymbol{r}')P(\boldsymbol{r})P(\boldsymbol{r}')+k_BT\sum_{\boldsymbol{r}}[P(\boldsymbol{r})\ln(P(\boldsymbol{r}))+(1-P(\boldsymbol{r}))\ln(1-P(\boldsymbol{r}))]$$

➢ 晶体相场模型



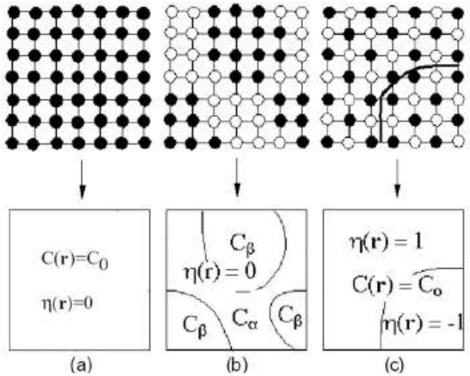




$$\frac{\partial\psi}{\partial t}=\Gamma\nabla^2\frac{\delta F}{\delta\psi}$$

$$F\left[\psi(\vec{r})\right]=\int d\vec{r}\left\{\frac{1}{2}\psi(\vec{r})\left[-\varepsilon+\lambda\prod_{m=1}^{n}\left(\left(k_m^2+\nabla^2\right)^2+b_m\right)\right]\psi(\vec{r})-\frac{\tau}{3}\psi(\vec{r})^3+\frac{1}{4}\psi(\vec{r})^4\right\}$$

➢ 粗粒化相场模型

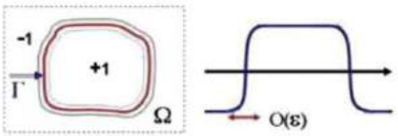


$$\frac{\partial c(\mathbf{r},t)}{\partial t}=M\nabla^2\frac{\delta F_{tot}}{\delta c(\mathbf{r},t)}+\xi\,(\mathbf{r},t)$$

$$\frac{\partial\eta_1(\mathbf{r},t)}{\partial t}=-\hat{L}_{1j}\frac{\delta F_{tot}}{\delta\eta_j(\mathbf{r},t)}+\xi_1(\mathbf{r},t)$$

➢生物膜泡相场

$$\mathcal{E}_b=\int_\Gamma H^2\,\mathrm{d}s.\qquad \mathcal{E}_\epsilon^b(\psi)=\frac{1}{\epsilon}\int_\Omega\left(\epsilon\Delta\psi+\frac{1}{\epsilon}\psi(1-\psi^2)\right)^2\mathrm{d}\Omega$$



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✓ 非线性相场(PRE 86, 051609 (2012))

$$F=\frac{1}{v_m}\int_V\left[f(\xi,\eta)+\frac{1}{2}\kappa(\nabla\xi)^2\right]dV \quad \frac{\partial\xi}{\partial t}=-RTk_n\left[\exp\left(\frac{\alpha\,\delta F/\delta\xi}{RT}\right)-\exp\left(-\frac{\beta\delta F/\delta\xi}{RT}\right)\right]$$

✓ 多相、非平衡相变与多过程耦合

✓ 相场与DFT等微观模型的结合

✓ 相场模型与相图计算的结合

✓ 相场模型应用场景的扩展（断裂、位错、能源材料、辐照微结构…）

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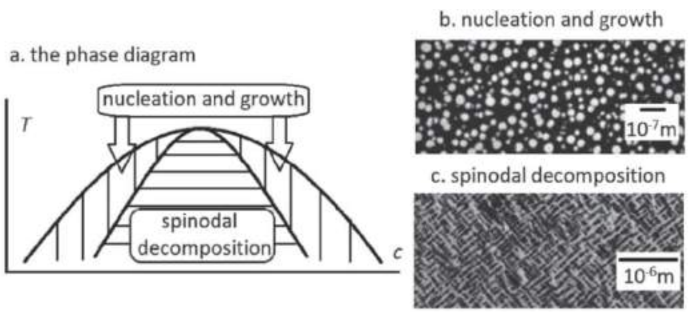
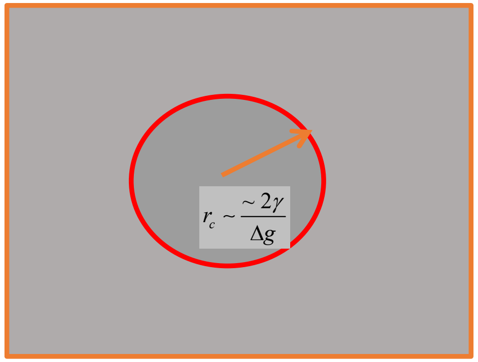
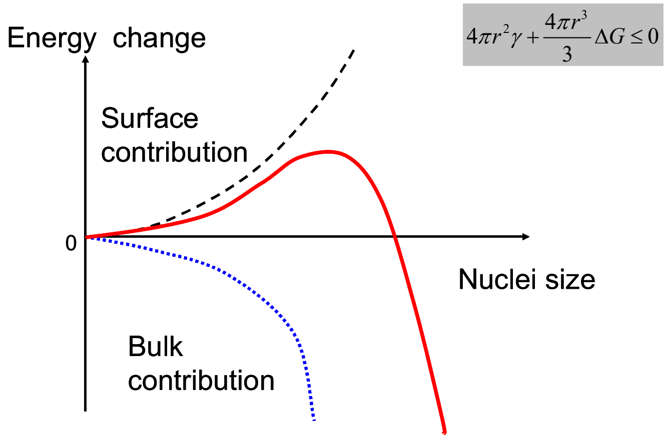
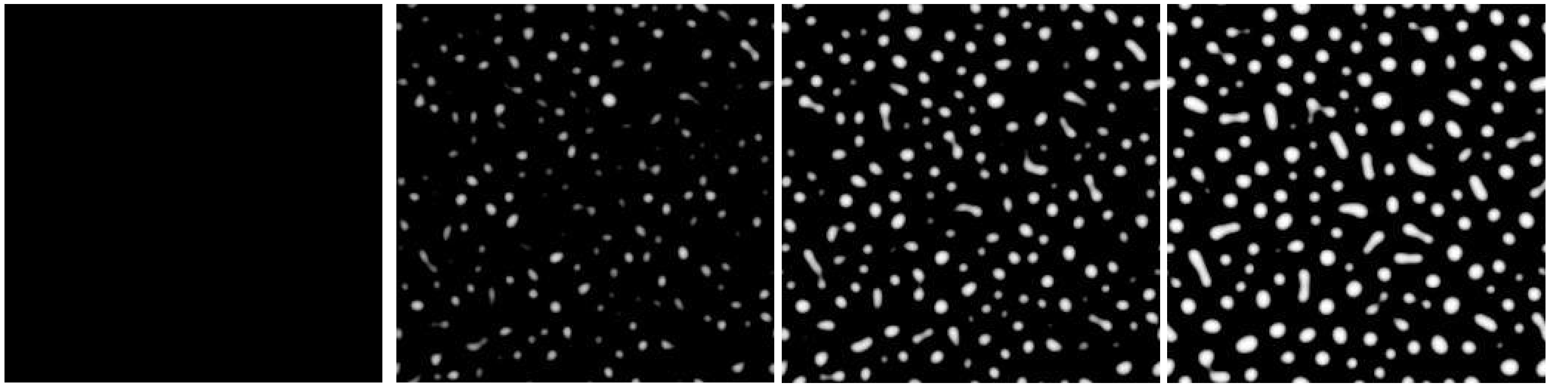
相分离：成核生长模式





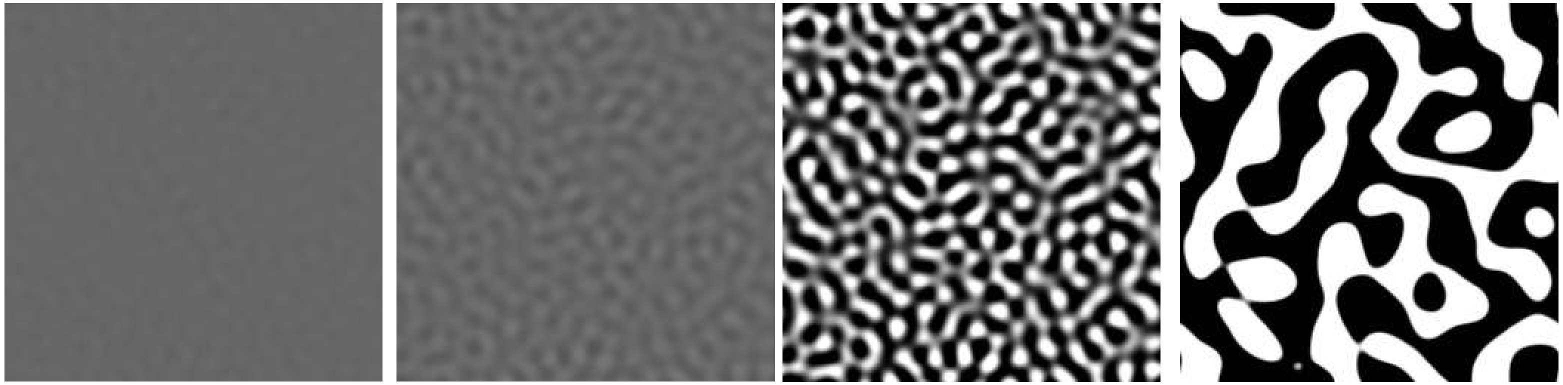


基于Cahn-Hilliard方程的相场模拟

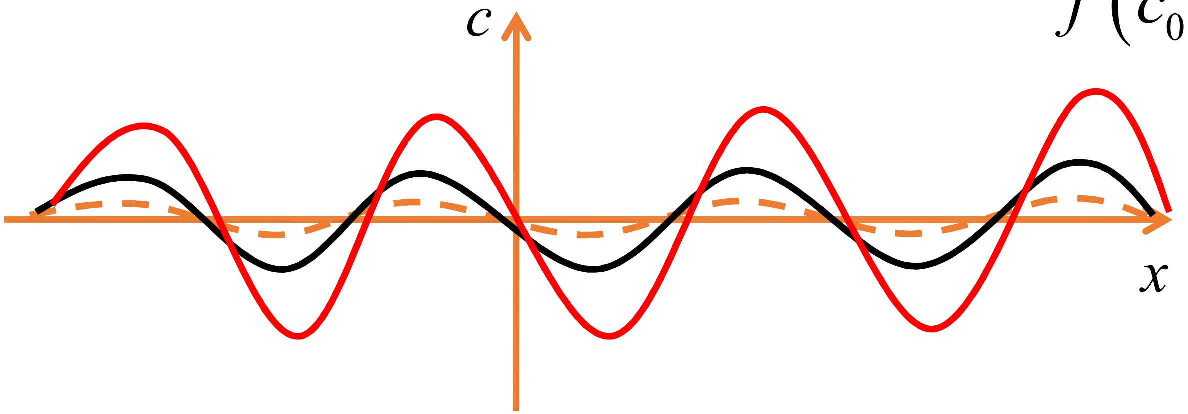


time

基于Cahn-Hilliard方程的相场模拟



time



$$f\left(c_0+\Delta c\right)+\beta\left[\nabla\left(c_0+\Delta c\right)\right]^2$$

$$\Delta c=\delta\sin\frac{2\pi}{\lambda}x$$

$$\lambda_c\sim 2\pi\sqrt{-\beta\Big/\frac{\partial^2 f}{\partial c_0^2}}$$

相分离：旋节分解模式

（Spinodal decomposition）

管状有序多级结构的形成与演化

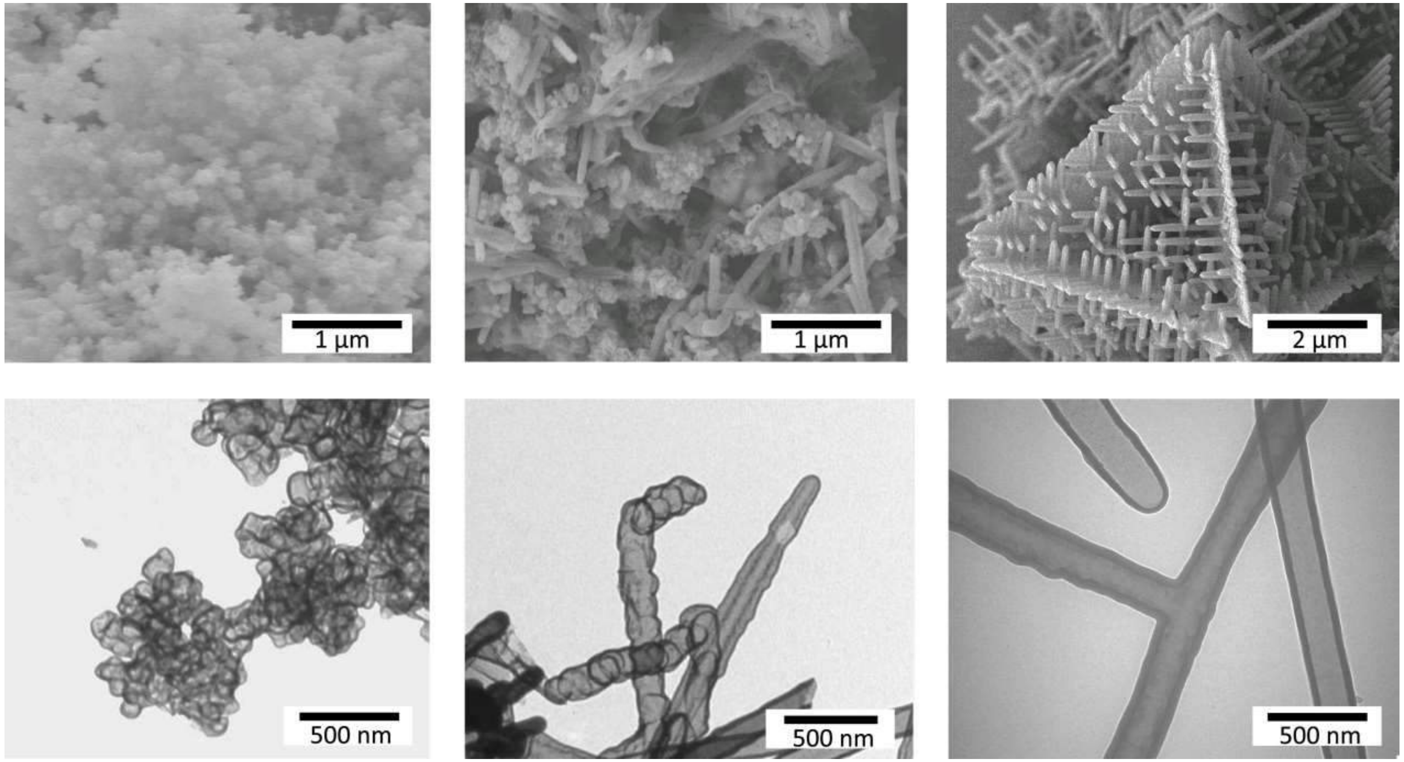


Fig. 1. The morphology of PN with different reaction time. (a), (b) and (c) SEM images of PN with reaction time of 1h, 3h and 9h, respectively. (d), (e) and (f) TEM images of PN with reaction time of 1h, 3h and 9h, respectively.

曲率弹性驱动空心球融合为纳米管

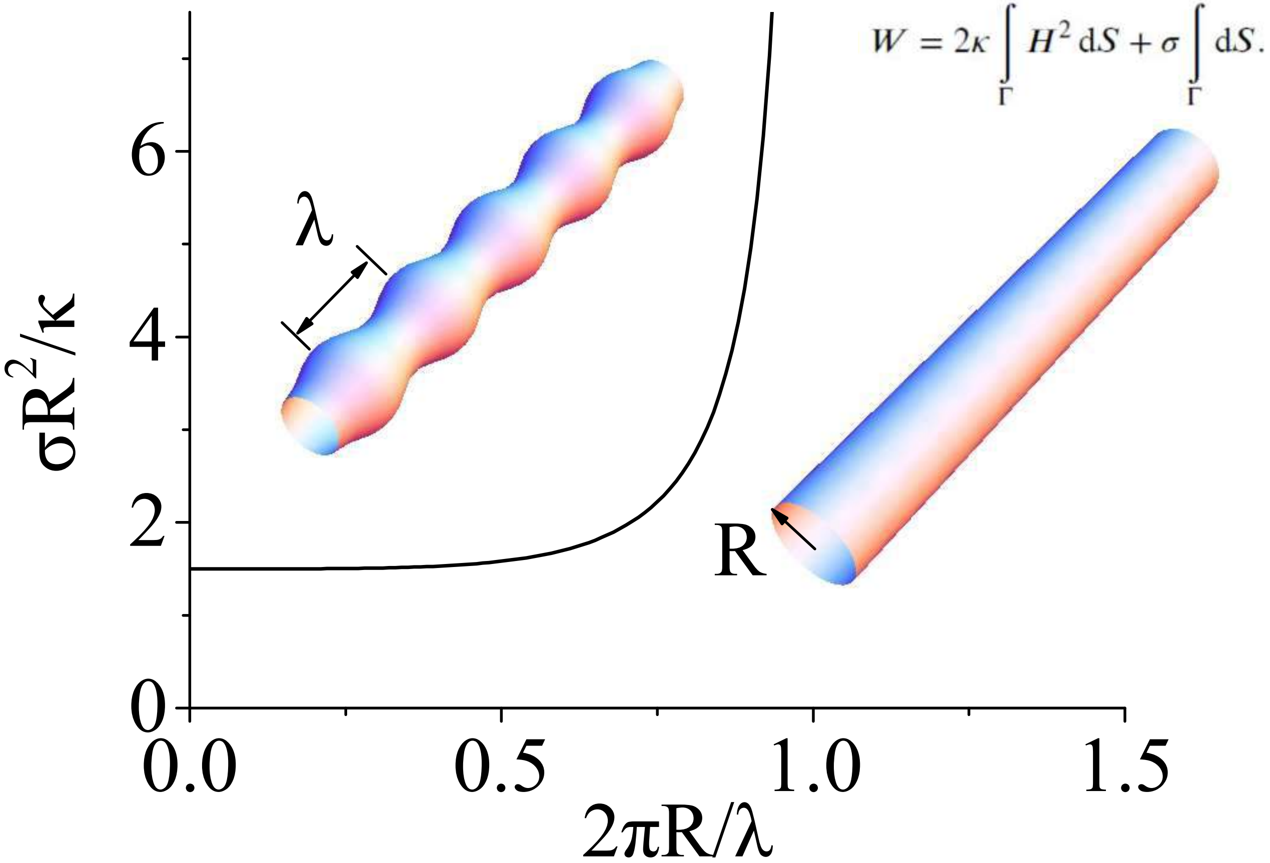
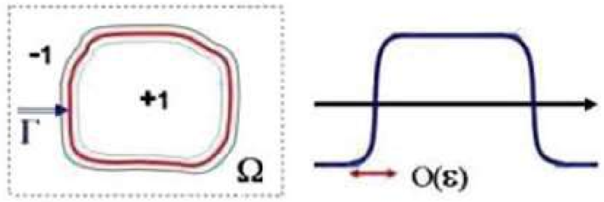


Fig.2 Phase diagram showing the transition from straight tube to pealing tubular state with respect to two dimensionless parameters $\sigma R_0^2/\kappa$ and $2\pi R_0/\lambda$

相场模型

引入相场函数

$$\phi(x)=\begin{cases}-1 & outside\, of\ the\, membrane\\ 1 & inside\, of\ the\, membrane\end{cases}$$



Du,et al. Journal of Computational Physics,2006

曲率弹性能

$$E(\phi)=\frac{3}{2\sqrt{2}}\int_\Omega \kappa\varepsilon\left(\Delta\phi-\frac{1}{\varepsilon^2}(\phi^2-1)(\phi+C\varepsilon)\right)^2 dx$$

表面张力能

$$S(\phi)=\frac{3}{2\sqrt{2}}\int_\Omega \sigma\left(\frac{\varepsilon}{2}|\nabla\phi|^2+\frac{1}{4\varepsilon}(\phi^2-1)^2\right)dx$$

总能量

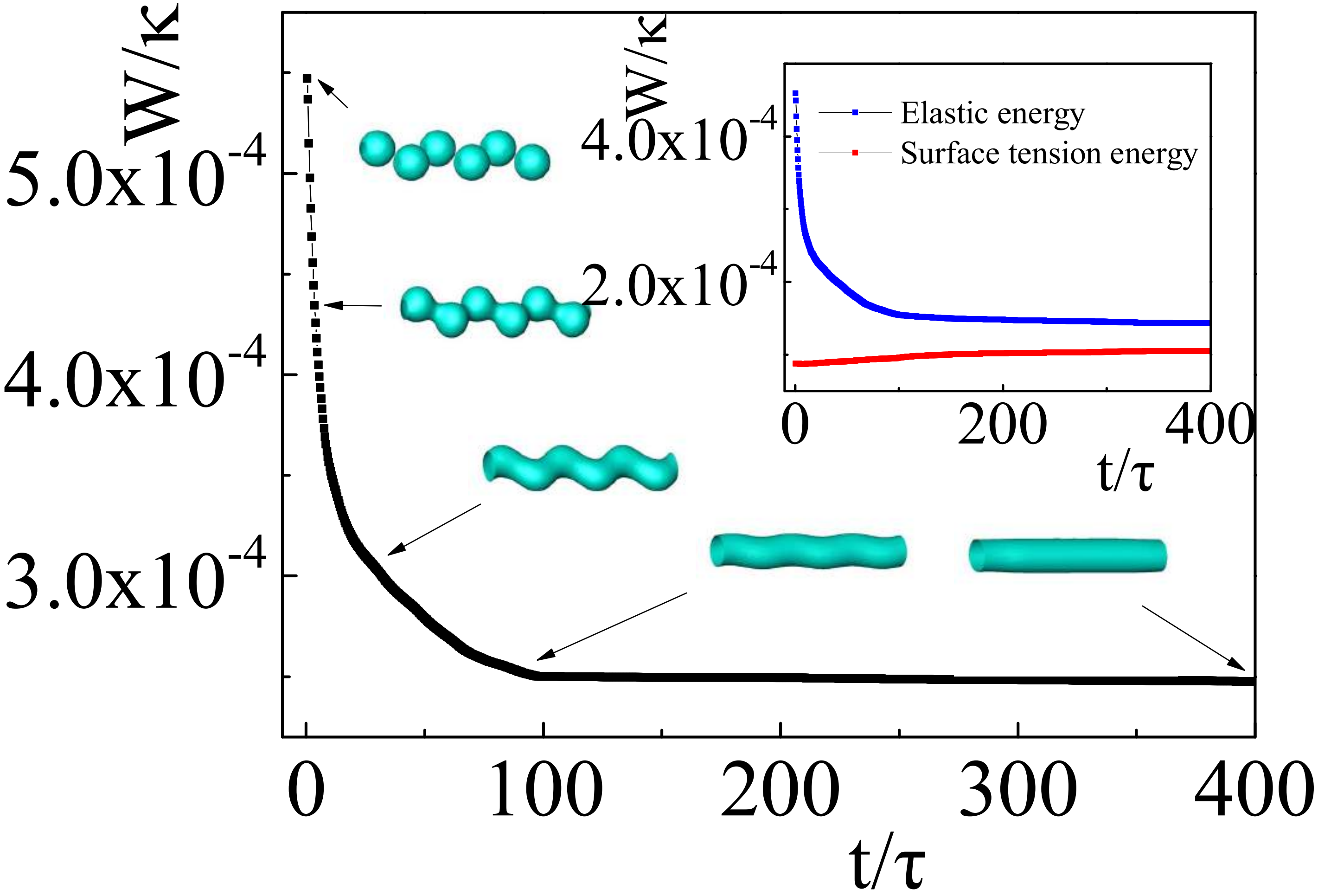
$$W(\phi)=E(\phi)+S(\phi)$$

演化方程

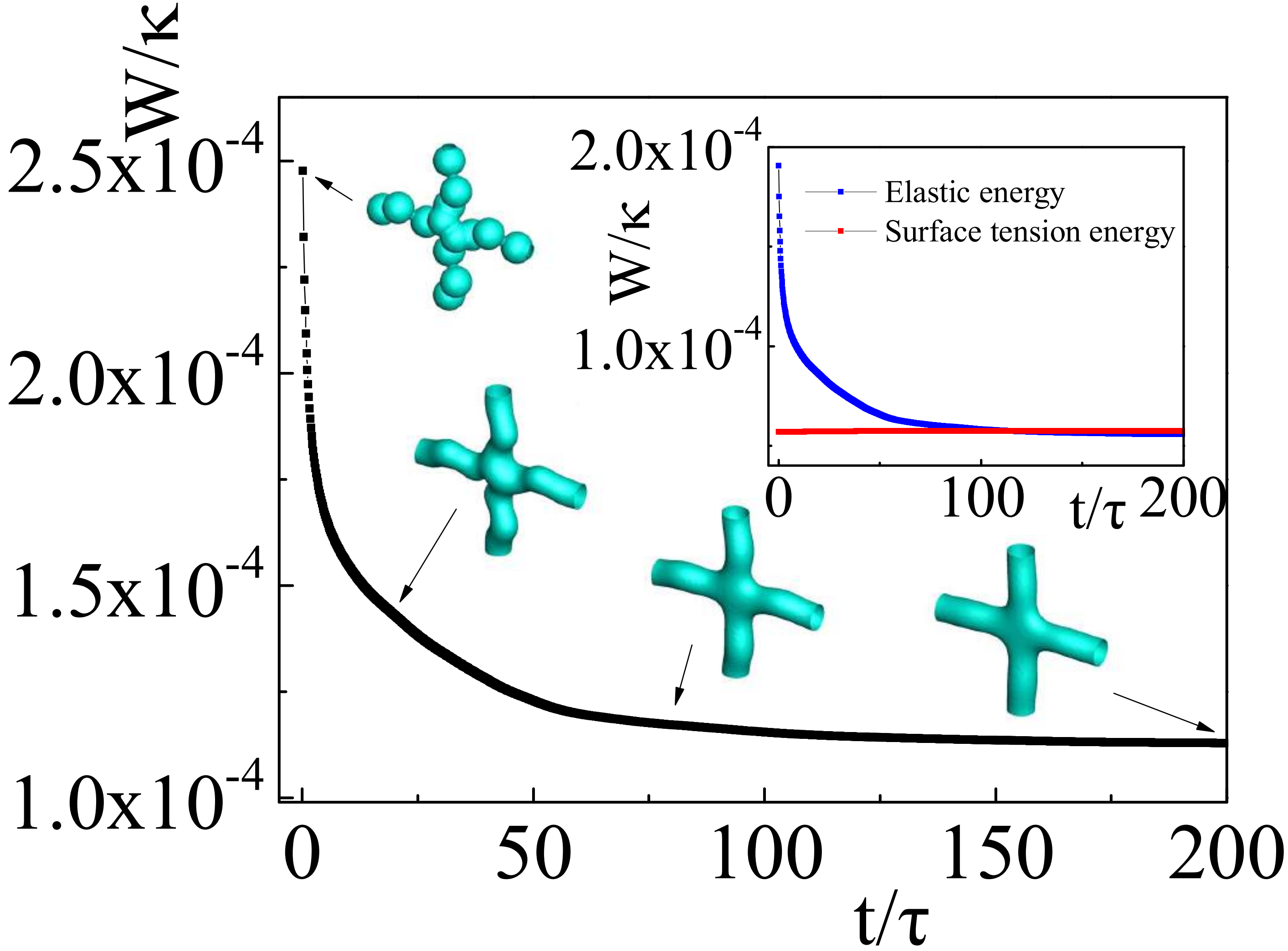
$$\frac{\partial\phi}{\partial t}=\nabla^2\left(\frac{\delta W}{\delta\phi}\right)$$

离散格式：半隐格式的Fourier谱方法

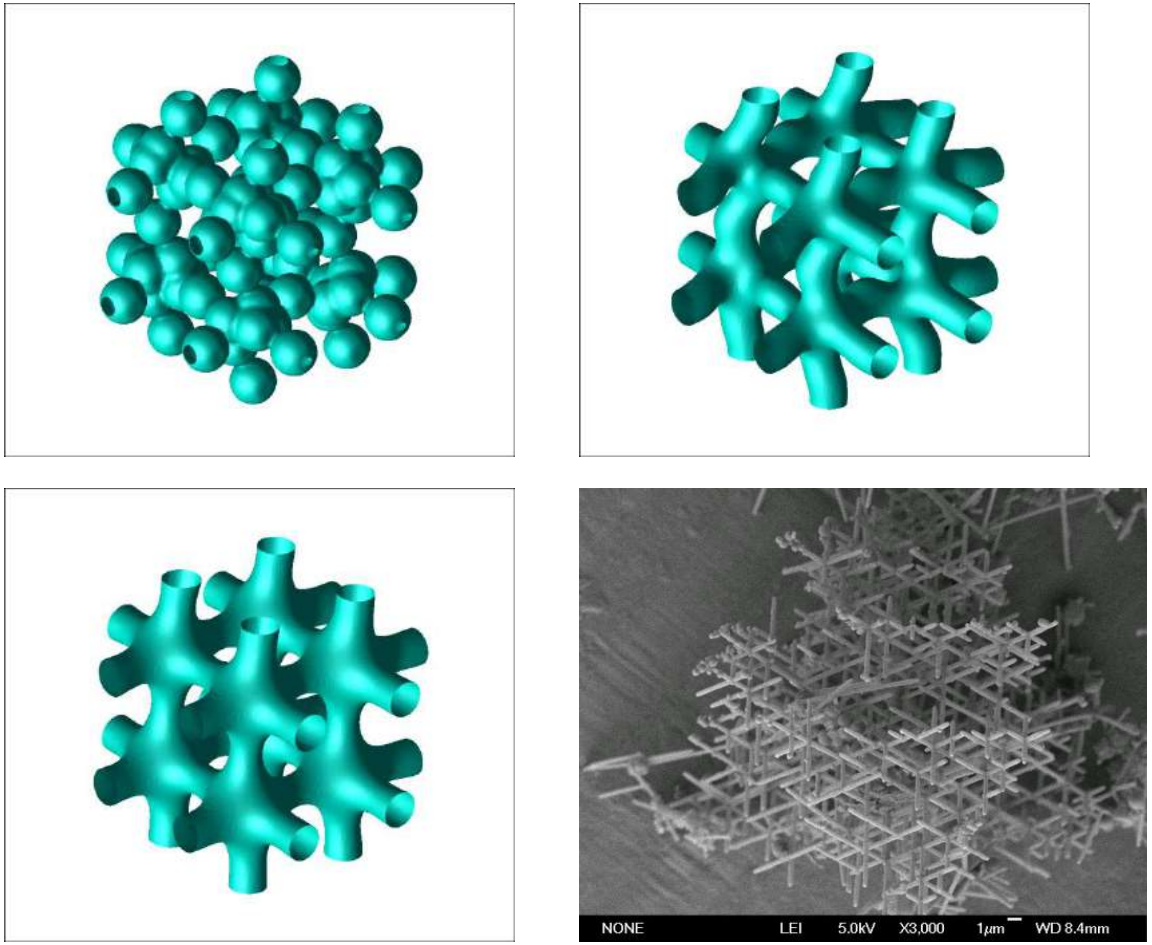
空心球融合为纳米管的相场模拟



空心球融合为正交管状结构的相场模拟

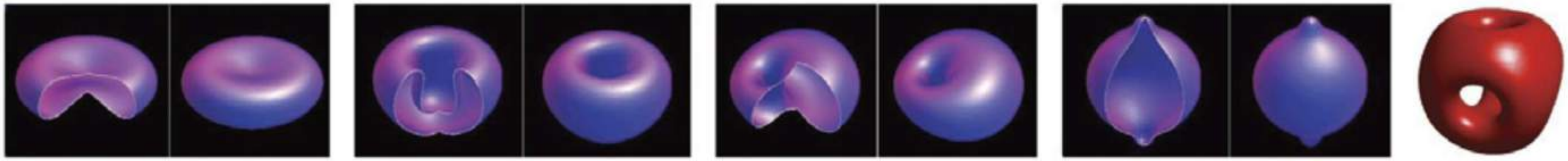


随机分布的空心球融合组装为三维有序网络结构的相场模拟

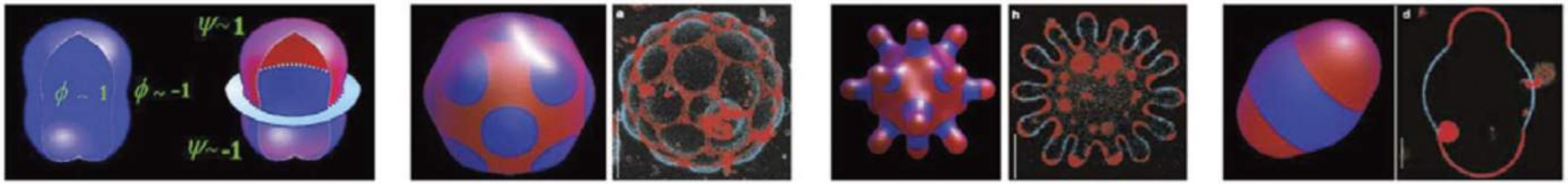


ACS nano 11 (3), 2928-2933(2017)

复杂膜泡形状的相场模拟



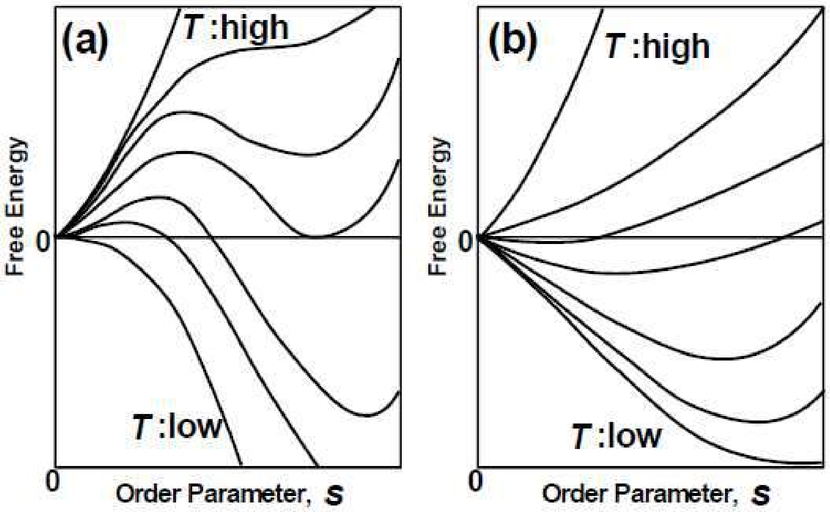
单相膜泡形状

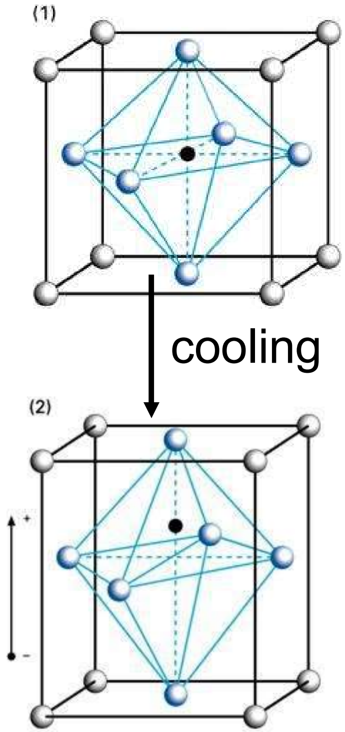


双相膜泡形状

Du, Q. Phase field calculus, curvature-dependent energies, and vesicle membranes. Philosophical Magazine, 91(1), 165-181(2011).

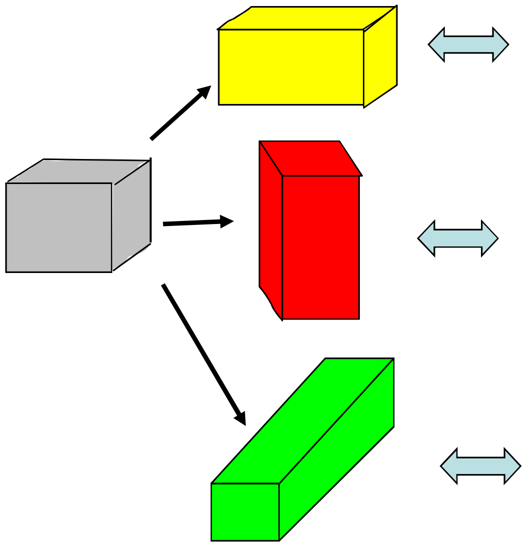
位移型相变





corresponding transformation strain

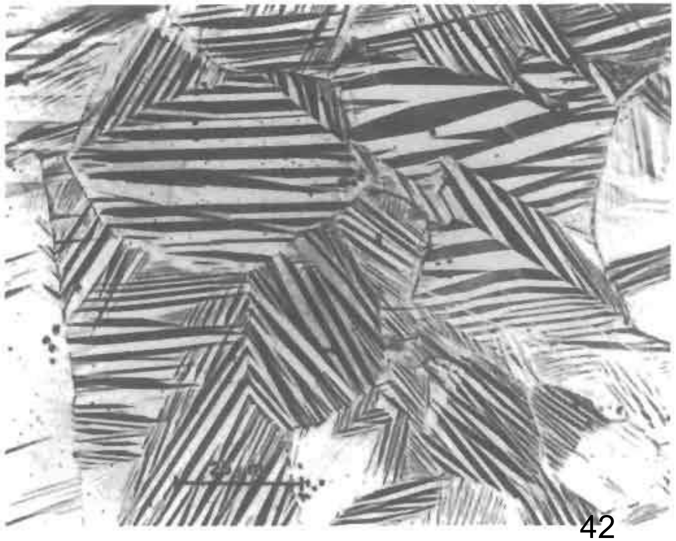
$$\varepsilon_{ij}^{o}(\boldsymbol{r}) = \sum_{p=1}^{3} \varepsilon_{ij}^{oo}(p)\eta_p(\mathbf{r},t)$$



$$\begin{pmatrix} \varepsilon_c & 0 & 0 \\ 0 & \varepsilon_a & 0 \\ 0 & 0 & \varepsilon_a \end{pmatrix}$$

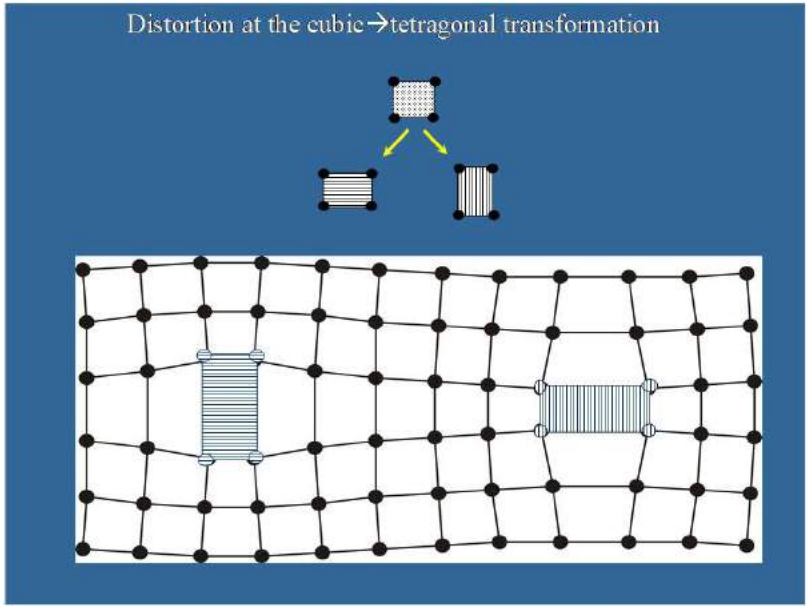
$$\begin{pmatrix} \varepsilon_a & 0 & 0 \\ 0 & \varepsilon_a & 0 \\ 0 & 0 & \varepsilon_c \end{pmatrix}$$

$$\begin{pmatrix} \varepsilon_a & 0 & 0 \\ 0 & \varepsilon_c & 0 \\ 0 & 0 & \varepsilon_a \end{pmatrix}$$

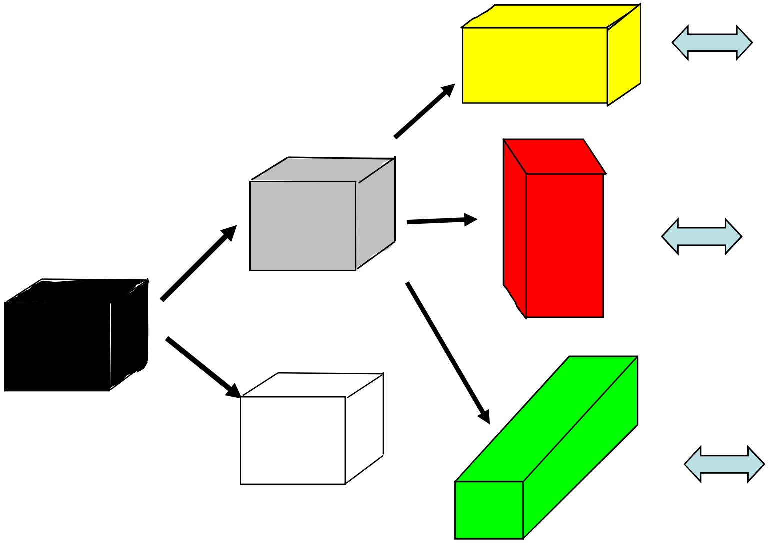


立方→四方相分解：位移型相变与扩散型相变的耦合

*



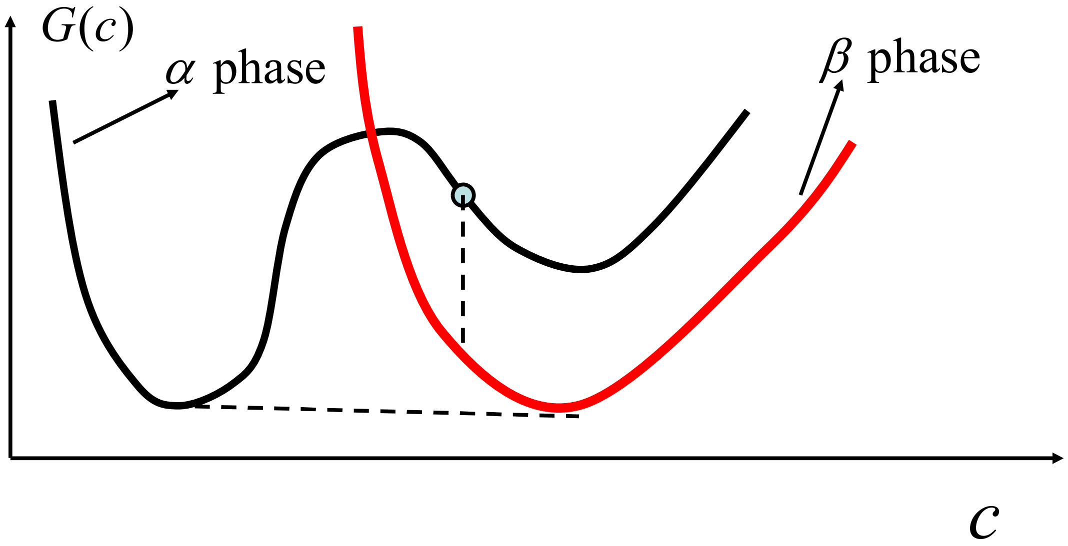
corresponding transformation strain



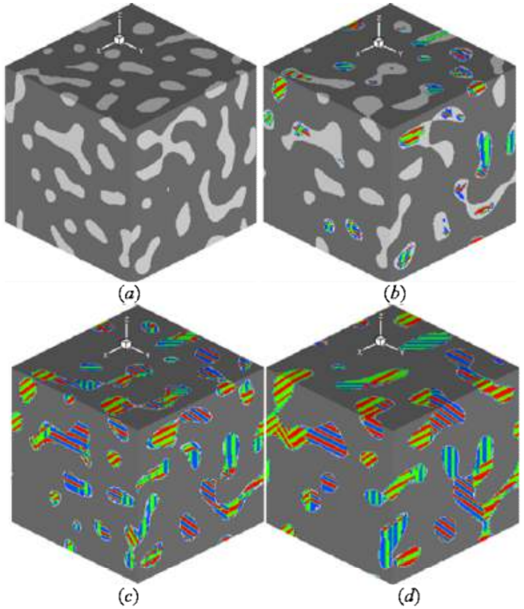
$$\begin{pmatrix} \varepsilon_c & 0 & 0 \\ 0 & \varepsilon_a & 0 \\ 0 & 0 & \varepsilon_a \end{pmatrix}$$

$$\begin{pmatrix} \varepsilon_a & 0 & 0 \\ 0 & \varepsilon_a & 0 \\ 0 & 0 & \varepsilon_c \end{pmatrix}$$

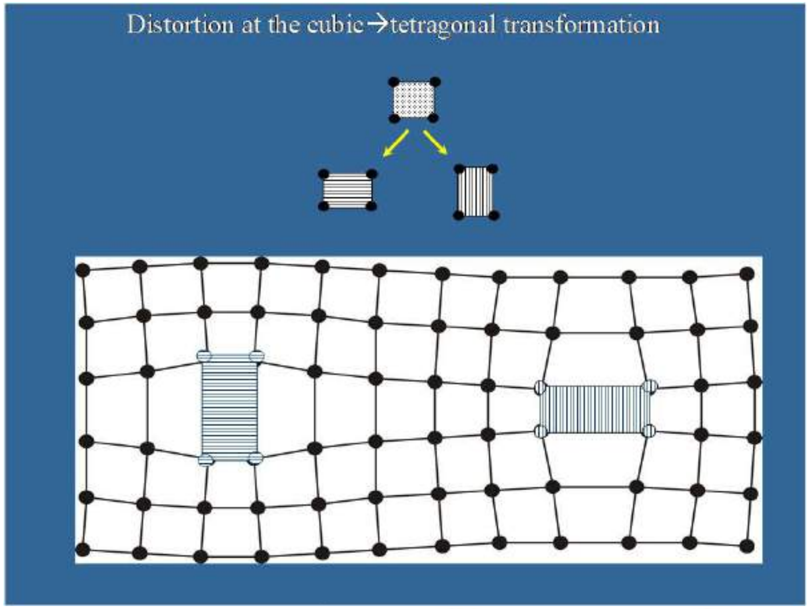
$$\begin{pmatrix} \varepsilon_a & 0 & 0 \\ 0 & \varepsilon_c & 0 \\ 0 & 0 & \varepsilon_a \end{pmatrix}$$

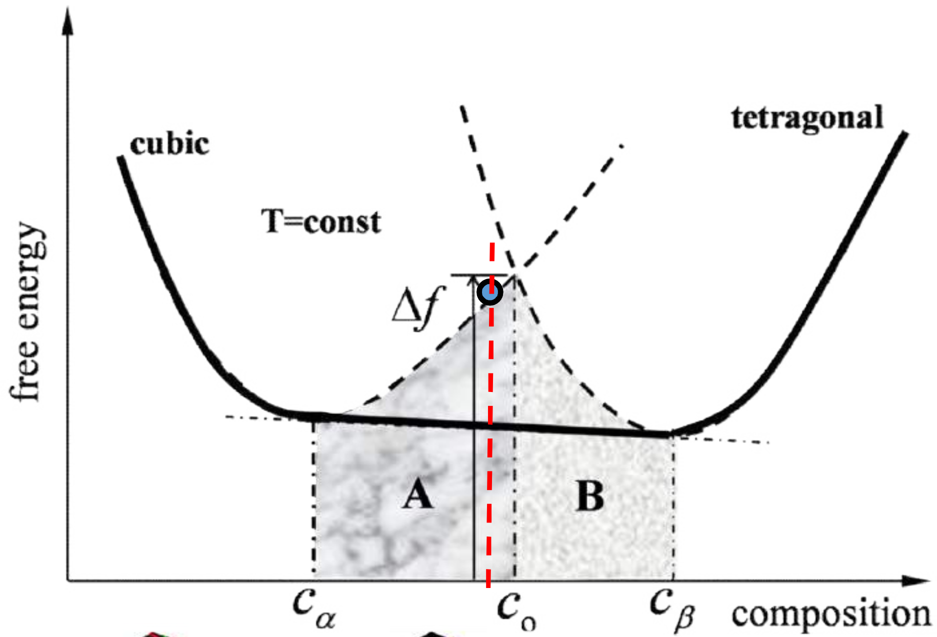


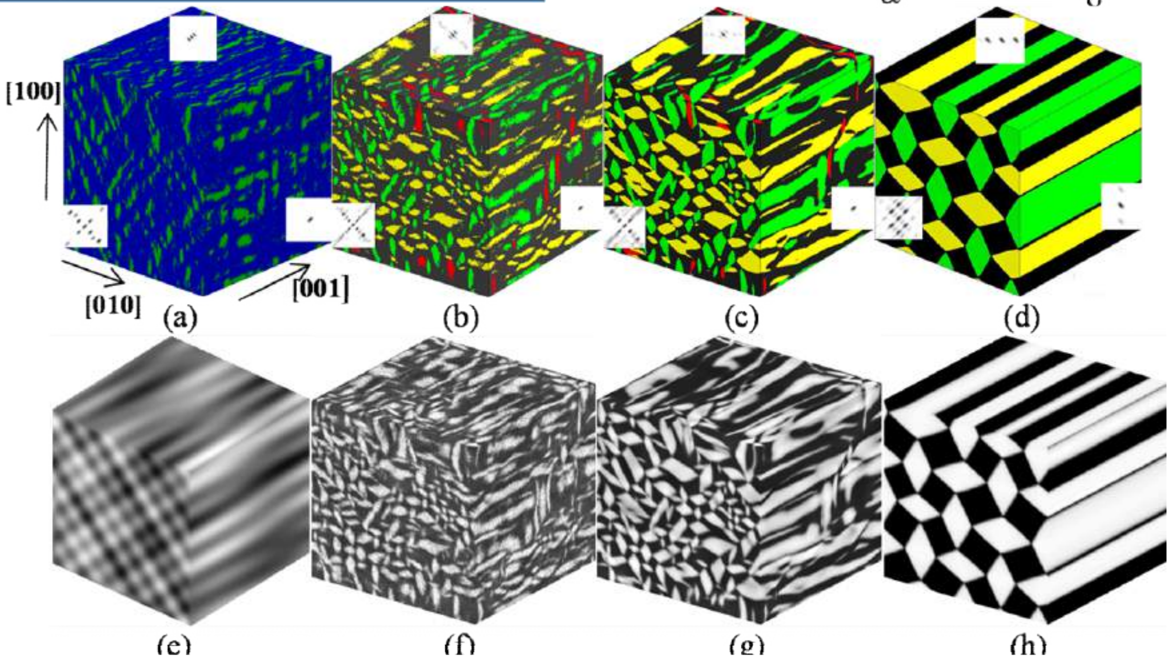
A schematic free energy curve vs composition



赝旋节分解相变模态（Pseudospinodal decomposition）

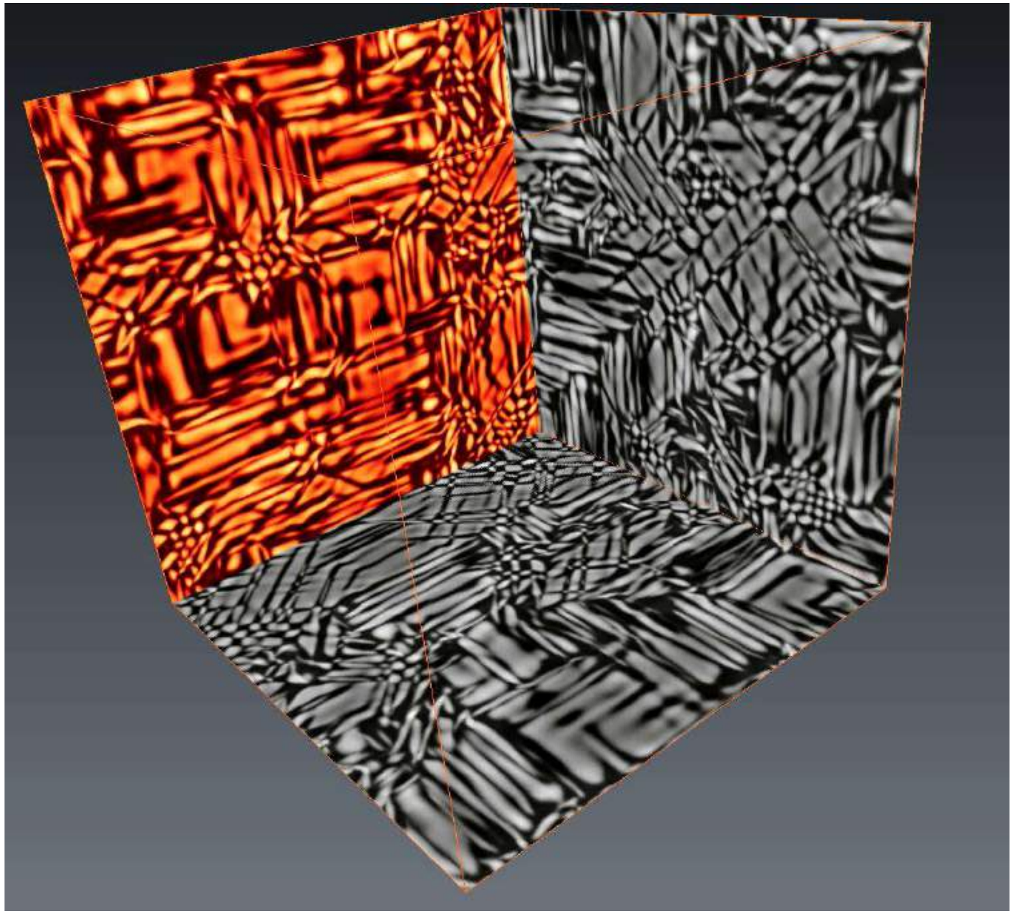


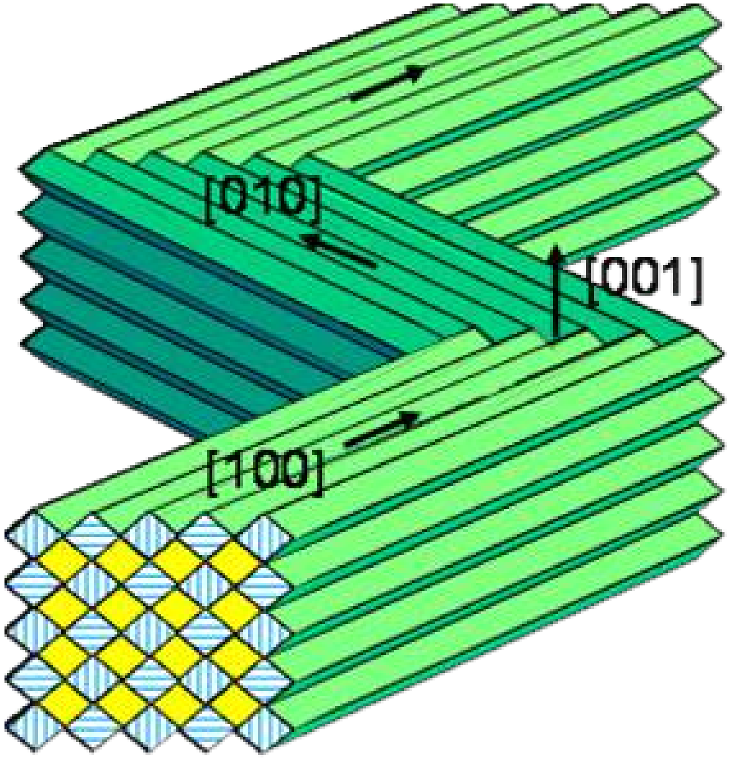




*

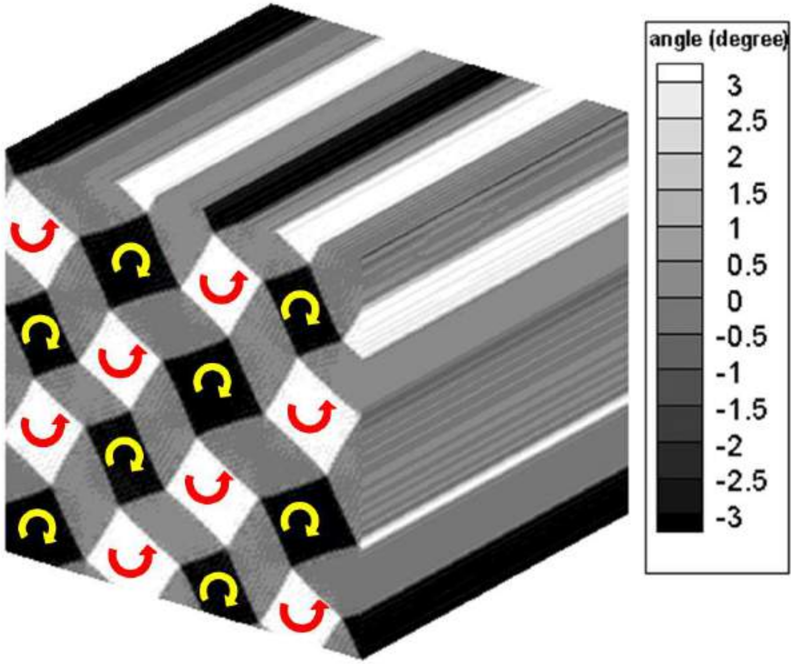
棋盘状纳米畴结构的形成

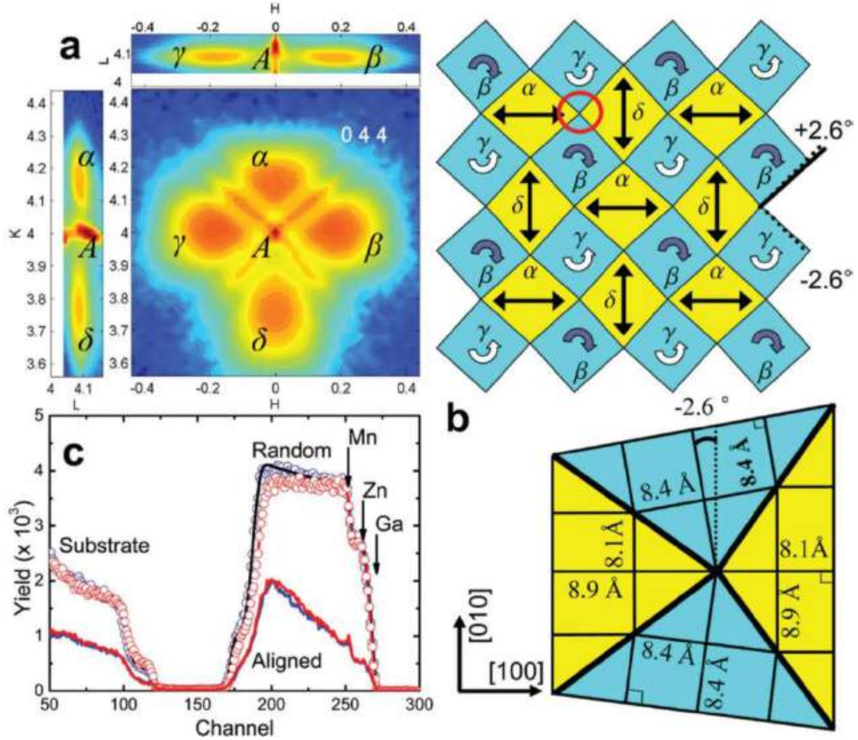




Nature Materials 8, 410-414 (2009).

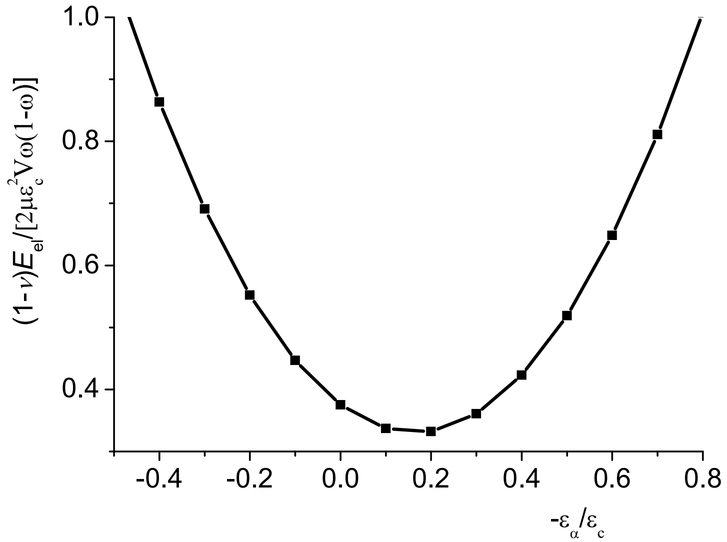
棋盘纳米畴结构的晶体学特征

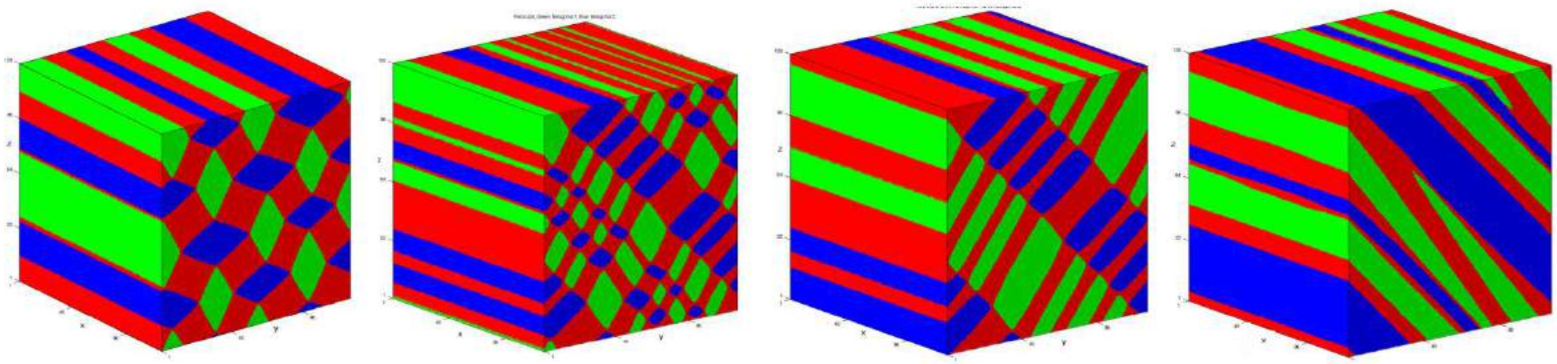




S. Park, et al. *Nano Lett*. **2007**, 8, 720.

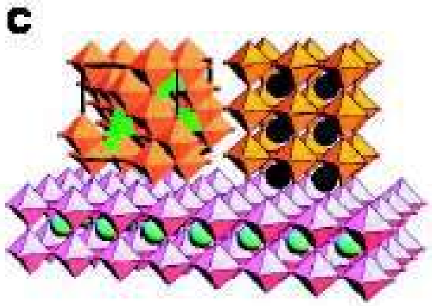
晶体学参数对棋盘纳米结构形成的影响

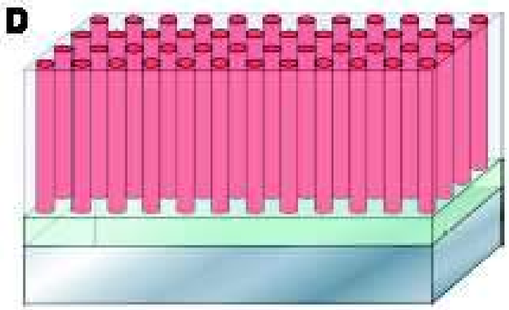


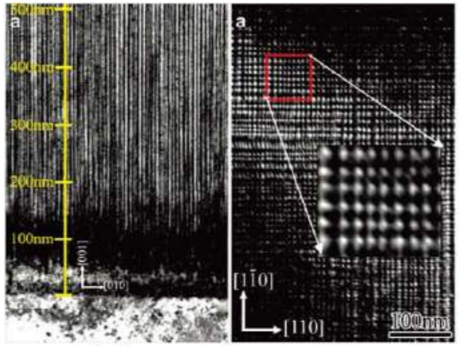


$\xi = 0.2$ $\xi = 0.3$ $\xi = 0.35$ $\xi = 0.4$

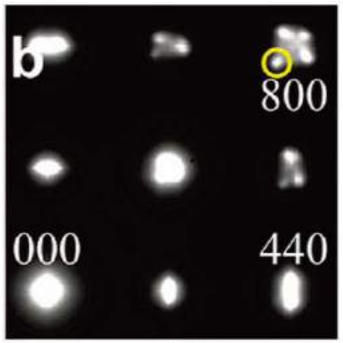
棋盘状纳米结构薄膜:优化的生长条件



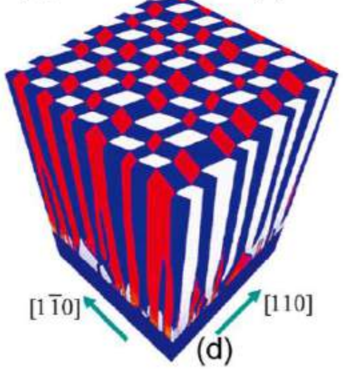




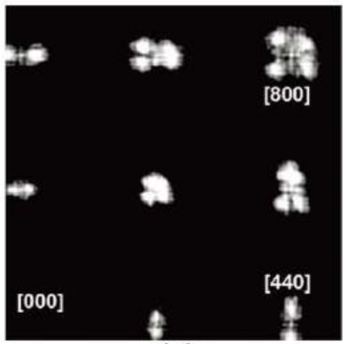
(a) (b)



(c)



(d)



(e)

优化温度与组分

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

优化晶体学参数一

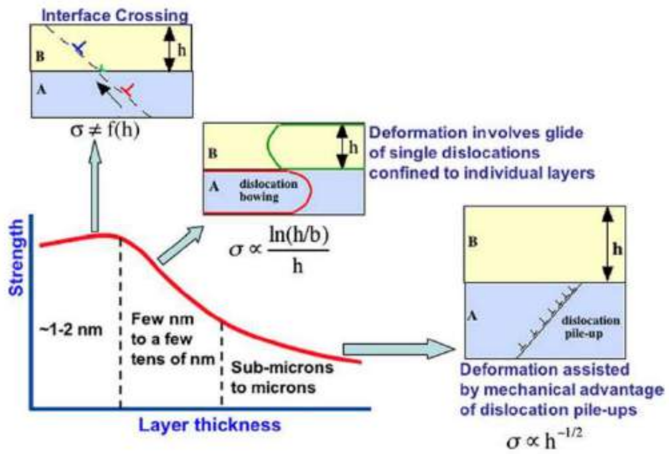
$$\xi_0 = \frac{a_c - a_t}{c_t - a_t} = \frac{1+4\nu}{11+8\nu}$$

优化晶体学参数二

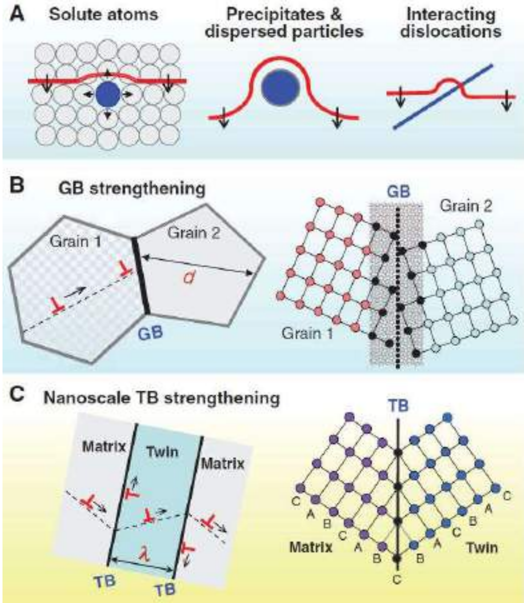
$$\rho = \frac{\bar{a}^f}{a_s} = \frac{2a_c + c_t + a_t}{4a_s} \rightarrow 1$$

Nano Letter, 9,3275(2009)

高强高韧纳米晶材料

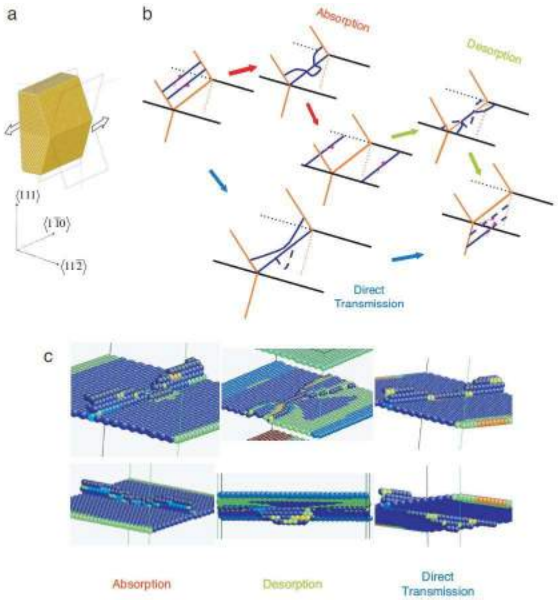


(Misra et. al, Acta Mater. 2005)



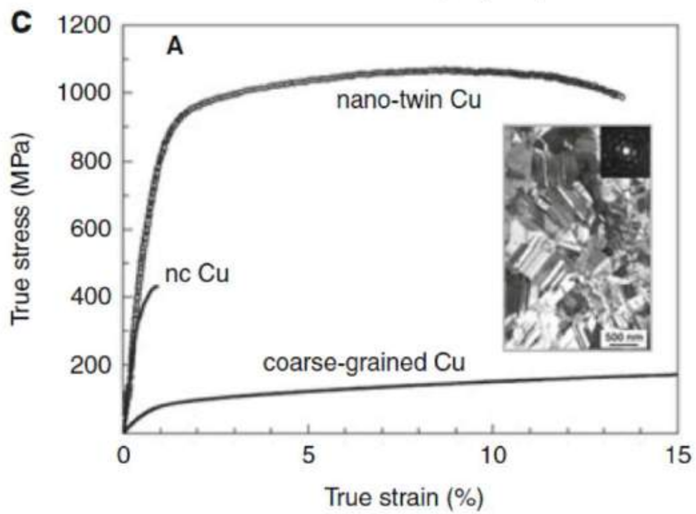
Interface as a barrier

(Lu K. et. al, Science 2009)



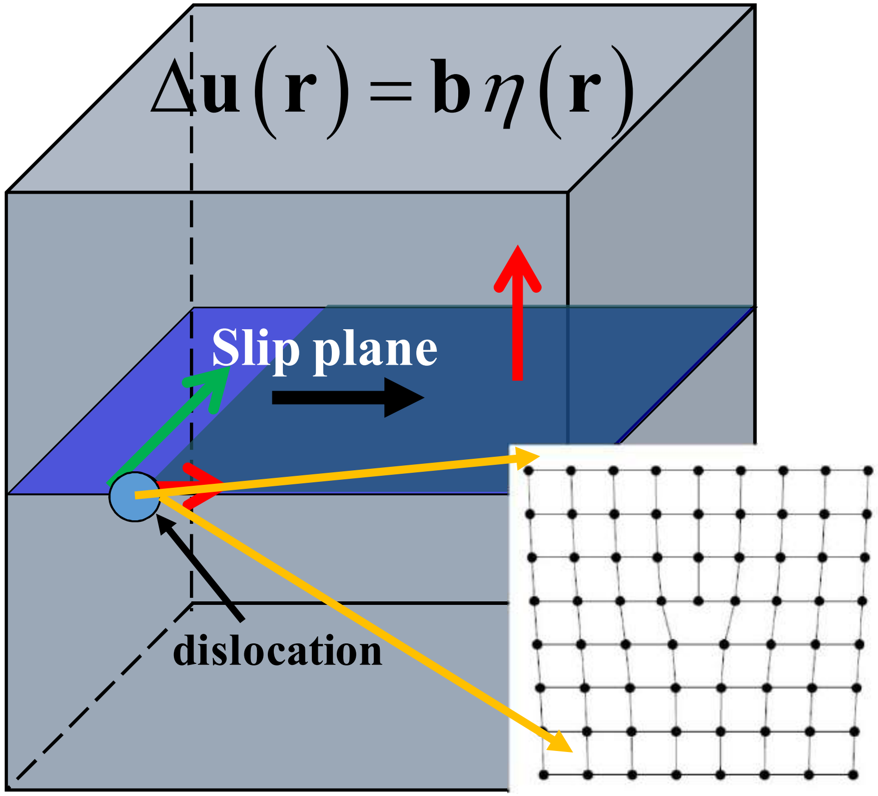
Interface as a source

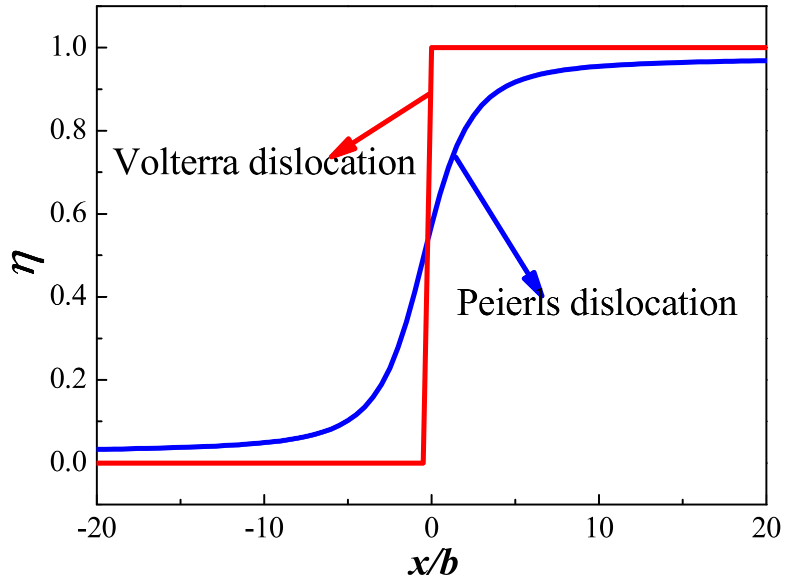
(Zhu et. al, PNAS 2007)



(Shen YL et. al, Script Mater. 2005)

Peierls-Nabarro 位错模型

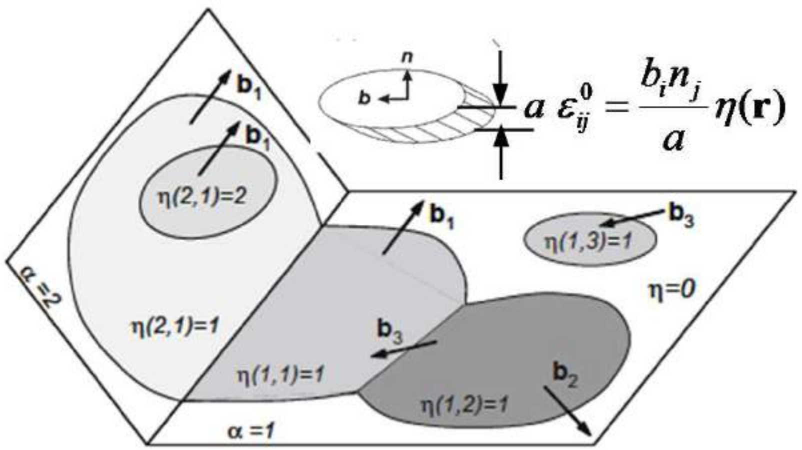


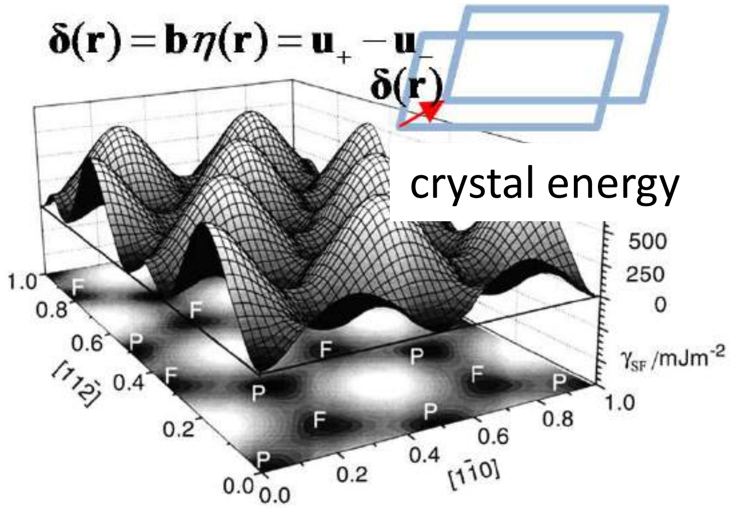


Minmization of $E^{\text{tot}} = E^{\text{cryst}} + E^{\text{elas}} + E^{\text{ext}}$

$$\boxed{E^{\text{cryst}} = \int \sum_{\alpha, m_\alpha} \Phi\left(\Delta\mathbf{u}_\alpha^{m_\alpha}(\mathbf{r})\right) \mathrm{d}^3 r,}$$

位错相场：广义的Peierls-Nabarro 位错模型





$$\text{Minmization of } E^{\text{tot}} = E^{\text{cryst}} + E^{\text{elas}} + E^{\text{ext}}$$

Ginzburg-Landau equations

$$\frac{d\eta_i(\mathbf{r})}{dt} = -L_{ij}\frac{\partial E\left[\eta_j(\mathbf{r})\right]}{\partial \eta_j(\mathbf{r})}$$

hard ⇦ dislocation movement ⇨ easy

strengthening toughening

from atomistic simulation to phase field to discrete dislocation simulation

⇨ time and space scales increase

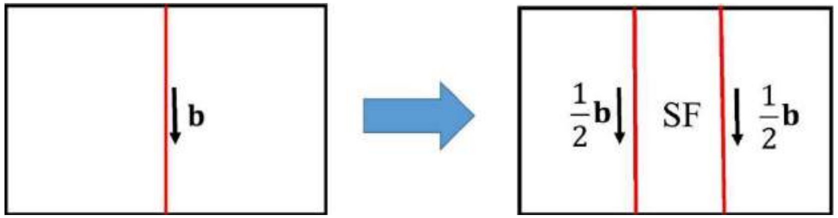
Y. Wang et al., Acta Mater. (2001); Y.Z.Wang Acta Mater. (2010)

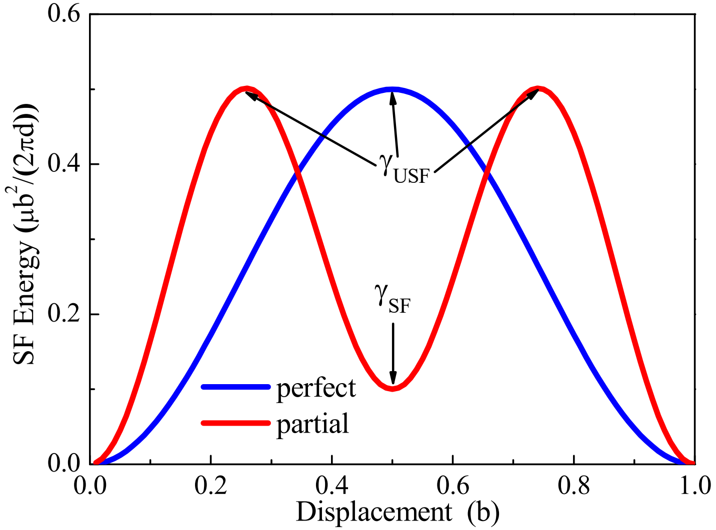
位错相场模拟：层错能参数如何影响位错分解

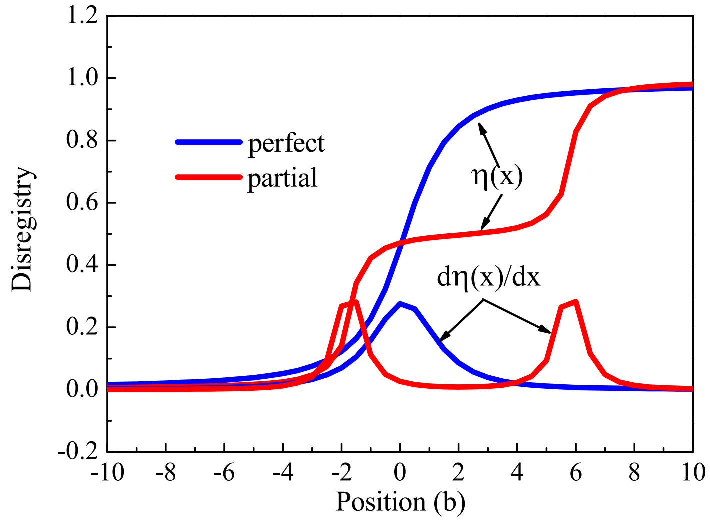
perfect $\rightarrow$ $\phi(r) = \gamma_{USF} \sin^2(\pi\eta)$

partial $\rightarrow$ $f(r) = \gamma_{SF} \sin^2(\pi\eta) + (\gamma_{USF} - \gamma_{SF}/2)\sin^2(2\pi\eta)$

只考虑一个方向

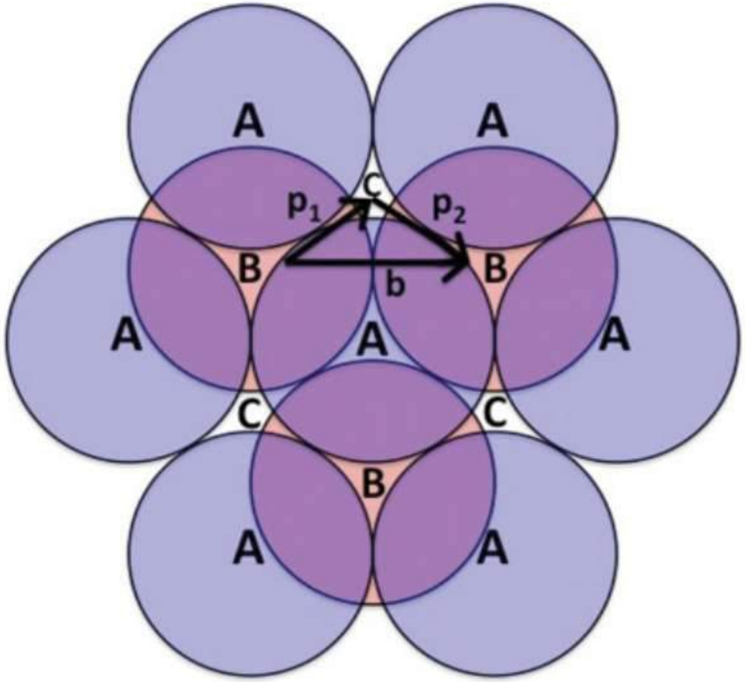


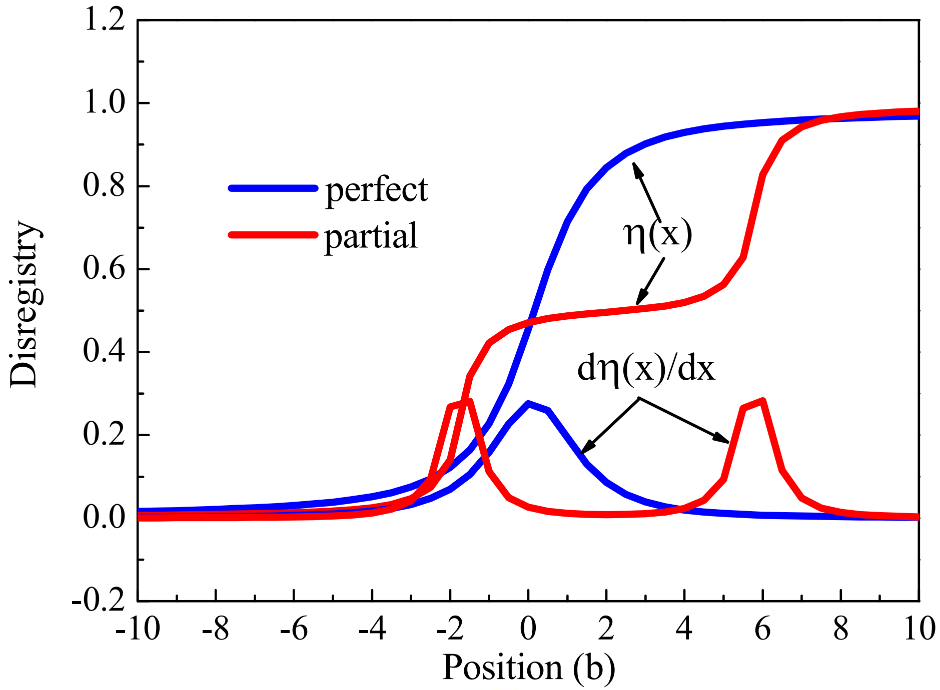




位错相场模拟：（111）面上的位错结构

FCC：(111) plane





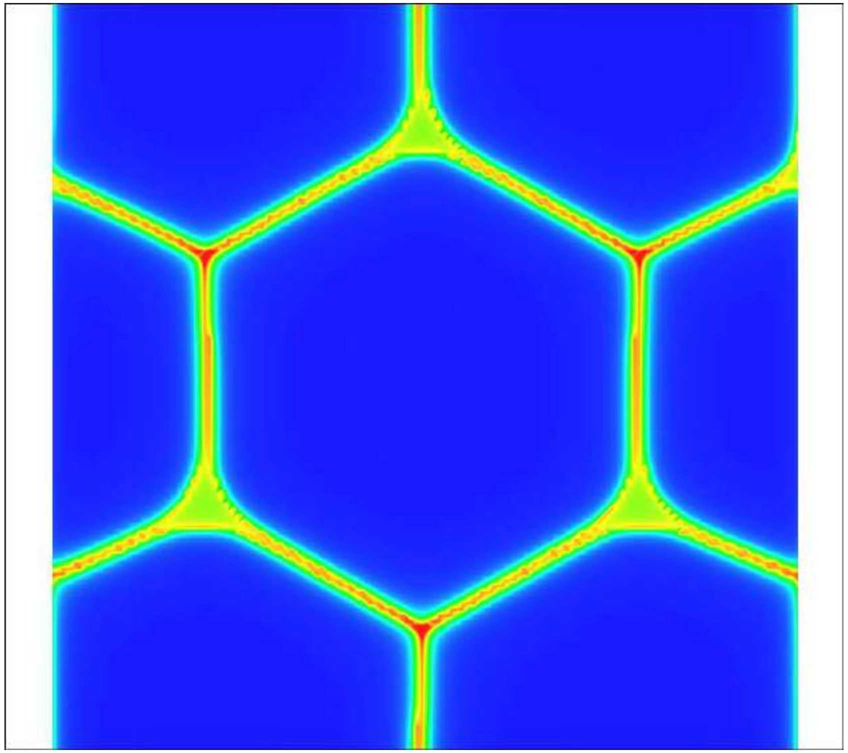
$$\frac{a}{2}[110] \rightarrow \frac{a}{6}[211] + \frac{a}{6}[12\bar{1}]$$

Perfect dislocation ⟶ partial dislocation + stacking fault (SF) + partial dislocation

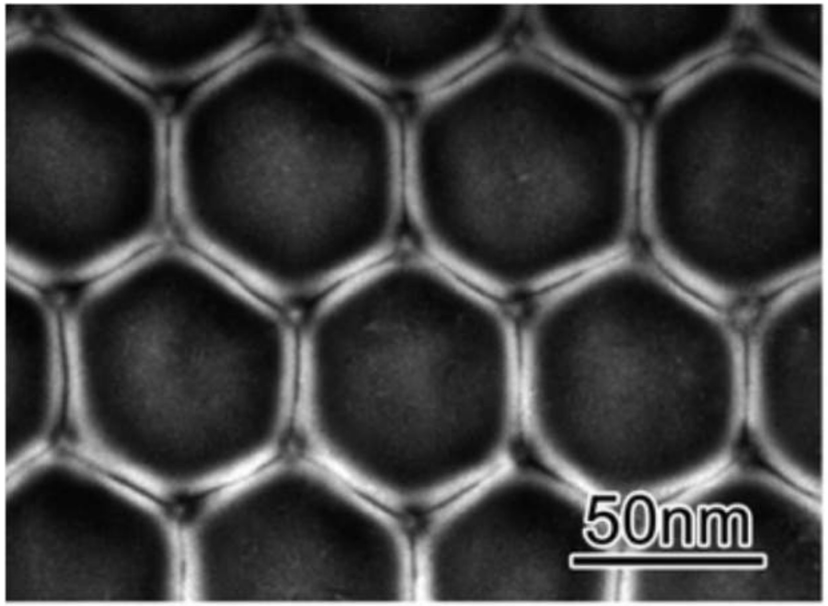
C.Shen and Y.Z. Wang, Acta Mater. (2003)；(2004)；(2014)

位错相场模拟：（111）面上的位错结构

$$\theta = 0.78^{\circ}$$



Phase field simulation



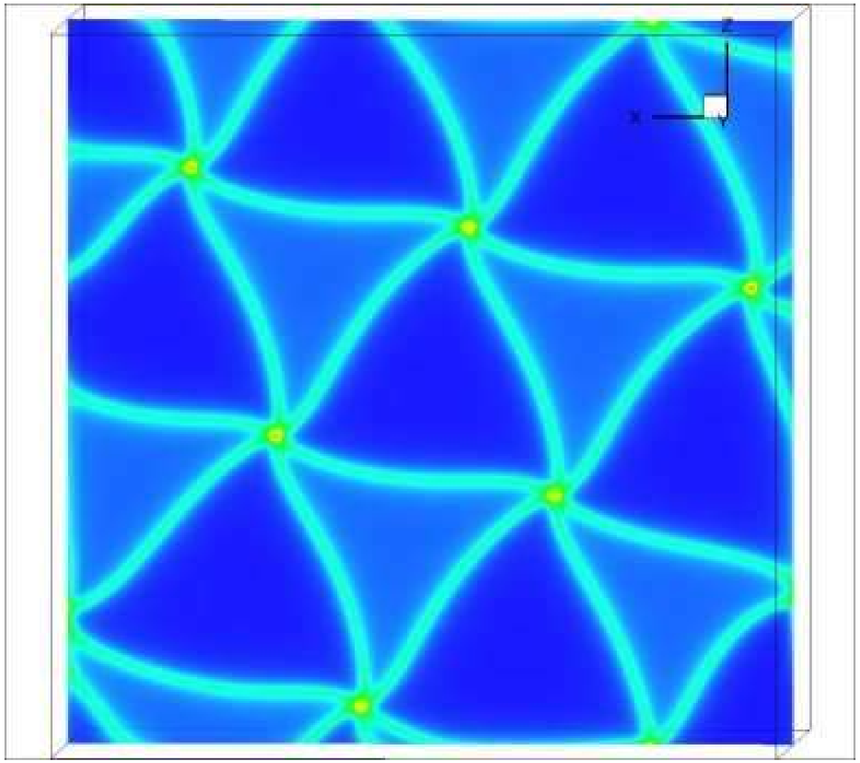
Experimental observation

Tochigi, et al., Acta Mater. (2012)

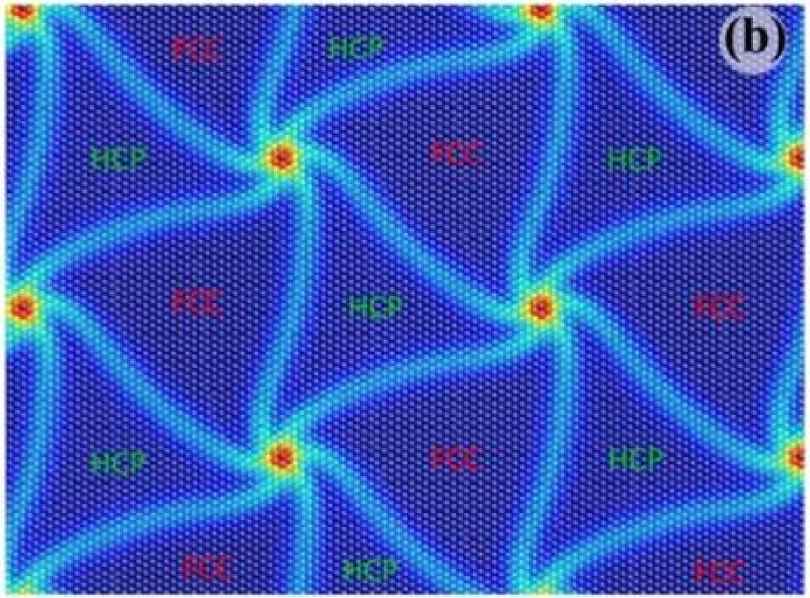
Twist GB in Al

位错相场模拟：（111）面上的位错结构

$$\theta = 0.78^{\circ}, \varepsilon_{mis} = 0.005$$



Phase field simulation

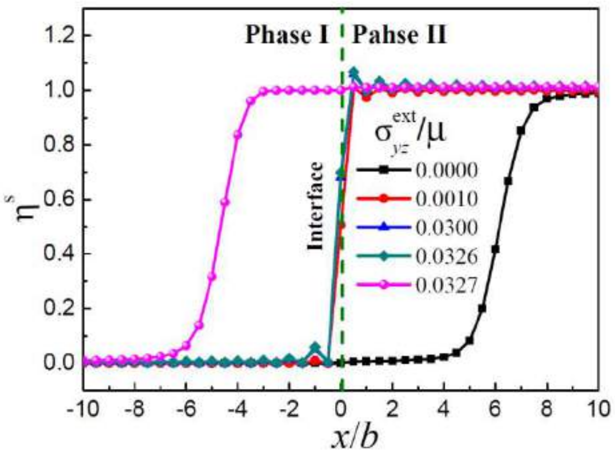


Molecular dynamic simulation

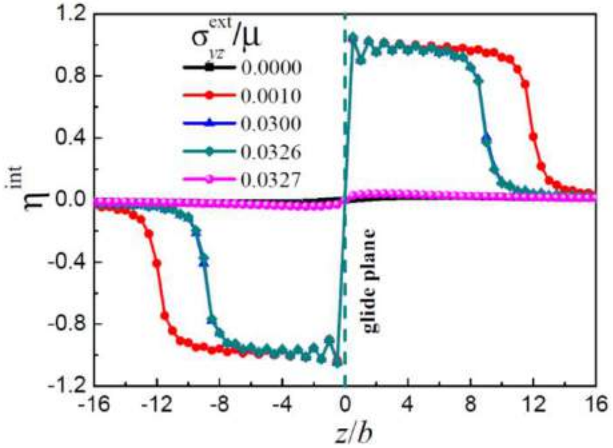
J. Wang, et al., Sci. Rep. (2014)

GB in Cu

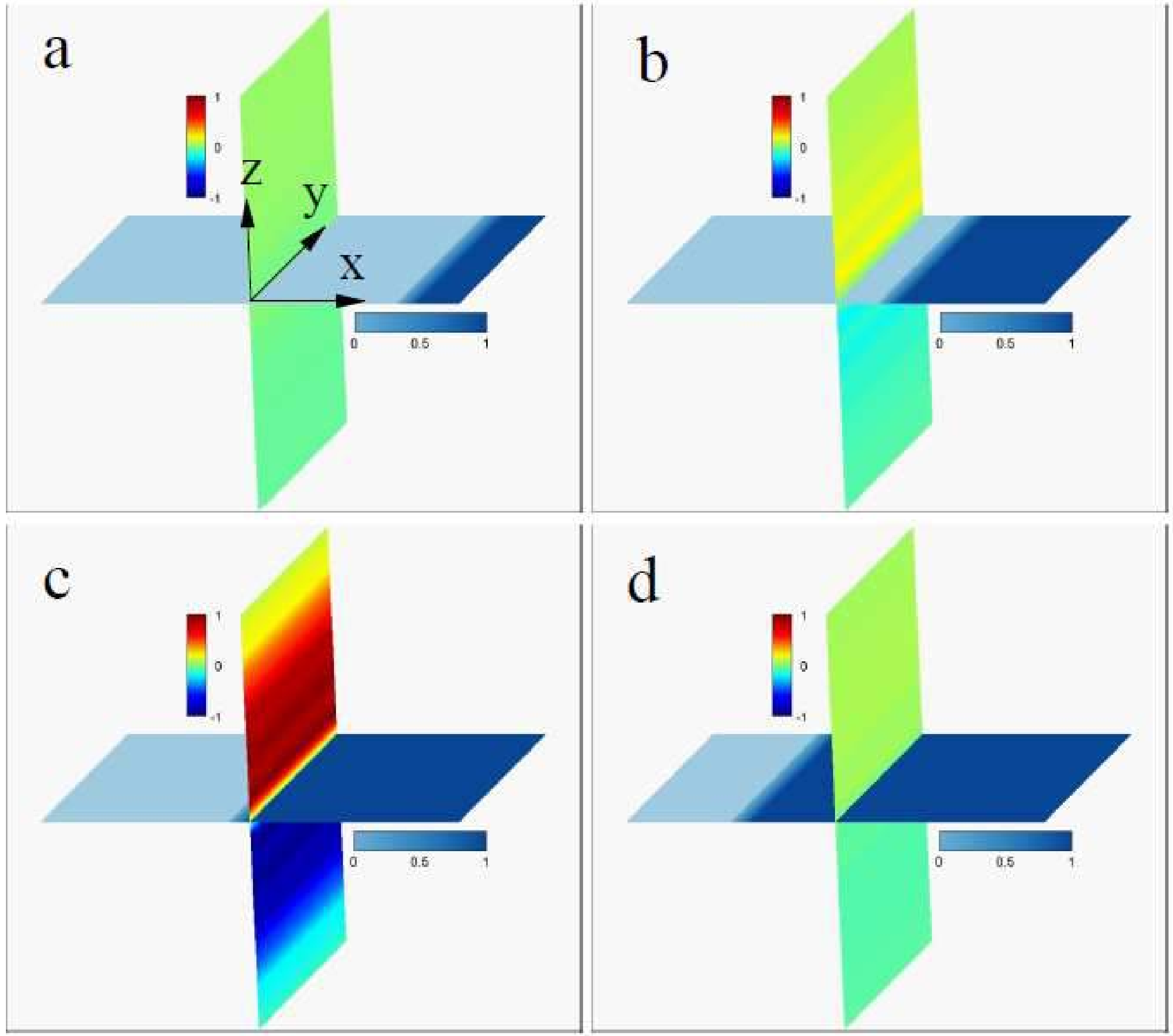
位错相场模拟：位错穿越界面



slipping profile on
the glide plane



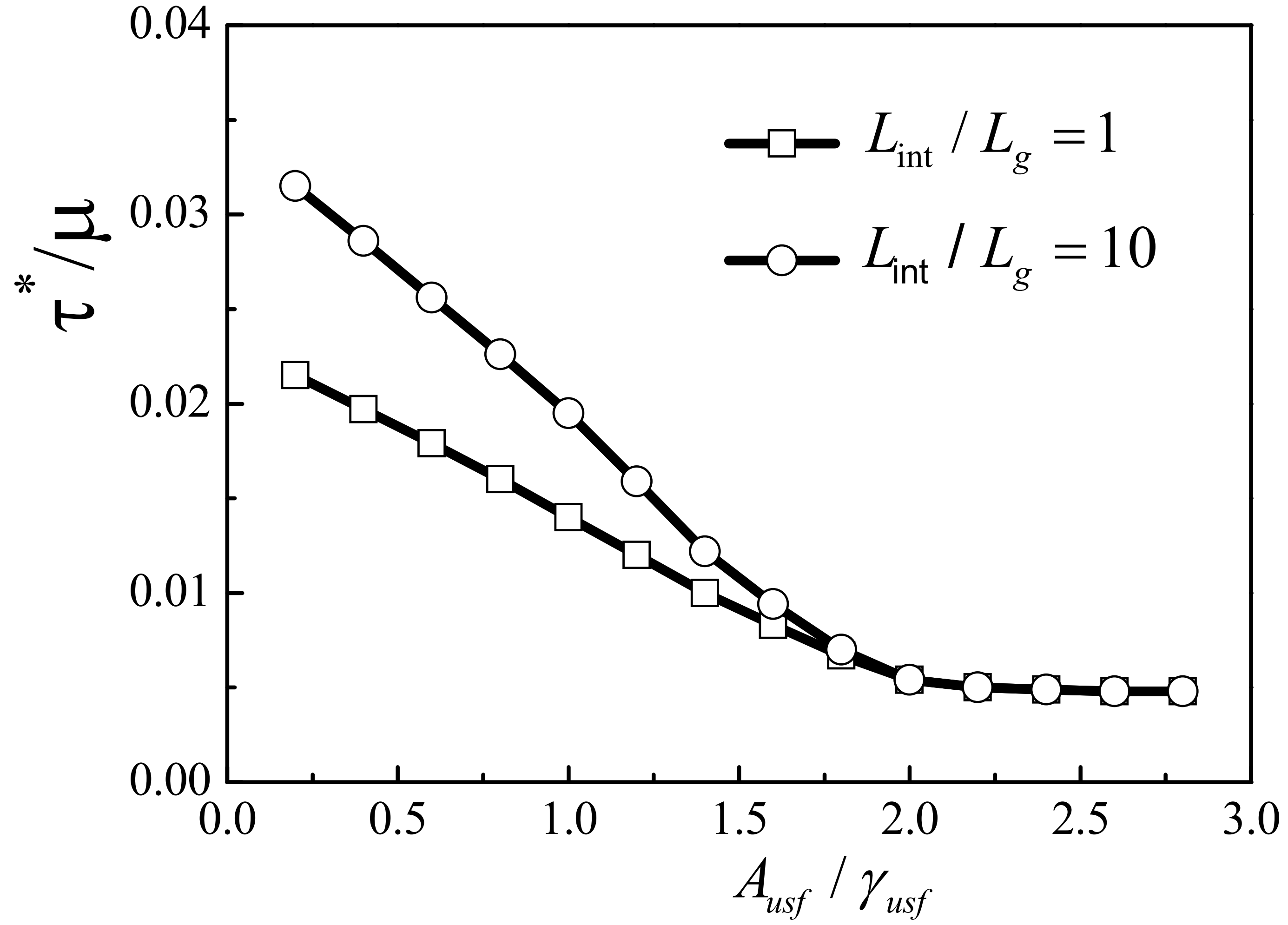
slipping profile on
the interface



transmission process for the sliding interface

位错相场模拟：位错穿越界面

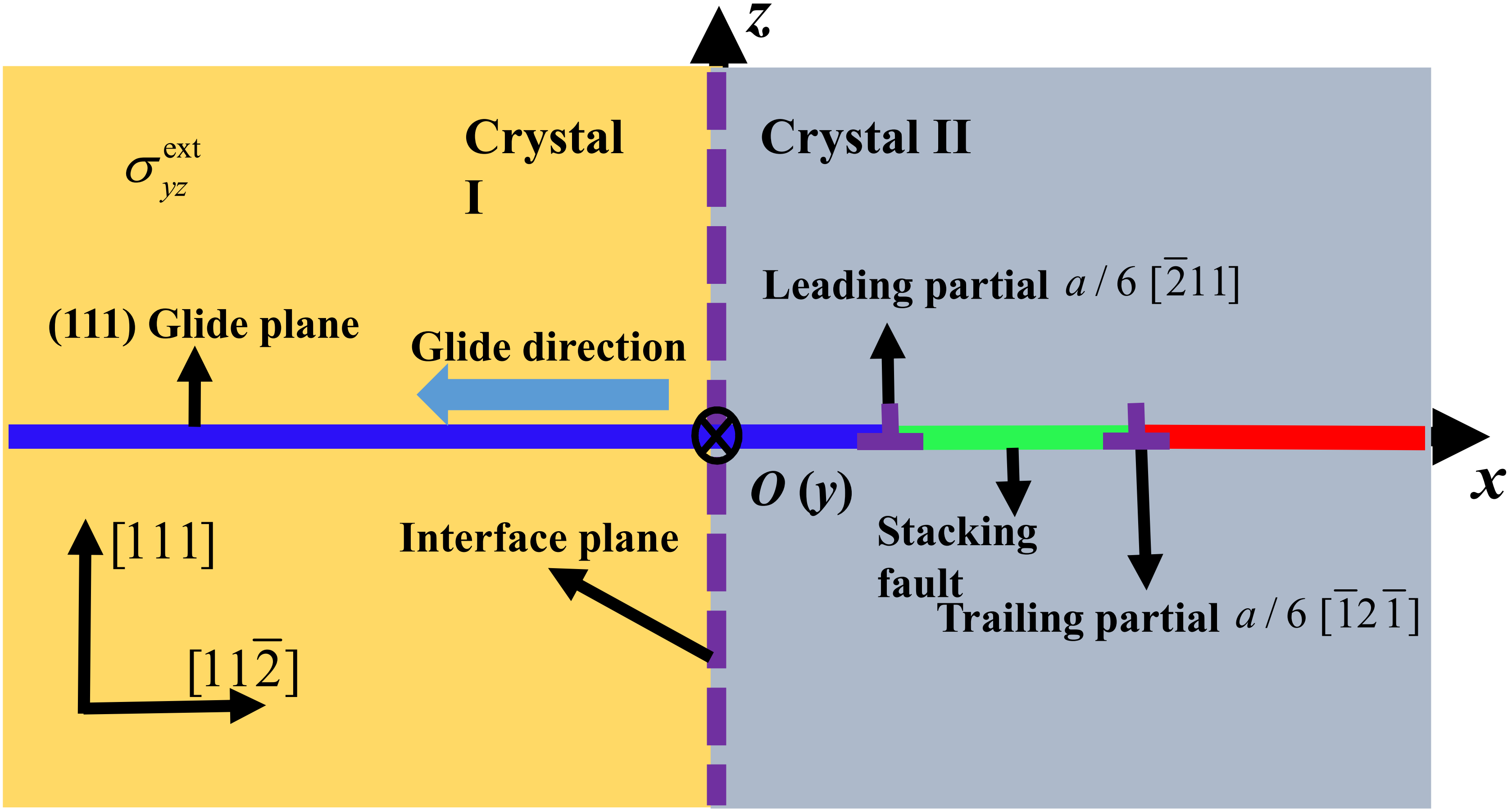
Rate dependent weak-interface strenghening



Modelling Simul. Mater. Sci. Eng. 23, 035002(2015)

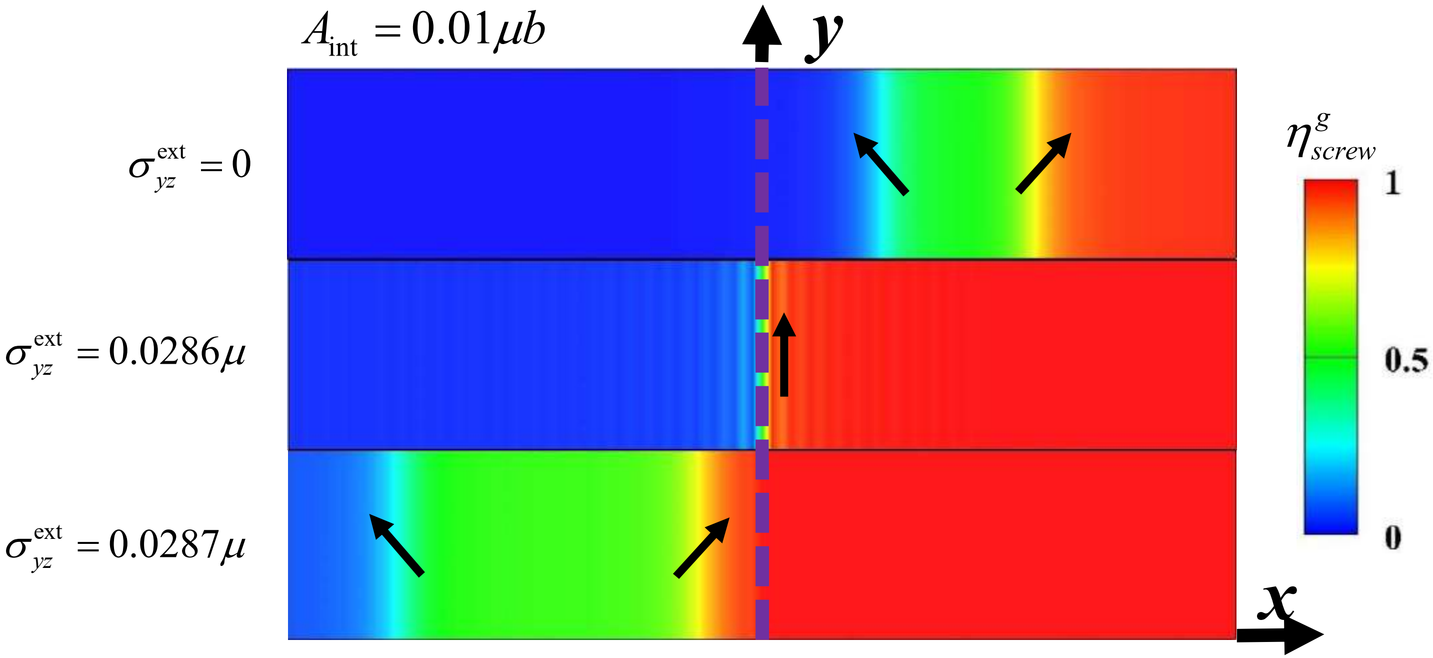
位错相场模拟：位错穿越界面

<u>An extended dislocation across a sliding interface</u>



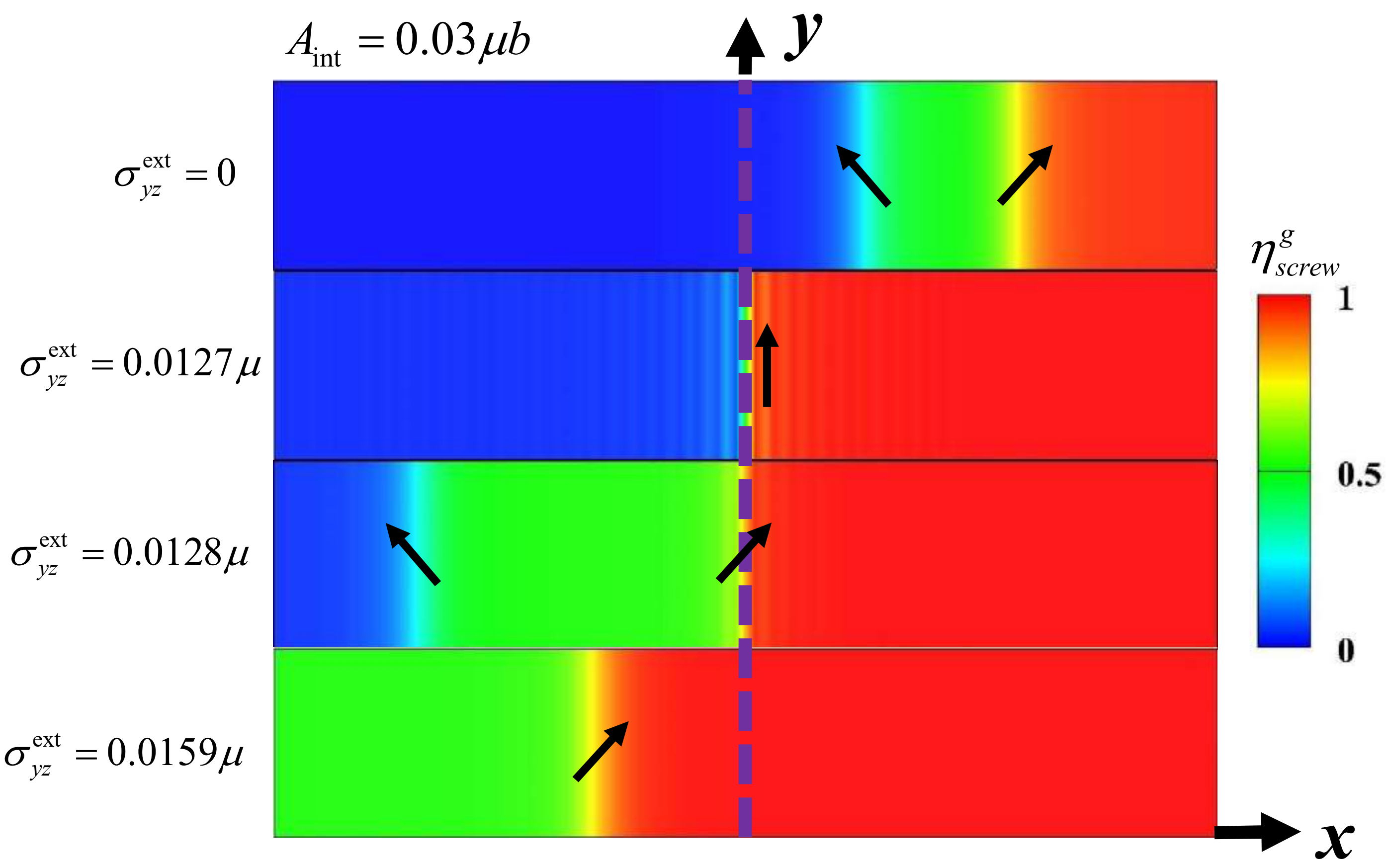
位错相场模拟：位错穿越界面

Transmission mode:full transmission



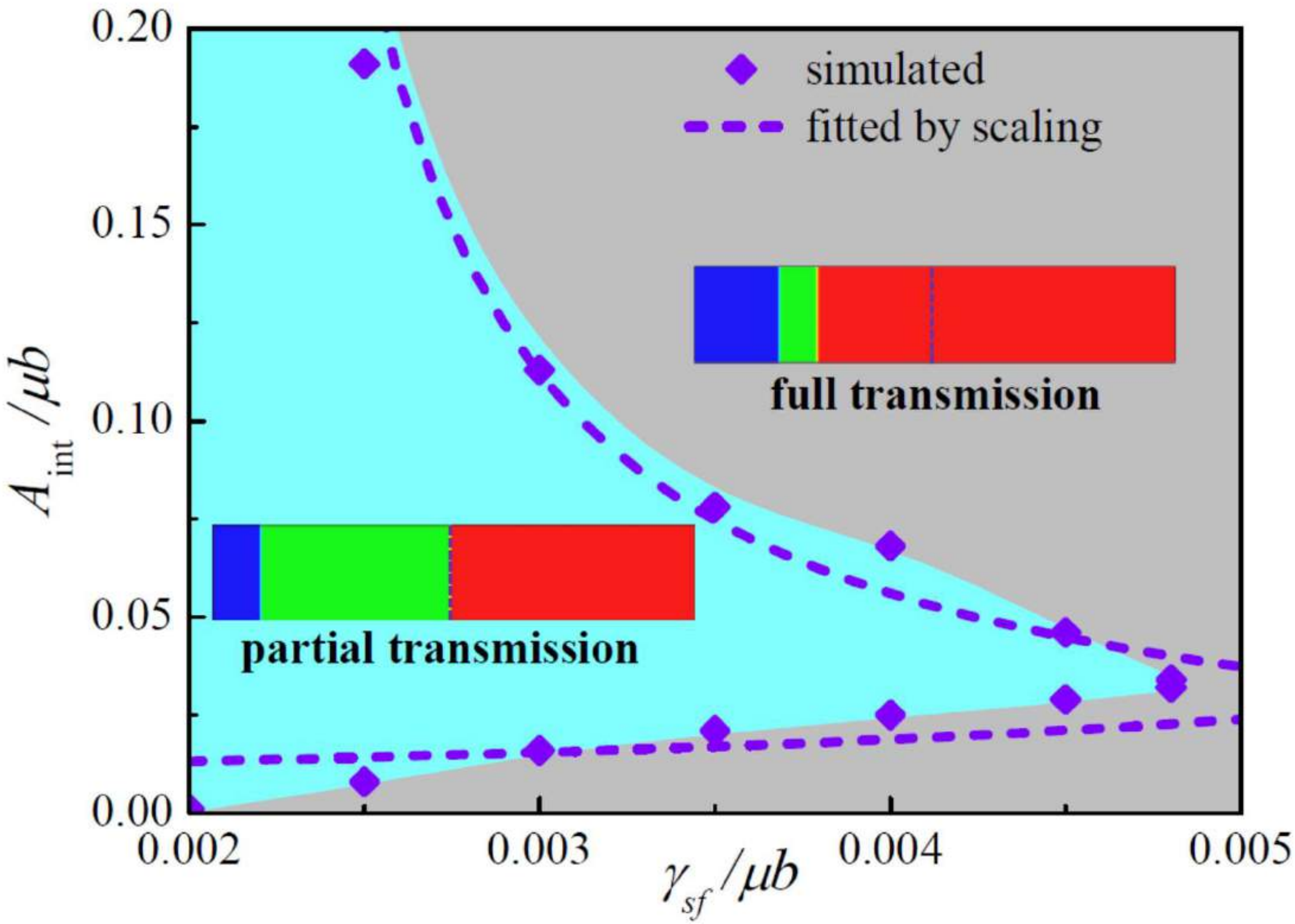
位错相场模拟：位错穿越界面

Alternative transmission mode:partial transmission



位错相场模拟：位错穿越界面

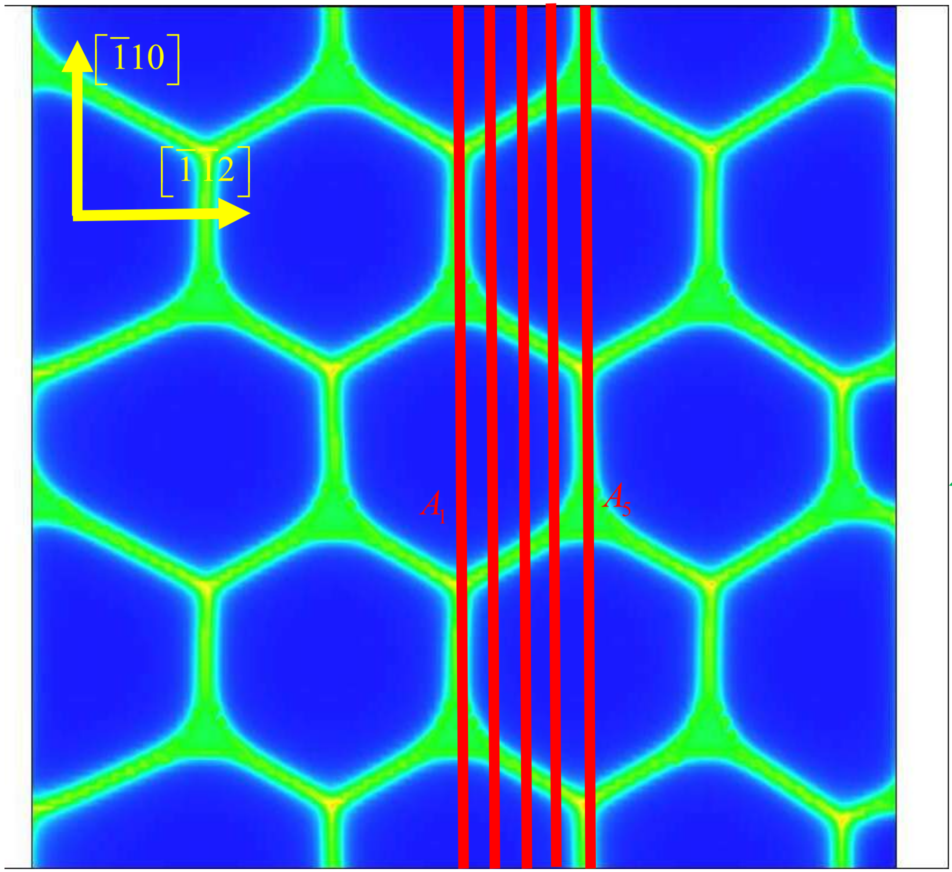
Phase diagram of the transmission modes

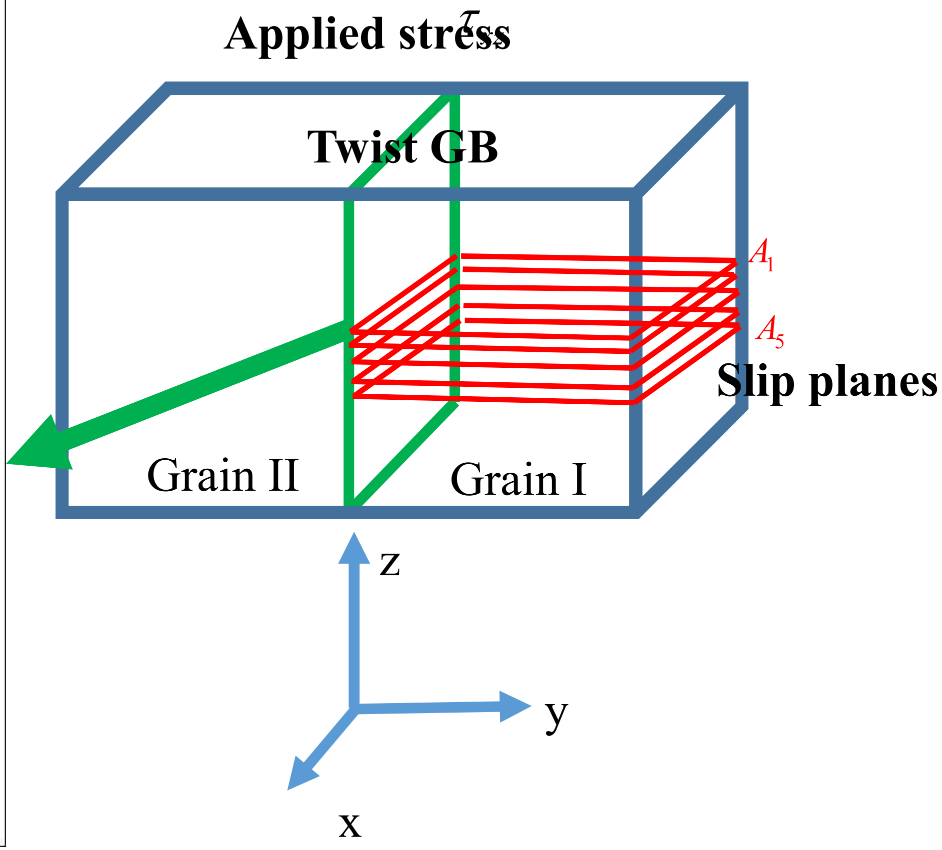


J. Phys. D. 48,395301(2015)

位错相场模拟：位错穿越界面

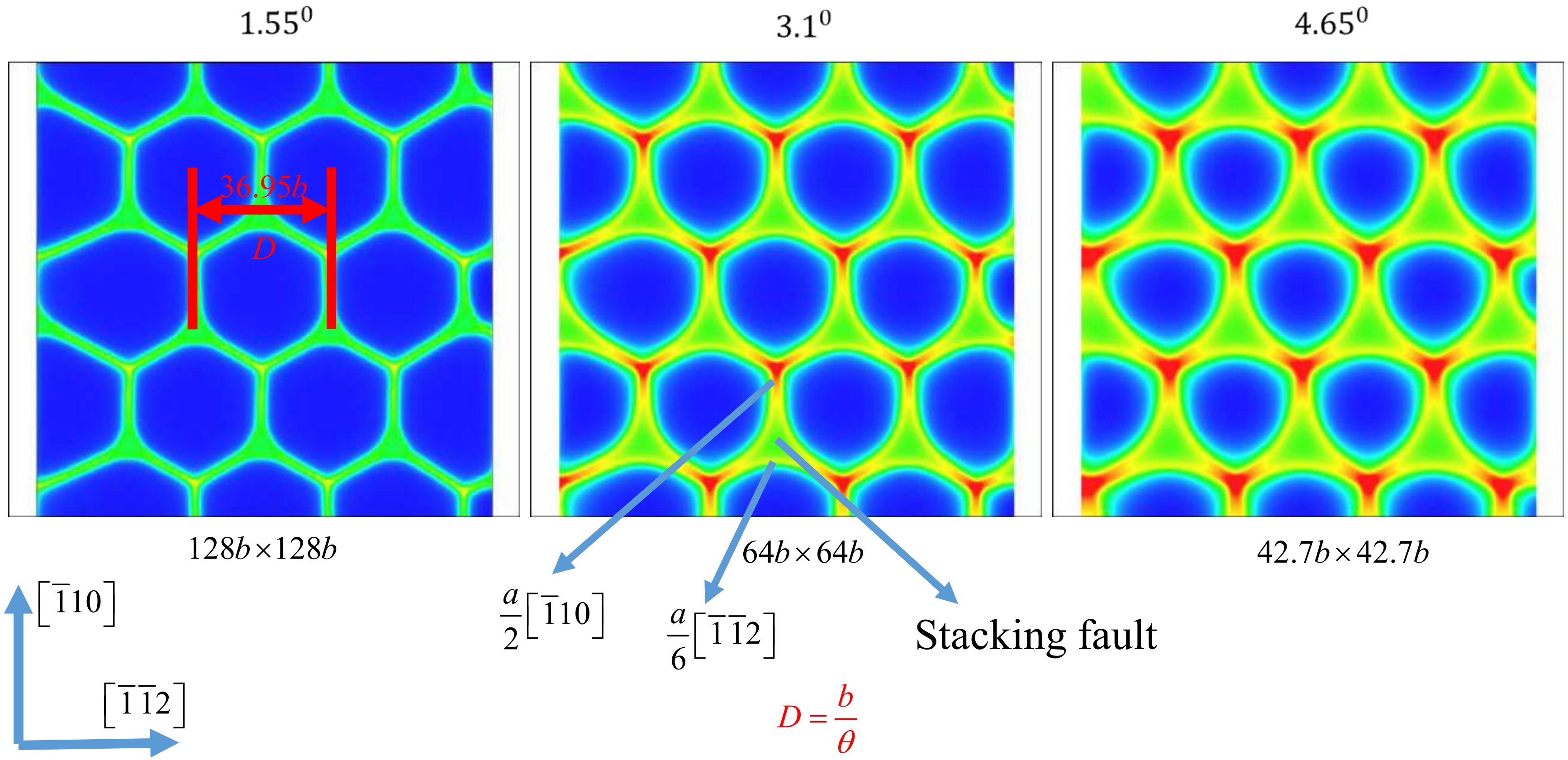
Glide dislocation acrosss the twist GB





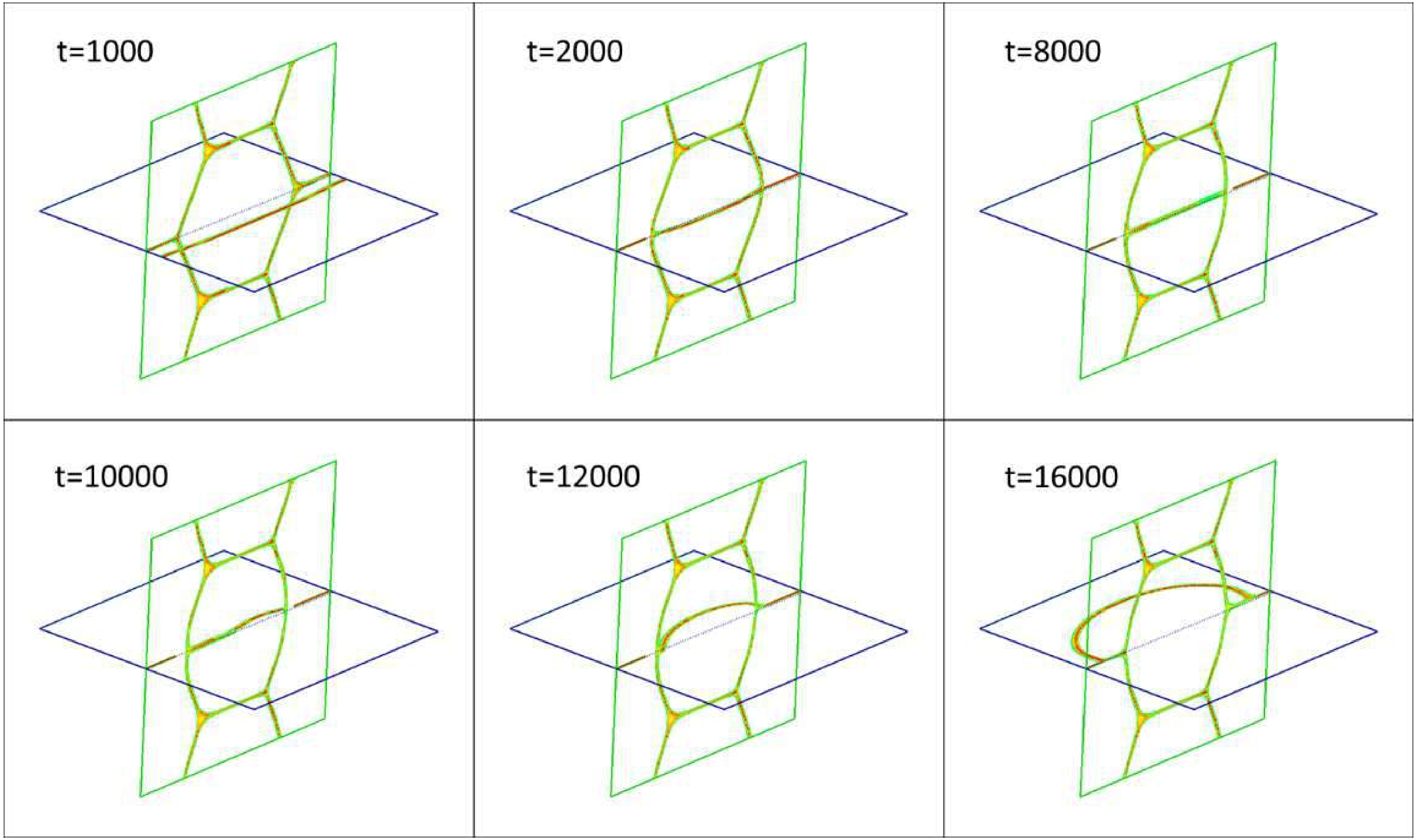
位错相场模拟：位错穿越界面

Twist GB in Al with different twist angle



位错相场模拟：位错穿越界面

Glide dislocation across the twist GB in Al

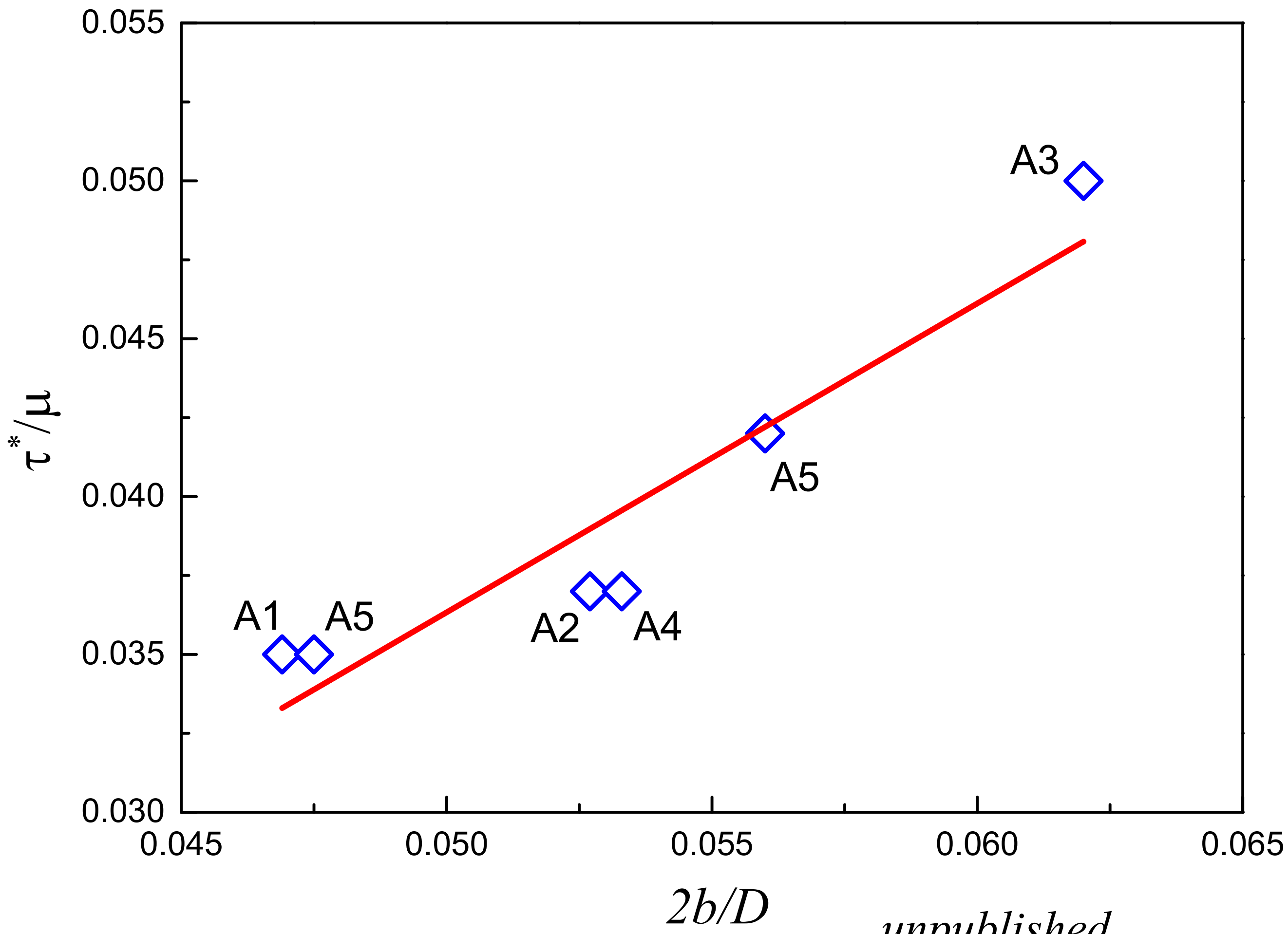


Unpublished

位错相场模拟：位错穿越界面

Glide dislocation across the twist GB in Al

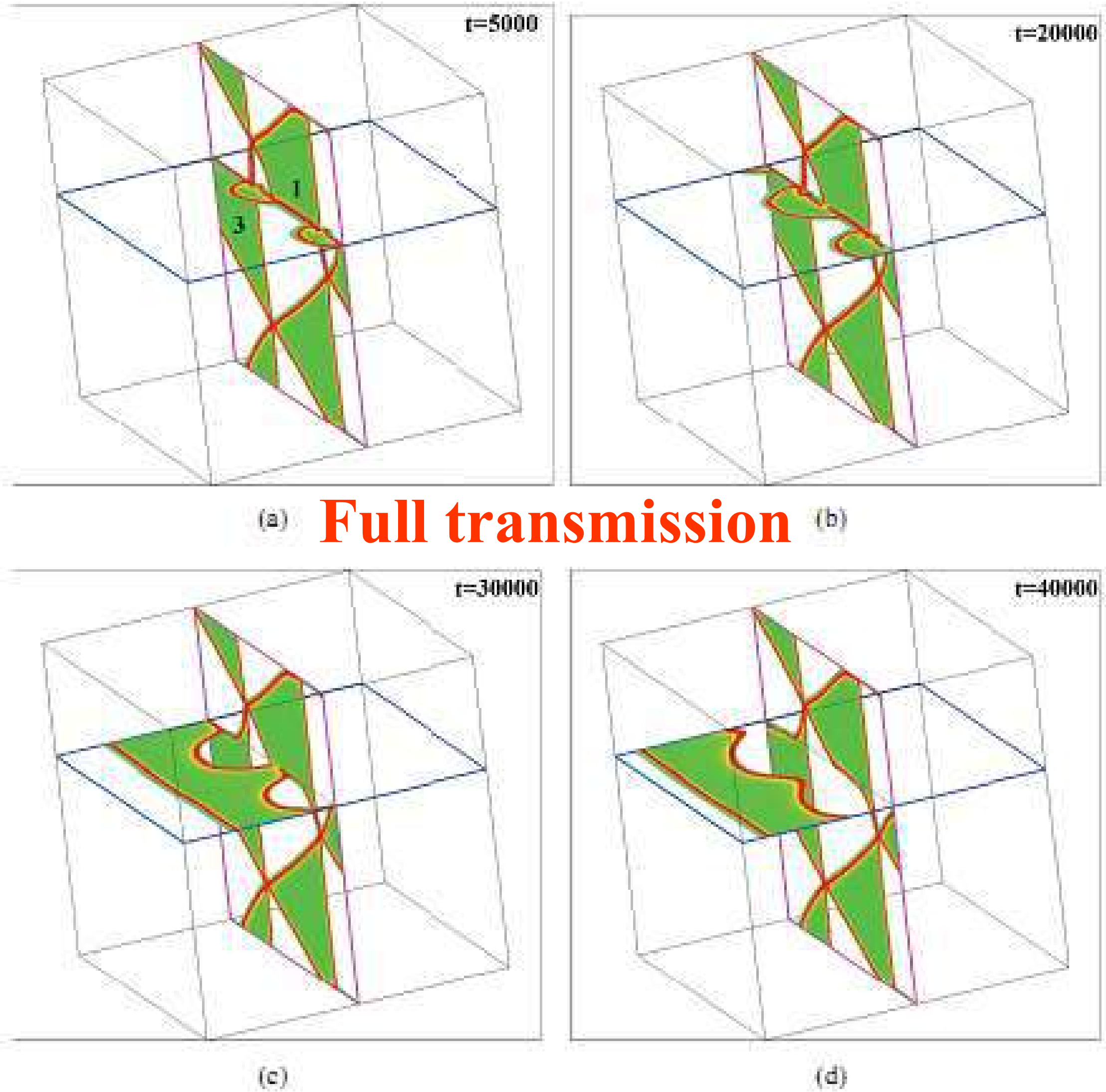
Line tension model $\tau^* \sim \frac{2\mu b}{D}$



unpublished

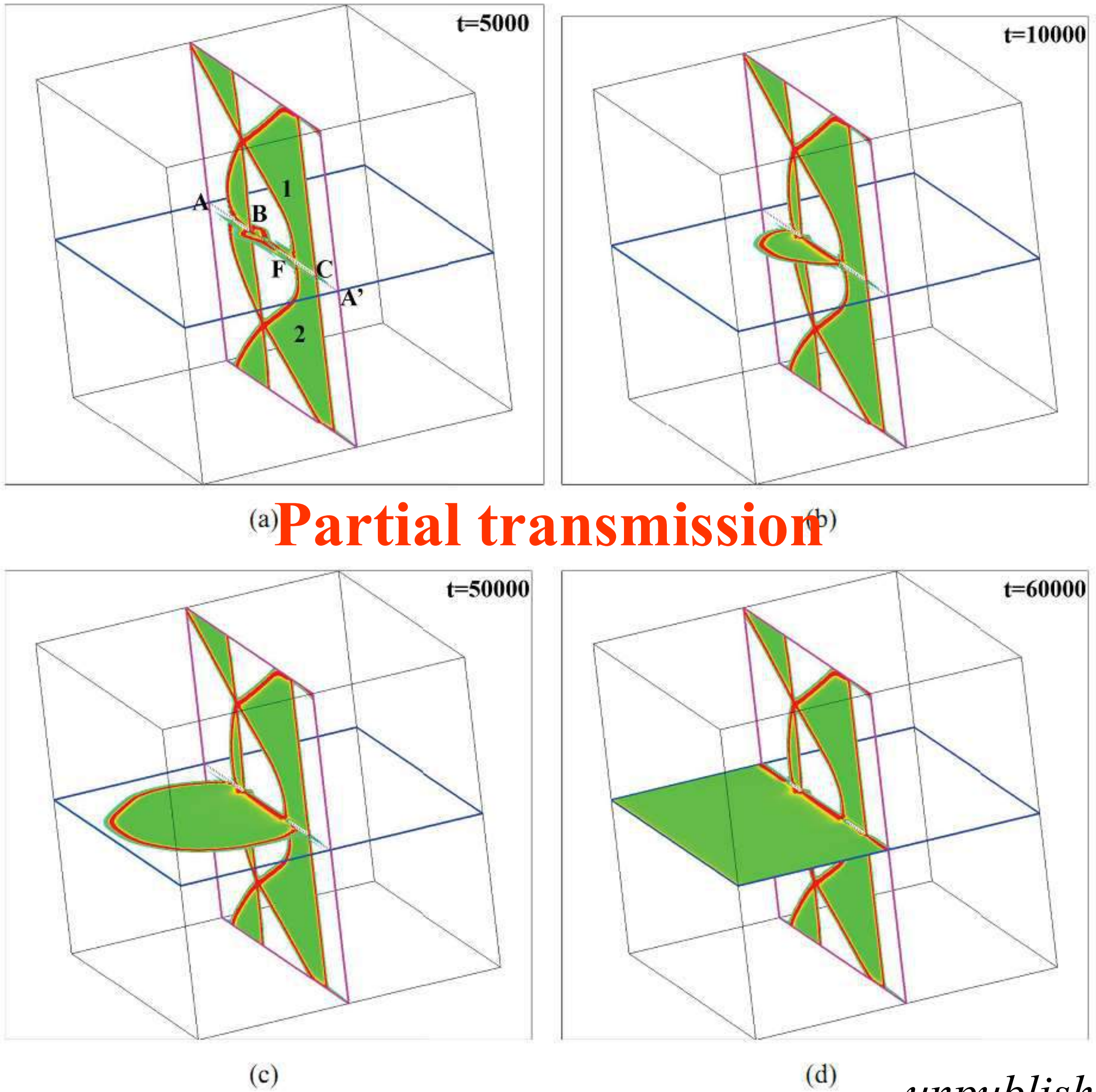
位错相场模拟：位错穿越界面

Glide dislocation across the twist GB in Cu



位错相场模拟：位错穿越界面

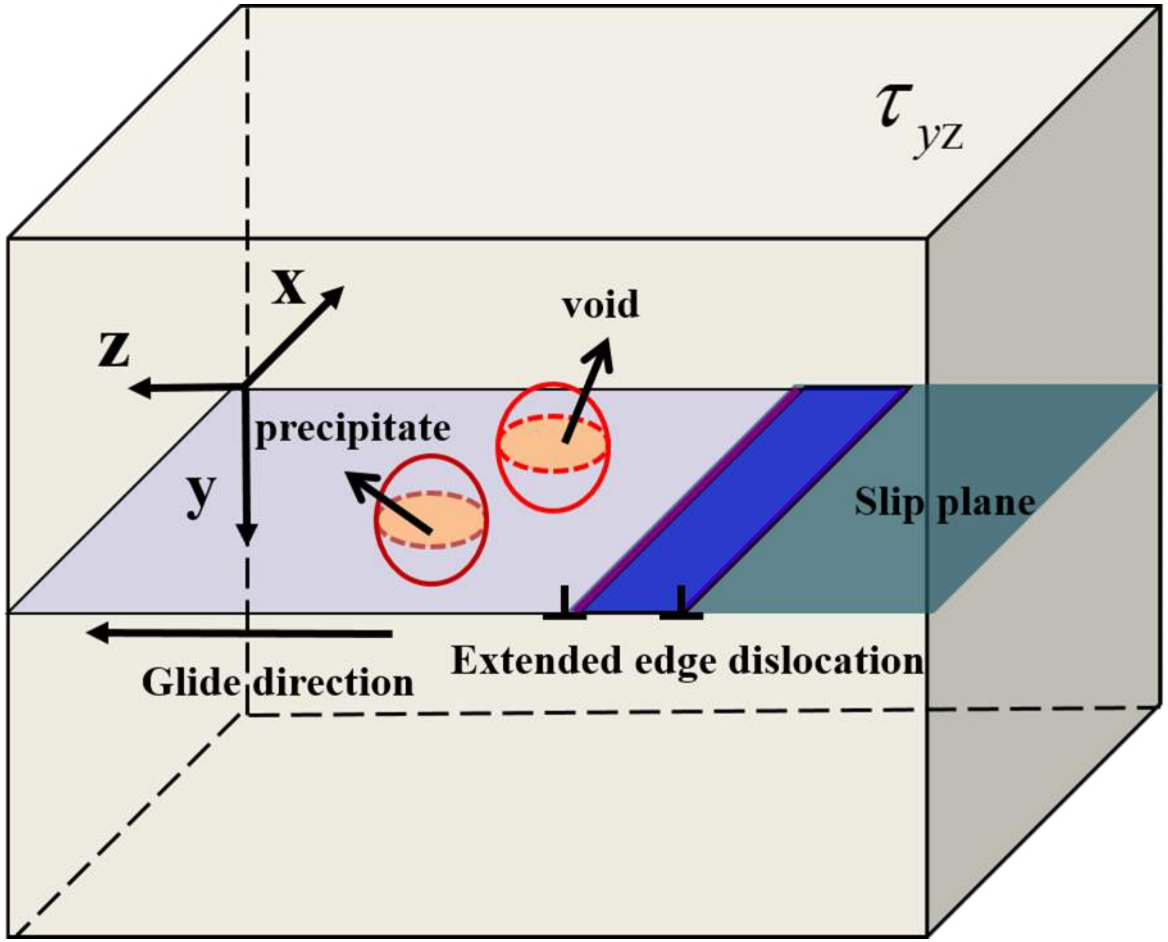
Glide dislocation across the twist GB in Cu



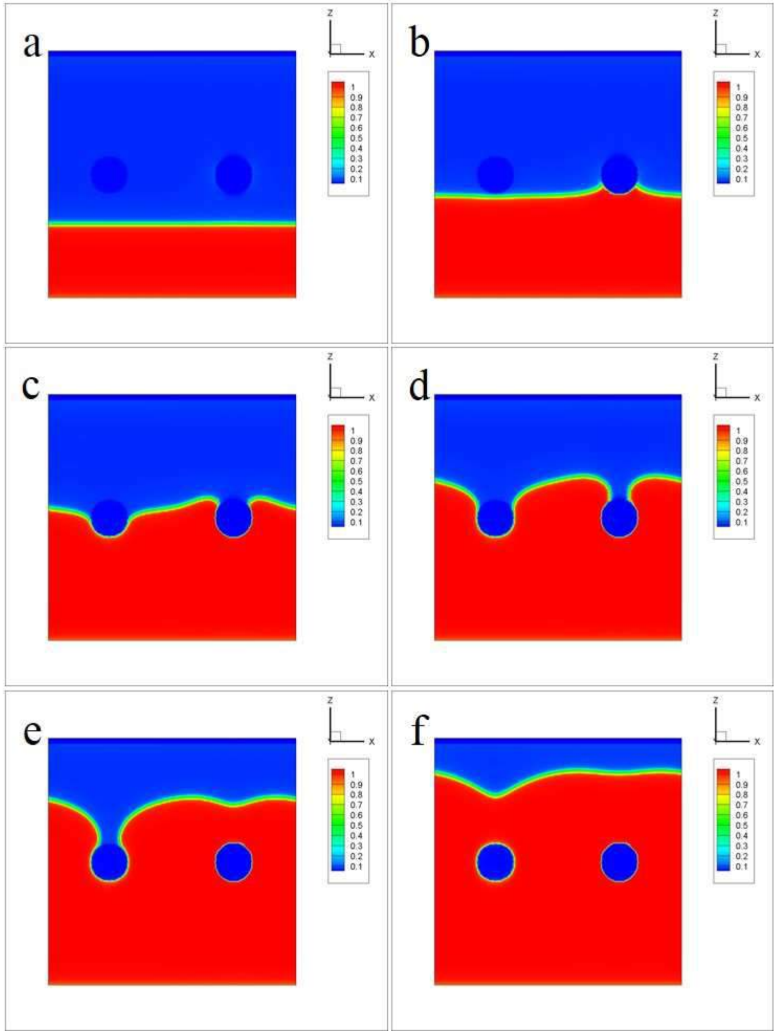
Partial transmission

unpublished

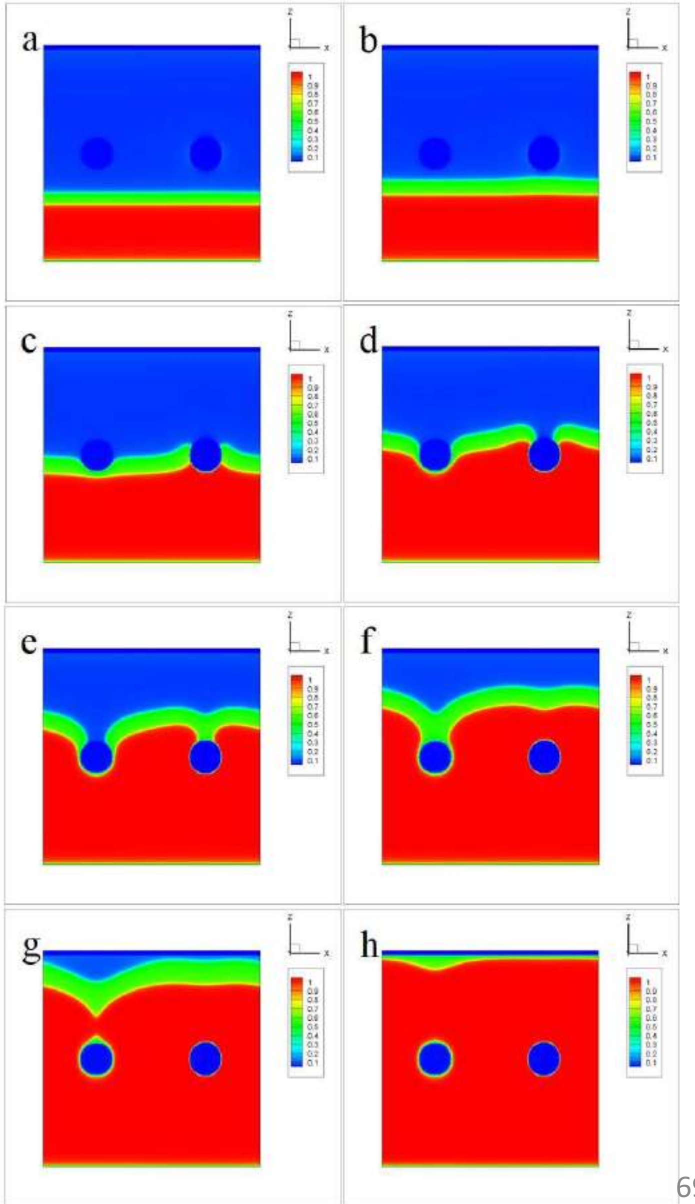
剪切应力下扩展位错穿越孔洞和夹杂相



刃型位错同时穿越孔洞和夹杂相的过程

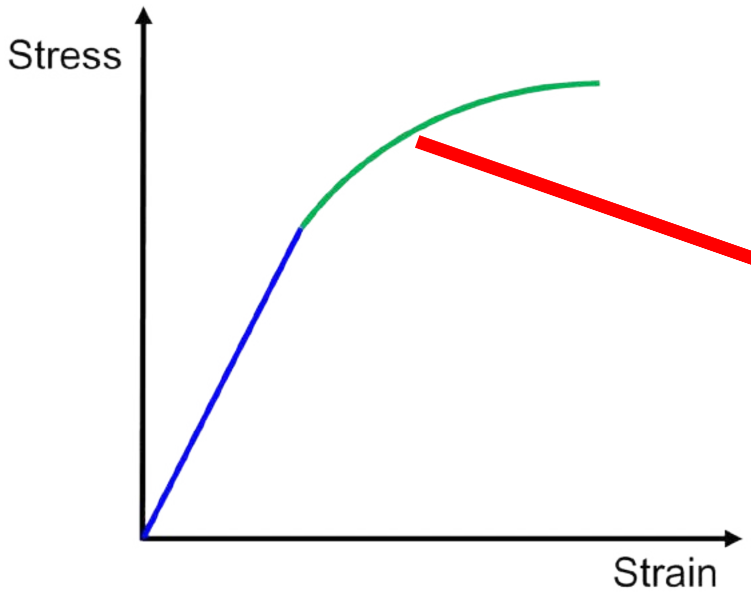


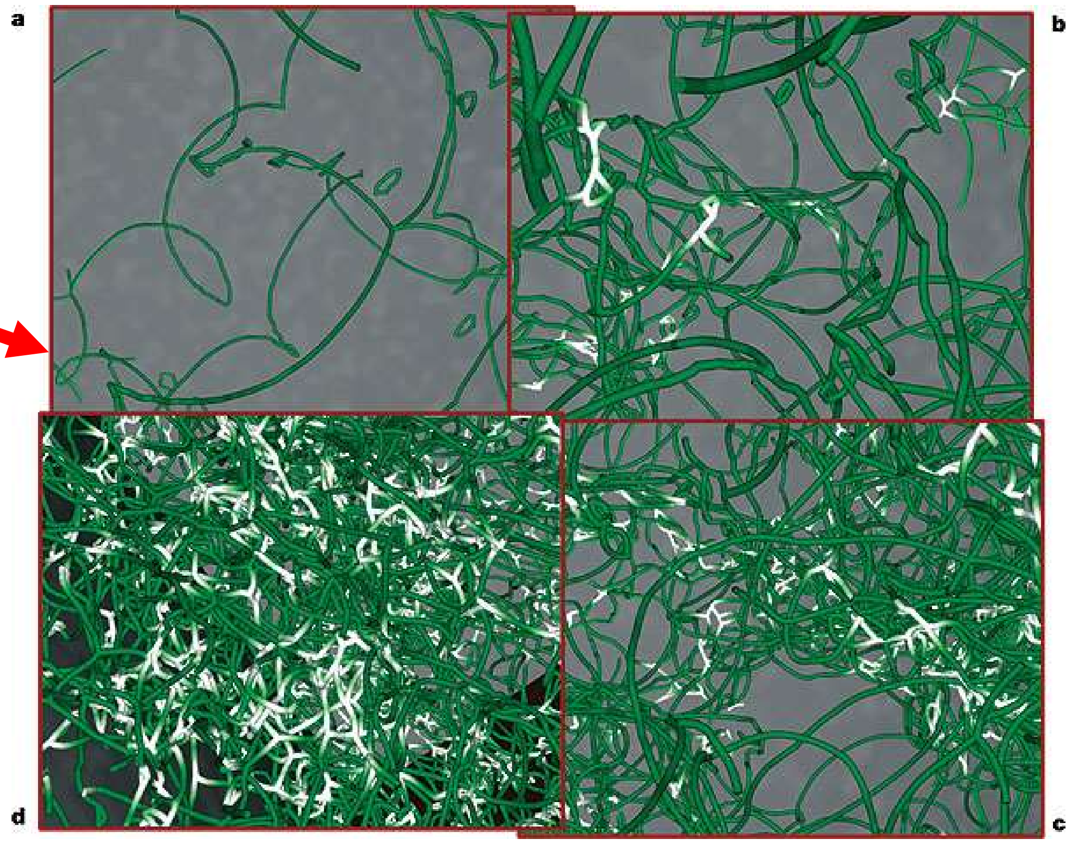
高层错能情况：铝



低层错能情况：铜

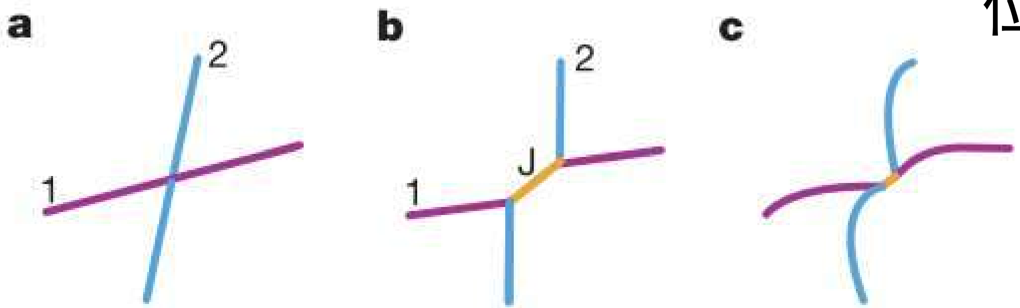
位错反应、位错网络与应变硬化





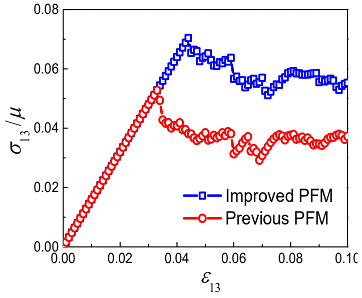
位错网络

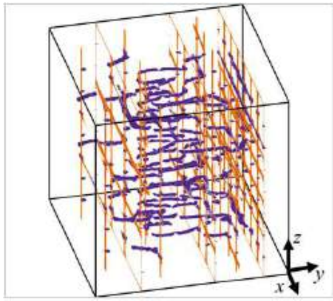
位错结

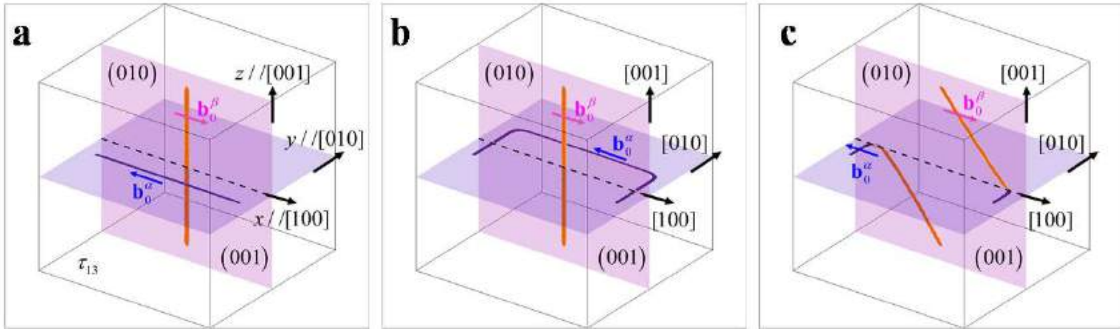


Bulatov et al, Nature 2006

复杂芯结构反应的位错相场模型







涉及芯结构变化的位错反应

传统位错相场无法捕捉芯结构变化

改进位错相场捕捉复杂芯结构变化

提出相交平面的层间滑移势，改进位错相交的相场模型

$$E_{cry} = \int_{\alpha-\alpha\cap\beta} f_{cry}^{\alpha} d^3r + \int_{\beta-\alpha\cap\beta} f_{cry}^{\alpha} d^3r + \int_{\alpha\cap\beta} f_{cry}^{\alpha\cap\beta} d^3r$$

$$E_{cry}^{\alpha\cap\beta} = \int_{\alpha\cap\beta} f_{cry}^{\alpha\cap\beta} d^3r = \int_{\alpha\cap\beta} A\left(1-\cos 2\pi\frac{b_i^{\alpha\cap\beta}}{a}\cos 2\pi\frac{b_j^{\alpha\cap\beta}}{a}\cos 2\pi\frac{b_k^{\alpha\cap\beta}}{a}\right)d^3r.$$

$$\begin{aligned}\mathbf{b}(\mathbf{r}) &= \eta_1^{\alpha}(\mathbf{r})\mathbf{b}_1^{\alpha} + \eta_2^{\alpha}(\mathbf{r})\mathbf{b}_2^{\alpha} + \eta_3^{\alpha}(\mathbf{r})\mathbf{b}_3^{\alpha} + \\ &\quad \eta_1^{\beta}(\mathbf{r})\mathbf{b}_1^{\beta} + \eta_2^{\beta}(\mathbf{r})\mathbf{b}_2^{\beta} + \eta_3^{\beta}(\mathbf{r})\mathbf{b}_3^{\beta} \\ &= b_i^{\alpha\cap\beta}\mathbf{i} + b_j^{\alpha\cap\beta}\mathbf{j} + b_k^{\alpha\cap\beta}\mathbf{k},\end{aligned}$$

npj Computational Materials

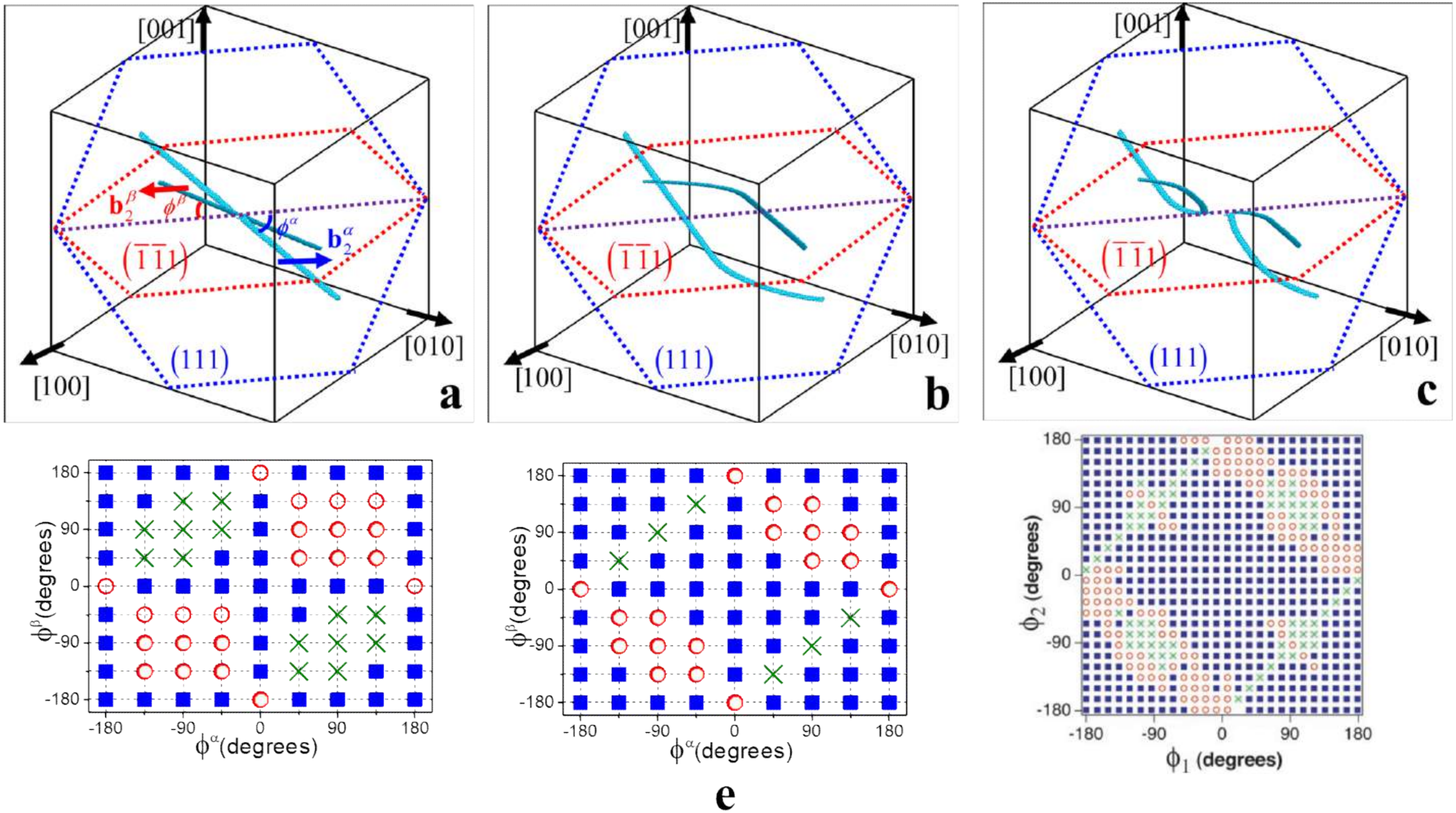
2018, 4, 20

ARTICLE OPEN

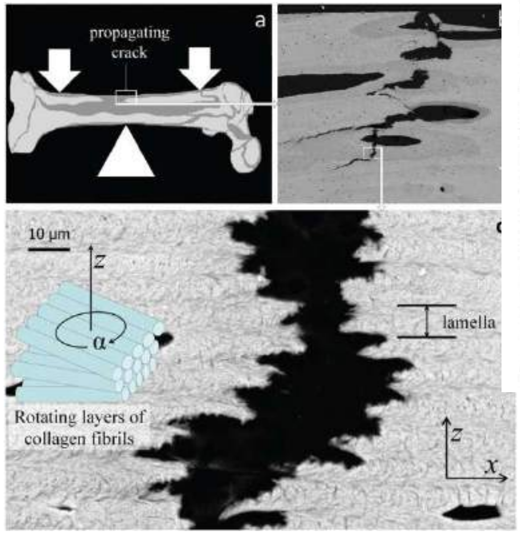
Improved phase field model of dislocation intersections

Songlin Zheng[1,2], Dongchang Zheng[1], Yong Ni[1] and Linghui He[1]

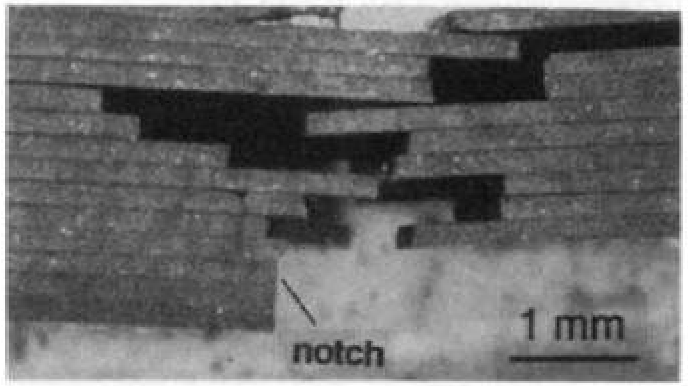
捕捉复杂的共线位错结结构



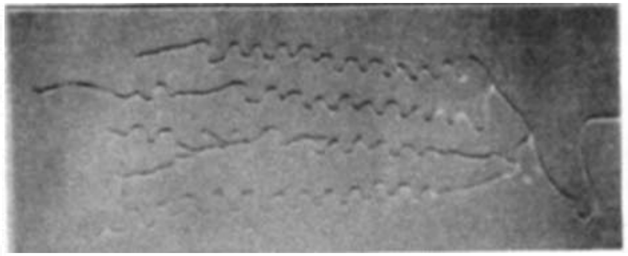
裂纹扩展路径问题



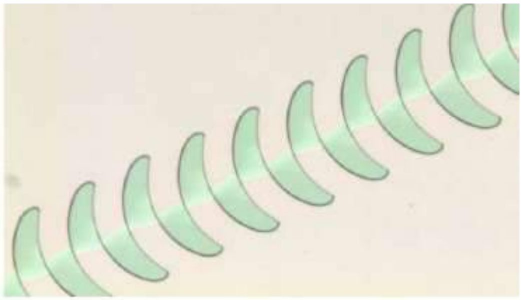
Chem. Soc. Rev., 2016, **45**, 252–267



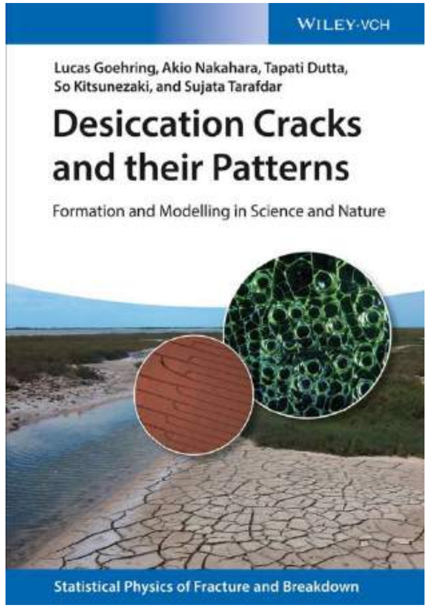
NATURE · VOL 347 · 4 OCTOBER 1990



NATURE · VOL 362 · 25 MARCH 1993



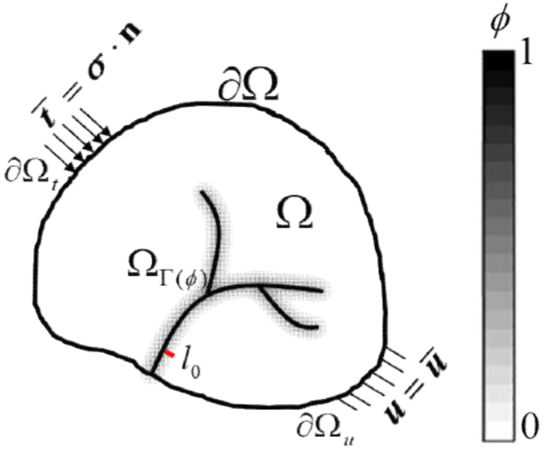
PRL **113**, 085502 (2014)



关键问题：

- ◆ 运动边界问题
- ◆ 裂纹斑图动力学
- ◆ 多裂纹相互作用与强度、疲劳、韧性、失效关联
- ◆ 裂纹与微结构演化相互作用：竞争、协同、关联

典型相场断裂模型



$$\Pi = \int_\Omega \left[g(\phi)\psi_e^+(\varepsilon) + \psi_e^-(\varepsilon) \right] d\Omega + \int_\Omega G_c \left[\frac{\phi^2}{2l_0} + \frac{l_0}{2} |\nabla\phi|^2 \right] d\Omega$$

$$- \int_\Omega \mathbf{f} \cdot \boldsymbol{u} \, d\Omega - \int_{\partial\Omega} \bar{\boldsymbol{t}} \cdot \boldsymbol{u} \, d\partial\Omega$$

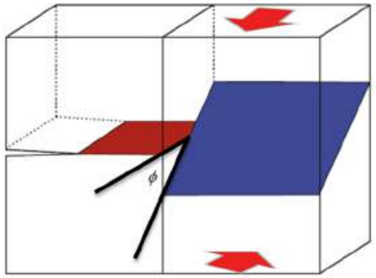
$$\int_\Gamma G_c d\Gamma \approx \int_\Omega G_c \left[\frac{\phi^2}{2l_0} + \frac{l_0}{2} |\nabla\phi|^2 \right] d\Omega \qquad g(\phi) = (1-\phi)^2 + \kappa$$

$$\boldsymbol{\varepsilon}_\pm = \sum_{i=1}^{i=d} \langle \varepsilon_i \rangle_\pm \boldsymbol{n}_i \otimes \boldsymbol{n}_i \qquad \psi_e^\pm(\varepsilon) = \frac{\lambda}{2} \langle tr(\varepsilon) \rangle_\pm^2 + \mu tr(\varepsilon_\pm^2) \qquad \psi_e(\varepsilon) = g(\phi)\psi_e^+(\varepsilon) + \psi_e^-(\varepsilon)$$

力学平衡方程和相场演化方程
$$\begin{cases} Div(\sigma) + \mathbf{f} = 0 \\ \dfrac{\partial\phi}{\partial t} = -L \left[\dfrac{G_c}{l_0} (\phi - l_0^2 \Delta\phi) - 2(1-\phi)\psi_e^+ \right] \end{cases}$$

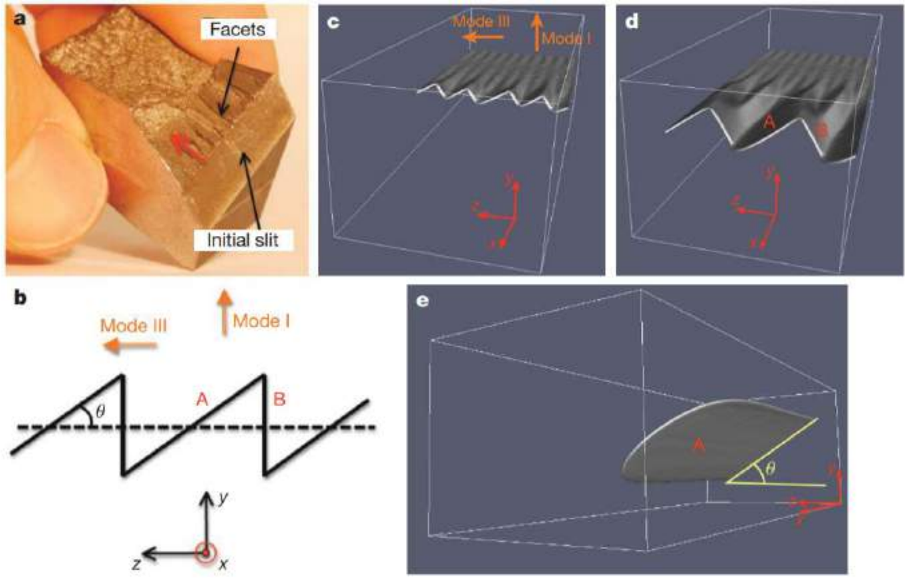
Wu, J. Y., Nguyen, V. P., Nguyen, C. T., Sutula, D., Bordas, S., & Sinaie, S. (2018). Phase field modeling of fracture. Advances in applied mechancis: multi-scale theory and computation, 52.（综述文献）

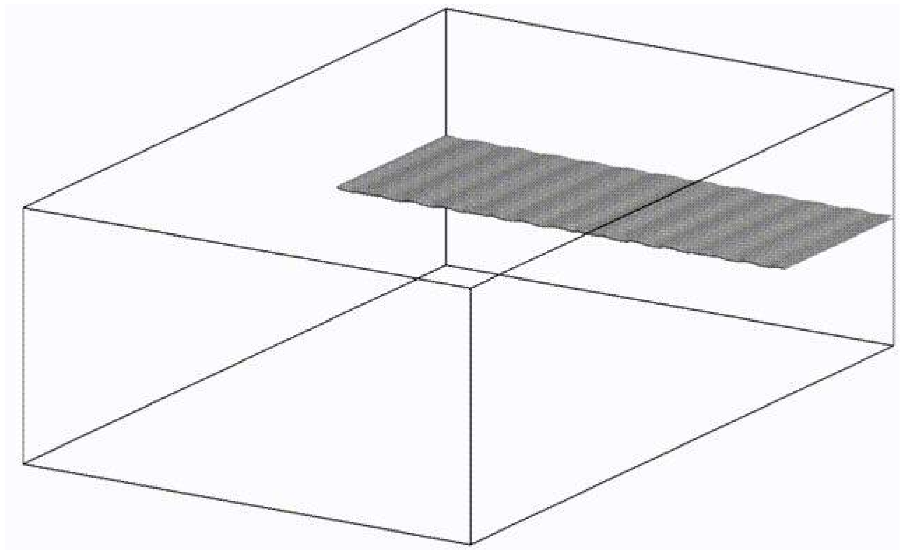
Helical crack-front instability in mixed-mode fracture



$$\Pi(u,\phi)=\int_{\Omega}\left\{\frac{\rho}{2}\left(\partial_t \mathbf{u}\right)^2+\frac{\kappa}{2}\left|\nabla\phi\right|^2+g(\phi)\left[\psi_0-\psi_c\right]\right\}dx$$

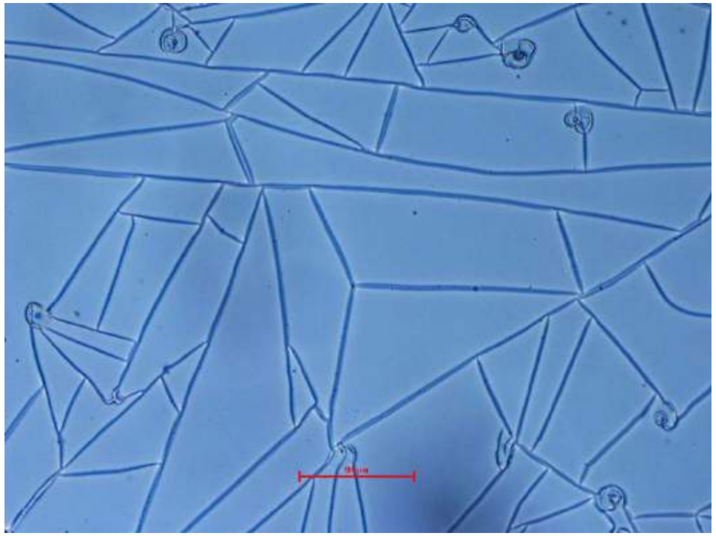
$$\partial_t\phi=-\chi\delta\Pi/\delta\phi \qquad \rho\partial_t^2 u_i=-\delta\Pi/\delta u_i$$

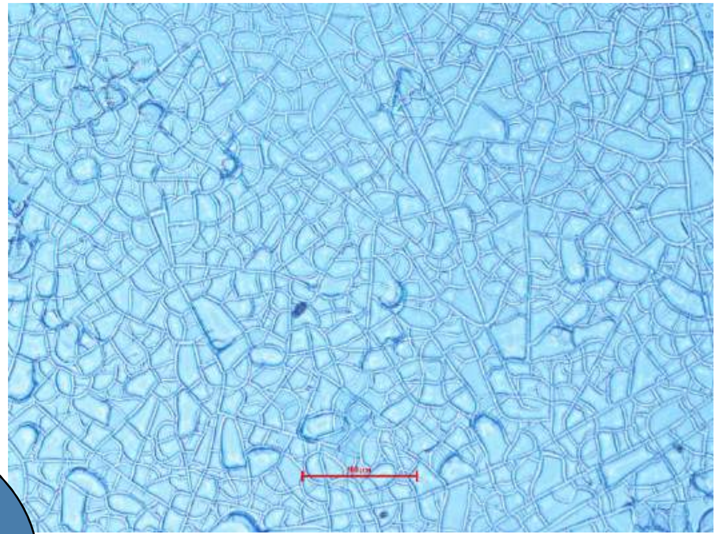


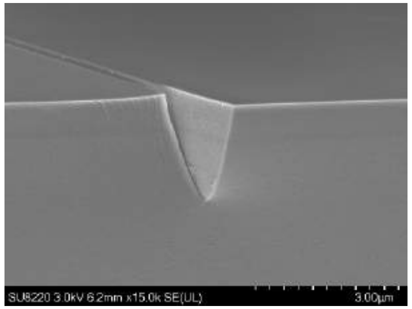


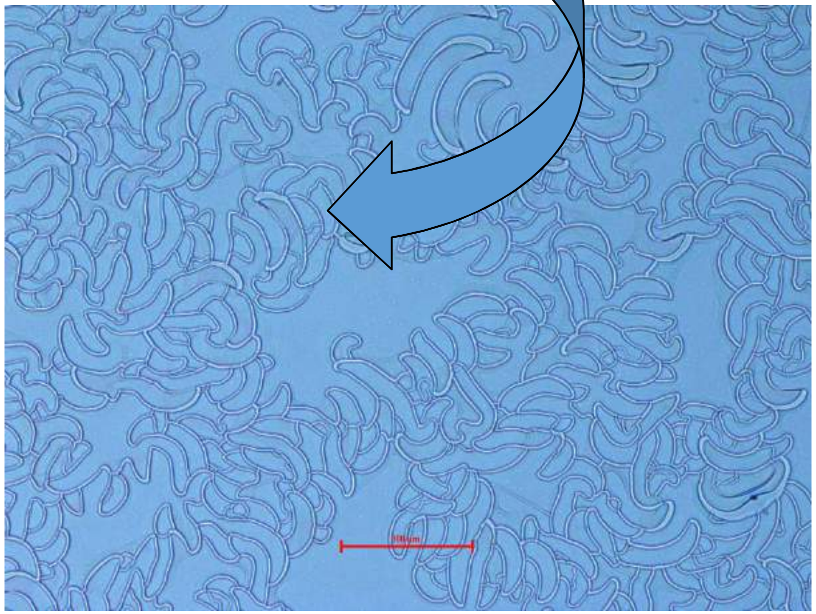
Pons, A., Karma, A. ***Nature*** 464, 85–89 (2010).

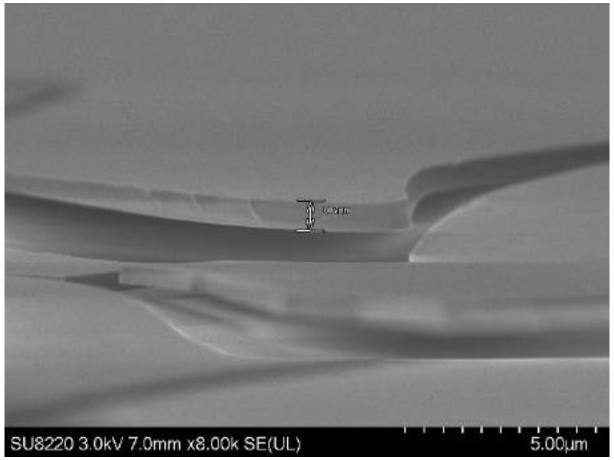
玻璃基底上氧化硅中的裂纹网络：开裂与界面脱层协同











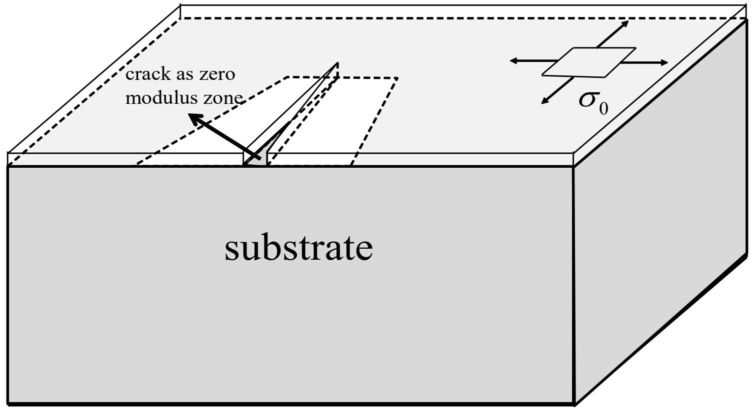
含复杂薄膜裂纹的脱层动力学:相场模拟

场变量：　位移跳跃 $\Lambda_\alpha\left(x_1,x_2,t\right)$, $(\alpha=1,2)$

即薄膜与基底界面上切向位移差

总能量：　$U^{tot}(\Lambda_\alpha)=U^{film}+U^{sub}+U^{\text{int}}$

当总能量取得极小值时，系统达到平衡态构型。



静态裂纹+脱层过程

➤ 含预应变的弹性板理论描述薄膜变形

$$U^{film}=\frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}N_{\alpha\beta}e_{\alpha\beta}dx_1dx_2,$$

$$e_{\alpha\beta}=\frac{1}{2}\left(u_{\alpha,\beta}+u_{\beta,\alpha}\right)-\varepsilon^0_{\alpha\beta},$$

$\varepsilon^0_{\alpha\beta}$ 为预应变（本征应变）

$$U^{\text{int}}=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\int_0^{\Lambda_\alpha}T_\alpha\left(\Lambda_\alpha\right)d\Lambda_\alpha\right)dx_1dx_2$$

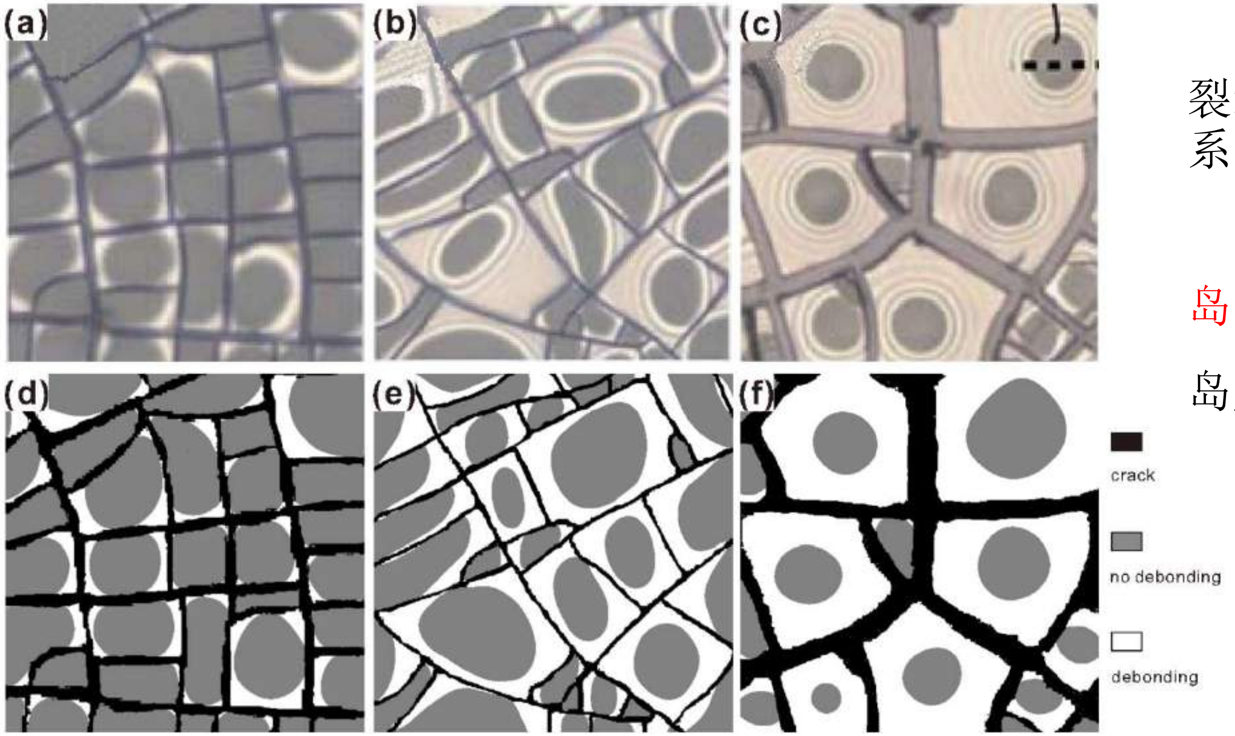
$$U^{sub}=\frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}T^s_\alpha u^s_\alpha dx_1dx_2,$$

$$\frac{\partial\Lambda_\alpha}{\partial t}=-\Gamma_{\Lambda_\alpha}\frac{\delta U^{tot}}{\delta\Lambda_\alpha}=-\Gamma_{\Lambda_\alpha}\left(T_\alpha-T^s_\alpha\right).\quad(\alpha=1,2)$$

$$\frac{\partial\varepsilon^0_{\alpha\beta}}{\partial t}=-\Gamma_{\varepsilon^0_{\alpha\beta}}hC^0_{\alpha\beta\delta\gamma}\left(\varepsilon^0_{\alpha\beta}-\frac{1}{2}\int_{|\xi|\neq0}\frac{i\left(\xi_\alpha\tilde{G}_{\beta k}+\xi_\beta\tilde{G}_{\alpha k}\right)\tilde{\rho}_k e^{i\xi\cdot r}}{(2\pi)^2}d^2\xi\right)$$

Eng. Fract. Mech., 177:123 (2017)

不同厚度下含多裂纹薄膜的脱层行为



裂纹间距与薄膜厚度关系：

$$\lambda_c = 2h\sigma^* / \tau_m$$

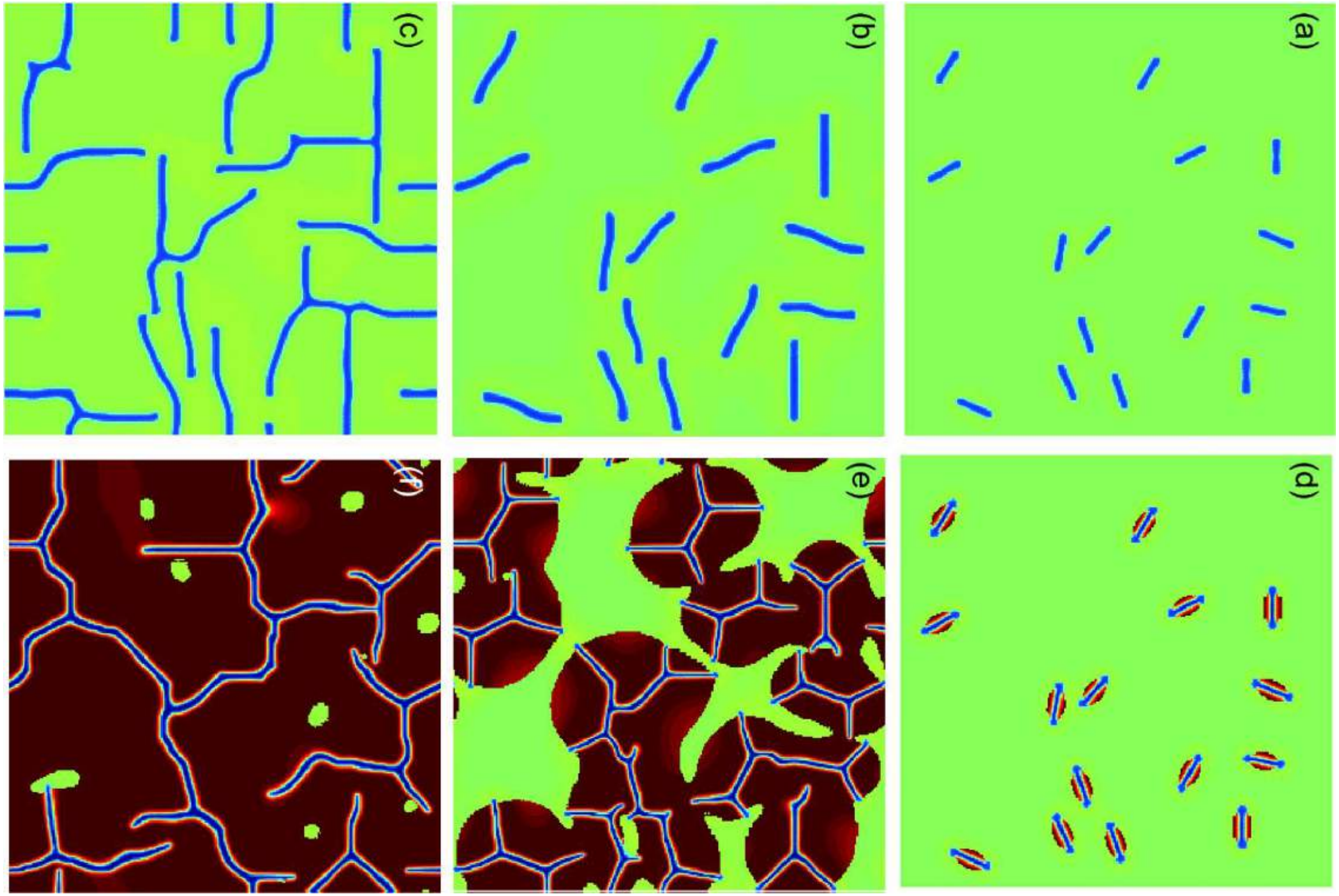
岛结构的尺寸由裂纹间距决定。

岛脱层的临界尺寸：

$$\lambda_d = \sqrt{\frac{4h\mu_f\gamma_t}{\left(1-\nu_f\right)\tau_m^2}}$$

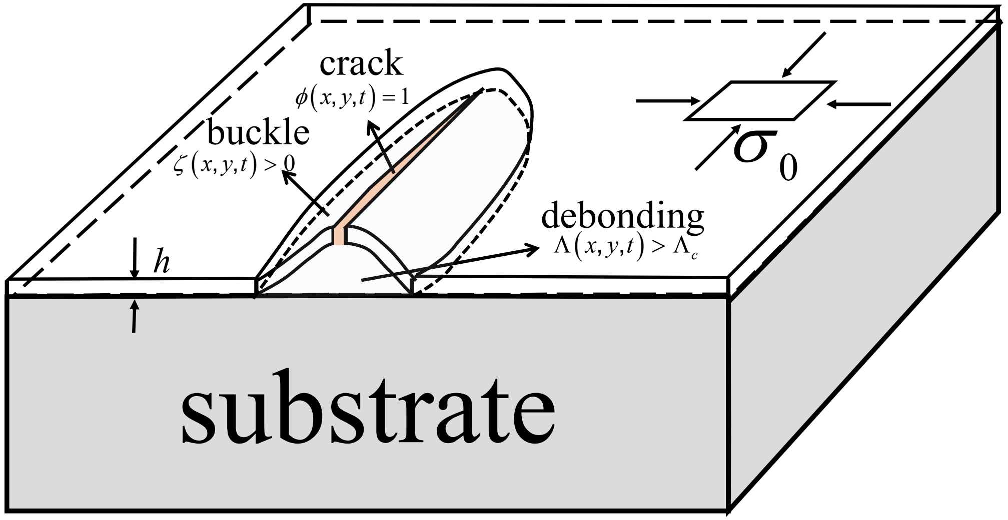
Eng. Fract. Mech. 177,123(2017).

开裂与界面脱层协同生长的相场模拟



中国科学，物理、力学、天文学 48(9), 094614 (2018),（邀请文章）

薄膜结构中翘曲耦合裂纹扩展的相场模型

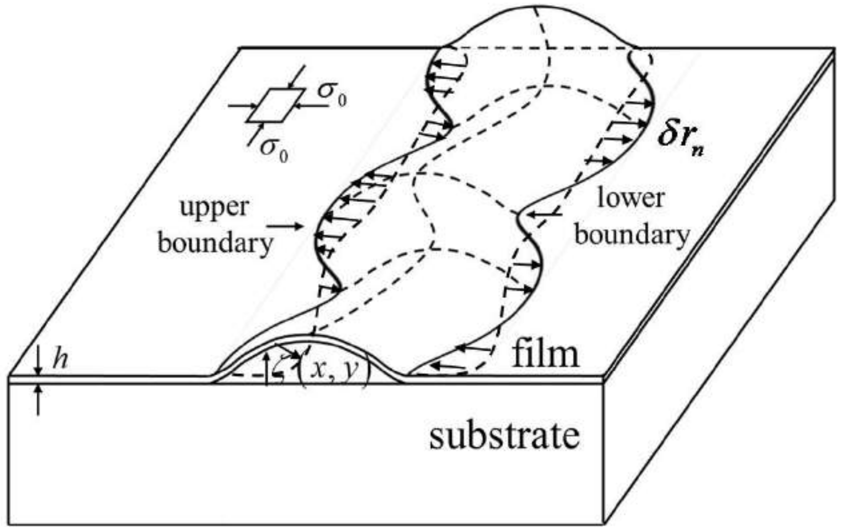


$$N_{\alpha\beta}=h\left[C^{0}_{\alpha\beta\delta\gamma}\phi(r)\left(\varepsilon_{\delta\gamma}(r)-\varepsilon^{*}_{\delta\gamma}(r)\right)\right]$$

$$\phi(r)=\begin{cases}0 & \text{crack}\\ 1 & \text{no crack}\end{cases}$$

$$\frac{\partial\phi}{\partial t}=-L\frac{\delta F^{\text{tot}}_{\text{inhom}}}{\delta\phi}$$

$$\frac{\partial\Lambda_i}{\partial t}=-\Gamma_{\Lambda_i}\frac{\delta F^{tot}}{\delta\Lambda_i}$$

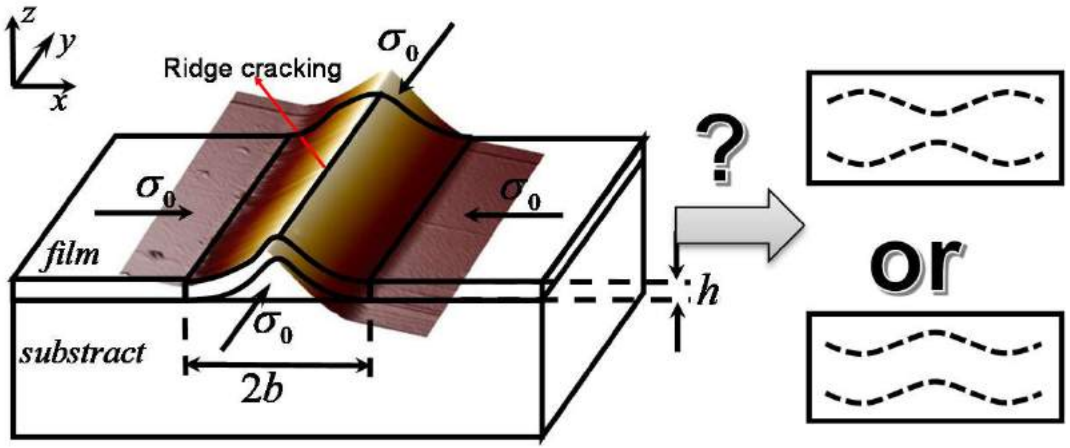


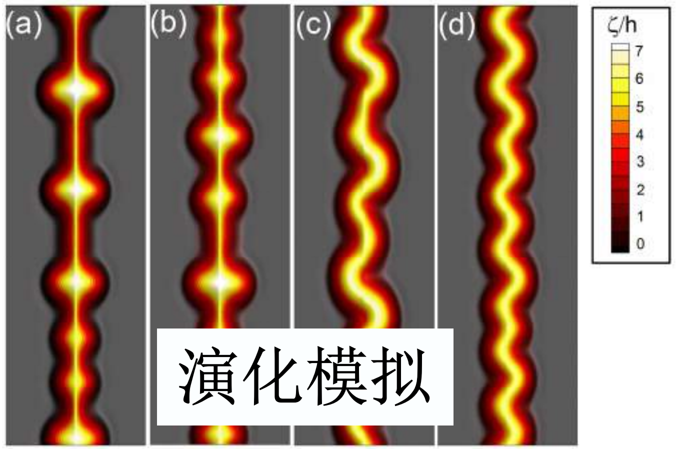
$$\frac{\partial\zeta}{\partial t}=-\Gamma\left[\Delta D(\phi,x_i)\Delta\zeta-\left(N_{\alpha\beta}\zeta_{,\alpha}\right)_{,\beta}+T^{s}_{3}\right]$$

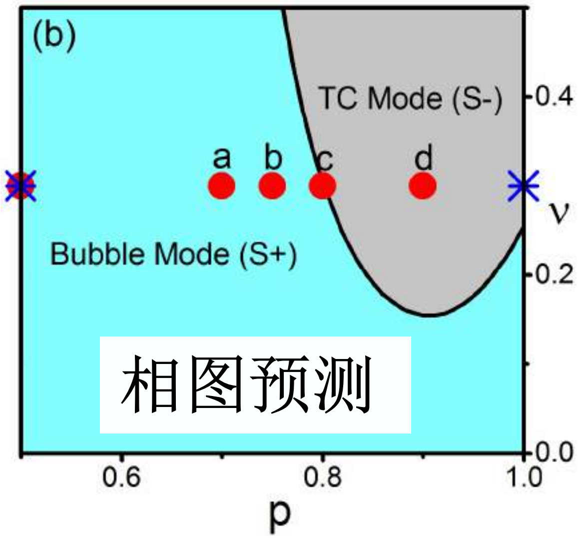
Acta Mater., 69,37 (2014)； Acta Mater., 127,220 (2017)

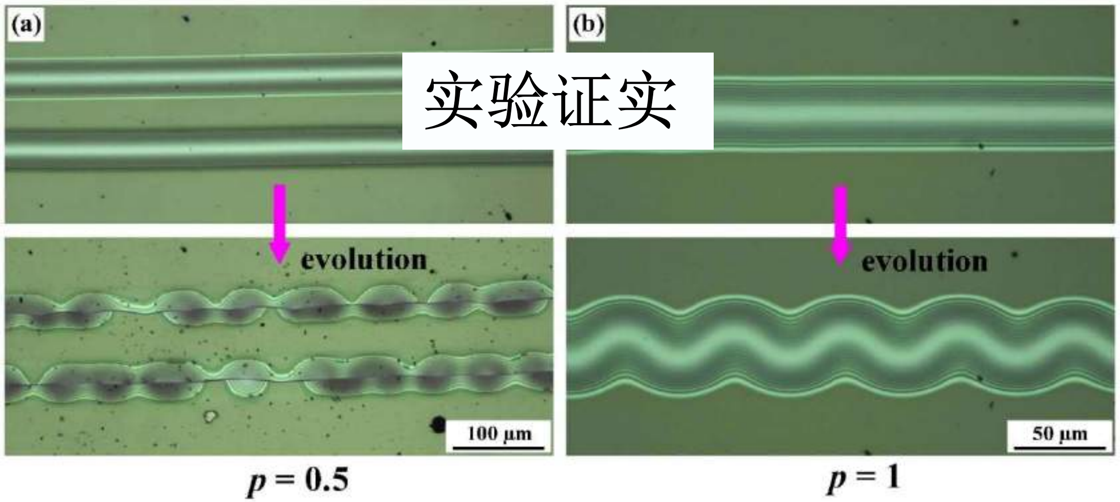
应力对薄膜结构中翘曲失效复杂模态与演化的作用机制

顶部开裂有利于“直边”翘曲形貌发生对称失稳模式









JMPS, 112,637(2018)

提纲

1. 相场方法基本思想与发展历史

1.1材料微结构演化现象：相变与动边界问题

1.2相场模拟基础：相场变量的选择，总自由能、动力学方程的构建，动力学方程的数值求解格式

1.3相场模型的分类：粗粒化相场、晶体相场和生物膜泡相场

1.4相场方法的发展趋势

2. 相场方法的应用举例

2.1相分离

2.2膜泡形状

2.3结构相变

2.4位错

2.5裂纹

yni@ustc.edu.cn

3. 相场方法的上机实践

Fifth International Symposium on Phase-Field Modelling in Materials Science