

《工业中的多尺度力学方法》讲习班

位错动力学方法及应用

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提纲

1 力学响应的位错机理

2 位错基本理论

3 位错动力学方法DDD

4 DDD与原子模拟和连续介质力学的联系

5 应用举例

6 DDD代码介绍及上机指导

1 力学响应的位错机理

1.1 什么是位错？

1.2 为何材料的理论强度>真实强度？

1.3 位错如何影响力学响应？

1.4 为何材料变形呈现温度依赖性？

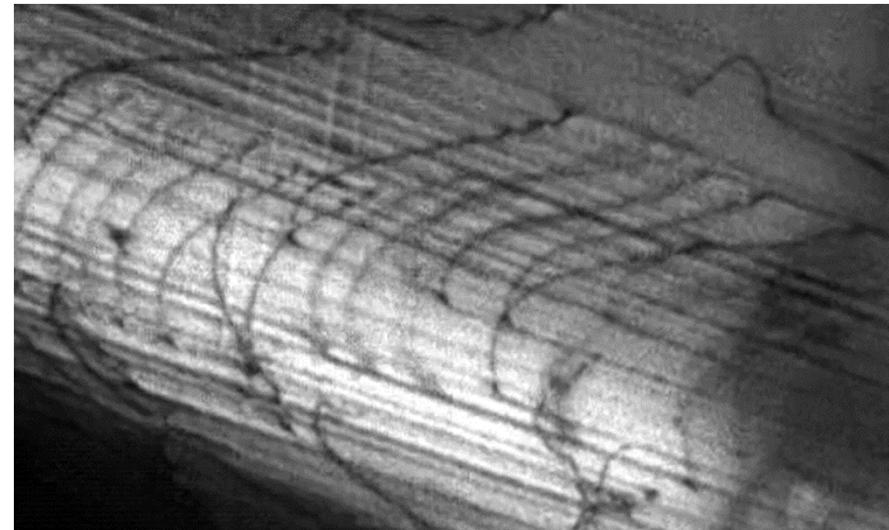
1.5 如何通过调控位错机理，实现材料强韧化？

1 力学响应的位错机理

冷冰冰的金属



电镜下“会跳舞”的位错



J Kacher et al., Acta Mater., 2012, 19(60)

1 力学响应的位错机理

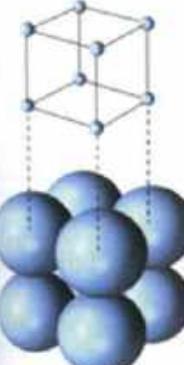
Q1：什么是位错？

位错是晶体材料中的线缺陷

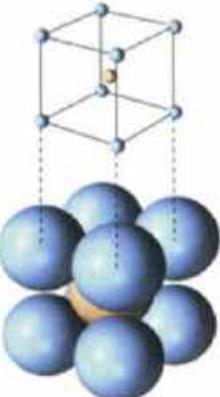
Q：什么是晶体？

晶体中原子形成有序结构。
取决于电子性质，
不同材料呈现出不同的晶体结构。

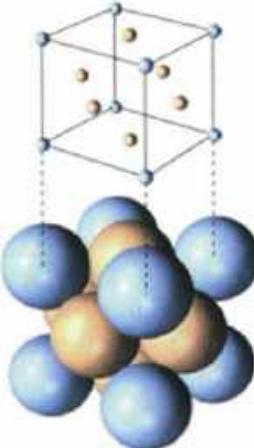
简单立方



体心立方

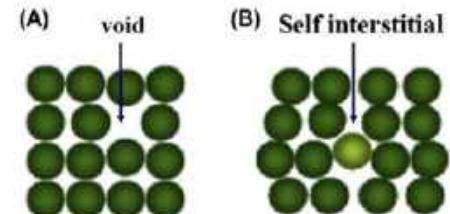


面心立方

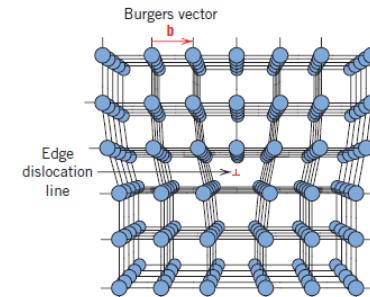


Q：什么是线缺陷？

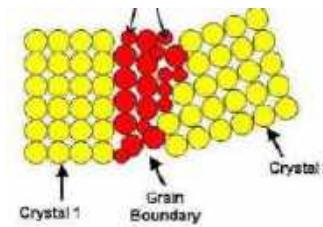
点缺陷



线缺陷



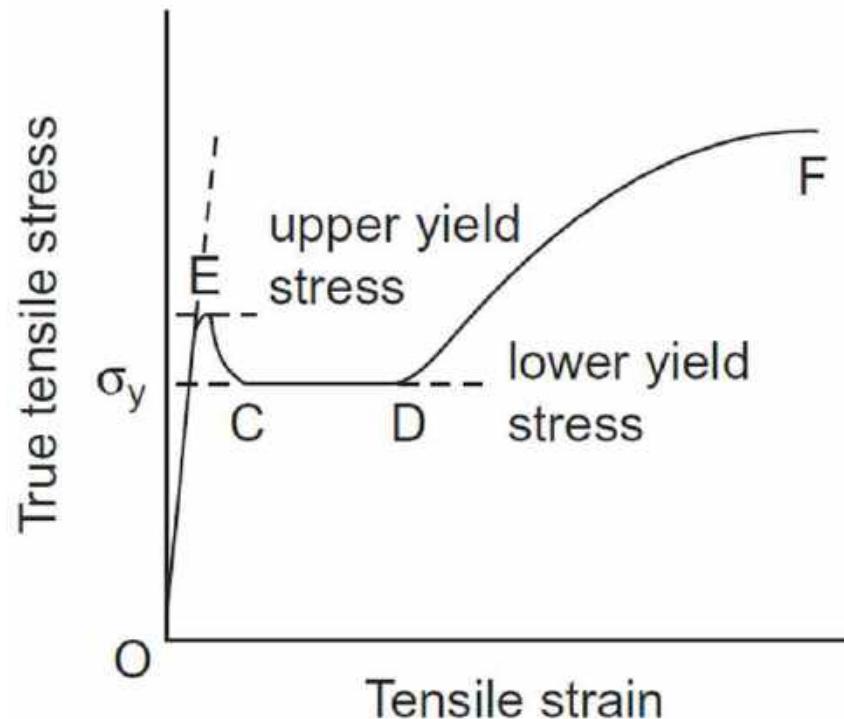
面缺陷



1 力学响应的位错机理

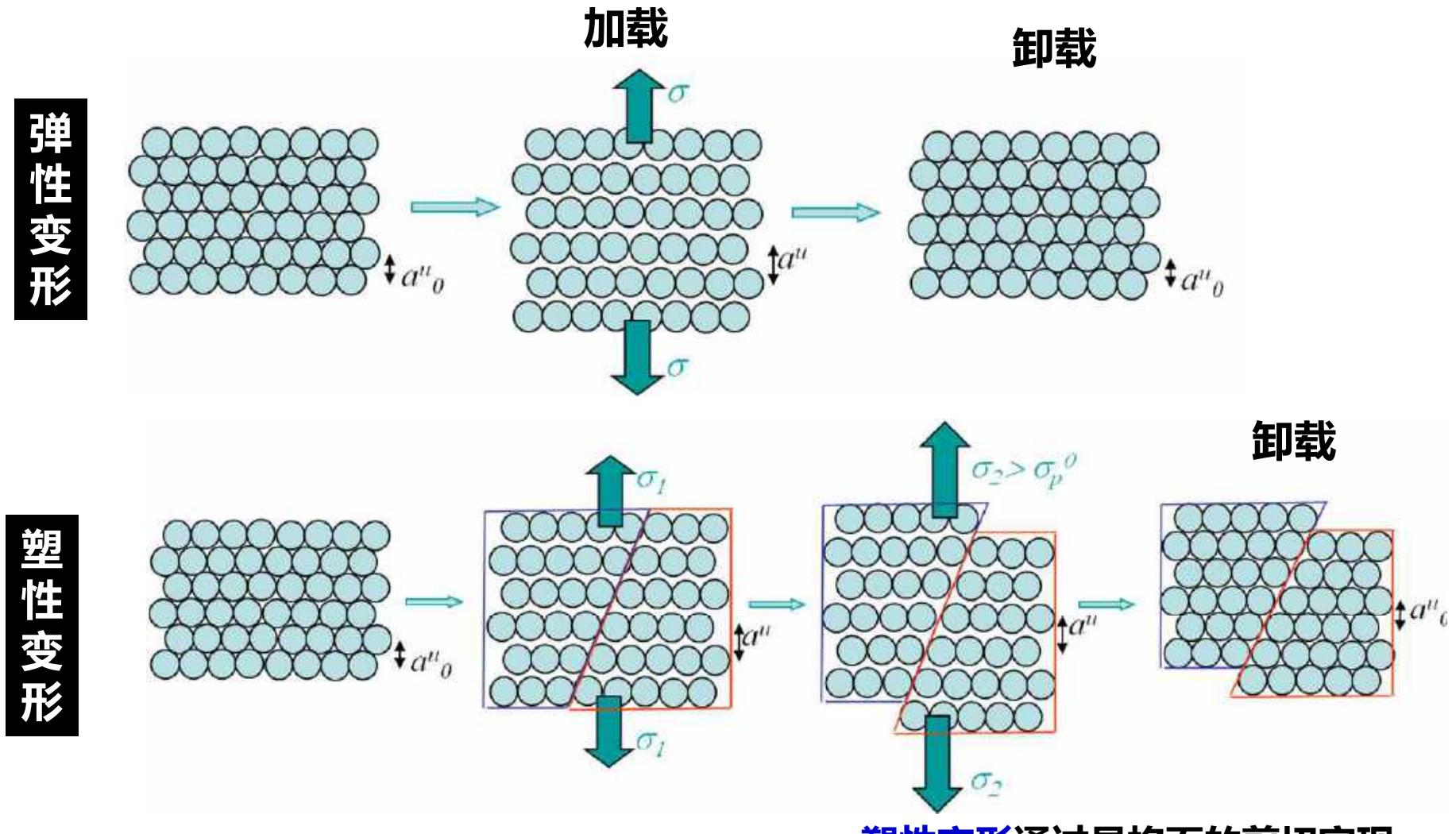
Q2：位错在塑性力学中有何作用？

Yield strength, hardening, ductile/brittle;
Temperature dependence;
Strain rate dependence
(from creep to shock loading).....



1 力学响应的位错机理

Q: 什么是弹性变形？什么是塑性变形？



1 力学响应的位错机理

理想强度：使两个晶格面发生剪切所需要的力

Q: 怎么估计材料的理想强度？

作为近似，假设剪应力随运动距离呈现正弦关系

$$\tau = \tau_{crit} \sin \frac{2\pi u}{b}$$

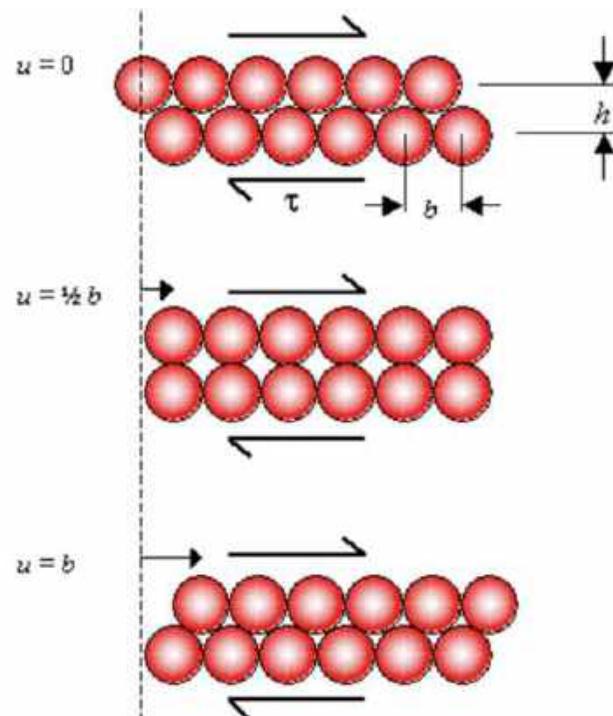
最大值发生在 $u = b/4$

根据 $\tau = G\gamma, \quad \gamma = u/h$

小变形时 $\sin x \sim x \quad \frac{\tau}{\gamma} = G = \frac{2\pi\tau_{crit}h}{b}$

密排结构 $b/h = 2/\sqrt{3}$

可得： $\tau_{crit} = \frac{Gb}{2\pi h} = \frac{G}{\sqrt{3}\pi} \approx \frac{G}{5}$



1 力学响应的位错机理

理想强度：使两个晶格面发生剪切所需要的力

$$\tau_{crit} \approx \frac{G}{5}$$

- 剪切模量大约20~150 GPa,
- 理想强度大约3~30GPa。

远远高于实验观察到的屈服强度 ($\sim G/1000$)

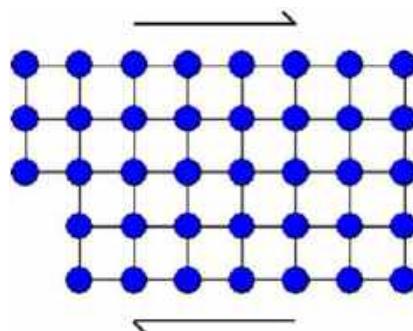
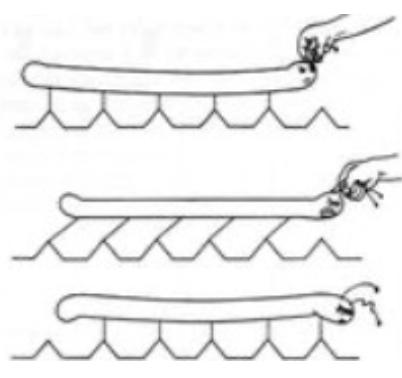
Material	Strength	
	Theoretical [MPa]	Experimental [MPa]
Al	4200	7-11
Cu	7700	50-100
Fe	13000	25-30
Al_2O_3	20000	19000
Diamond	46000	21000

Q:为什么存在这种差异性?

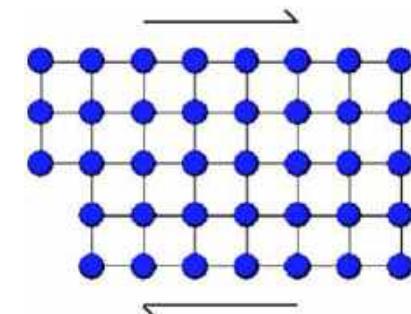
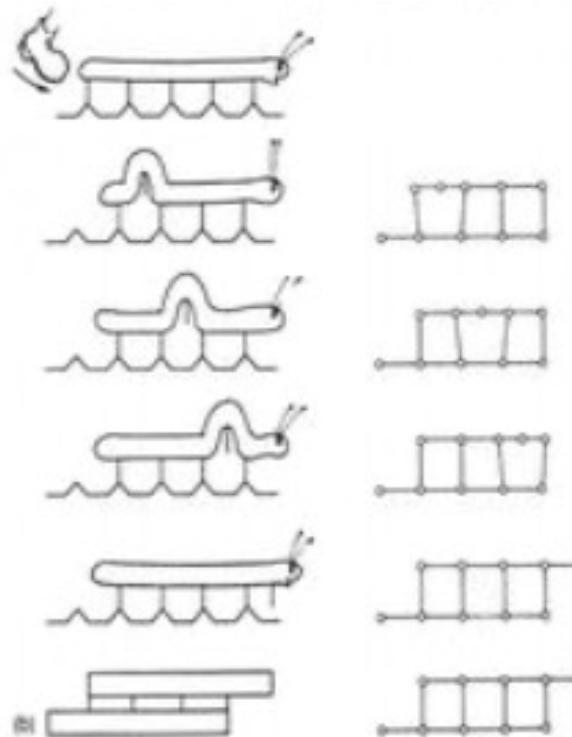
1 力学响应的位错机理

Q:为什么真实强度远低于理想强度?

理论强度



真实强度



晶体的真实强度是位错运动主导的

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1 力学响应的位错机理

晶体强度：不需要同时破坏滑移面之间的一层原子键合，只需要局部克服运动势垒。

晶格滑移阻力通常用Peierls-Nabarro 派纳力表示

派纳力：0K时位错滑移的最小阻力。

派纳力强烈依赖于晶体结构和键的类型
(金属键或共价键)。

派纳力计算很复杂，一个简单模型：

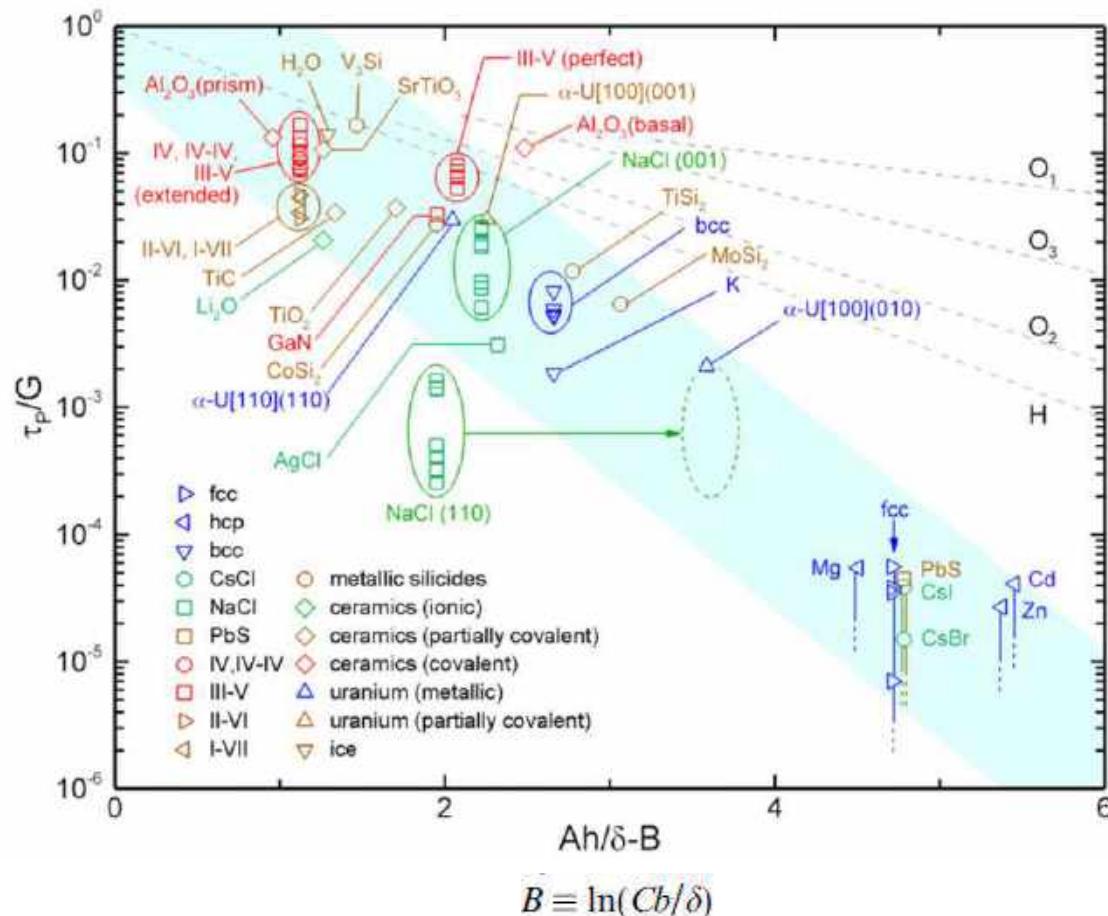
$$\tau_p = 3G \exp\left(-\frac{2\pi w}{b}\right)$$

假设 $w=b$ (位错的最小合理宽度为 b),得到最大值

$$\tau_p = 3G \exp(-2\pi) \approx \frac{G}{180}$$

1 力学响应的位错机理

派纳力



$$\frac{\tau_p}{G} = C \frac{b}{\delta} \exp \left(-A \frac{h}{\delta} \right)$$

h :滑移面间距

δ : 滑移方向的晶格周期

通常：

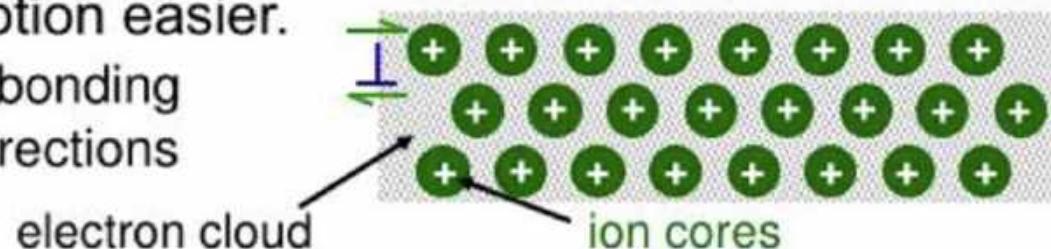
共价键>离子键>金属键

BCC>FCC

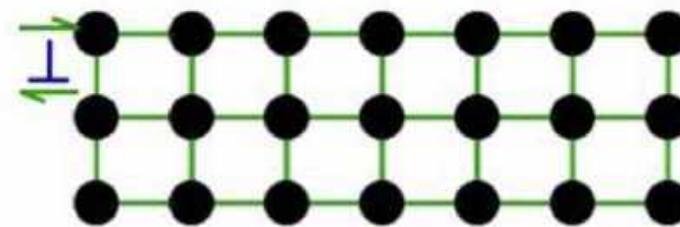
1 力学响应的位错机理

通常： 共价键>离子键>金属键

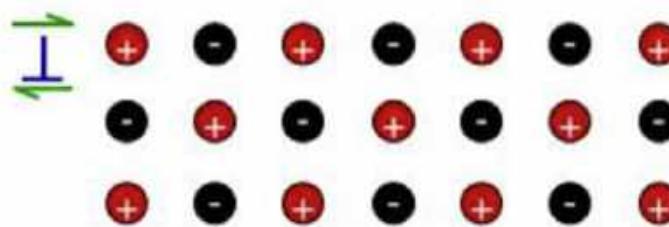
- Metals: Disl. motion easier.
 - non-directional bonding
 - close-packed directions for slip.



- Covalent Ceramics (Si, diamond): Motion hard.
 - directional (angular) bonding

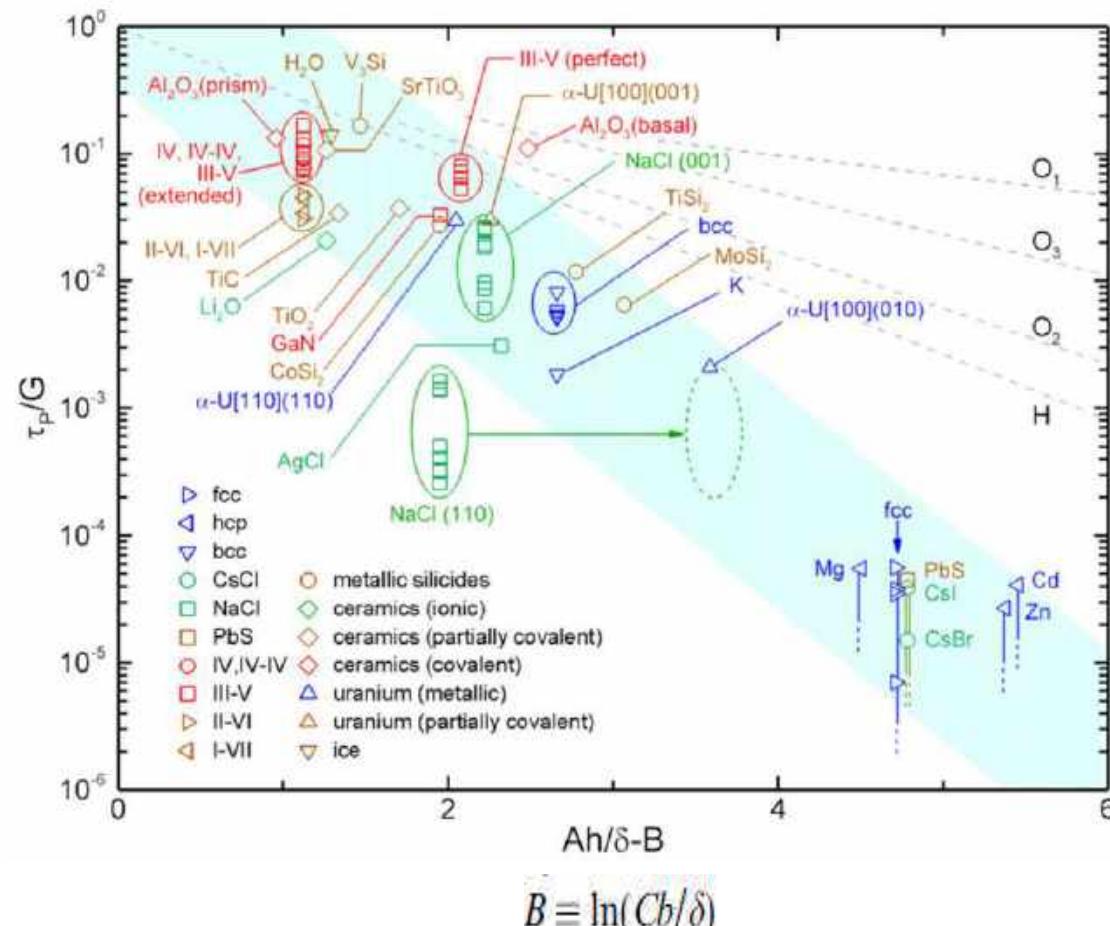


- Ionic Ceramics (NaCl): Motion hard.
 - need to avoid ++ and -- neighbors.



1 力学响应的位错机理

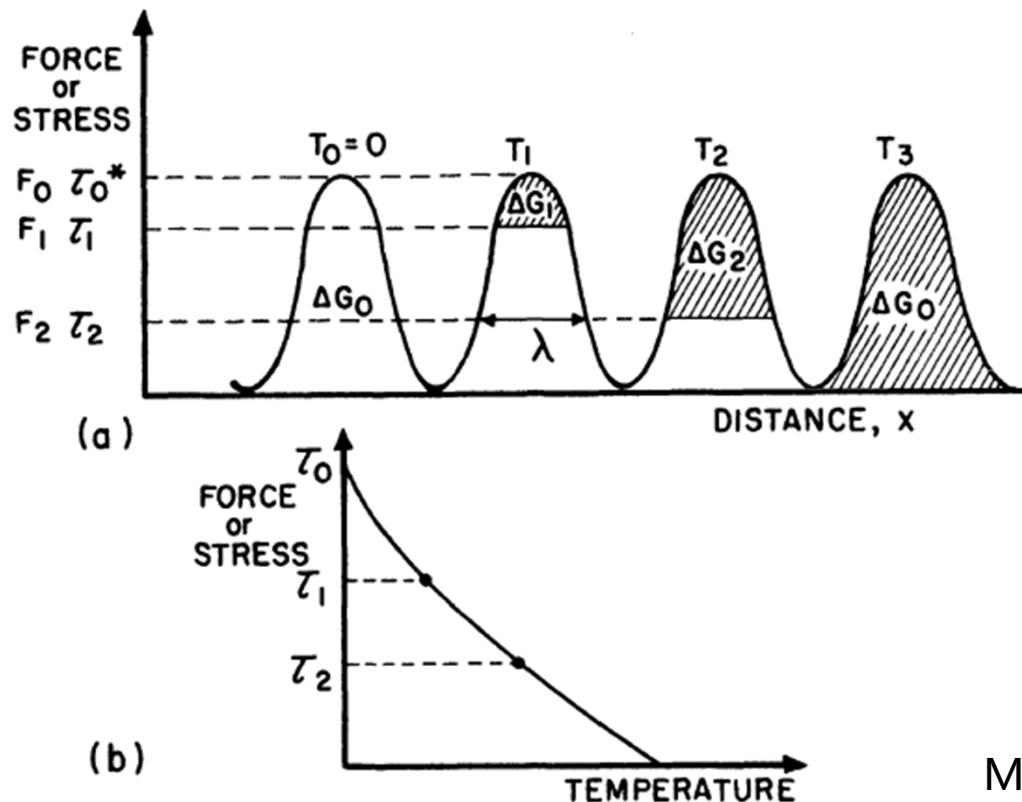
Q：如果材料的派纳力很大，其变形会呈现什么特征呢？



Y. Kamimura et al. 2013

1 力学响应的位错机理

派纳力很大，常需要热激活其克服派纳势垒。



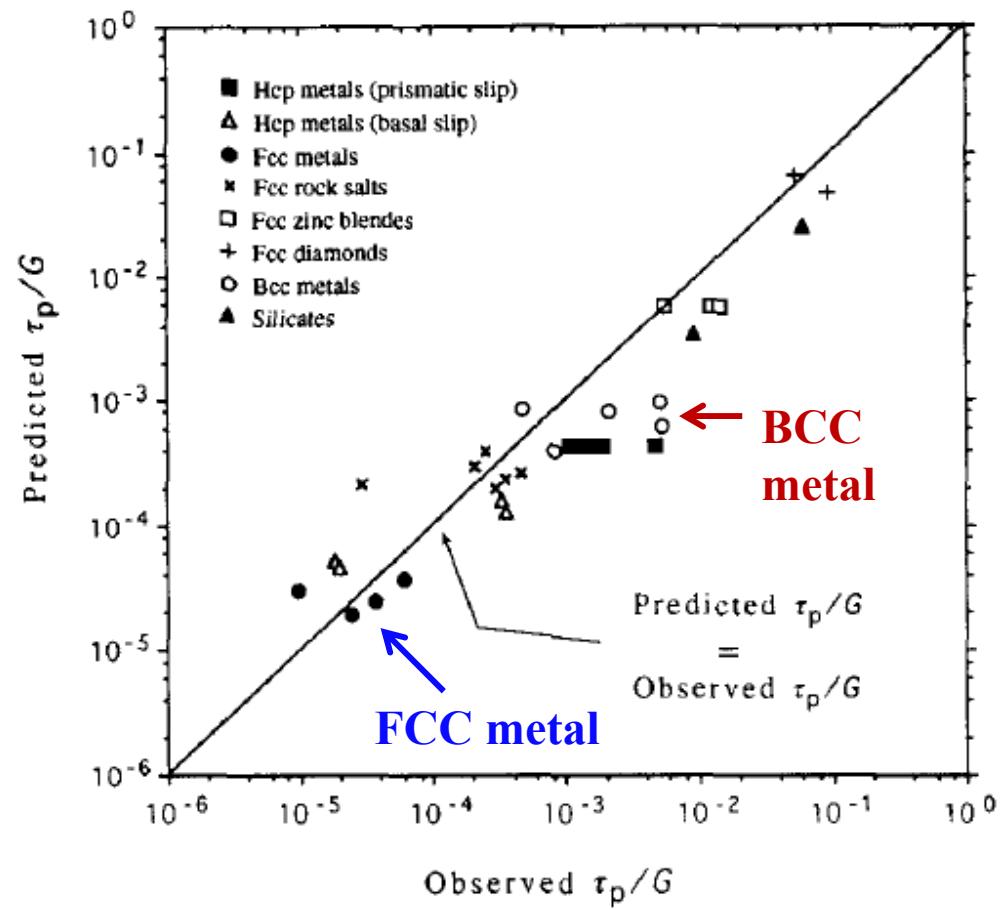
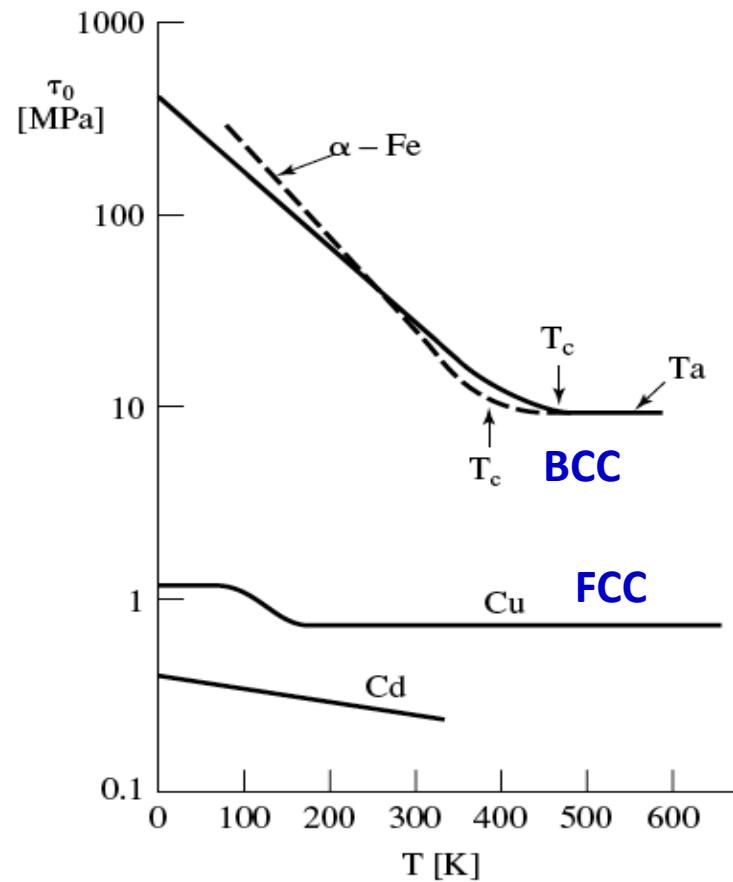
Mayer 1994

Q: 此时材料的力学行为会呈现什么特性?

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1 力学响应的位错机理

温度依赖性：材料的强度和塑性流动呈现出很强的温度依赖性。

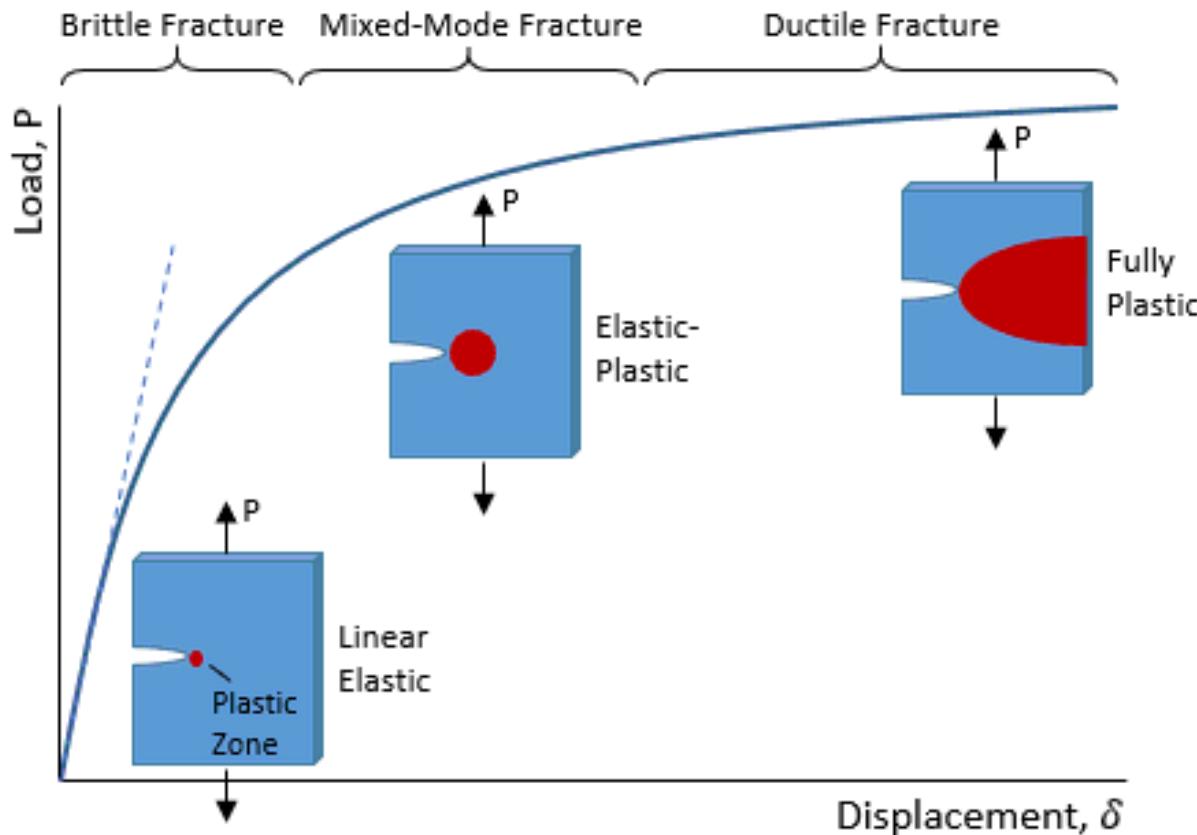


Q:为什么BCC温度依赖性更强?

Q:温度依赖性只影响塑性吗?

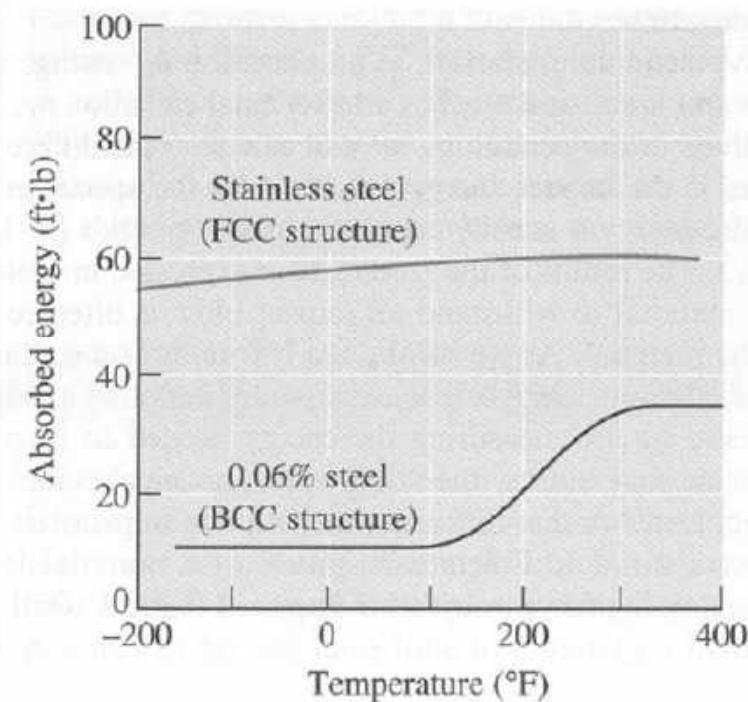
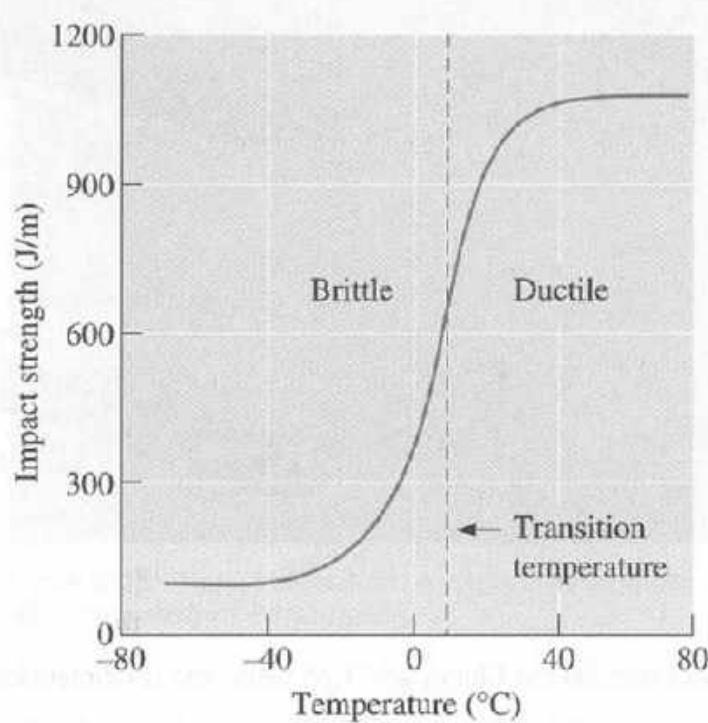
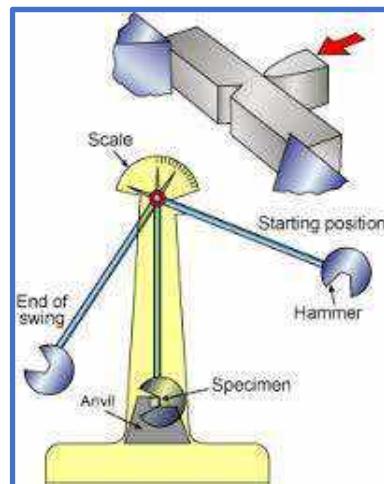
1 力学响应的位错机理

材料的断裂韧性取决于塑性变形能力
因此，位错机理对于材料脆韧转变同样起着主导作用。



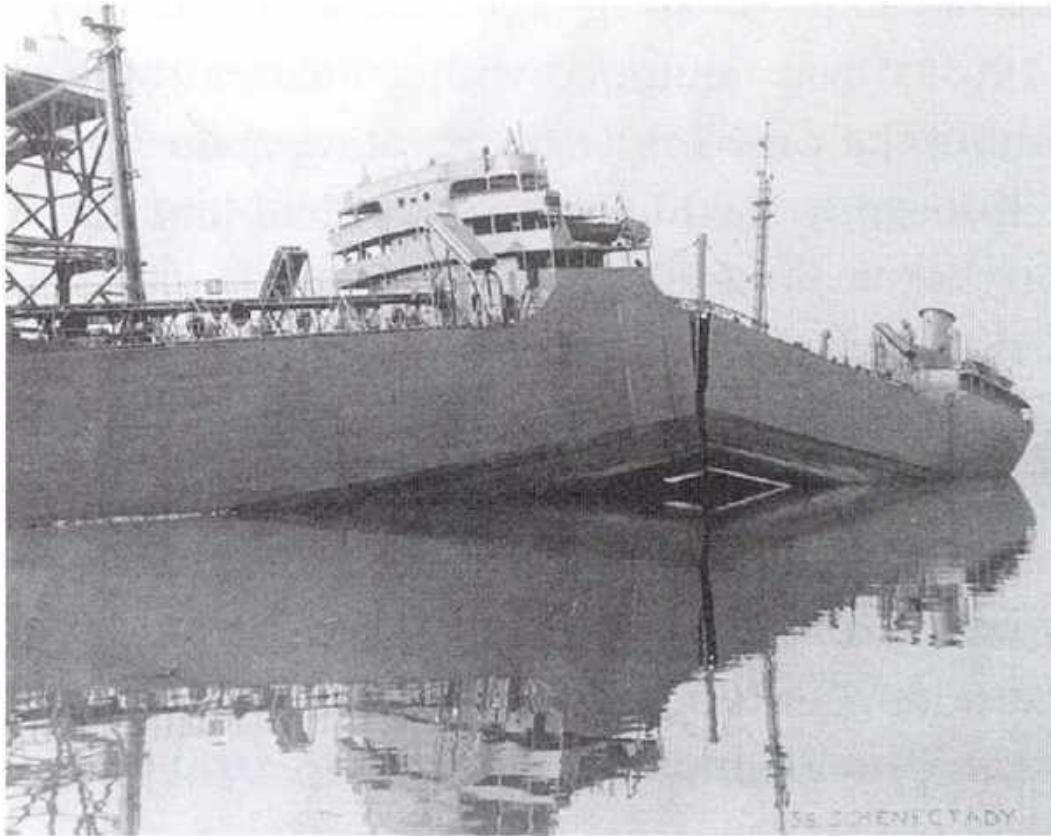
1 力学响应的位错机理

韧脆转变温度DBTT：断裂的温度依赖性



BCC的碳钢呈现明显的DBTT；
FCC的不锈钢韧性更好，无明显DBTT。

1 力学响应的位错机理



二战期间的船只由碳钢加工得到，DBTT接近海洋温度。
失效分析是基于韧性材料设计的，冷水下发生脆断。

1 力学响应的位错机理

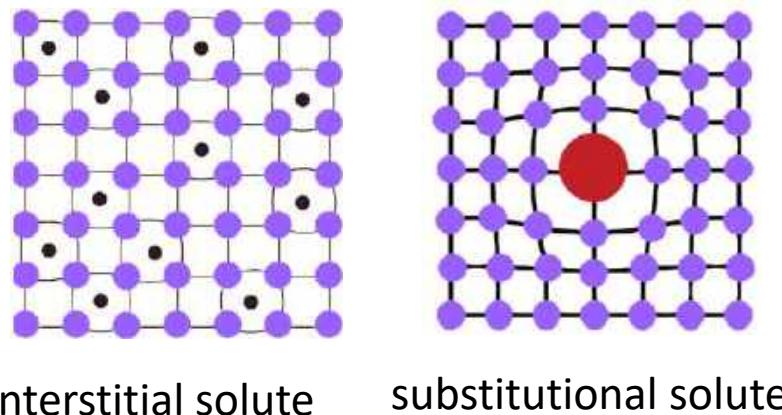
可见，位错演化通常决定着材料的塑性和断裂行为。

Q: 如何基于位错机理，提出材料强韧化方案呢？

调控位错演化（阻力，构型，外部效应……）

1 增加局部晶格扭转，增加派纳力

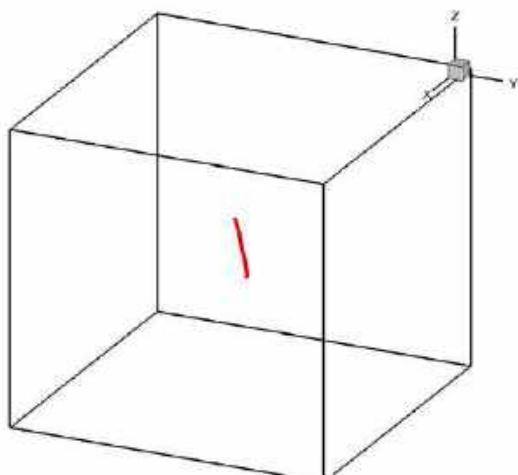
例如：合金化（固溶强化）



1 力学响应的位错机理

2 调控位错源特征长度

Frank-Read 位错源



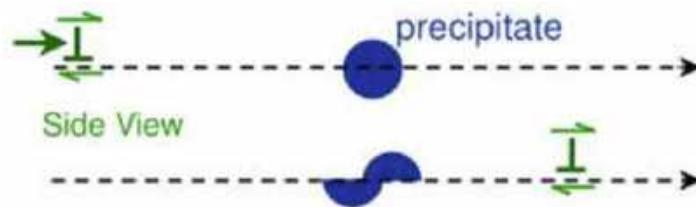
- 在韧型金属中派纳力很低，需要激活位错运动的力依赖于它们的“自由长度”

$$\tau = kGb/\lambda$$

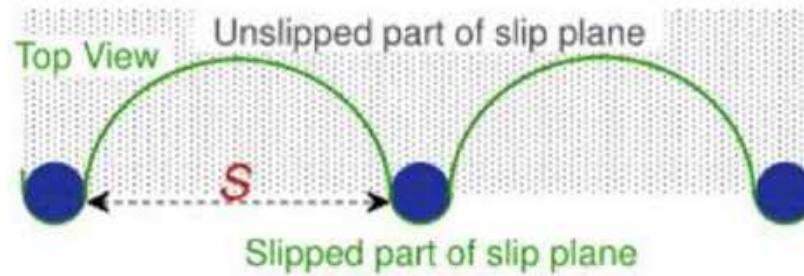
1 力学响应的位错机理

析出强化

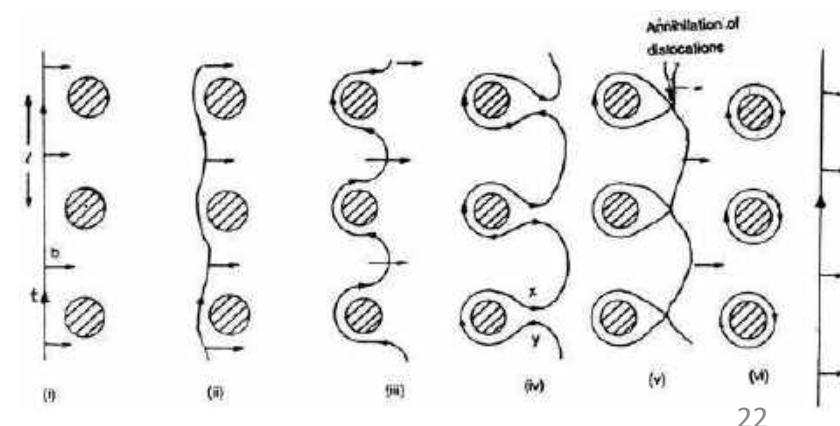
依赖于析出相的共格程度和强度：



➤ 析出相可能被位错切断



➤ 析出相被位错绕过

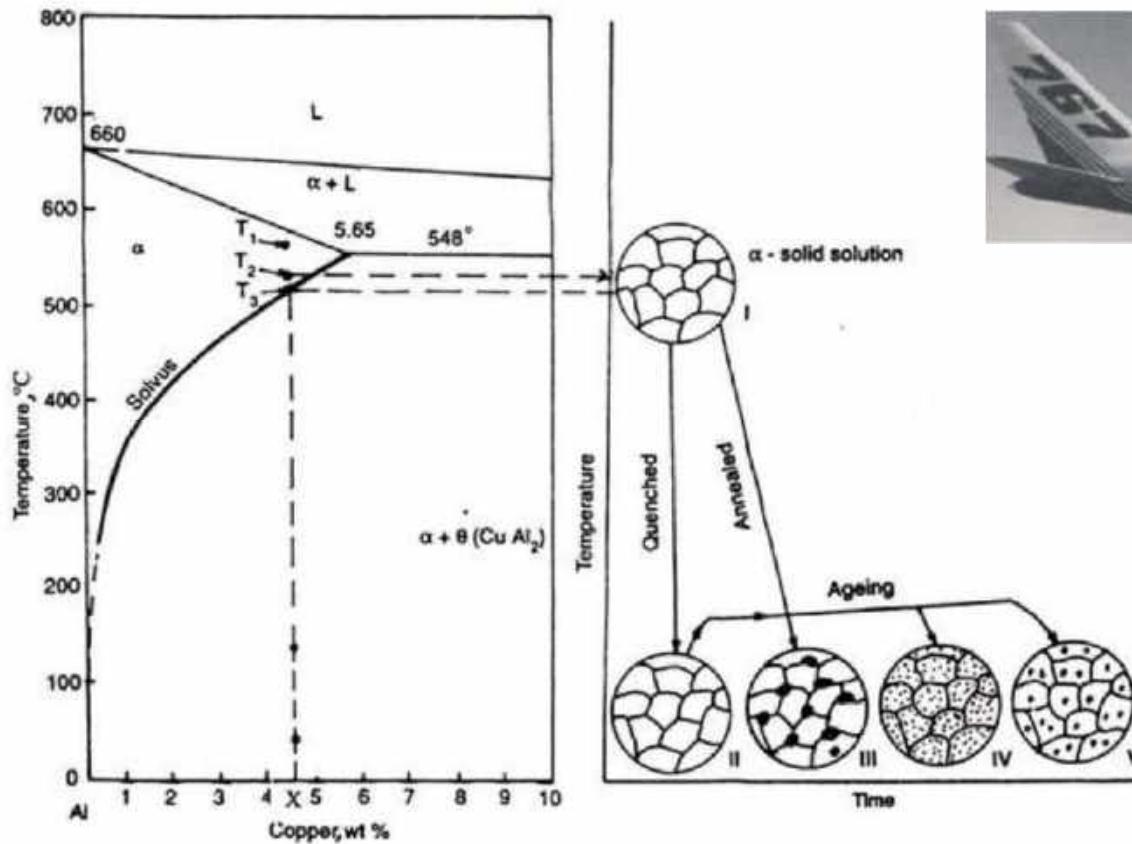


1 力学响应的位错机理

析出强化举例

自第二次世界大战以来，2000系列“硬铝”作为飞机机身。

拉伸强度：~ 270MPa (1000 series), 700MPa (7000 series)

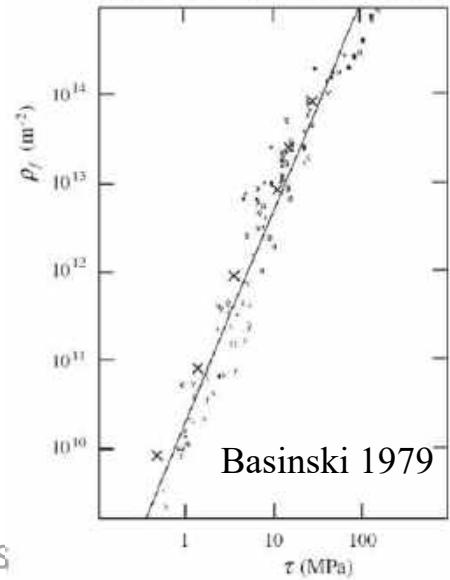


- I) Al-Cu 固溶
- II) 淬火，固溶体以过饱和的形式存在
- IV-V) 略高于室温的温度时效，在晶粒中析出弥散的Cu析出物。

1 力学响应的位错机理

3 林位错硬化

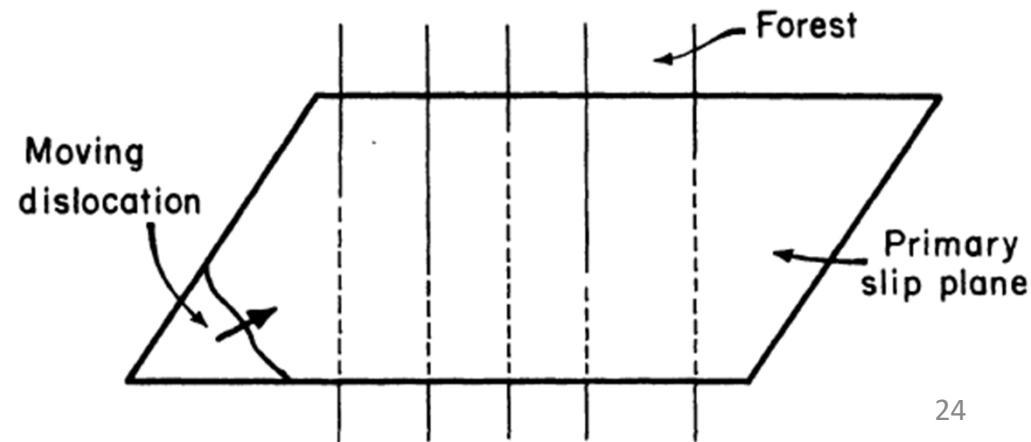
位错缠结，位错运动变得困难



- 随着塑性变形的进行，位错增殖，其密度增加

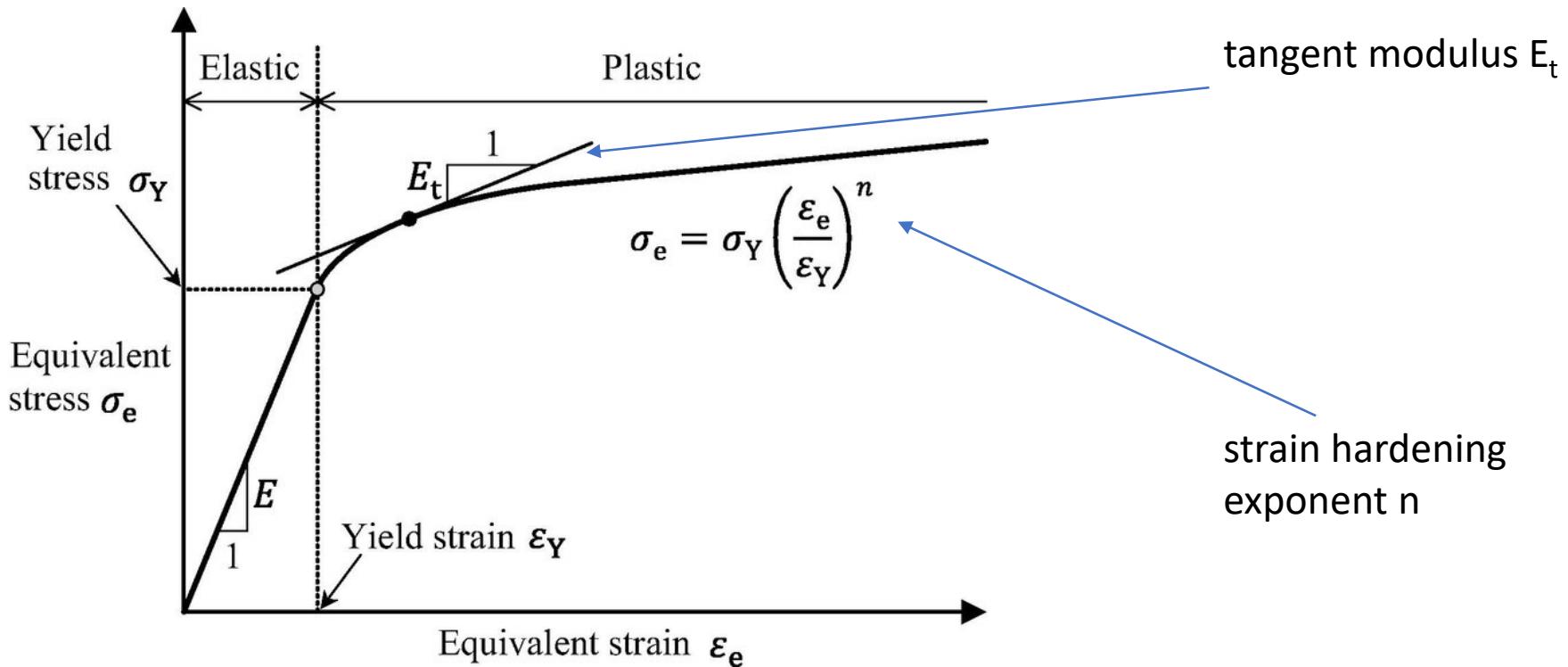
$$\rho = \frac{\text{total line length}}{\text{volume}}$$

$$\tau = kGb/\lambda = kGb\sqrt{\rho}$$



1 力学响应的位错机理

- 材料的流动应力随着塑性变形量的增加而增大的现象，称为应变硬化（加工硬化）

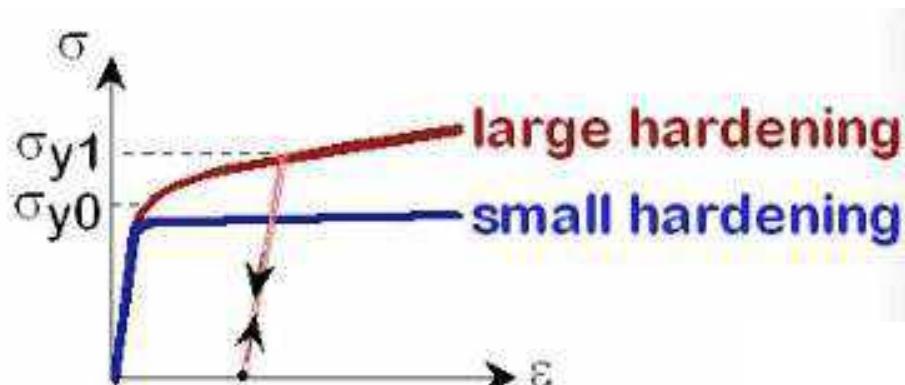
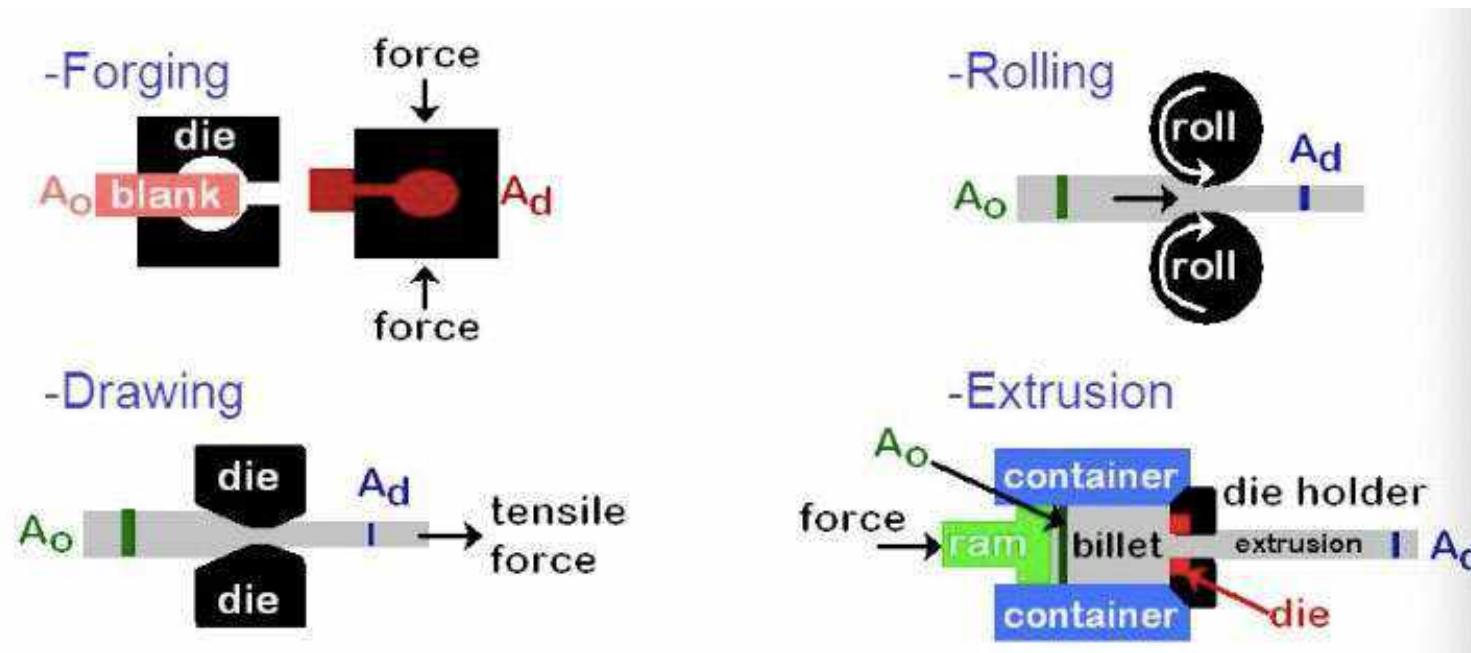


Q: 你知道什么加工硬化方式吗?

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1 力学响应的位错机理

加工硬化



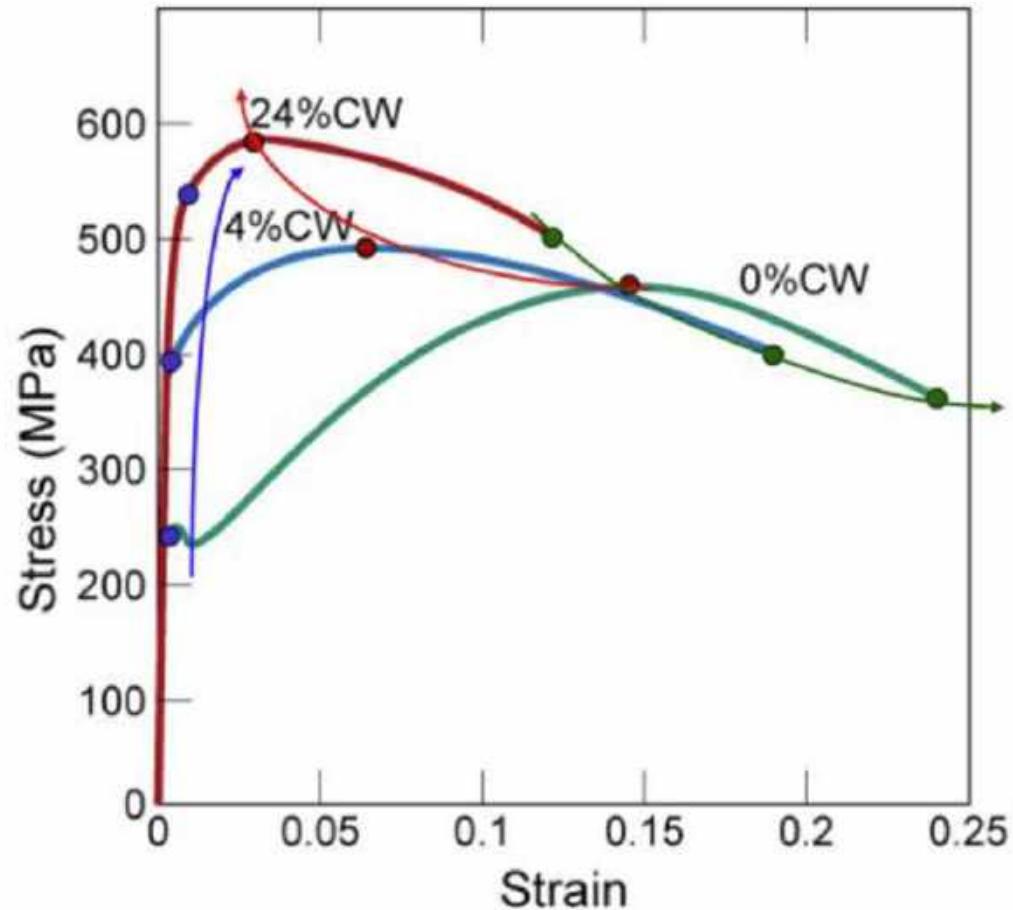
1 力学响应的位错机理

加工硬化都会影响什么呢？

屈服强度提高；

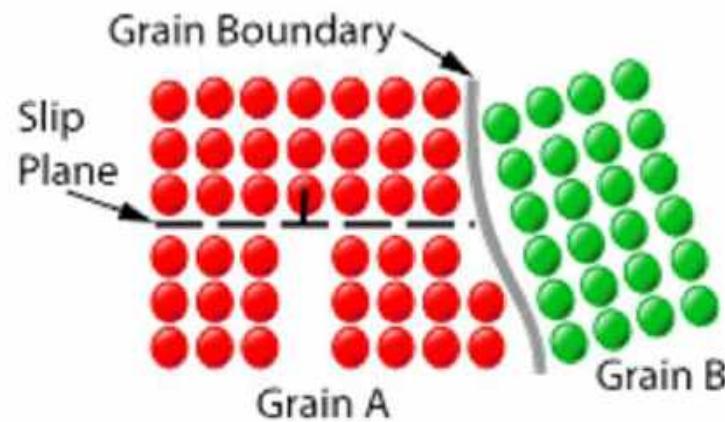
拉伸强度提高；

延伸率降低

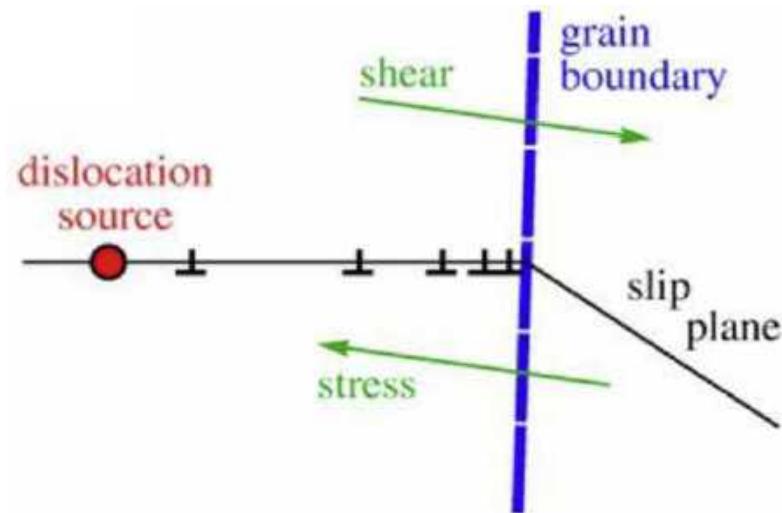


1 力学响应的位错机理

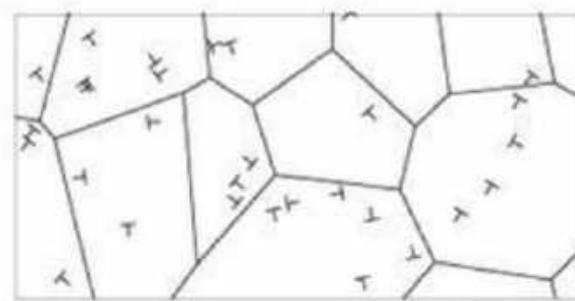
晶界强化



位错在晶粒处钉扎，引起强化



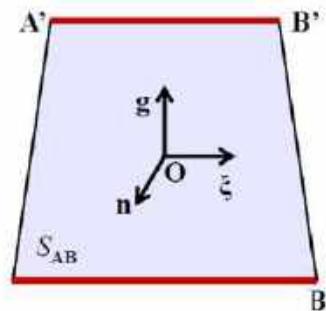
细化晶粒强化



1 力学响应的位错机理

位错

塑性变形的直接载体



$$\Delta\gamma = \frac{bS_{AB}}{V}$$

塑性变形率, 塑性旋转率

$$\mathbf{D}^p = \frac{1}{2V\Delta t} (\mathbf{b} \otimes \mathbf{A} + \mathbf{A} \otimes \mathbf{b})$$

$$\boldsymbol{\Omega}^p = \frac{1}{2V\Delta t} (\mathbf{b} \otimes \mathbf{A} - \mathbf{A} \otimes \mathbf{b})$$

强度 + 脆韧转变

派纳势垒

温度依赖性
应变率依赖性

运动阻力

尺寸效应

固溶强化

析出强化

林位错硬化

晶界硬化

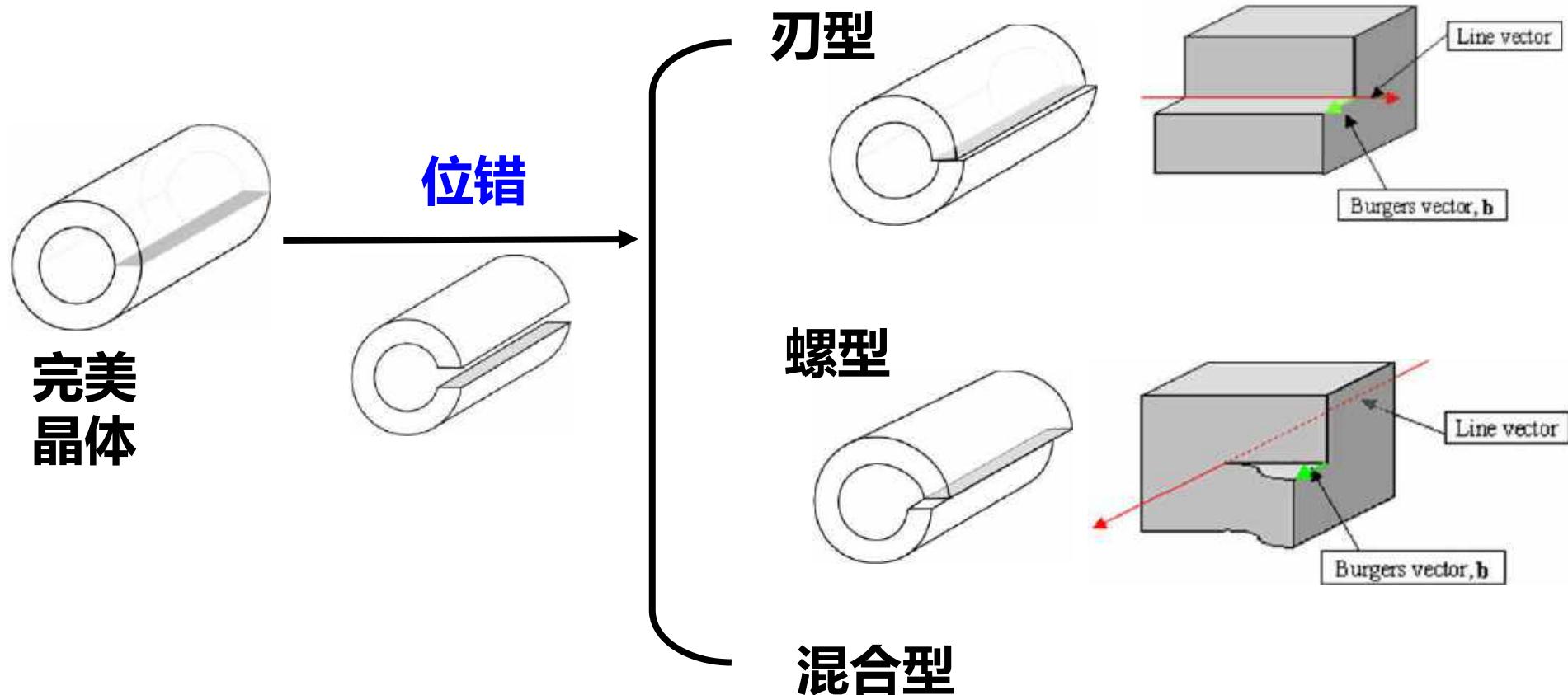
2 位错基本理论

2.1 位错的基本概念

2.2 位错的实验观察

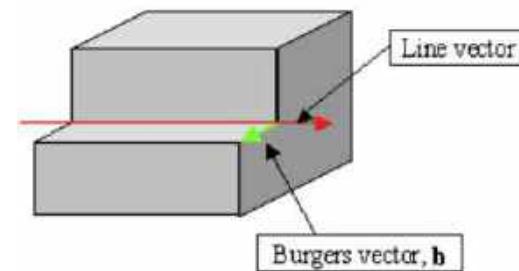
2 位错基本理论

位错的基本分类

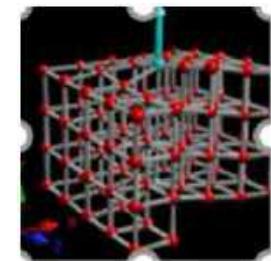
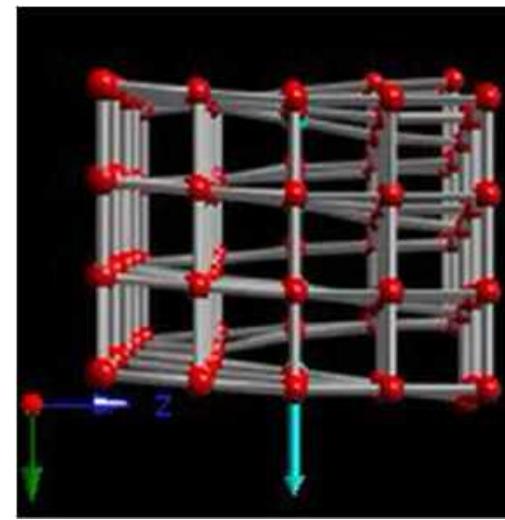
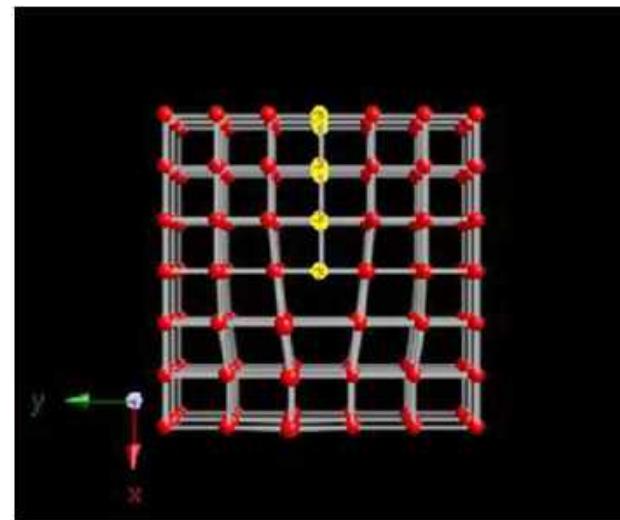
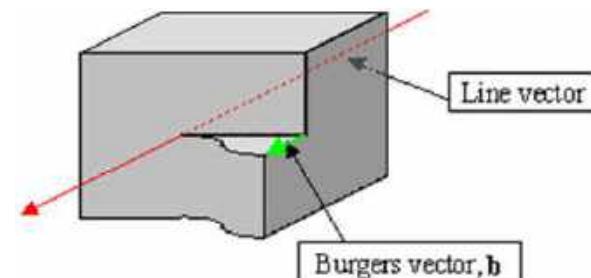


2 位错基本理论

刃位错

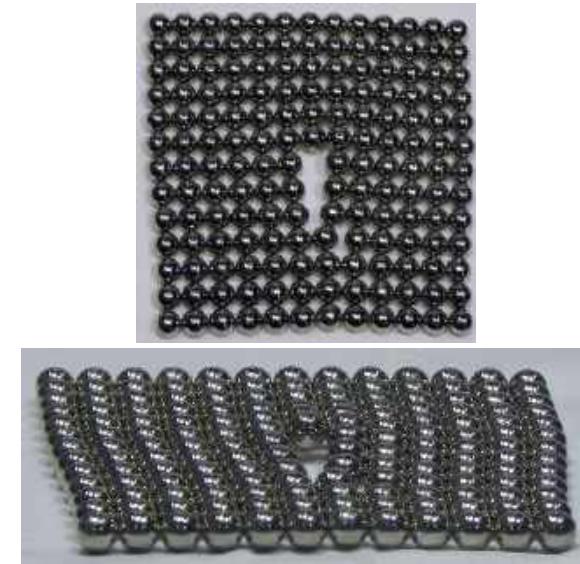
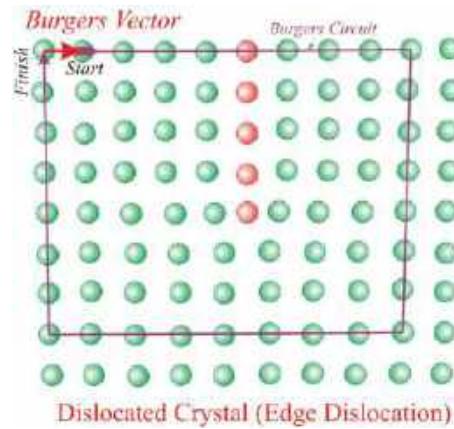
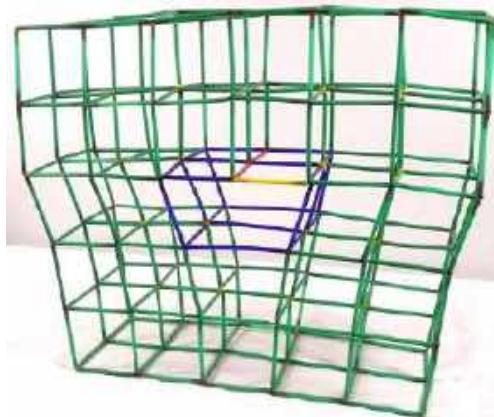


螺位错

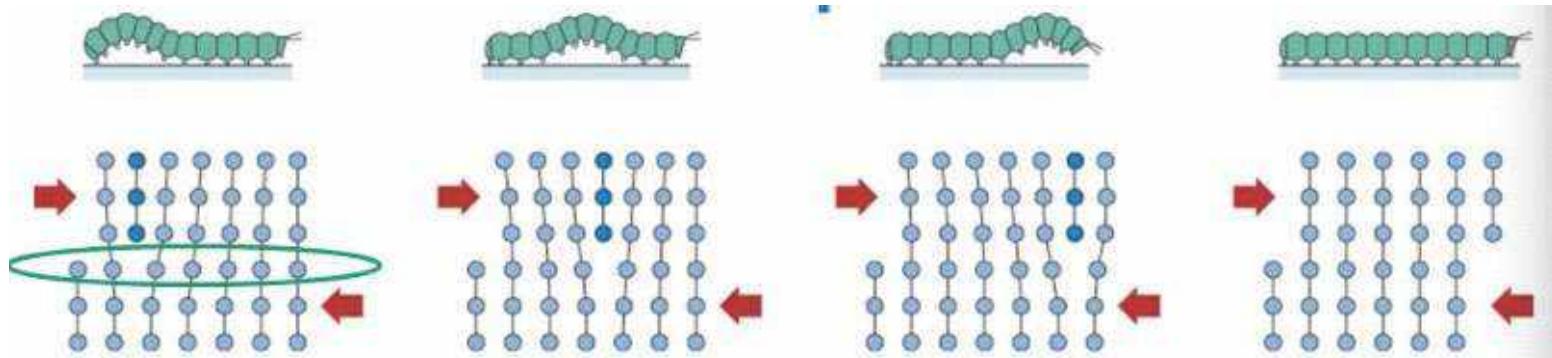


2 位错基本理论

刃位错



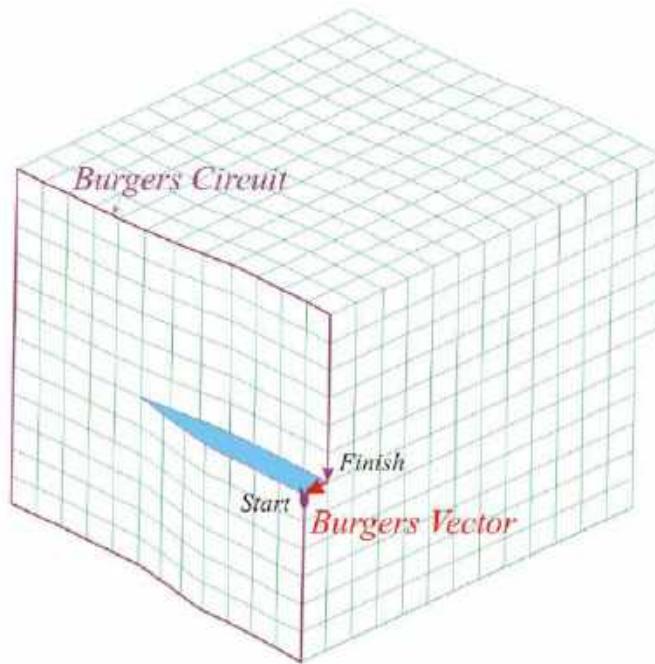
刃位错的运动



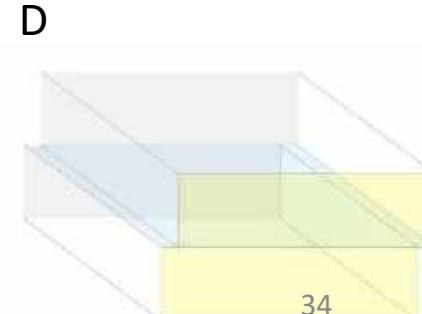
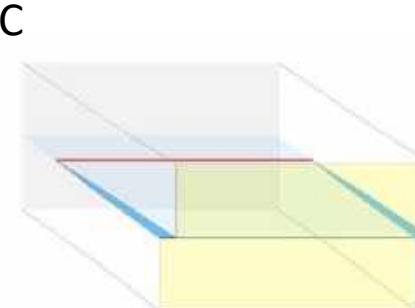
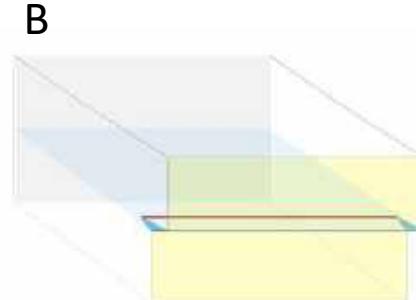
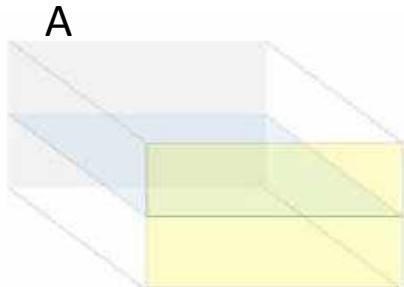
33

2 位错基本理论

螺位错



螺位错的运动



滑移面和滑移方向

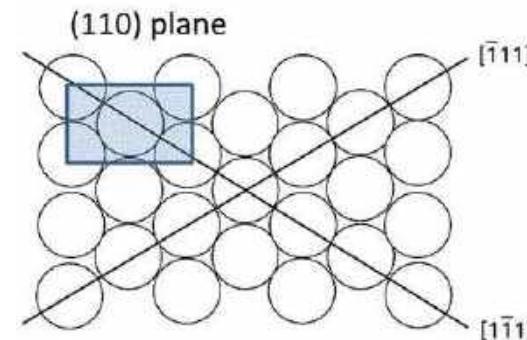
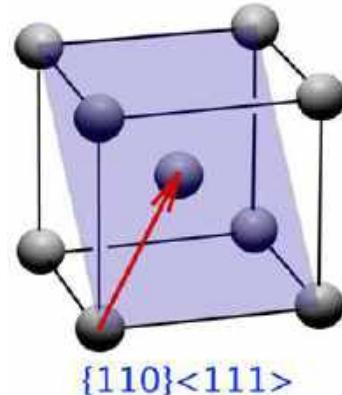
Q: 位错运动有什么约束条件吗?

	Simple cubic	Body-centered cubic (BCC)	Face-centered cubic (FCC)	Close-packed hexagonal (HCP)
Unit cell				
No real crystal				
Close packed Plane/ direction				

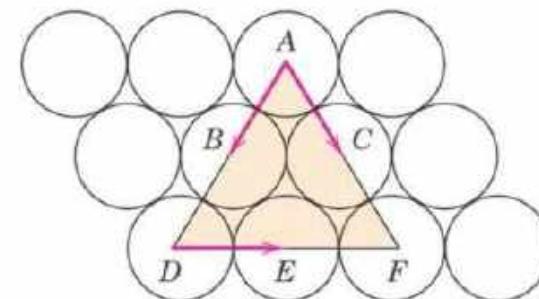
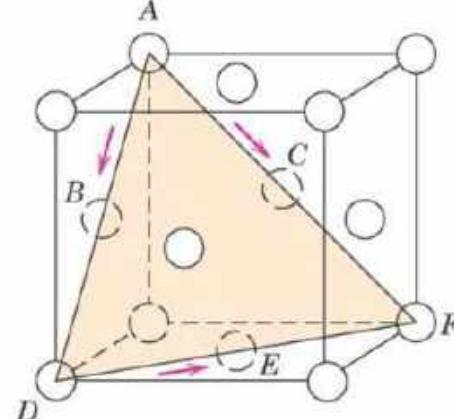
滑移面和滑移方向

BCC

$\langle 111 \rangle$ is close-packed, but $\{110\}$ plane is not close packed. Thus, additional planes that contain the $\langle 111 \rangle$ can also active.



FCC



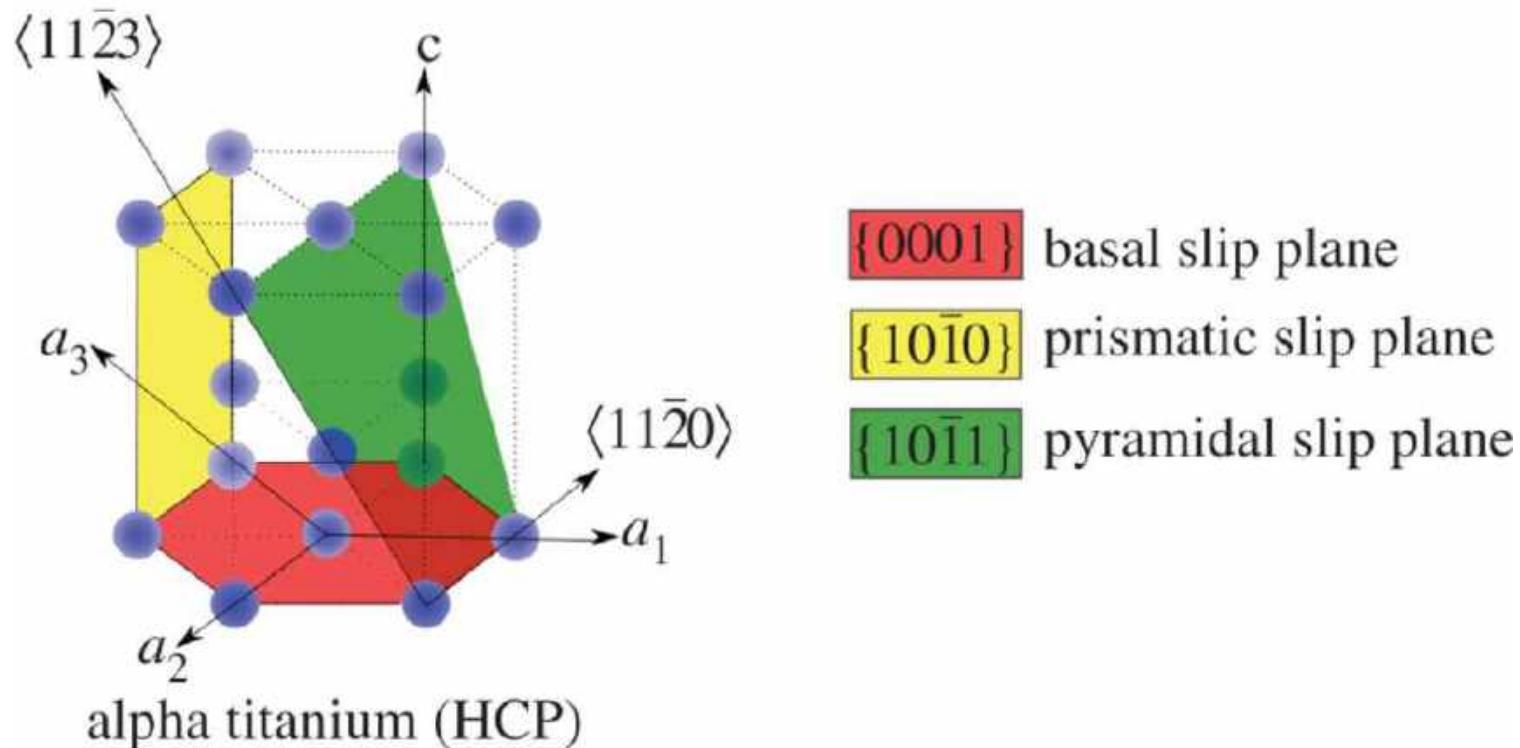
$\{111\}\langle 110 \rangle$

36

36

滑移面和滑移方向

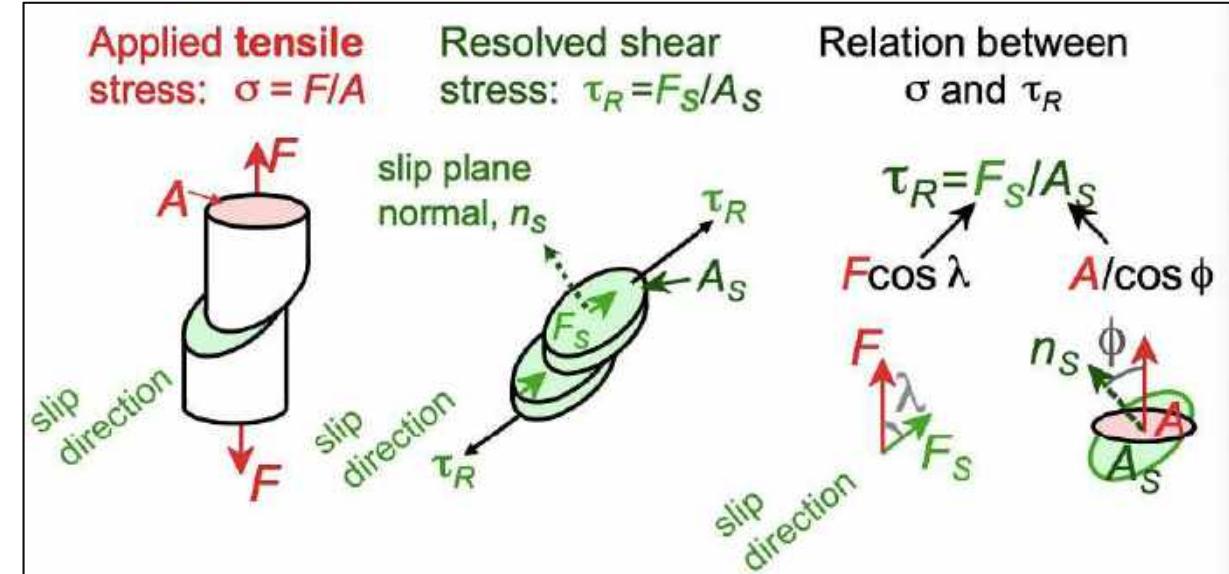
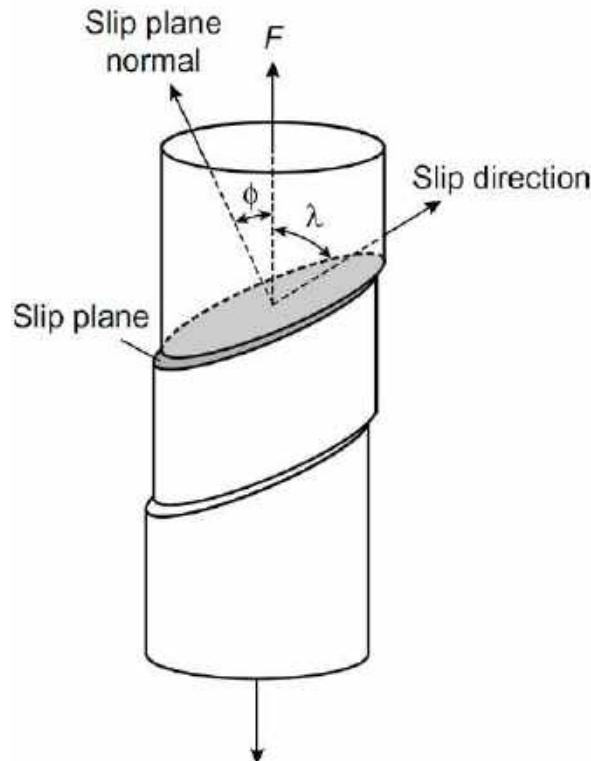
HCP



位错运动的驱动力

位错在滑移面上运动，其驱动力为合外力对应的分切应力

$$\tau_R = \sigma \cos \lambda \cos \phi$$



临界分切应力

只有分切应力大于临界分切应力，位错才能开动。

$$\tau_R > \tau_{CRSS}$$

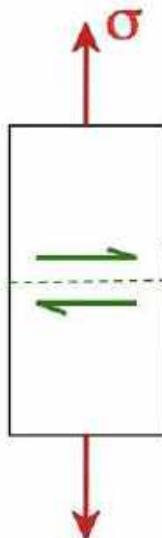
$$\tau_R = \sigma \cos \lambda \cos \phi$$

依赖于外力，微结构

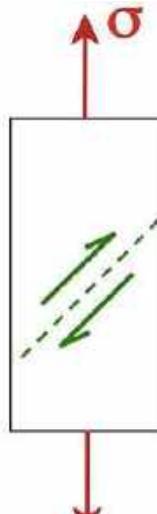
$$10^{-4} \text{ GPa to } 10^{-2} \text{ GPa}$$

依赖于材料类型，温度

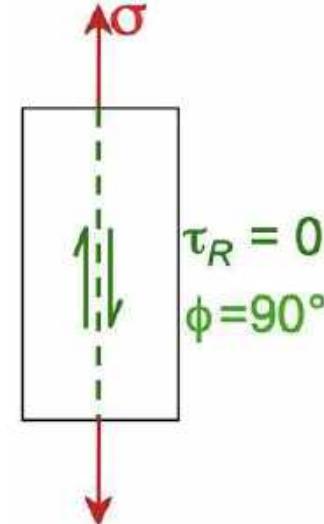
晶体取向，影响位错开动



$$\tau_R = 0$$
$$\lambda = 90^\circ$$



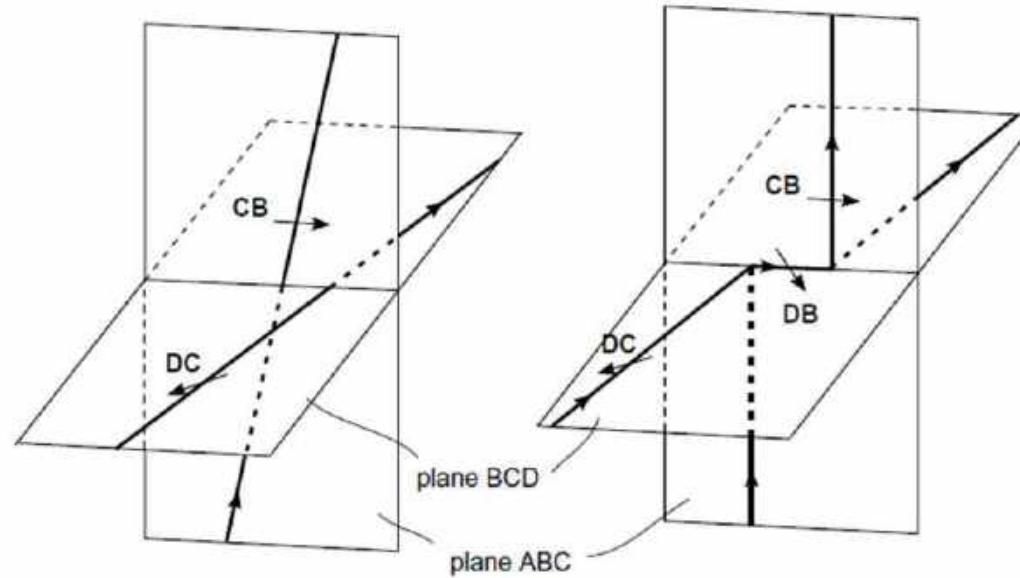
$$\tau \text{ maximum at } \lambda = \phi = 45^\circ$$



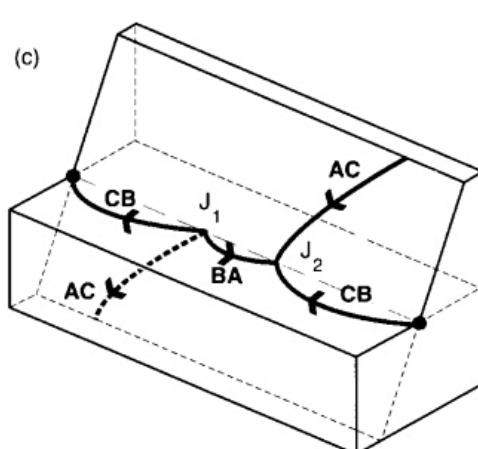
$$\tau_R = 0$$
$$\phi = 90^\circ$$

位错反应

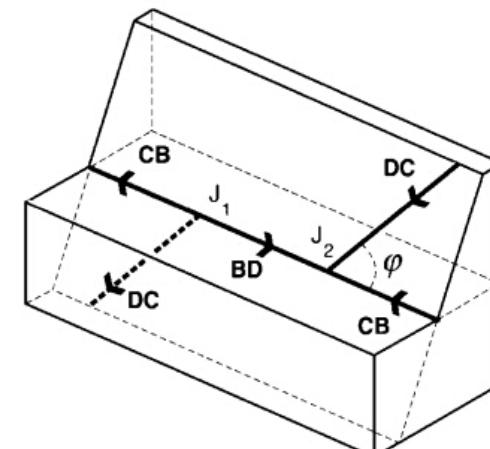
Junction formation



Glissile 位错锁

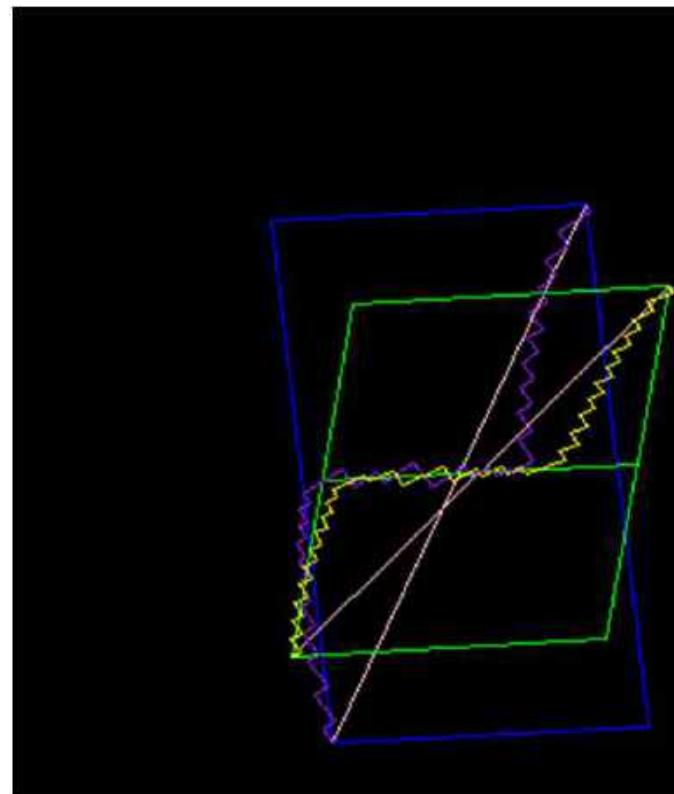


Lomer-Cottrell 位错锁



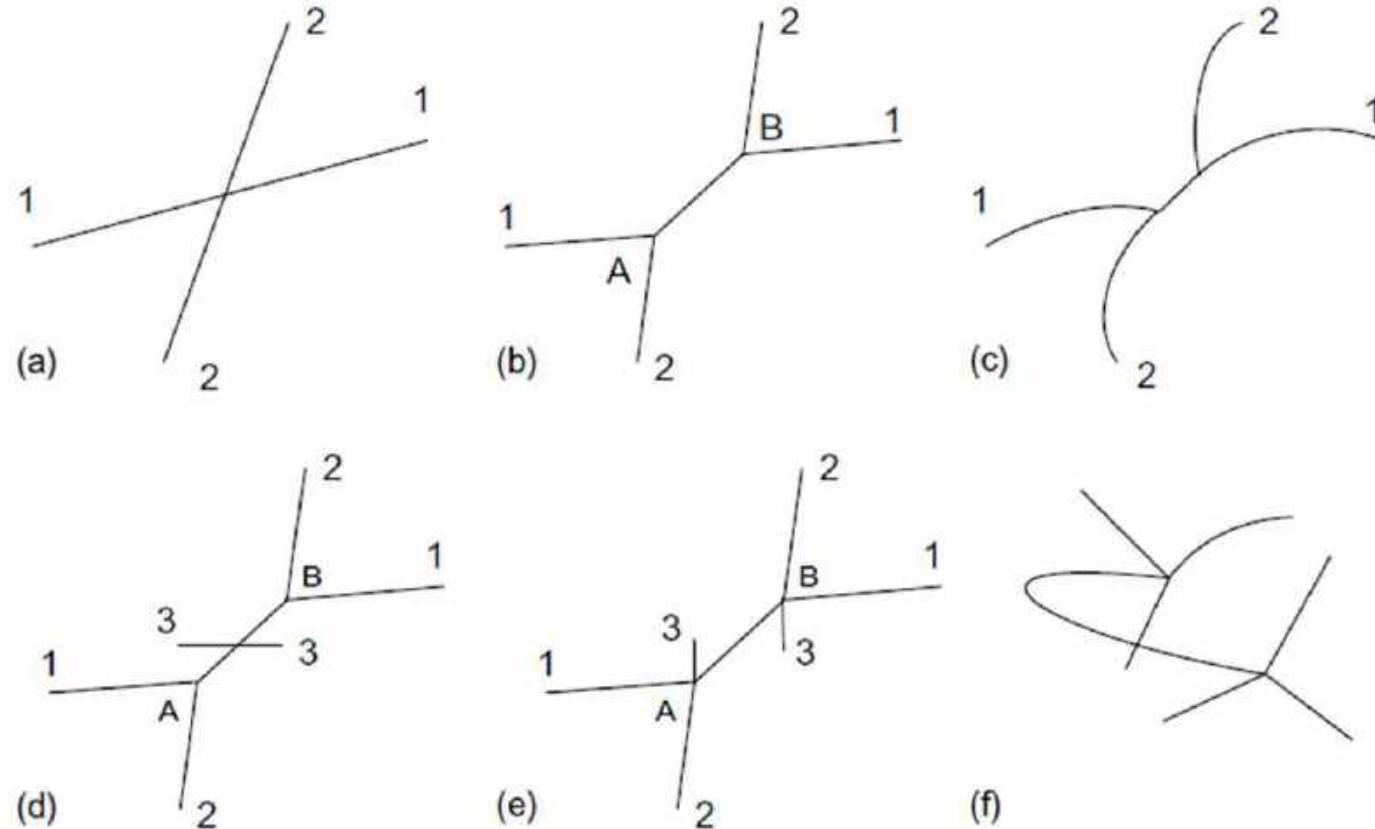
位错反应

Junction formation



位错反应

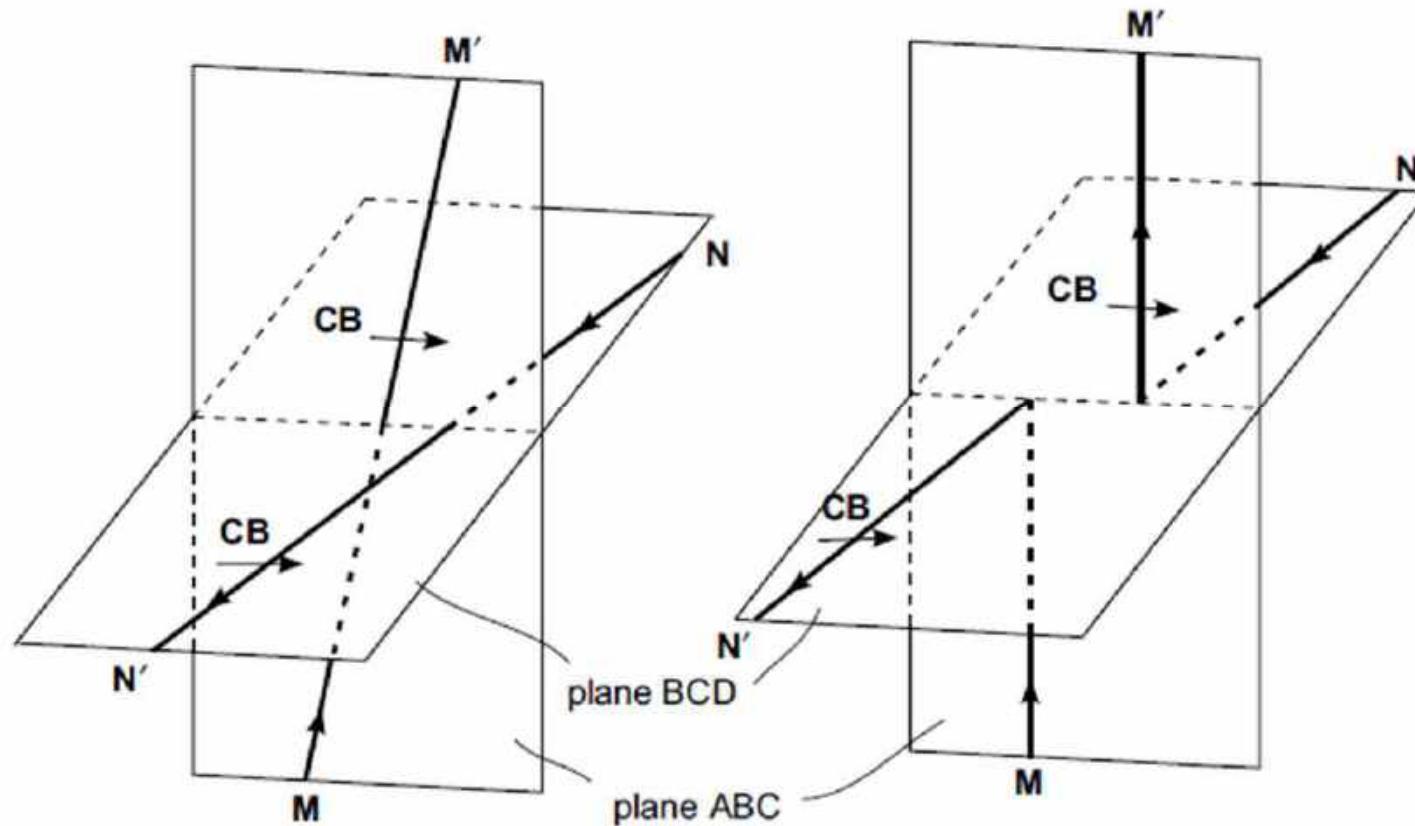
Junction formation



D Hull, 2011

位错反应

Collinear reaction



D Hull, 2011

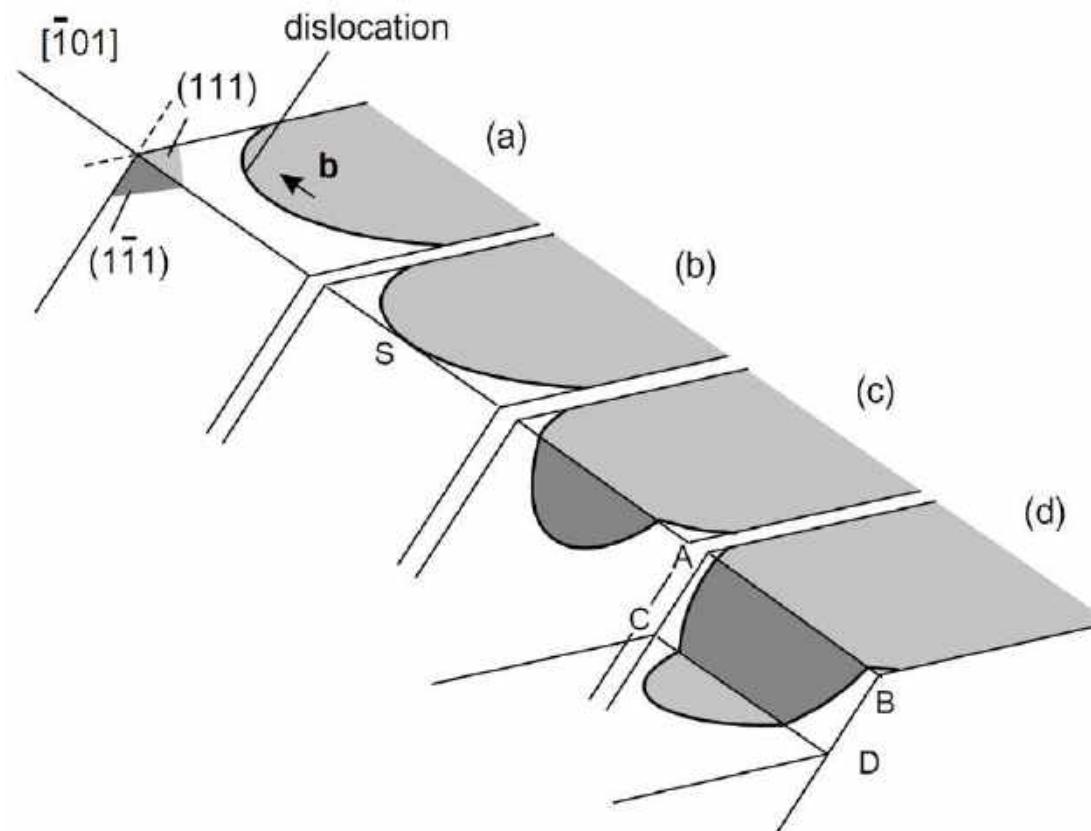
位错反应

Annihilation



位错交滑移

Cross slip



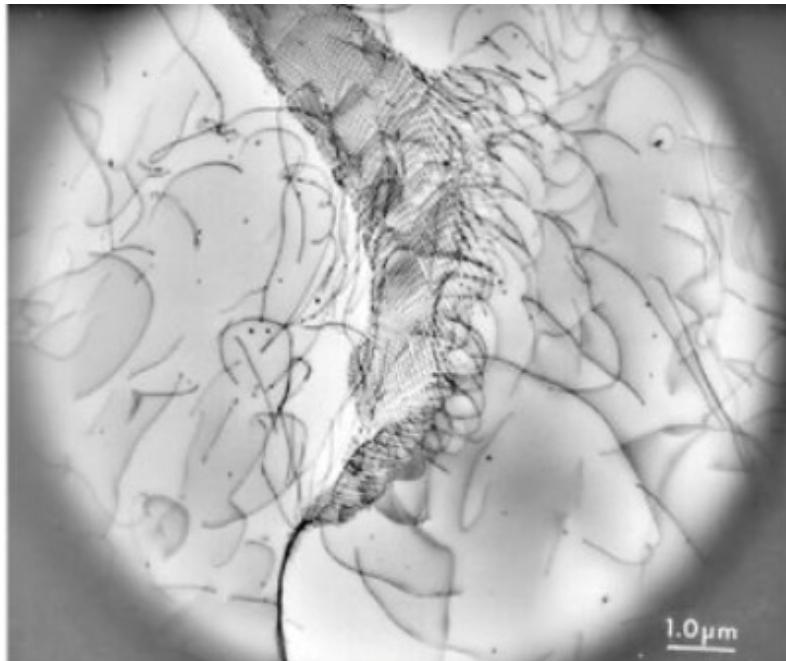
D Hull, 2011

2.2 位错的观察

1950第一次用TEM观察到位错

很多直接或间接方式观察位错:

e.g. ex-situ/in-situ transmission electron microscopy (TEM),
X-ray diffraction (XRD) methods
electron backscatter diffraction (EBSD)



P.H. Kitabjian: High Temperature Deformation Behavior of NiAl(Ti) Single Crystals. PhD thesis, Stanford University, 1998

单晶NiAl-2.5Ti在1200 °C蠕变条件下的TEM图像

2.2 可以看到他们的运动吗？

F-R源



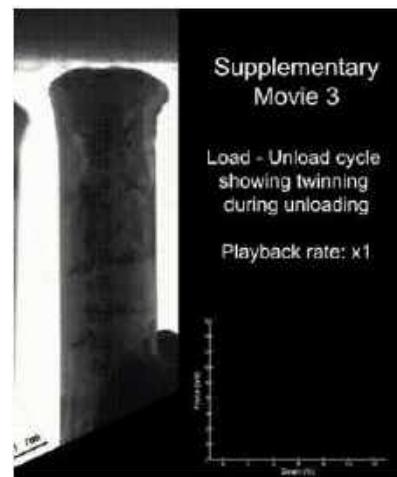
位错塞积



junction

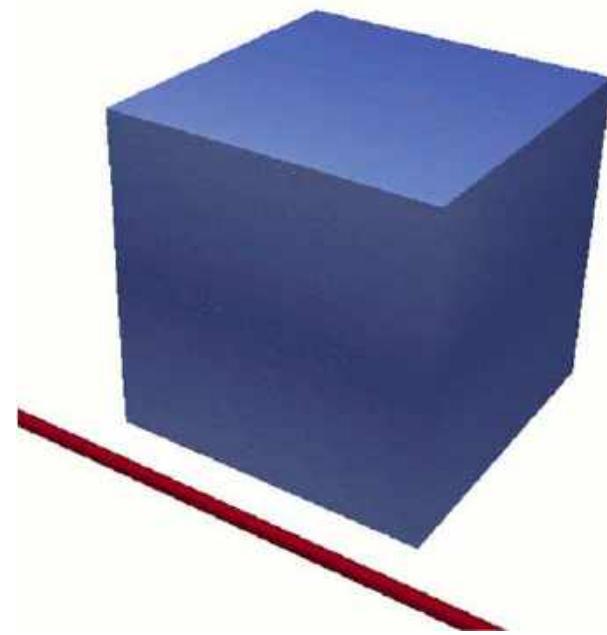
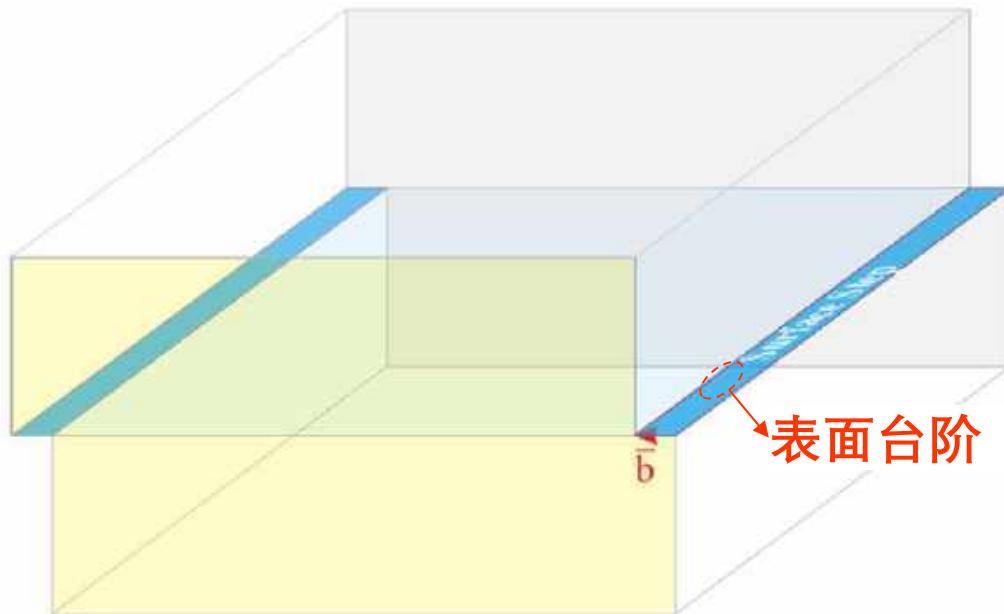


交滑移



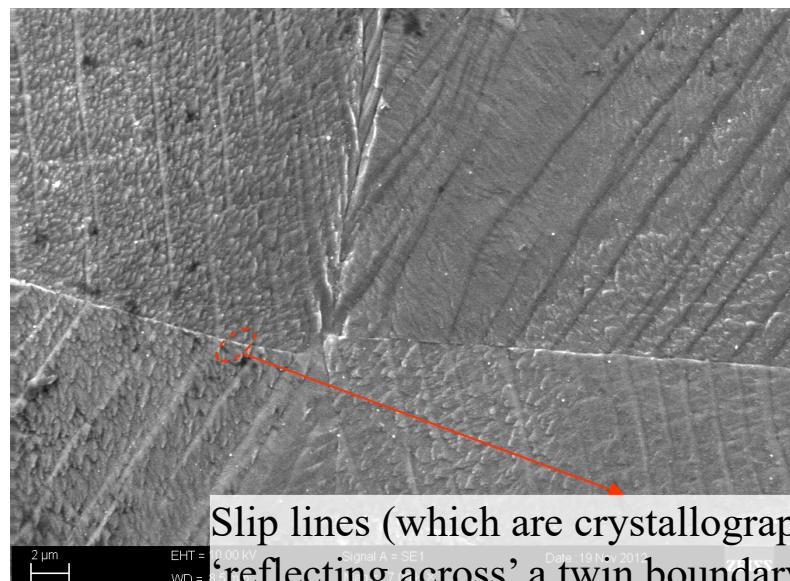
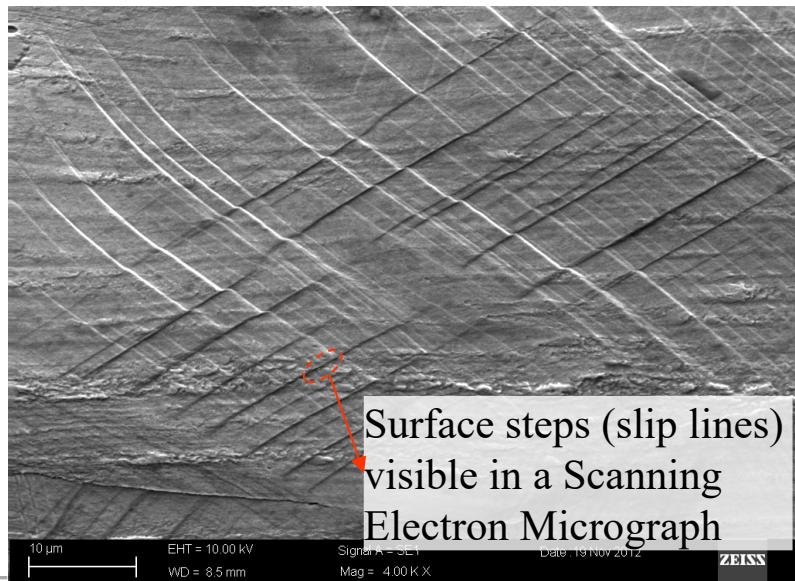
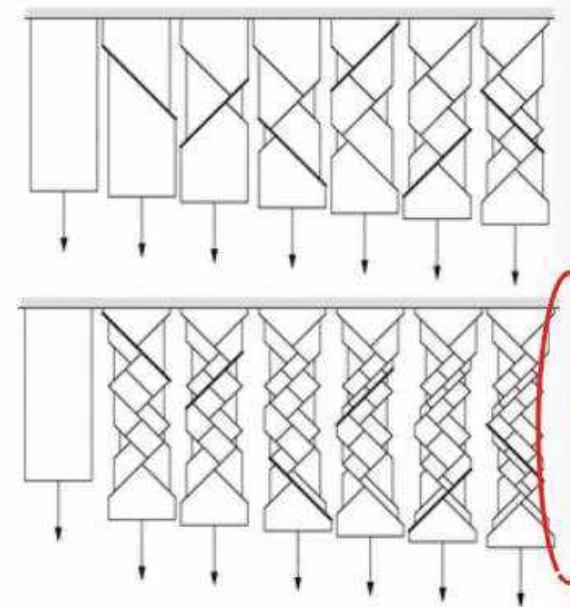
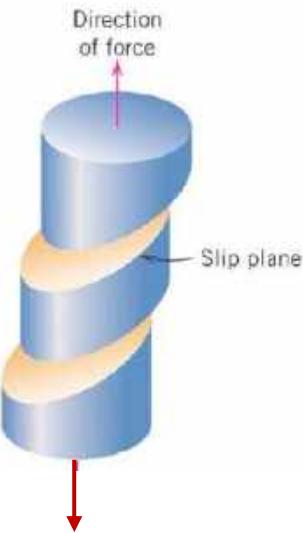
S Lee et al.
Nature comm. 2013

2.2 可以看到他们的运动吗？

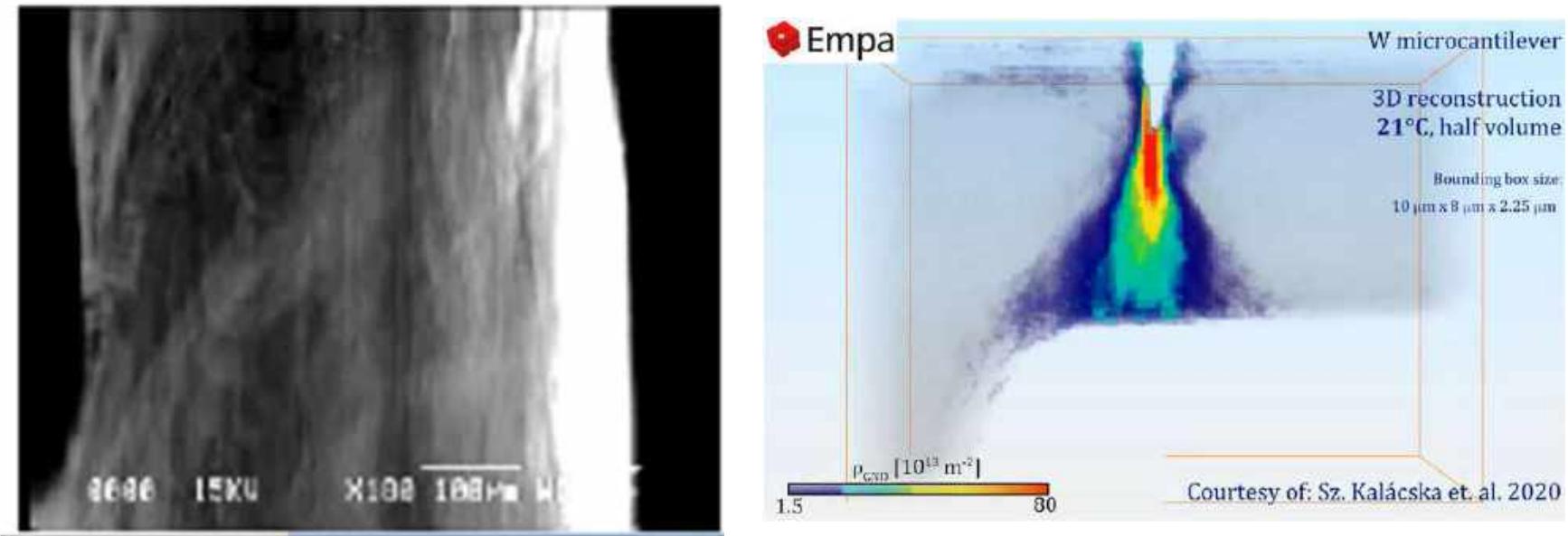


<http://www.numodis.fr/tridis/>
48

2.2 可以看到他们的运动吗？



2.2 塑性到断裂



3 位错动力学方法

Discrete Dislocation Dynamics (DDD)

3.1 2D DDD vs 3D DDD

3.2 3D DDD基本流程

离散化方案

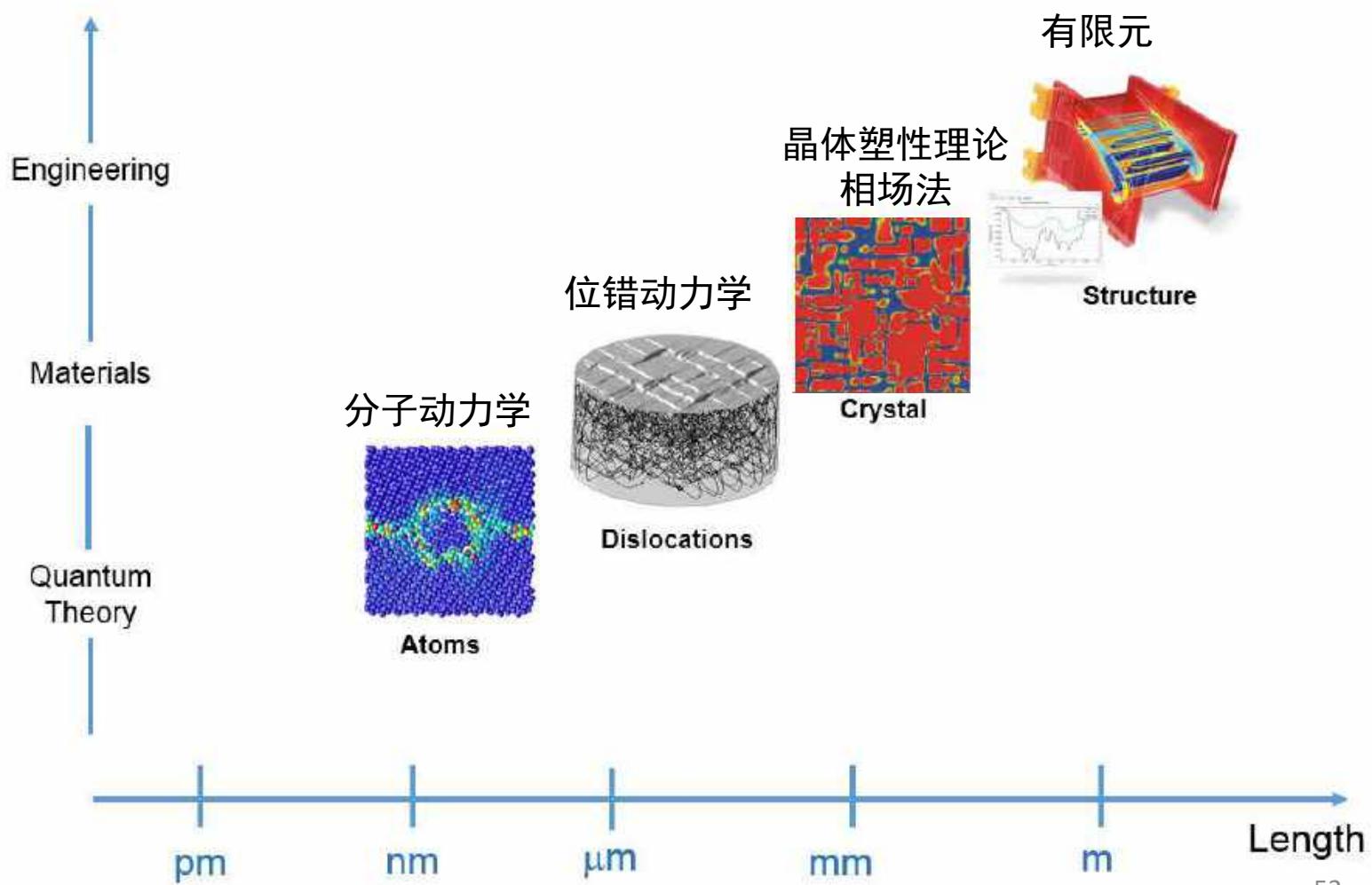
求解位错段受力

计算位错速度

计算塑性应变，更新应力

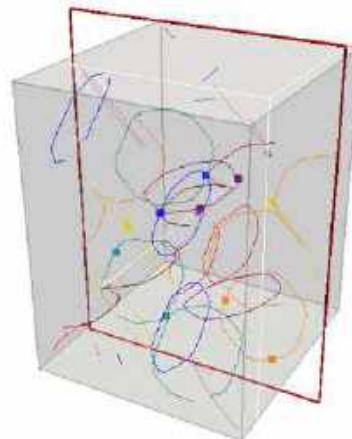
计算位错反应，交滑移，拓扑更新等

3 位错动力学方法

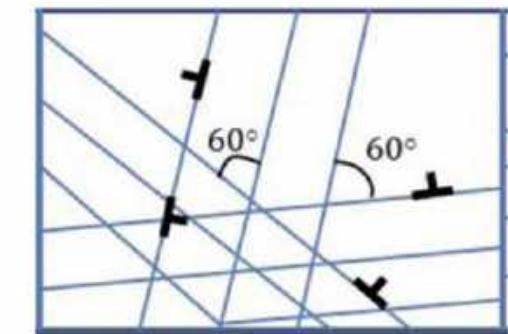
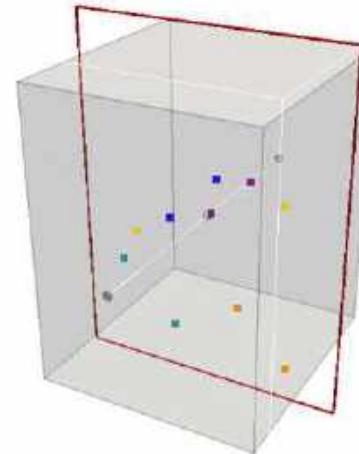


3 位错动力学方法

3D DDD

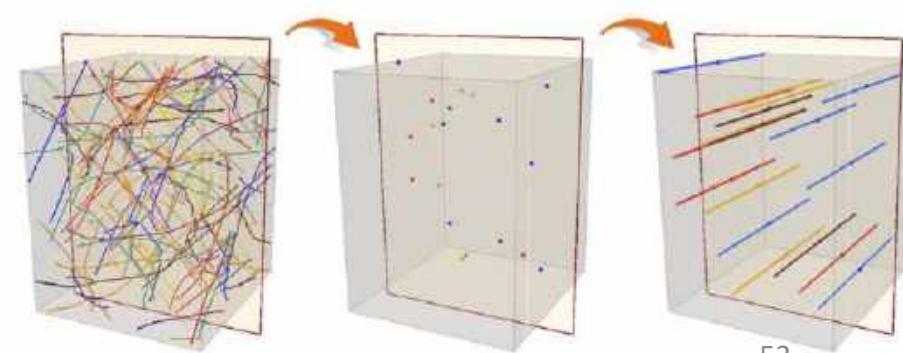


2D DDD



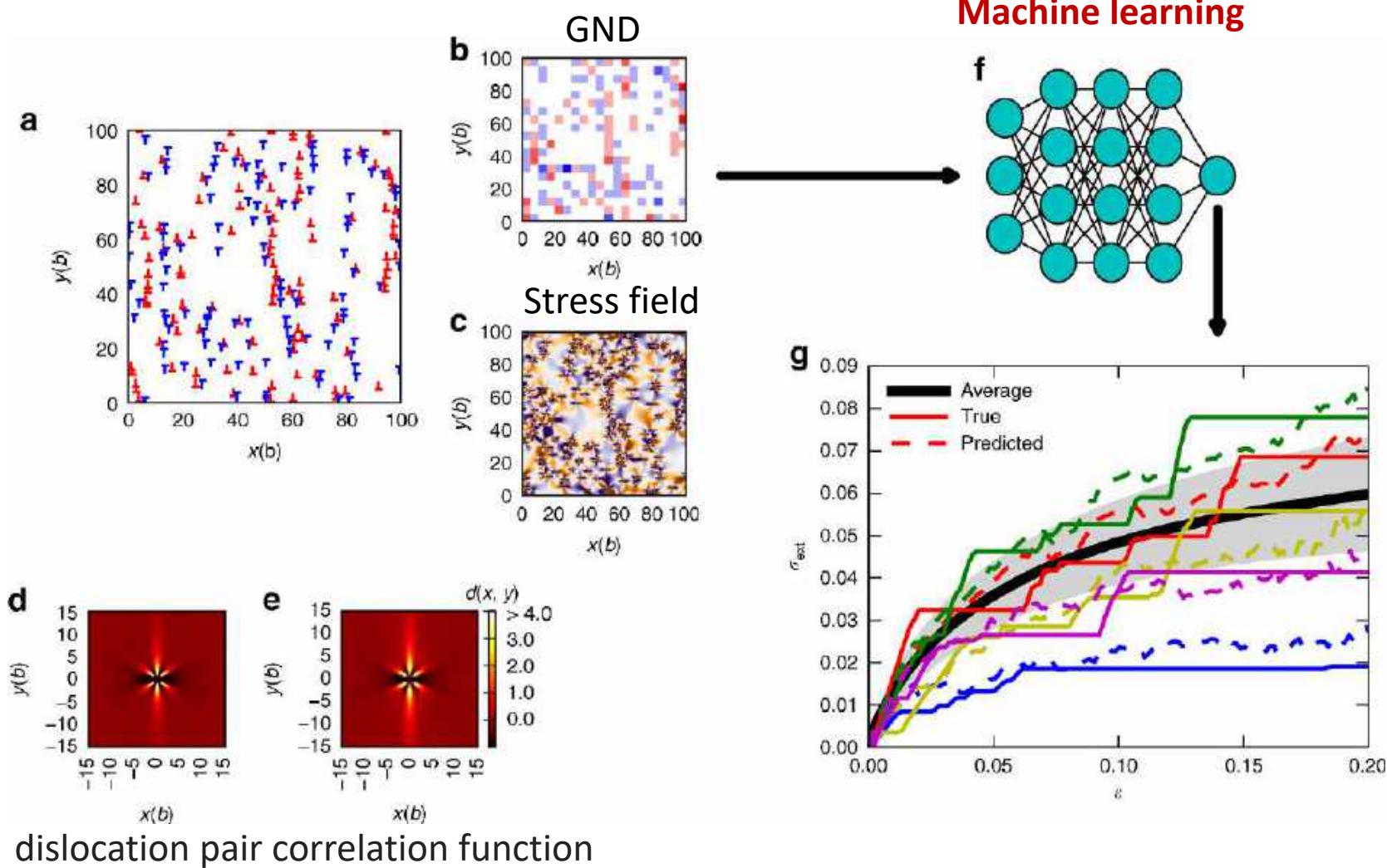
RHEOMAN WEBSITE

- edge dislocations \rightarrow plane strain
- screw dislocations \rightarrow anti-plane strain
- simple and fast simulation method
- useful for getting qualitative information



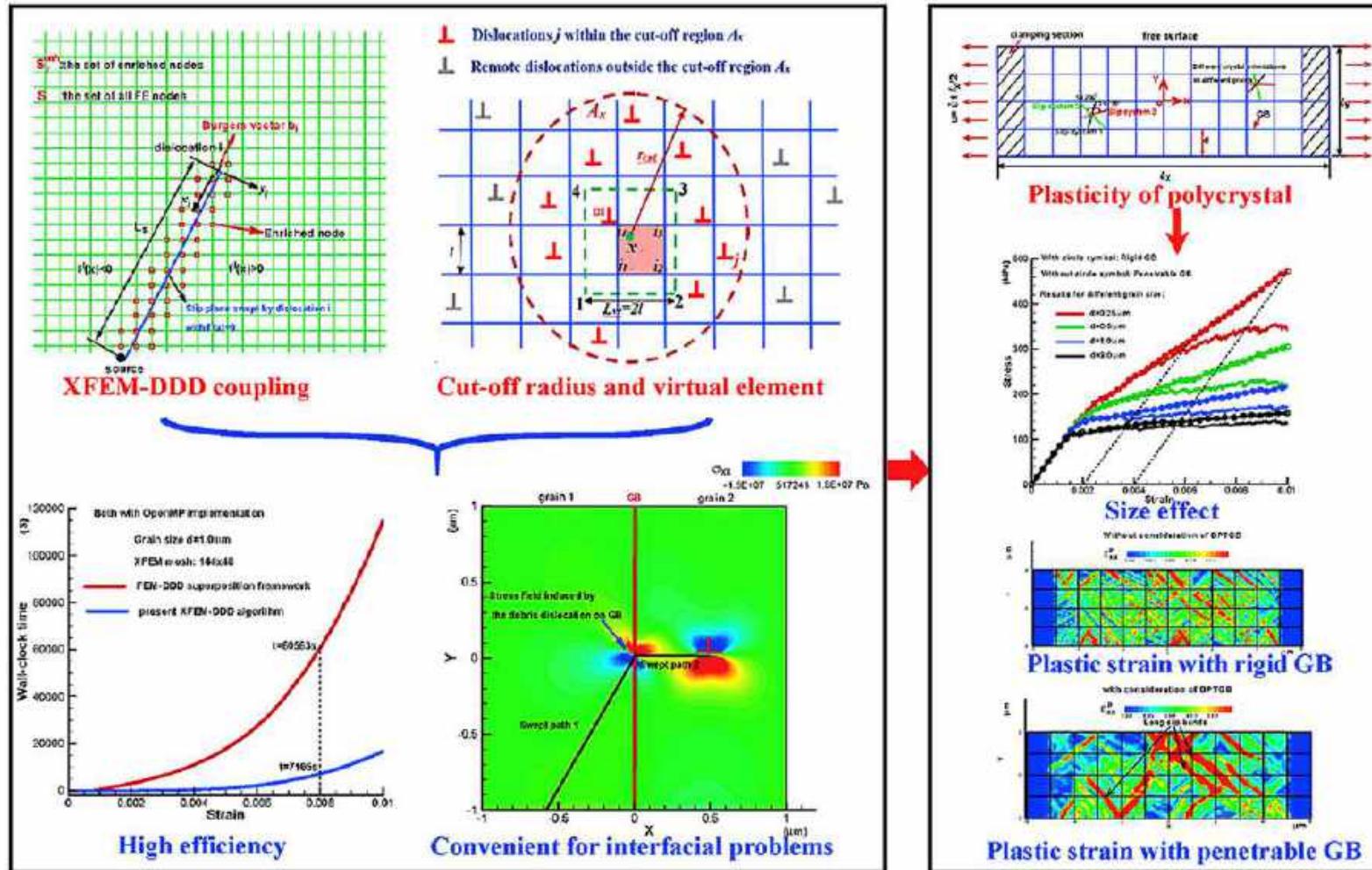
53

3 位错动力学方法



H SALMENJOKI, NATURE COMM. 2018

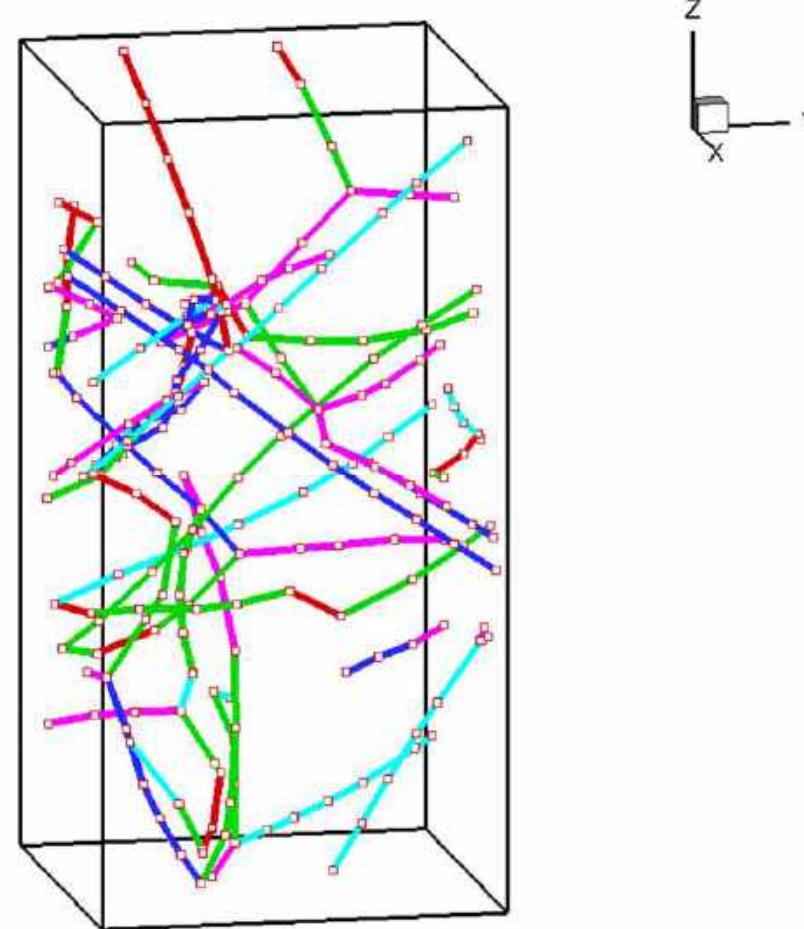
3 位错动力学方法



MS HUANG ET AL. IJP. 2020

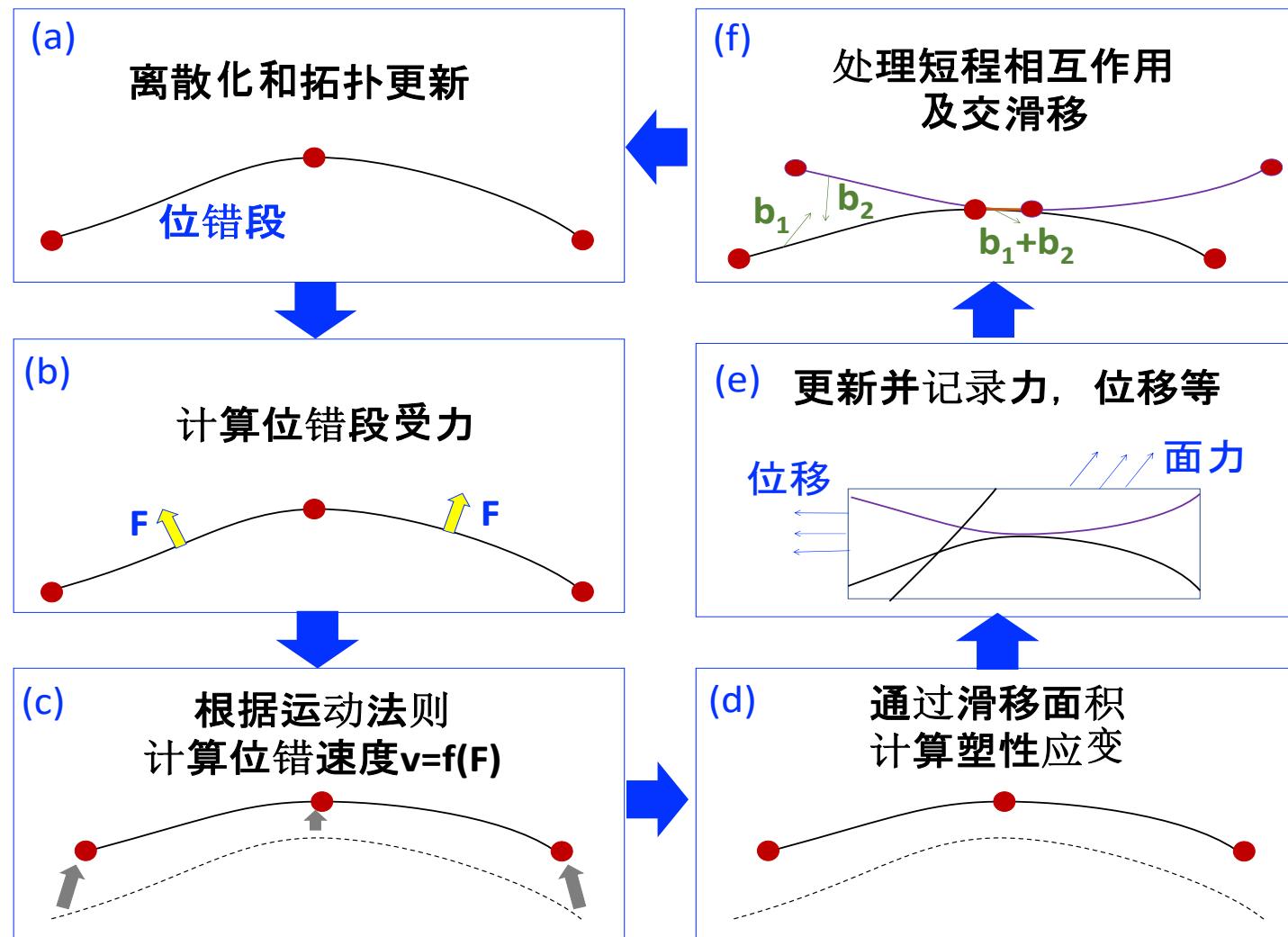
3 位错动力学方法

3D-DDD



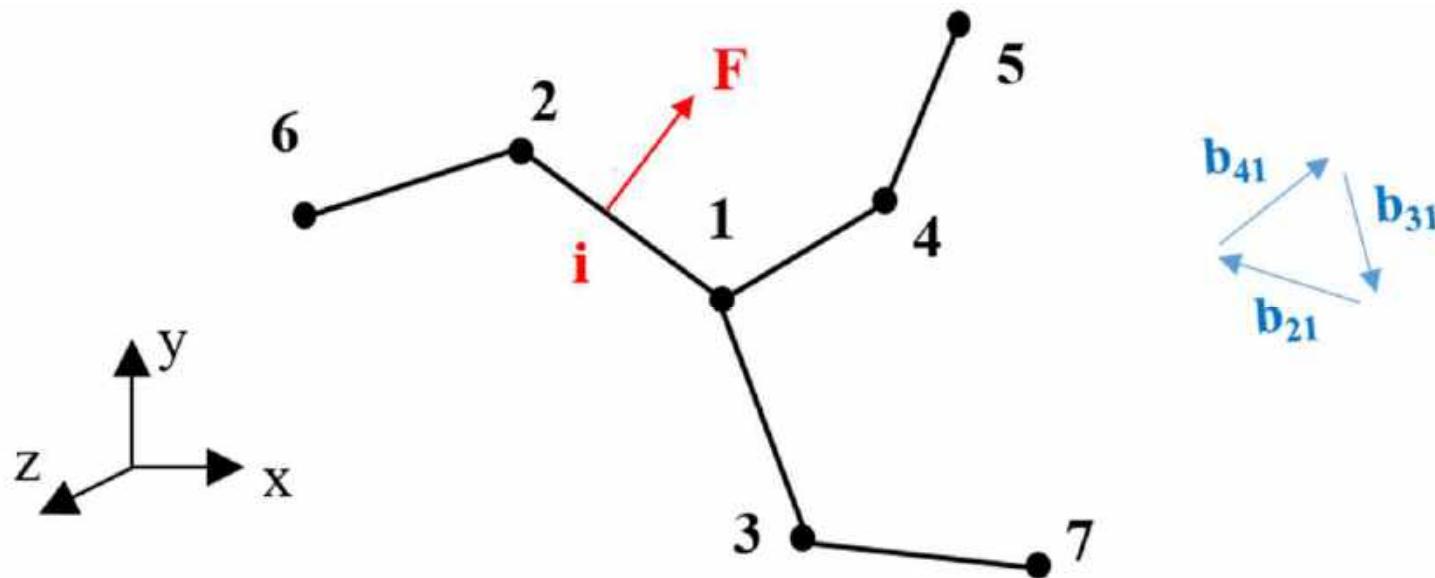
3位错动力学方法

基本流程



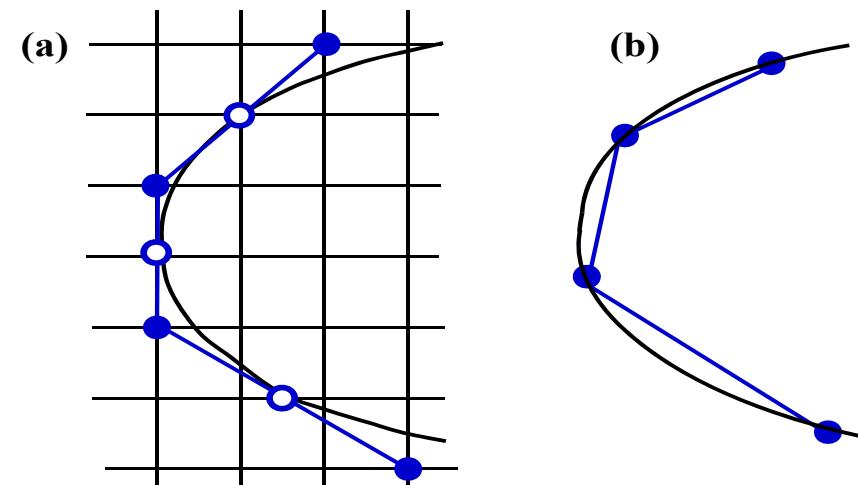
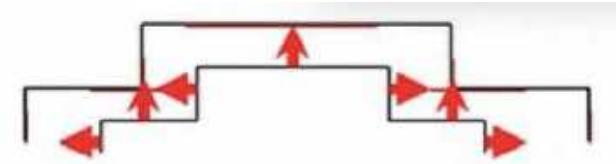
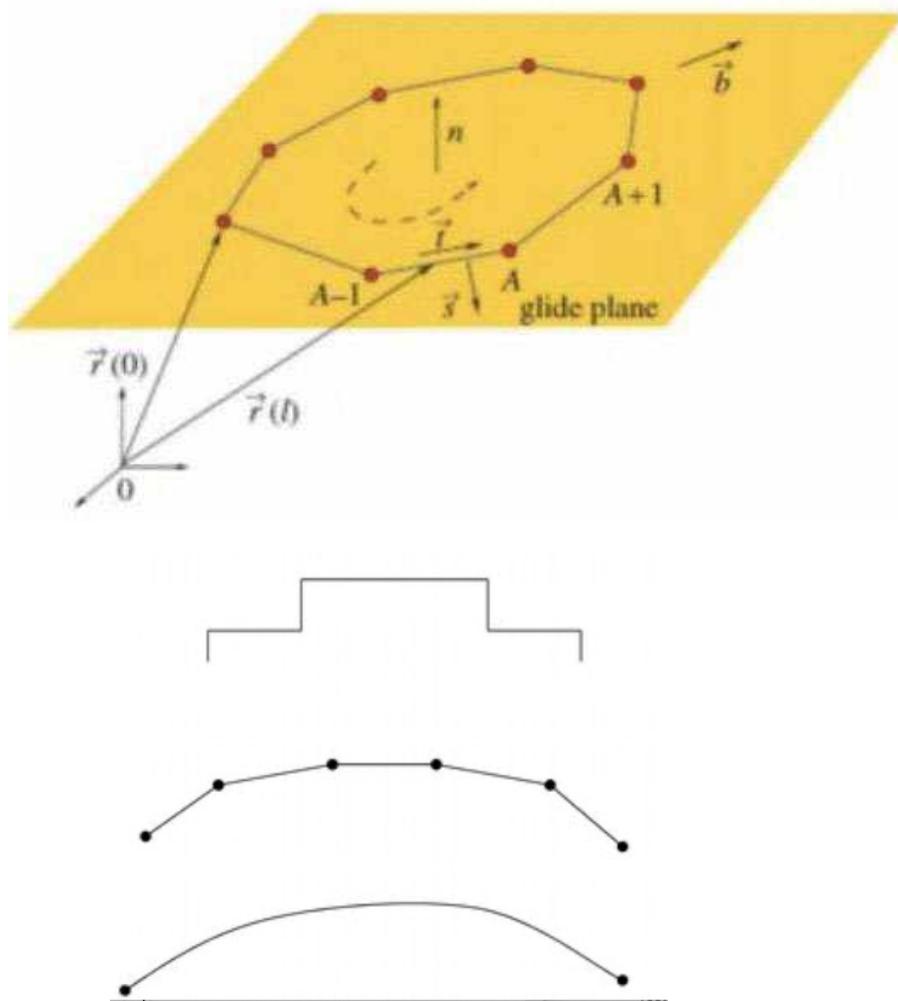
3 位错动力学方法

位错段离散化方案



3 位错动力学方法

位错段离散化方案

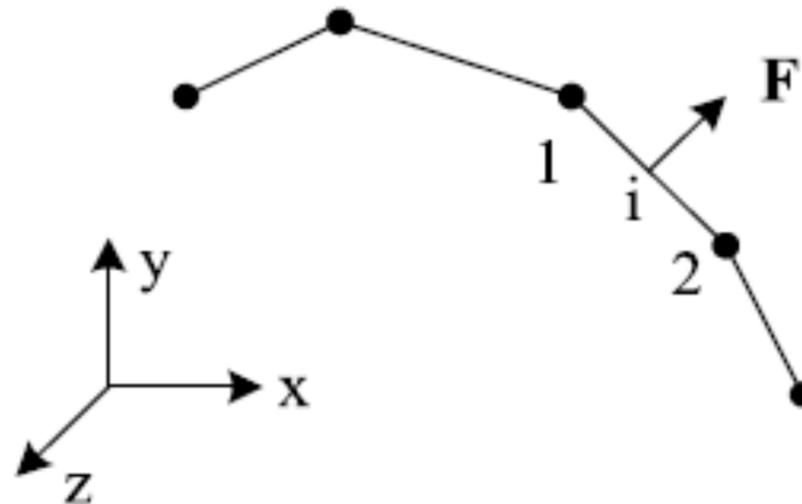


离散位错线的两种表述方式：(a) 基于离散晶格的描述；(b) 基于连续化的描述

3 位错动力学方法

(1) 位错段受力

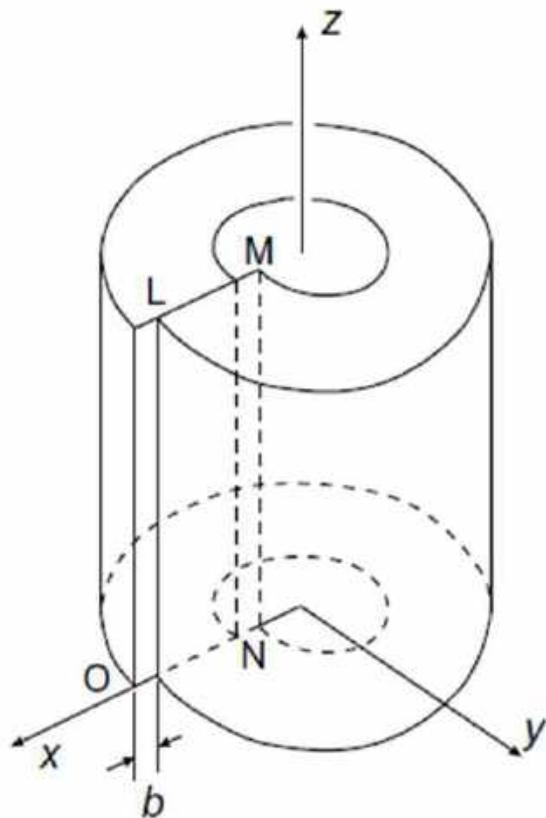
$$\tau_g^* = \tau_{self} + \tau_{ext} + \tau_{int} + \tau_{obs} + \tau_{im}$$



3 位错动力学方法

(1) 位错段受力

刃位错



$$\sigma_{xx} = -Dy \frac{(3x^2 + y^2)}{(x^2 + y^2)^2}$$

$$\sigma_{yy} = Dy \frac{(x^2 - y^2)}{(x^2 + y^2)^2}$$

$$\sigma_{xy} = \sigma_{yx} = Dx \frac{(x^2 - y^2)}{(x^2 + y^2)^2}$$

$$\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$$

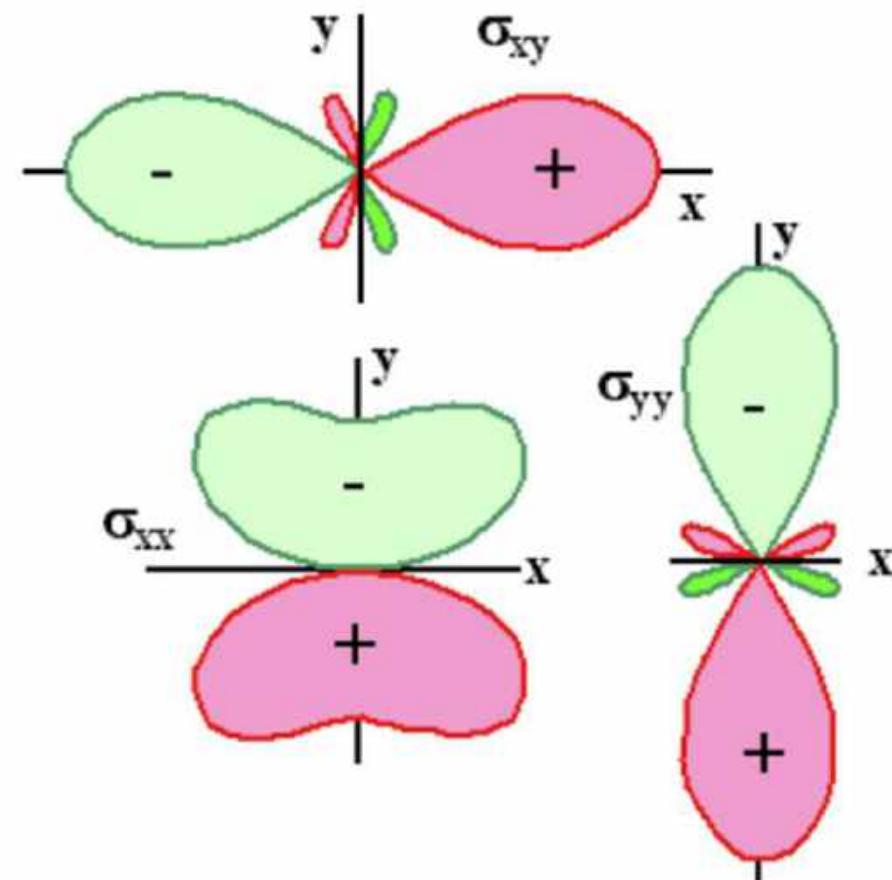
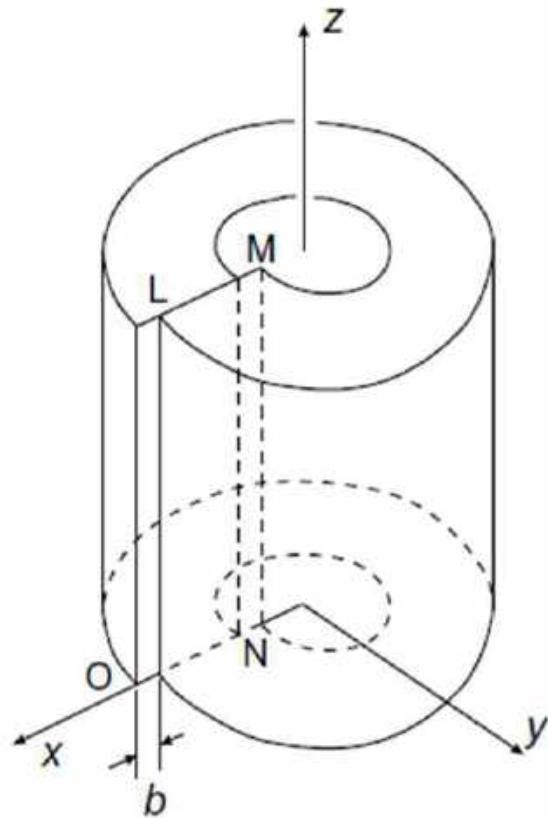
$$\sigma_{xz} = \sigma_{zx} = \sigma_{yz} = \sigma_{zy} = 0$$

$$D = \frac{Gb}{2\pi(1-\nu)}$$

3 位错动力学方法

(1) 位错段受力

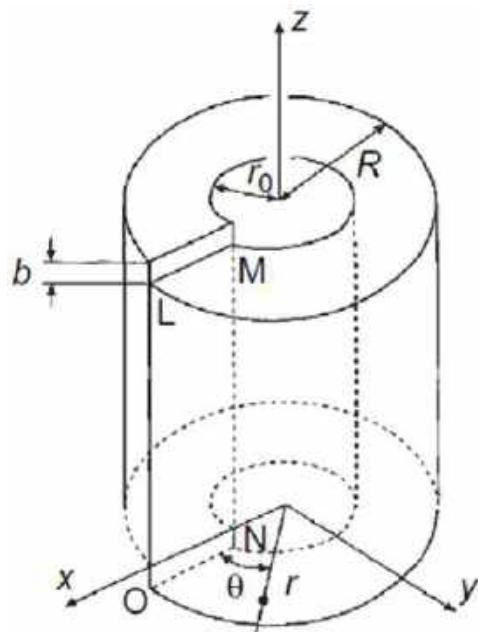
刃位错



3 位错动力学方法

(1) 位错段受力

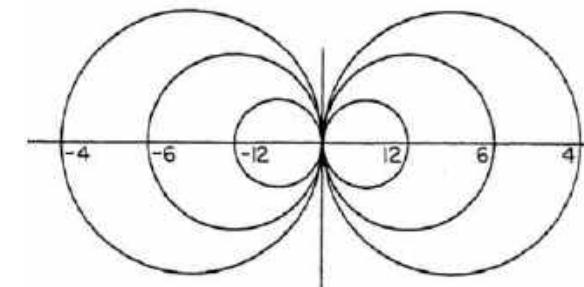
螺位错



$$\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \sigma_{xy} = \sigma_{yx} = 0$$

$$\sigma_{xz} = \sigma_{zx} = -\frac{Gb}{2\pi(x^2 + y^2)} \frac{\gamma}{r} = -\frac{Gb \sin \theta}{2\pi r}$$

$$\sigma_{yz} = \sigma_{zy} = \frac{Gb}{2\pi(x^2 + y^2)} \frac{x}{r} = \frac{Gb \cos \theta}{2\pi r}$$



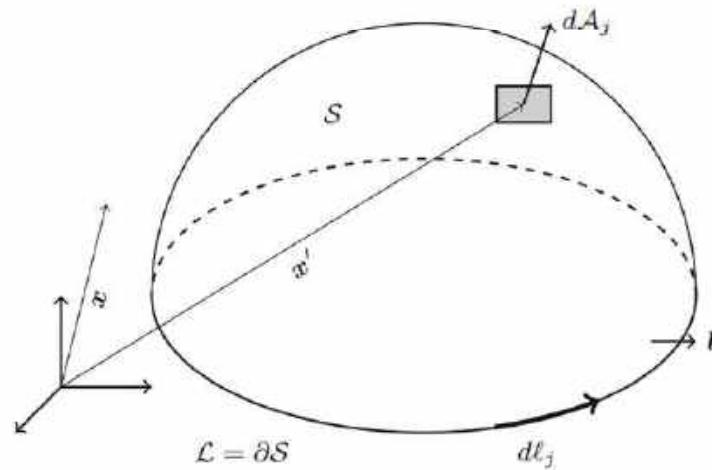
σ_{23}

3 位错动力学方法

(1) 位错段受力

任意位错环

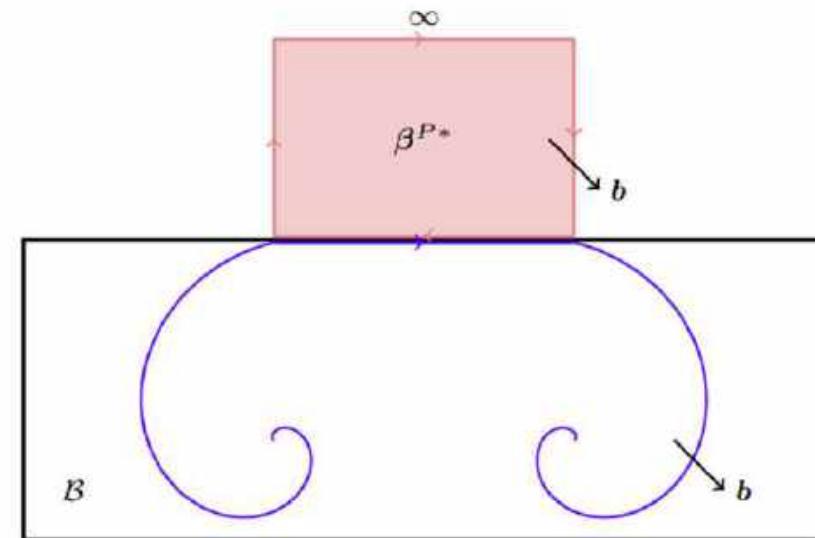
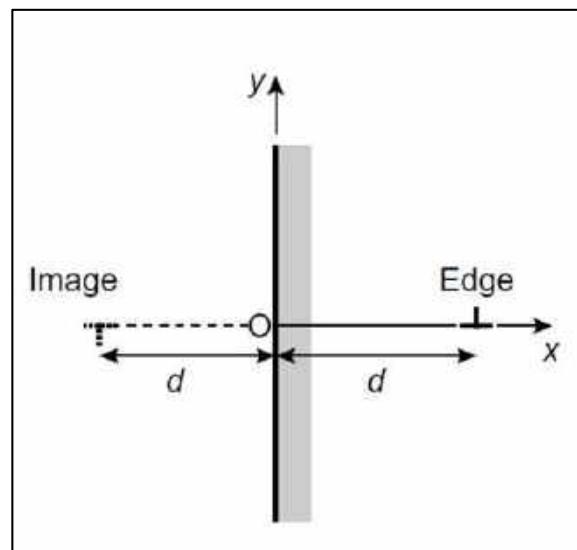
$$\sigma_{ij}(\mathbf{x}) = \frac{-\mu b_l}{4\pi(1-\nu)} \oint_{\mathcal{L}} \left\{ \frac{1-2\nu}{2R^3} (\delta_{il} R_k \epsilon_{jks} + \delta_{jl} R_k \epsilon_{iks} - R_i \epsilon_{jls} - R_j \epsilon_{ils}) \right. \\ \left. + \frac{3R_n R_l (R_i \epsilon_{jns} + R_j \epsilon_{ins})}{2R^5} + \frac{2\nu \delta_{ij} R_n \epsilon_{lns}}{R^3} \right\} \xi_s dL'.$$



3 位错动力学方法

(1) 位错段受力

镜像力

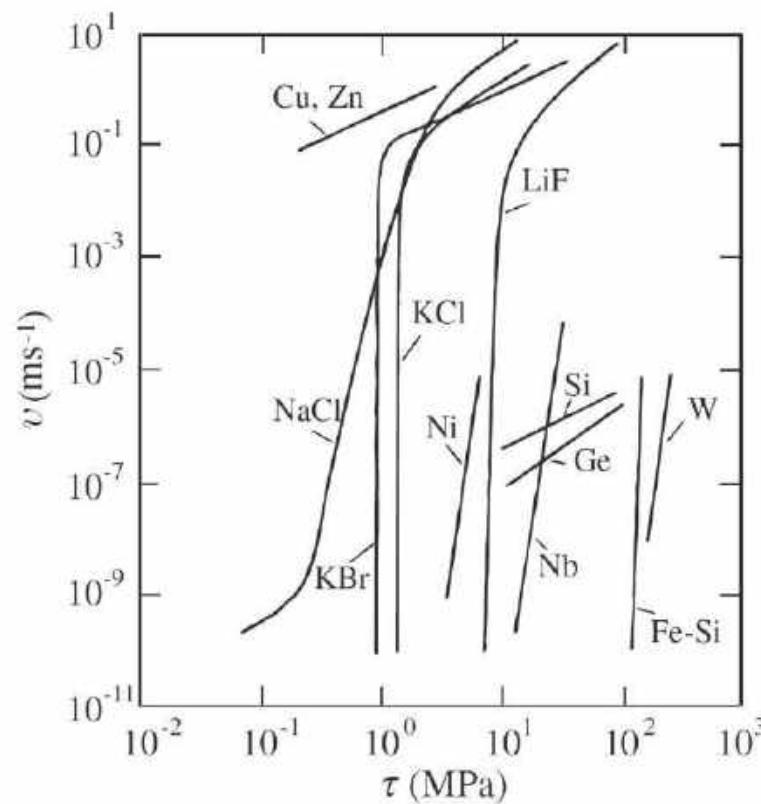


G Po, 2014

3 位错动力学方法

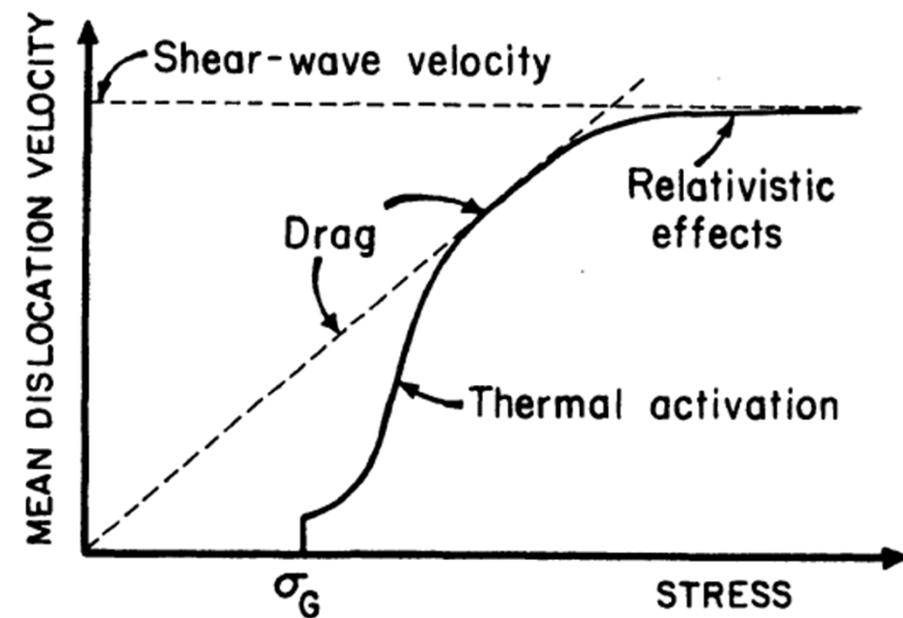
(2) 位错运动法则

$$v = f(\tau)$$



Haasen, Physical Metallurgy

Tsinghua university



Mayer 1994

3 位错动力学方法

(2) 位错运动法则

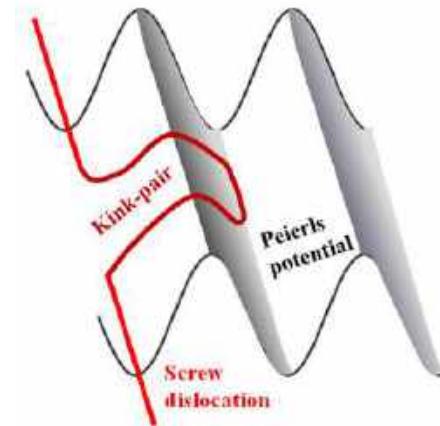
Thermal activation

Kink nucleation and motion is modeled through an Arrhenius-type equation:

$$v_s = \frac{\tau b}{A_s T} \exp\left(-\frac{\Delta G(\sigma, T)}{k_b T}\right)$$

The activation energy is written as (Kocks et al. 1975):

$$\Delta G(\sigma, T) = \Delta H - T \Delta S = \Delta H_0 \left[\left(1 - \left(\frac{\tau^\alpha}{\tau_p} \right)^p \right)^q - \frac{T}{T_c} \right]$$



τ^α is an effective stress that takes into account non-Schmid effects, following Groger and Vitek's work.

$$\tau^\alpha = \boxed{\boldsymbol{\sigma} : \mathbf{m}^\alpha \otimes \mathbf{n}^\alpha} + \boxed{a_1 \boldsymbol{\sigma} : \mathbf{m}^\alpha \otimes \mathbf{n}_1^\alpha} + \boxed{a_2 \boldsymbol{\sigma} : (\mathbf{n}^\alpha \times \mathbf{m}^\alpha) \otimes \mathbf{n}^\alpha + a_3 \boldsymbol{\sigma} : (\mathbf{n}_1^\alpha \times \mathbf{m}^\alpha) \otimes \mathbf{n}_1^\alpha}$$

Resolved shear stress Twining anti-twinning asymmetry Stress components that are not collinear with the Burgers vector change the dislocation core configuration modifying slip process

3 位错动力学方法

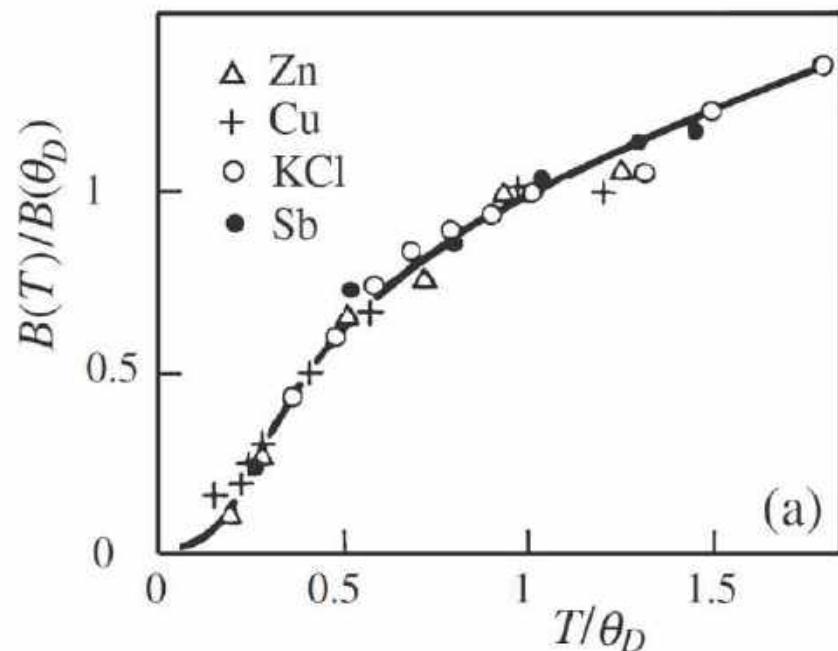
(2) 位错运动法则

Phonon drag mechanism

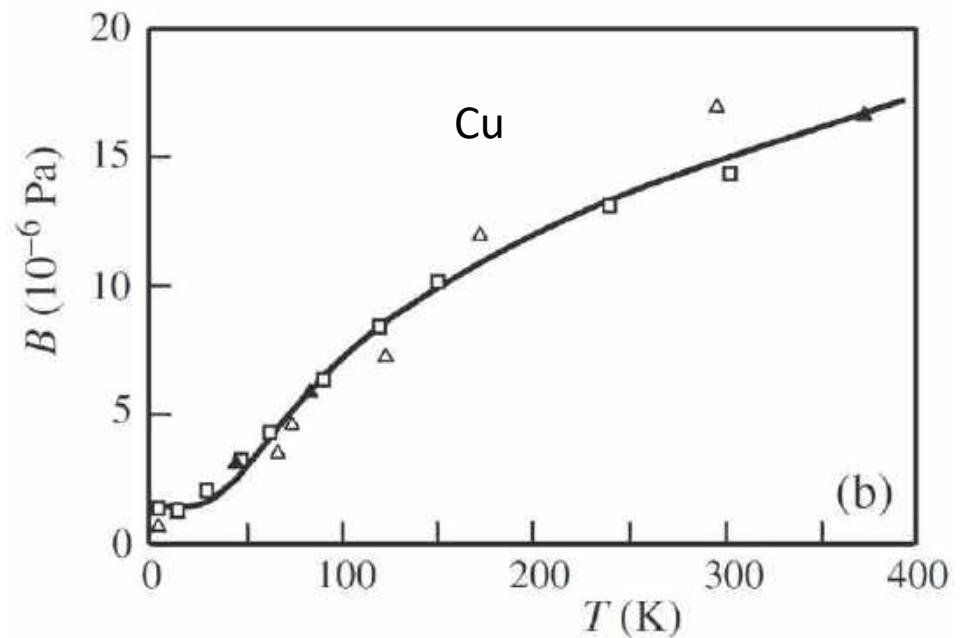
$$v = \frac{b}{B} \tau$$

Drag coefficient

(Experiments, MD, theory)



(a)



(b)

3 位错动力学方法

(2) 位错运动法则 High strain rate case

Inertia term

$$m_o \frac{dv}{dt} + Bv = \tau_a b$$

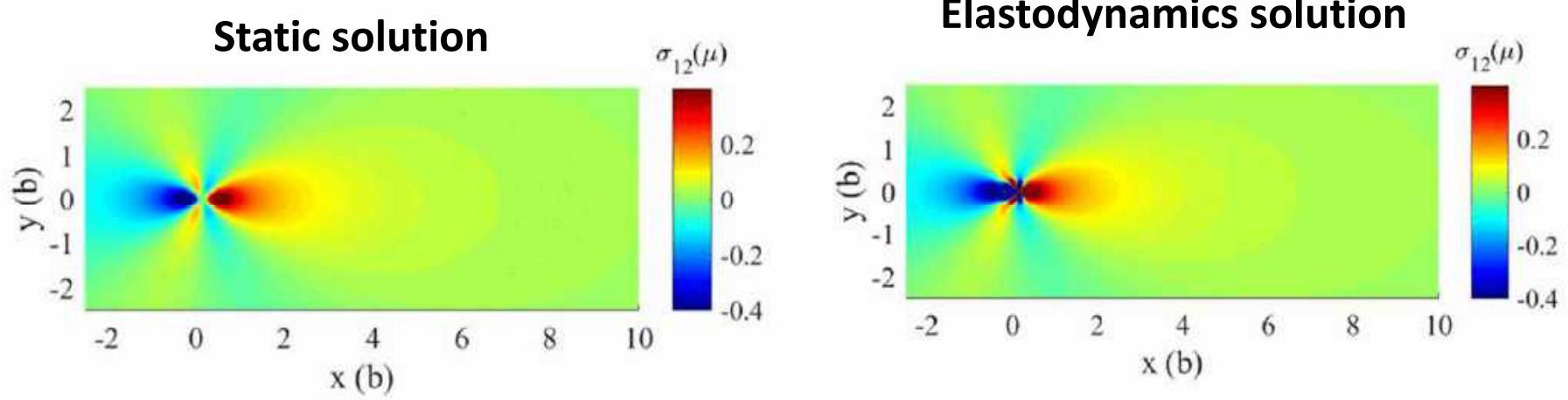
Calculate effective mass

$$(m_s)_{\text{screw}} = \frac{W_0}{v^2} (-\gamma^{-1} + \gamma^{-3}),$$

$$(m_s)_{\text{edge}} = \frac{W_0 C^2}{v^4} (-16\gamma_1 - 40\gamma_1^{-1} + 8\gamma_1^{-3} + 14\gamma + 50\gamma^{-1} - 22\gamma^{-3} + 6\gamma^{-5})$$

$$\gamma_1 = (1 - v^2/C_1^2)^{\frac{1}{2}}, \gamma = (1 - v^2/C^2)^{\frac{1}{2}}$$

3 位错动力学方法



$$\begin{aligned}\sigma_{\alpha\beta}(\mathbf{x}) = & \frac{\mu}{8\pi} \oint_C \partial_i \partial_\rho \partial_\beta R_a \left(b_m \epsilon_{im\alpha} dx'_\beta + b_m \epsilon_{im\beta} dx'_\alpha \right) \\ & + \frac{\mu}{4\pi(1-\nu)} \oint_C b_m \epsilon_{imk} \left(\partial_i \partial_\alpha \partial_\beta R_a - \delta_{\alpha\beta} \partial_i \partial_\rho \partial_\rho R_a \right) dx'_k\end{aligned}$$

$$\begin{aligned}v=0, & \quad t \leq 0; \\ v=0.8c_T, & \quad 0 < t \leq 6.25b/c_T; \\ v=0, & \quad t > 6.25b/c_T\end{aligned}$$

YN Cui et al., JMPS, 2019

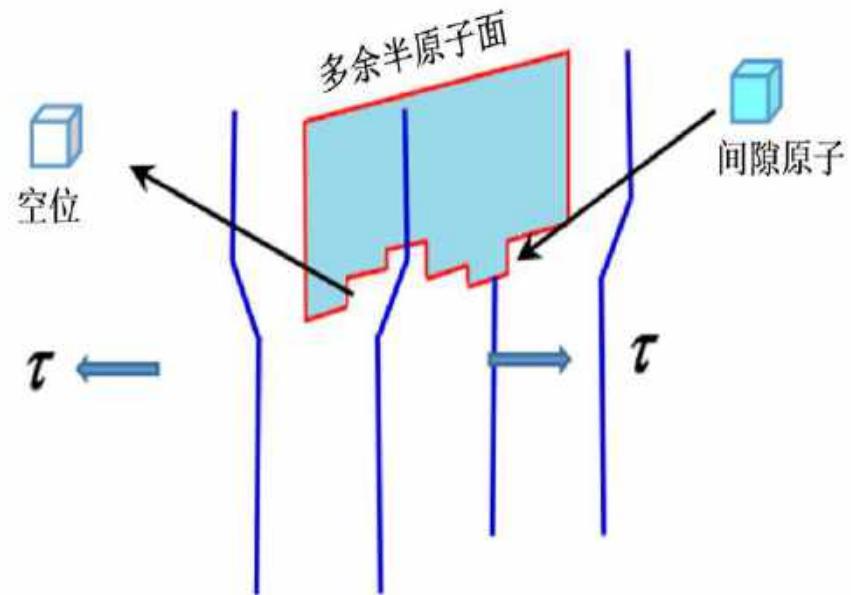
70

3 位错动力学方法

(3) 位错攀移

- 唯象的位错攀移模型

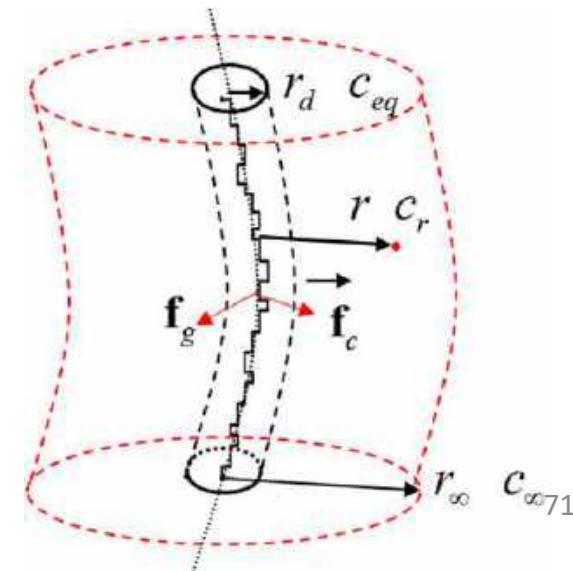
$$v_c^i = f(f_c^i)$$



- 基于点缺陷扩散理论的位错攀移模型

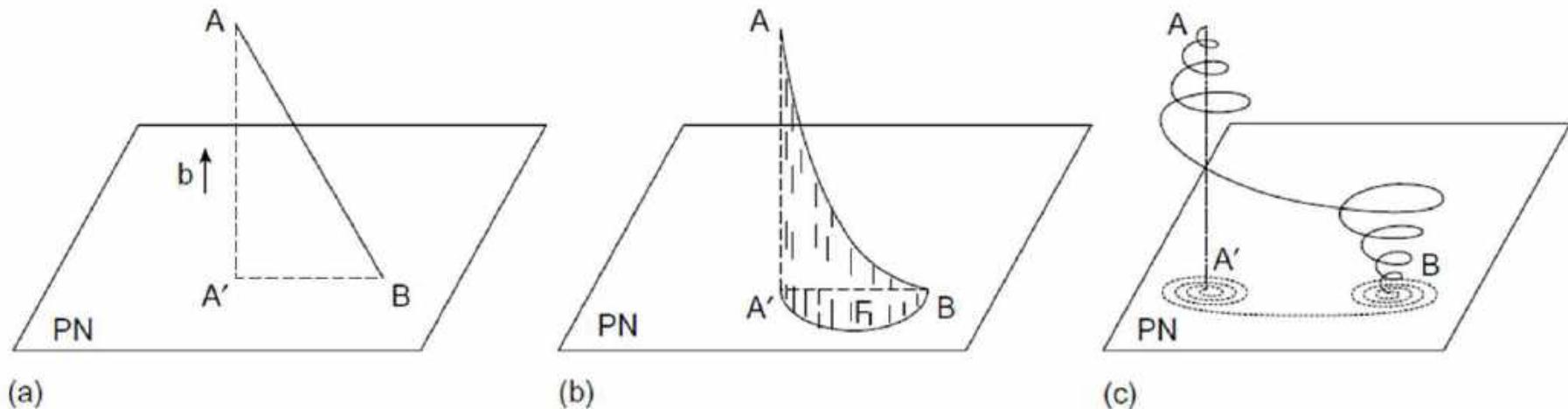
$$v_c^i = -\frac{2\pi r D_v}{b \sin \theta^i \ln(r_\infty / r_d)} (c_{eq}^i - c_\infty)$$

位错核平衡空位浓度 $c_{eq}^i = c_v^0 \exp\left(-\frac{f_c^i \Omega}{b \sin \theta^i kT}\right)$



3 位错动力学方法

Formation of a helical dislocation by climb of a straight dislocation with a screw component.



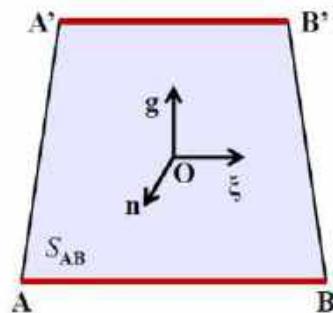
D Hull, et al. 2011

3 位错动力学方法

(4) 塑性变形计算及应力更新

L 速度梯度, 分解其对称和反对称部分

$$L = D + \Omega$$



$$\Delta\gamma = \frac{bS_{AB}}{V}$$

塑性变形率 $D^p = \frac{1}{2V\Delta t}(\mathbf{b} \otimes \mathbf{A} + \mathbf{A} \otimes \mathbf{b})$

塑性旋转率 $\Omega^p = \frac{1}{2V\Delta t}(\mathbf{b} \otimes \mathbf{A} - \mathbf{A} \otimes \mathbf{b})$

晶格坐标系中的旋转应力率 $\overset{\nabla}{\sigma}^e$

$$\overset{\nabla}{\sigma}^e = \mathbf{C}^e : \mathbf{D}^e$$

\mathbf{C}^e 是弹性切线模量张量,

$$\mathbf{D} = \mathbf{D}^e + \mathbf{D}^p$$

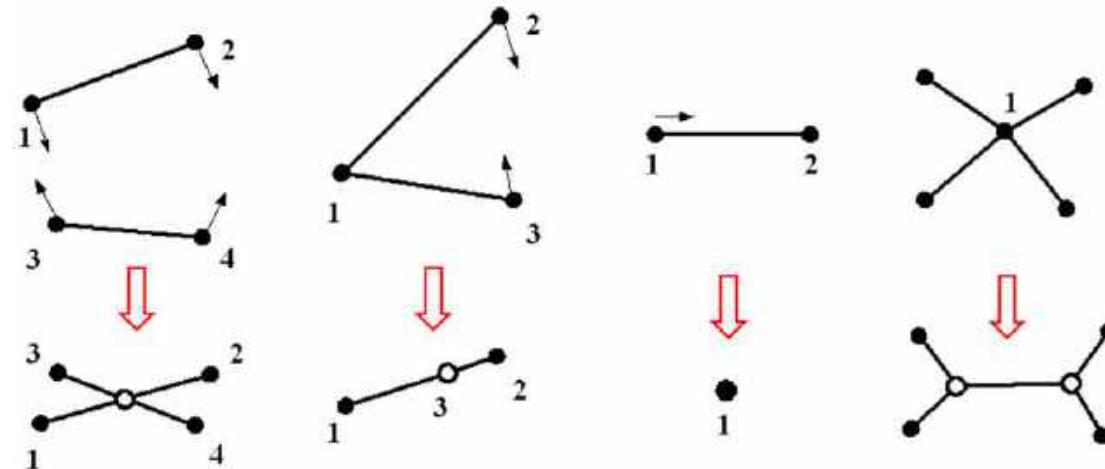
Cauchy应力的Jaumann率

$$\overset{\nabla}{\sigma} = \mathbf{C}^e : (\mathbf{D} - \mathbf{D}^p) - \Omega^p \cdot \overset{\nabla}{\sigma} + \overset{\nabla}{\sigma} \cdot \Omega^p$$

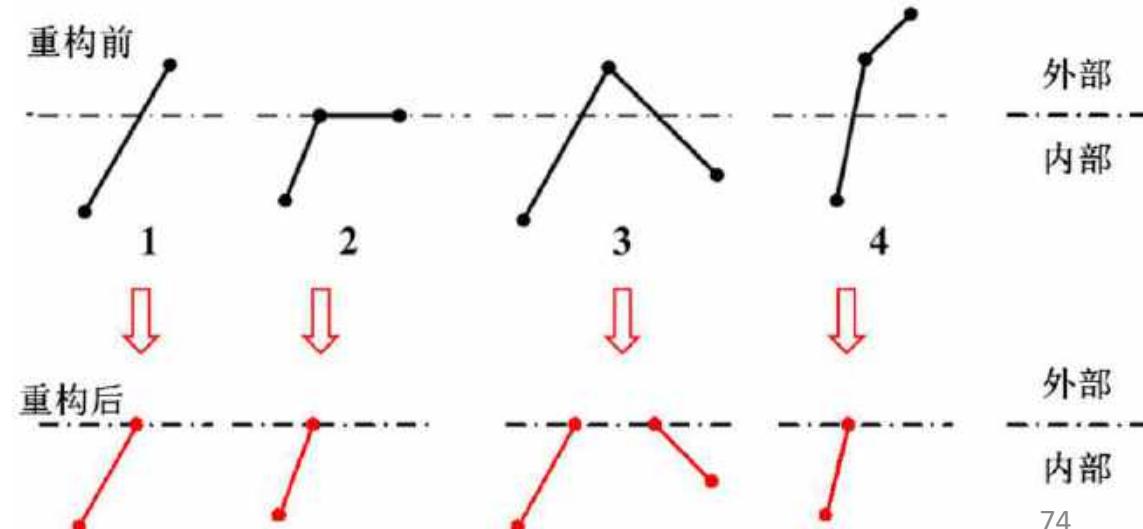
3 位错动力学方法

(5) 位错反应及拓扑处理

基本单元（位错段和节点）的拆分和合并

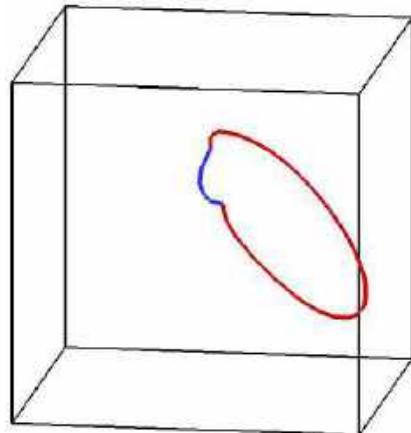


位错线与自由表面相互作用时的拓扑重构方案

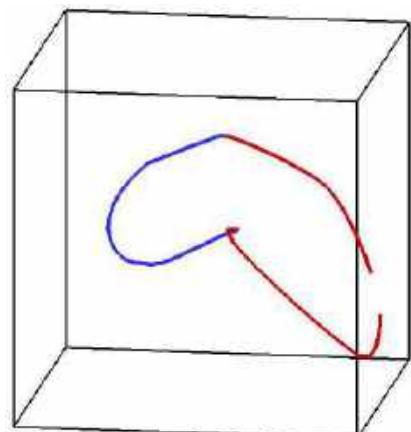


3 位错动力学方法

(6) 位错交滑移



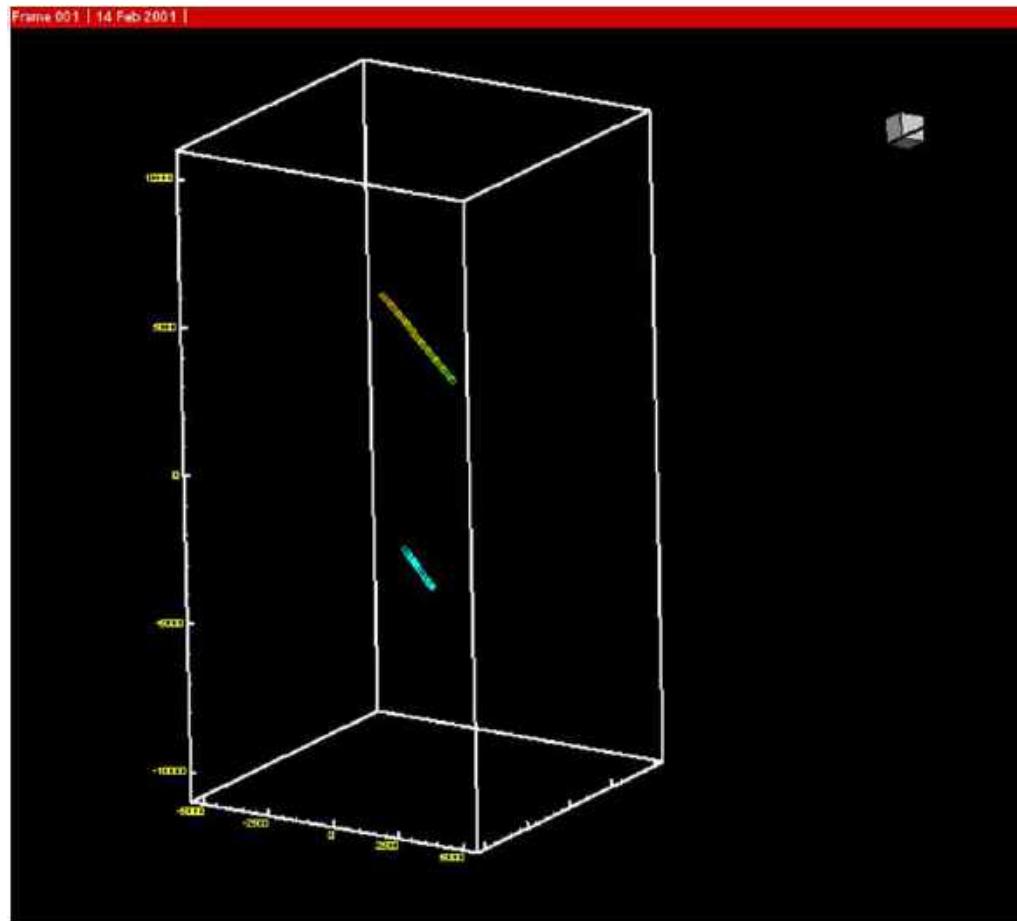
- 交滑移面上的分切应力需要大于原滑移面上的分切应力。这是因为交滑移的进
- 热激活模型



$$P = \beta \frac{L}{L_0} \frac{\delta t}{\delta t_0} \exp\left(V \cdot \frac{\tau - \tau_{III}}{kT}\right)$$

V 是激活体积，
 τ_{III} 是拉伸测试的第三阶段塑性变形开始时的分切应力，

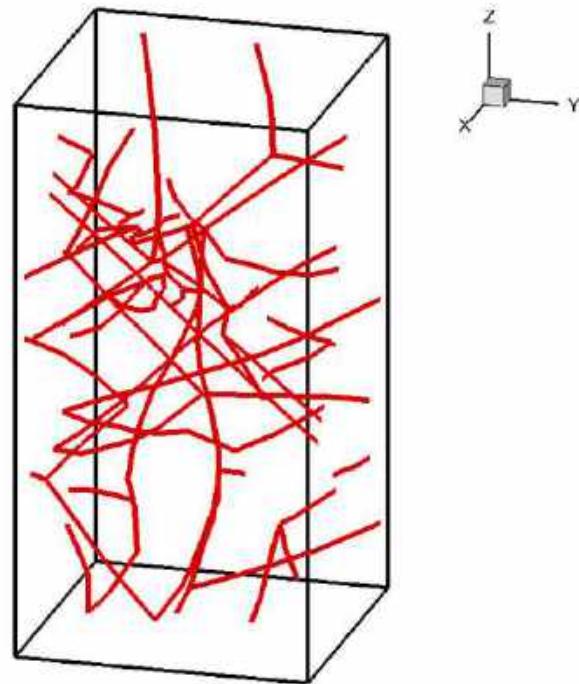
3 位错动力学方法



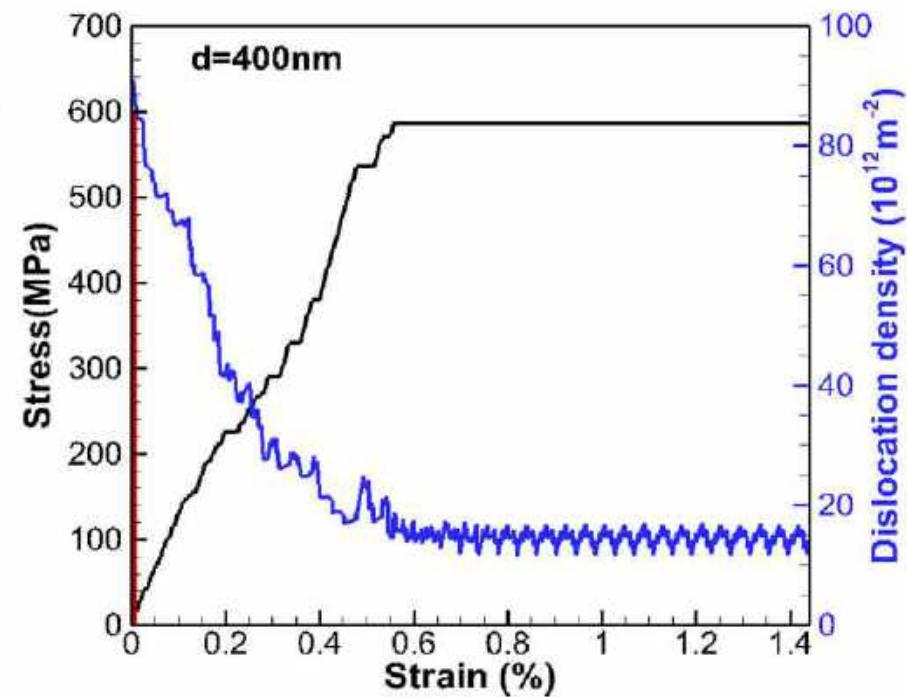
3 位错动力学方法

(7) 程序输出

微结构演化



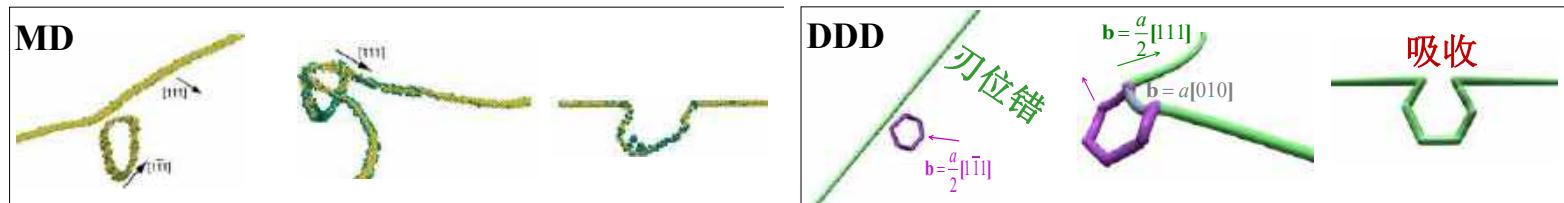
力学响应



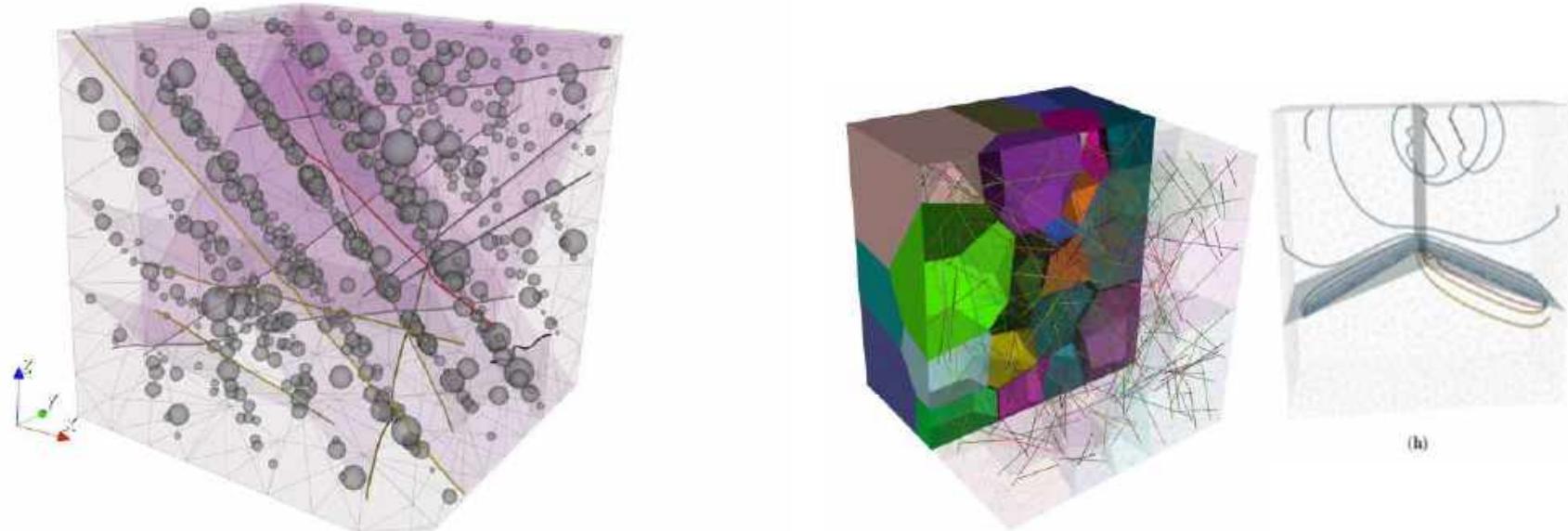
3 位错动力学方法

(7) 程序输出

多种微结构相互作用机理



YN Cui et al. Acta mater. 2017

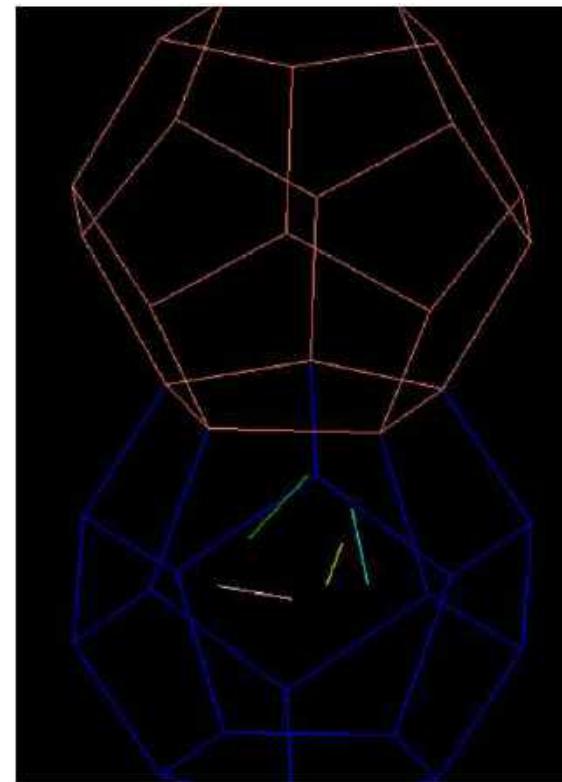
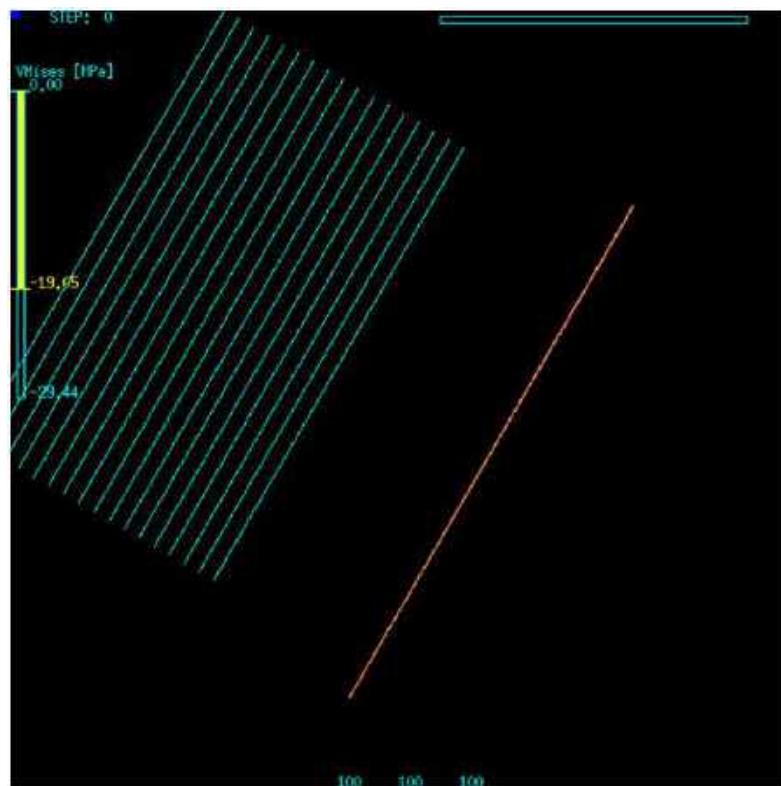


M Mahler et al. 2020
Tsinghua university

G Po et al. unpublished

3 位错动力学方法

(7) 程序输出

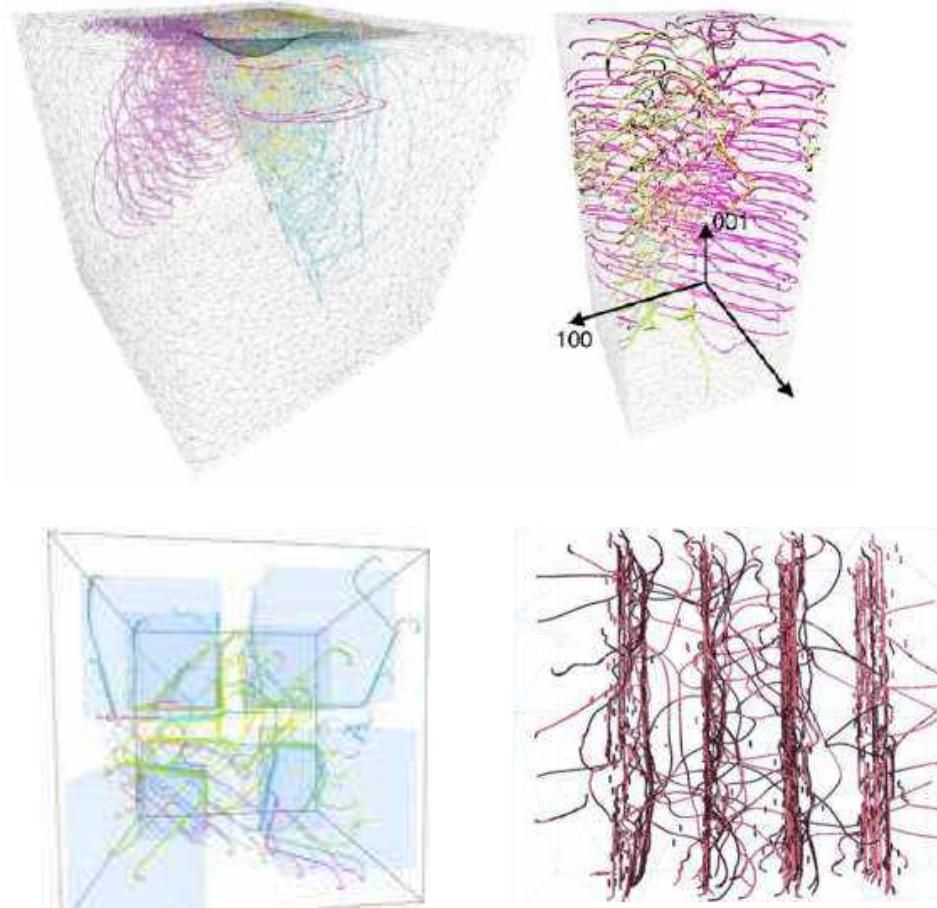


<http://www.numodis.fr/tridis>

3 位错动力学方法

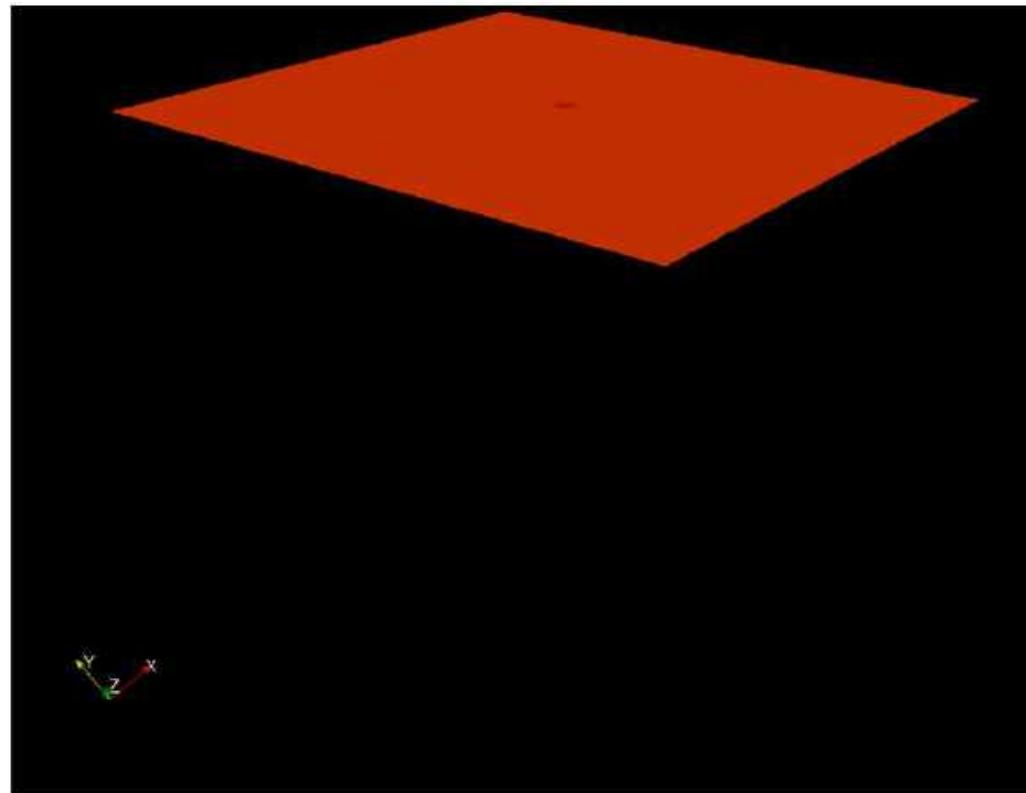
(7) 程序输出

复杂载荷

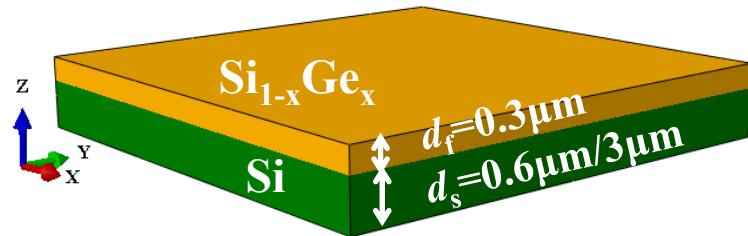


3 位错动力学方法

(7) 程序输出



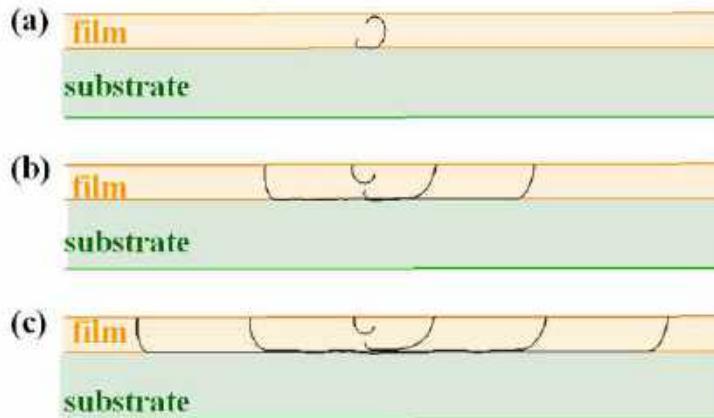
异质外延薄膜中的位错演化



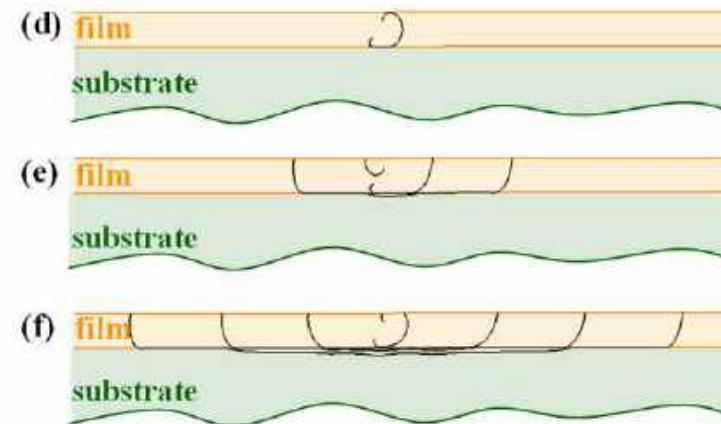
● 错配应变作用下的位错演化

位错影响Si电学响应

薄基底 ($d_f/d_s=1:2$)



厚基底 ($d_f/d_s=1:10$)



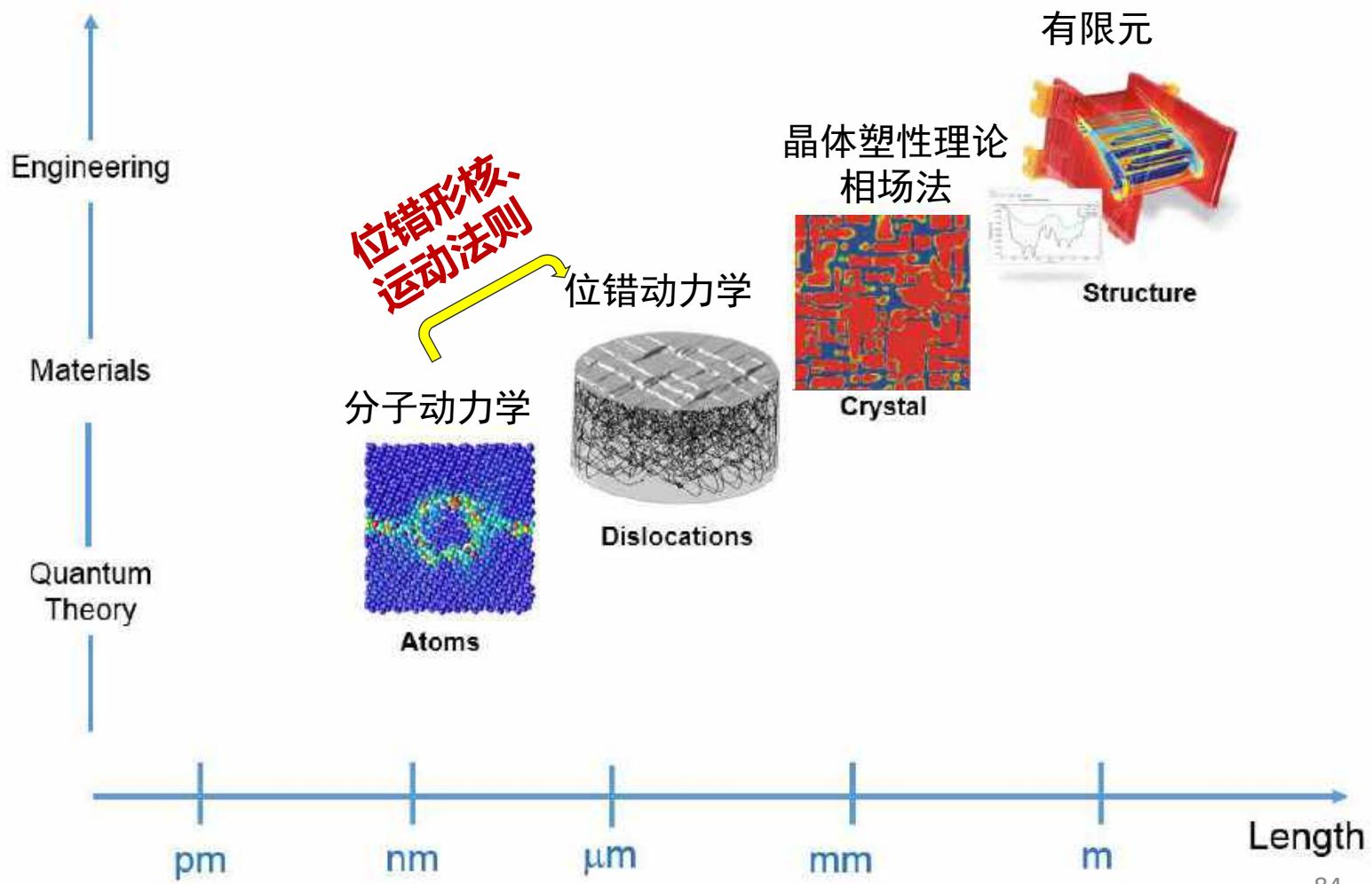
4 DDD与原子模拟及连续介质力学的联系

4.1 DDD与原子模拟的联系

4.2 DDD+FEM

4.3 基于DDD建立连续介质模型

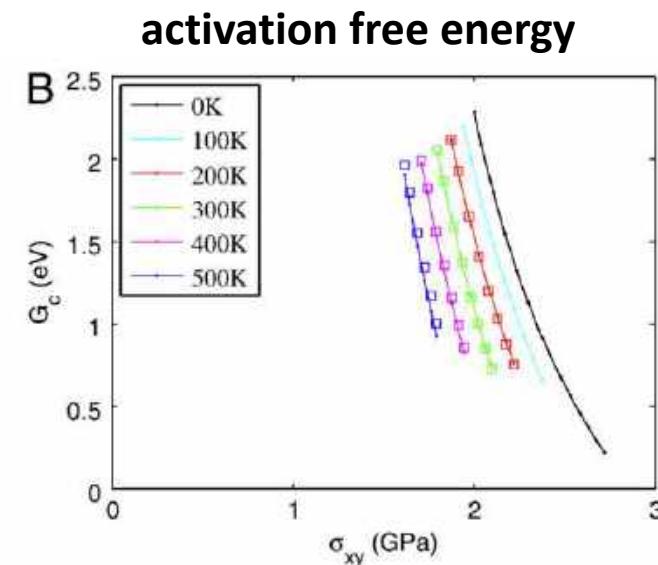
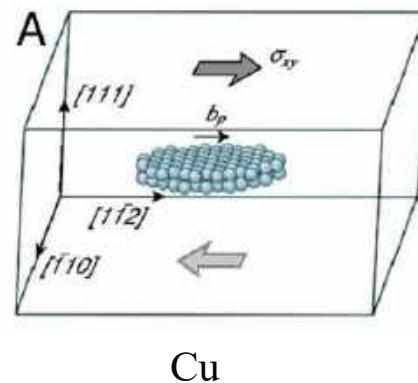
4.1 DDD与原子模拟的联系



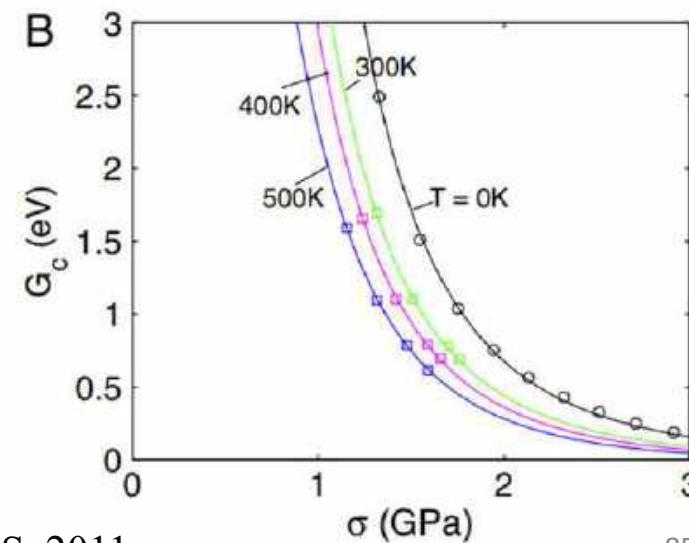
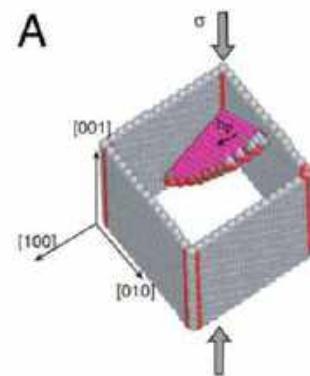
4.1 DDD与原子模拟的联系

位错形核

Homogeneous
dislocation
nucleation



Heterogeneous
dislocation
nucleation



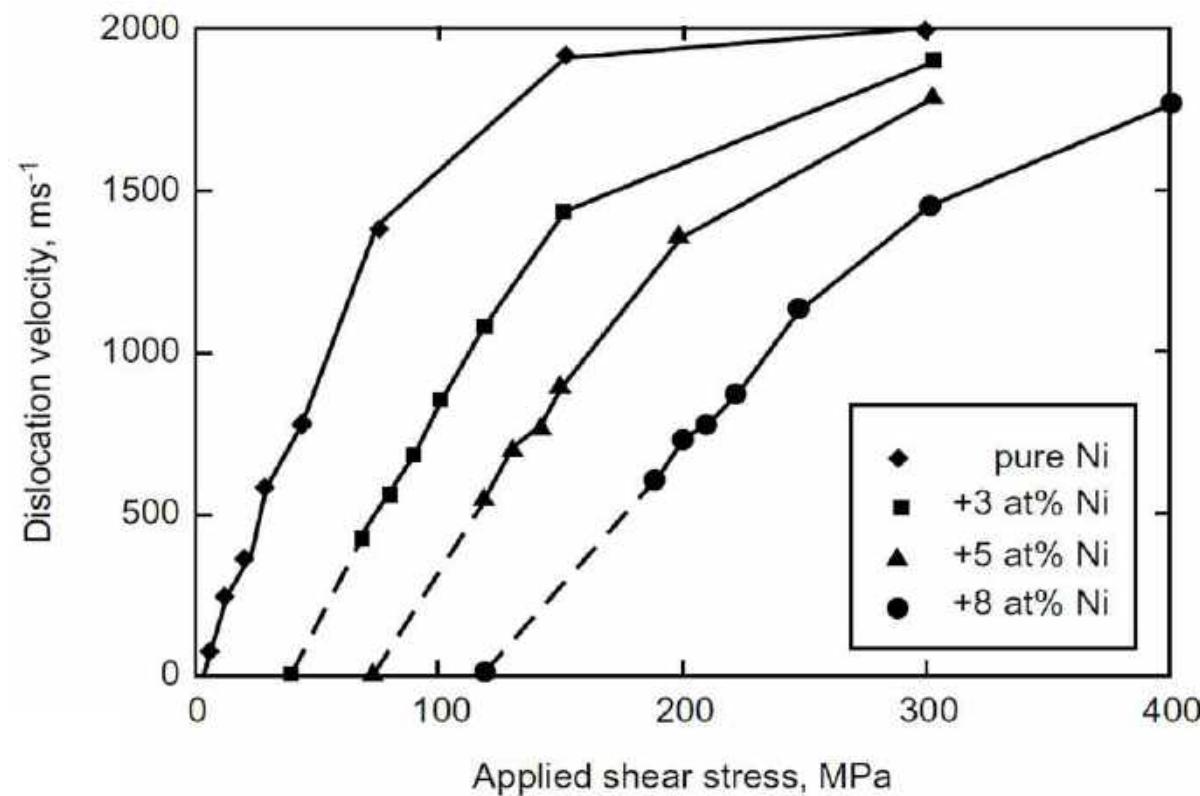
S Ryu et al. PNAS, 2011

85

4.1 DDD与原子模拟的联系

位错运动法则

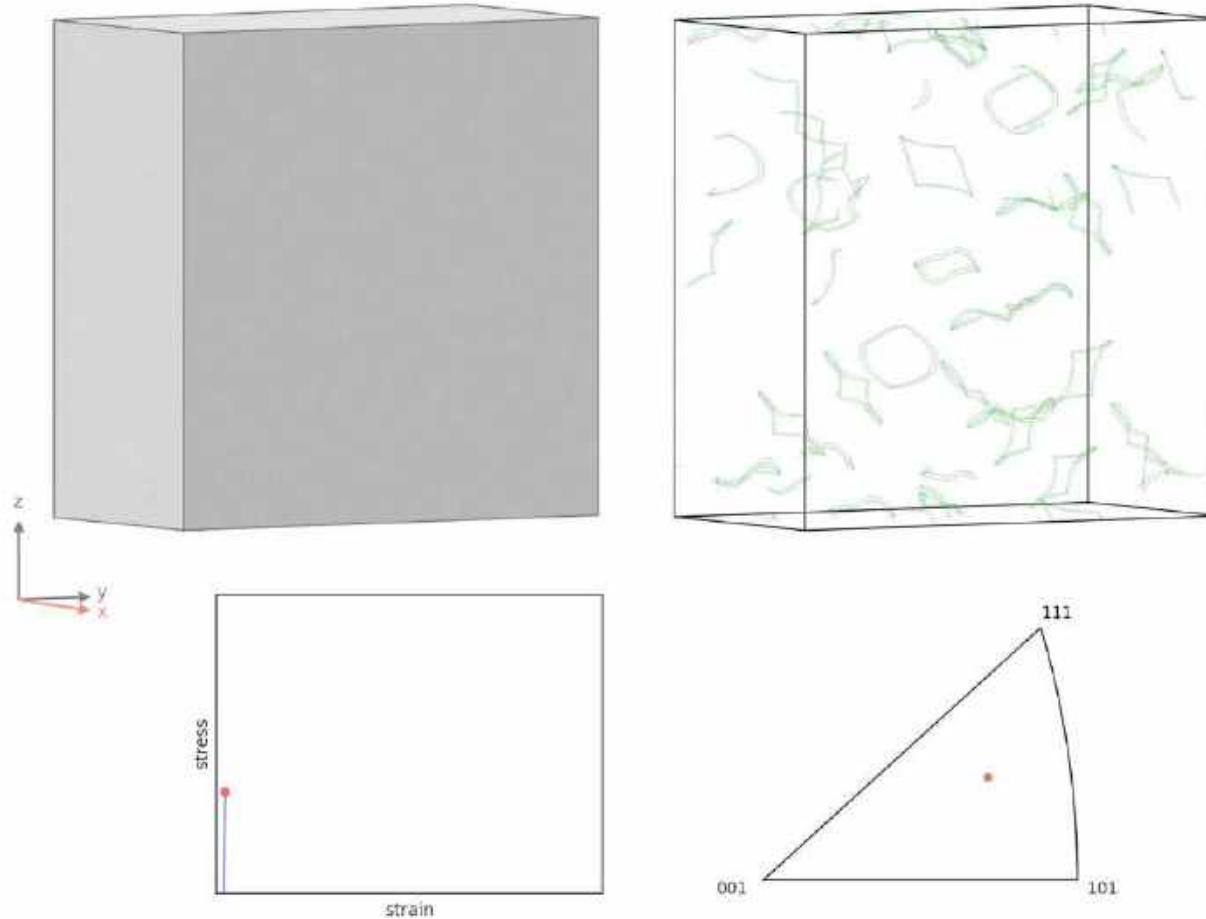
MD results on pure nickel
and Ni-Al solid solutions at 300 K



Rodary et al. 2004

86

4.1 DDD与原子模拟的联系



美国阿贡实验室，Lammps，AI，3亿原子， $5\text{e}7/\text{s}$ strain rate

LA Zepeda-Ruiz, Nature Mater, 2020

87

4.2 DDD+FEM

位错动力学 DDD

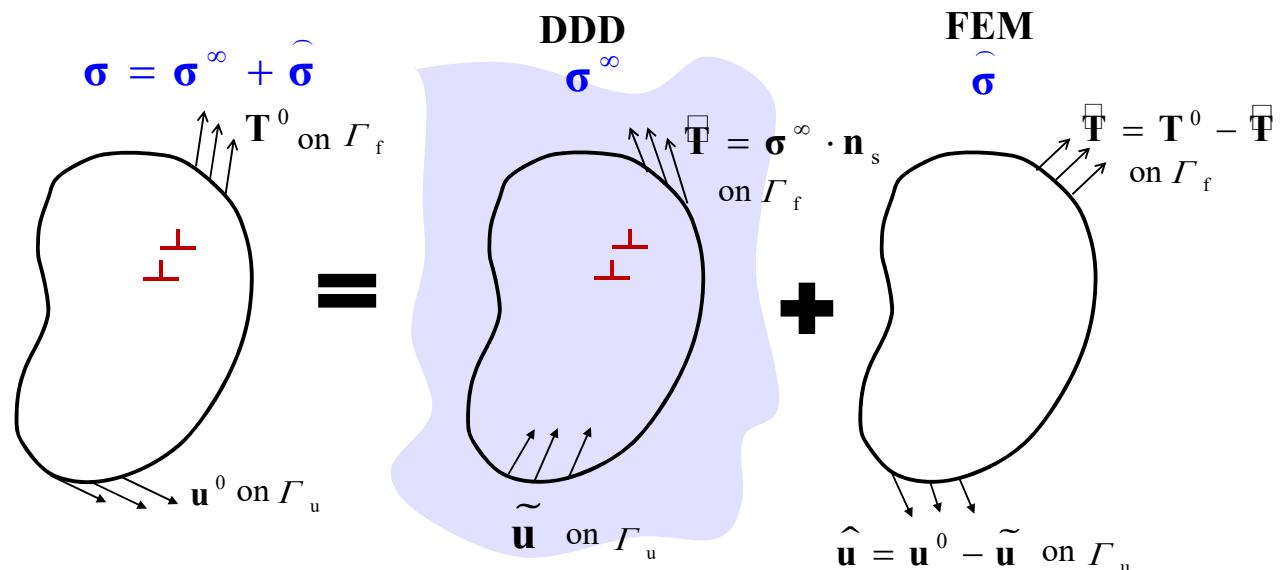
优点：

能物理的反映材料塑性变形机制

局限：

- 1 不能考虑计算模型的有限变形；
- 2 难以处理复杂边界条件和表界面效应。

Superposition Method (SPM)

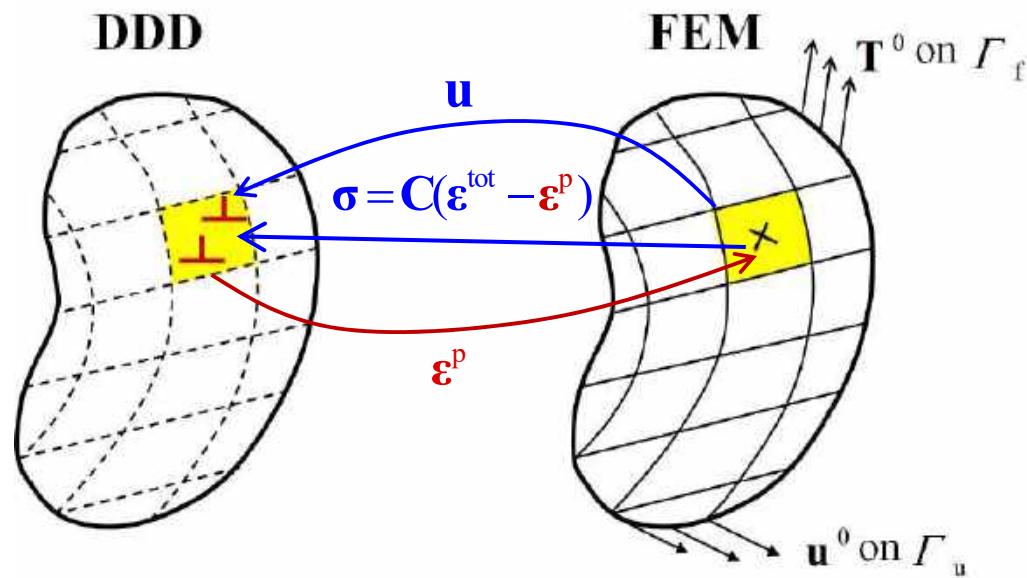


Van der Giessen and Needleman, 1995

- **优点：**准确捕捉短程相互作用
- **缺点：**没有直接体现‘塑性应变’的概念。

4.2 DDD+FEM

Discrete-Continuous Method (DCM)



◆ DD节点上位移

$$\mathbf{u}_I = \mathbf{u}_I^{DD} + \mathbf{u}_I^{FE}$$

位错演化

有限变形

$$\mathbf{u}_I^{DD} = \mathbf{v}_I^{DD} \Delta t$$

$$\mathbf{u}_I^{FE} = \frac{\sum_{i=1}^n w_i \mathbf{u}_i}{\sum_{i=1}^n w_i}$$

Tsinghua university

ZL. Liu et al., Int. J. Plasticity, 2009
YN Cui et al., Int. J. Plasticity, 2015

◆ 统一的有限元计算框架

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{f}^{int} = \mathbf{f}^{ext}$$

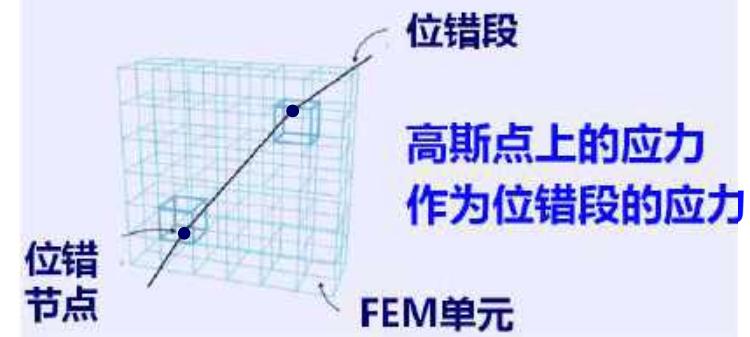
$$\mathbf{M} = \int_{\Omega} \rho \mathbf{N}^T \mathbf{N} d\Omega$$

$$\mathbf{f}^{int} = \int_{\Omega} \mathbf{B}^T \boldsymbol{\sigma} d\Omega$$

$$\mathbf{f}^{ext} = \int_{\Gamma} \mathbf{B}^T \mathbf{T}^0 d\Gamma + \int_{\Omega} \mathbf{B}^T \boldsymbol{\sigma}^0 d\Omega$$

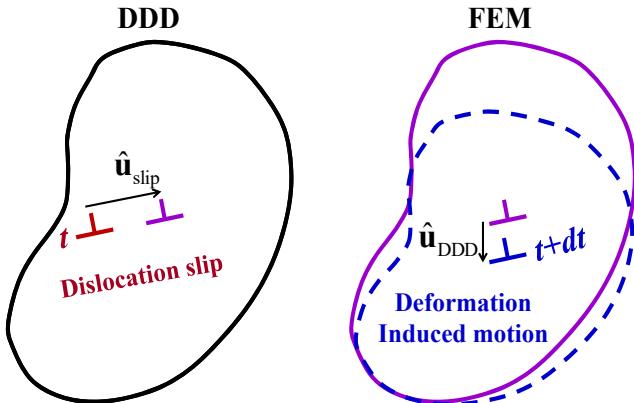
$$\mathbf{u} = \mathbf{u}^0 \quad \Gamma \in \Gamma_u$$

$$\mathbf{T} = \mathbf{T}^0 \quad \Gamma \in \Gamma_f, \quad \mathbf{T} = 0 \quad \Gamma \notin (\Gamma_u \cup \Gamma_f)$$



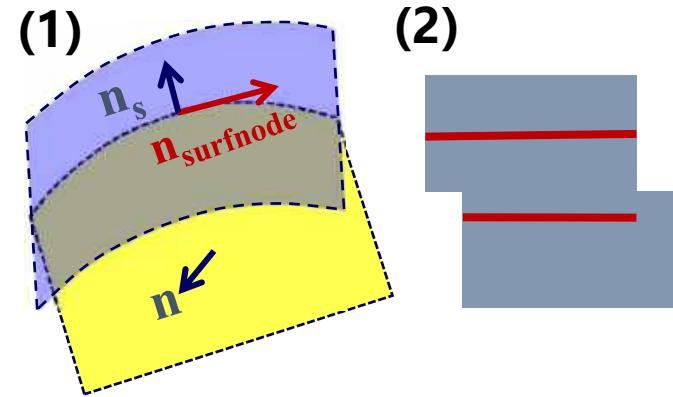
有限变形效应

变形场传递

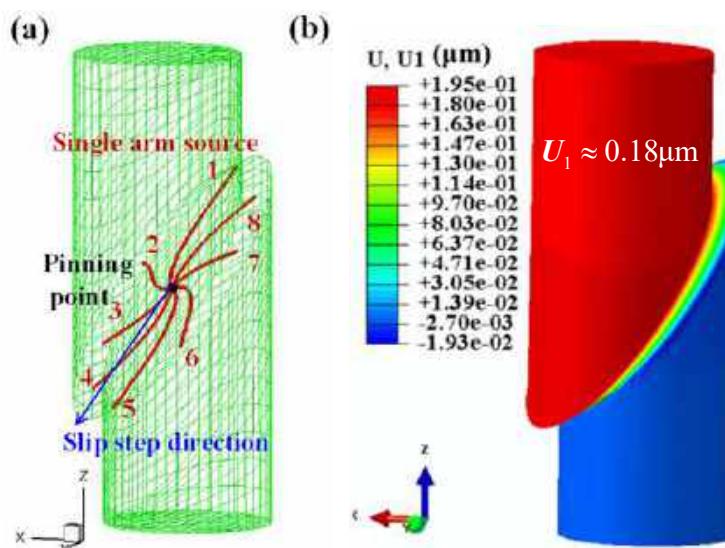


$$\hat{\mathbf{u}}^{(I)} = \hat{\mathbf{u}}_{\text{slip}}^{(I)} + \hat{\mathbf{u}}_{\text{DDD}}^{(I)}$$
$$\hat{\mathbf{u}}_{\text{DDD}}^{(I)} = \frac{\sum_{i=1}^n w_i \mathbf{u}_i}{\sum_{i=1}^n w_i}$$
$$w_i = 1 / d_{\text{seg-node}}^{(k)}$$

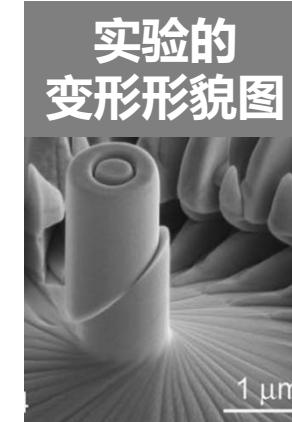
表面位错处理



位错源引起剪切带



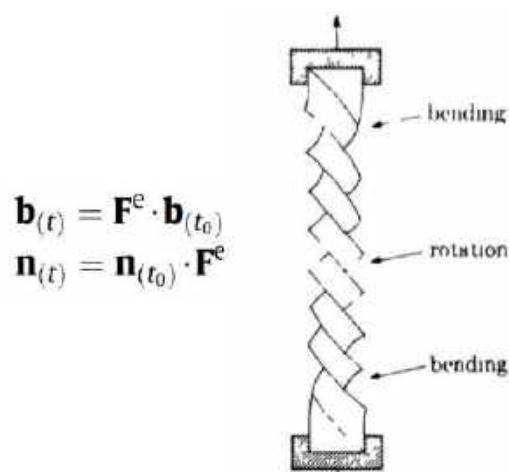
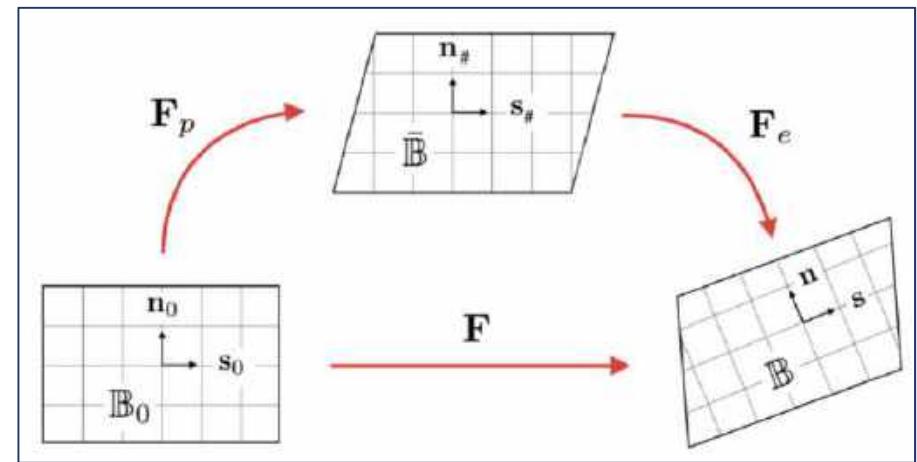
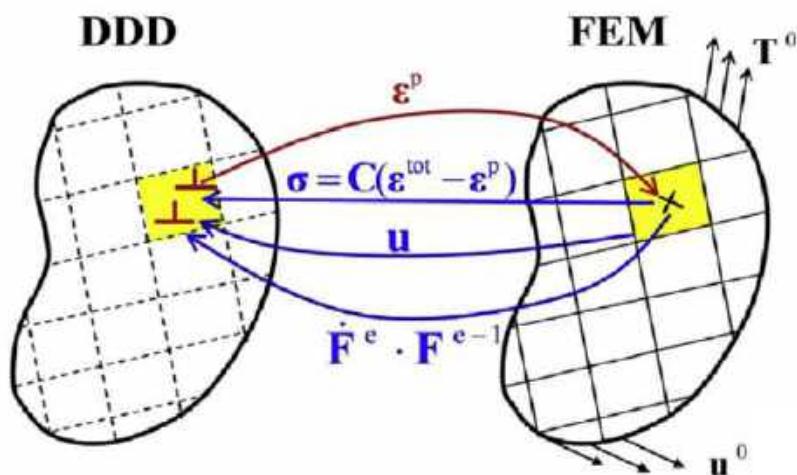
YN Cui et al., IJP, 2015



Dimiduk et al., 2005

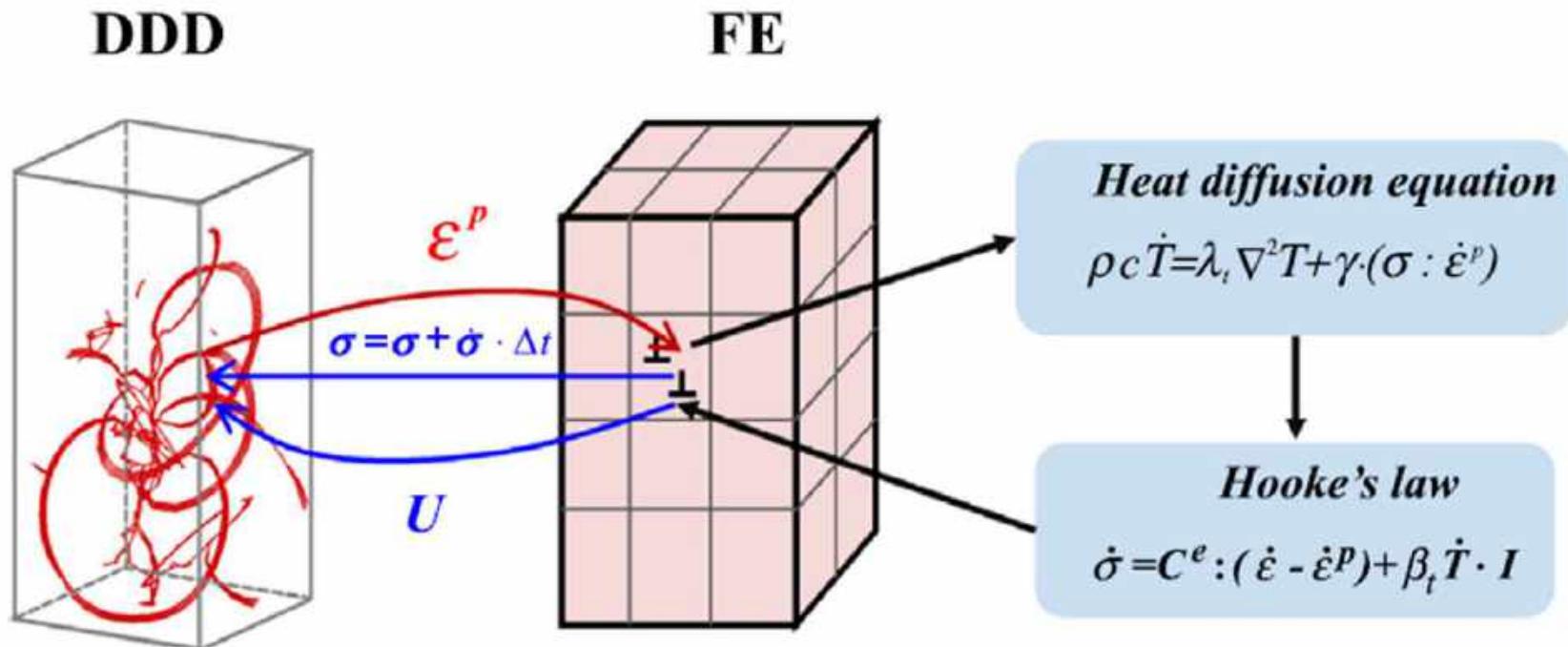
有限变形效应

晶格转动效应



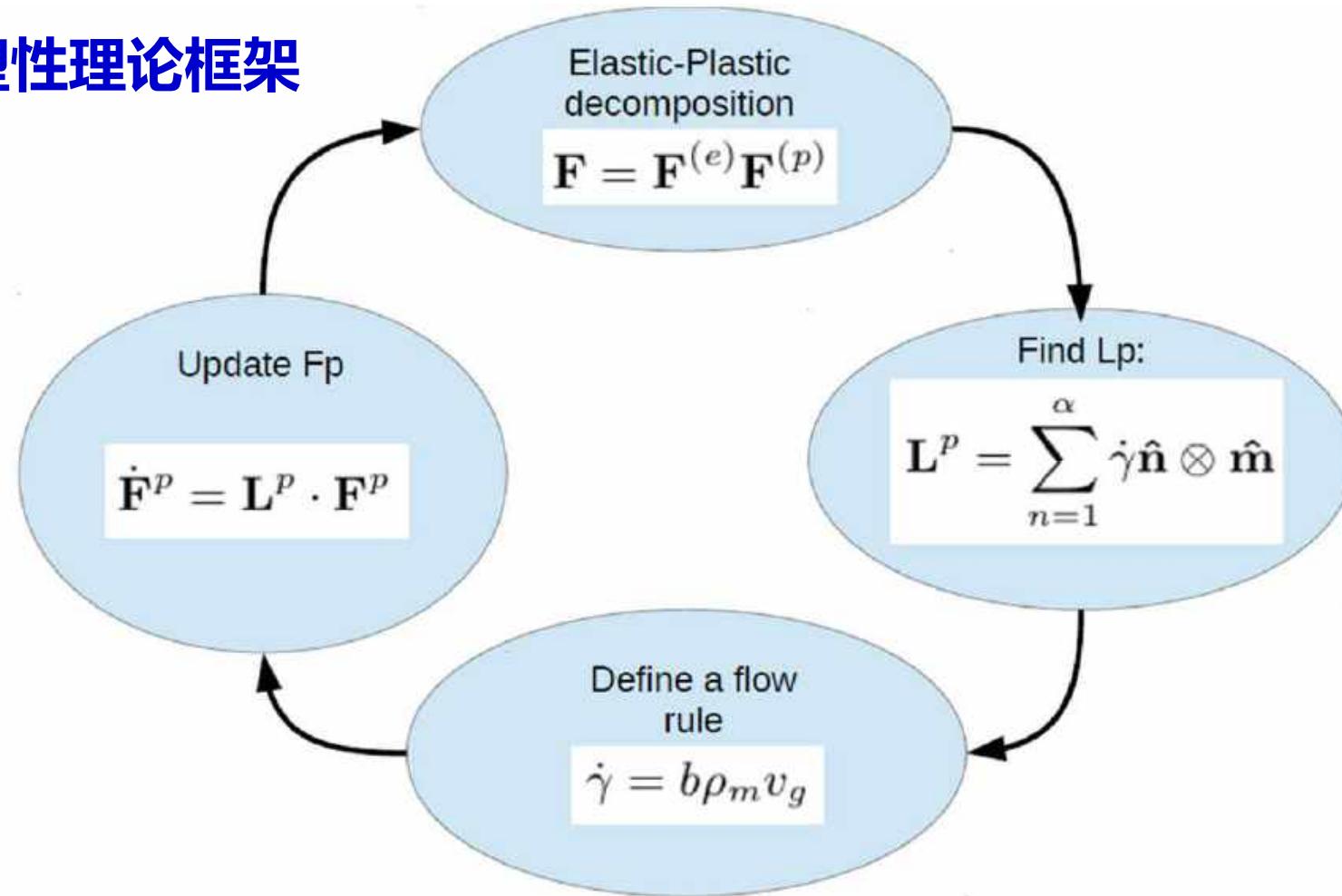
$$\begin{aligned} \mathbf{b}_{(t+\Delta t)} &= (\mathbf{I} + \dot{\mathbf{F}}^e \cdot \mathbf{F}^{e-1} \Delta t) \cdot \mathbf{b}_{(t)} \\ \mathbf{n}_{(t+\Delta t)} &= \mathbf{n}_{(t)} \cdot (\mathbf{I} - \dot{\mathbf{F}}^e \cdot \mathbf{F}^{e-1} \Delta t) \\ \dot{\mathbf{F}}^e \cdot \mathbf{F}^{e-1} &= \dot{\mathbf{F}} \cdot \mathbf{F}^{-1} - \mathbf{F} \cdot \mathbf{F}^{p-1} \cdot \dot{\mathbf{F}}^p \cdot \mathbf{F}^{-1}, \quad \dot{\mathbf{F}}^p = \mathbf{L}^p \cdot \mathbf{F}^p \\ \mathbf{F}^p_{(t+\Delta t)} &= \mathbf{F}^p_{(t)} + \dot{\mathbf{F}}^p_{(t)} \Delta t = (\mathbf{I} + \mathbf{L}^p \Delta t) \cdot \mathbf{F}^p_{(t)} \end{aligned}$$

温度效应



4.3 基于DDD的连续介质力学模型

晶体塑性理论框架



核心：确定塑性速度梯度 L^p



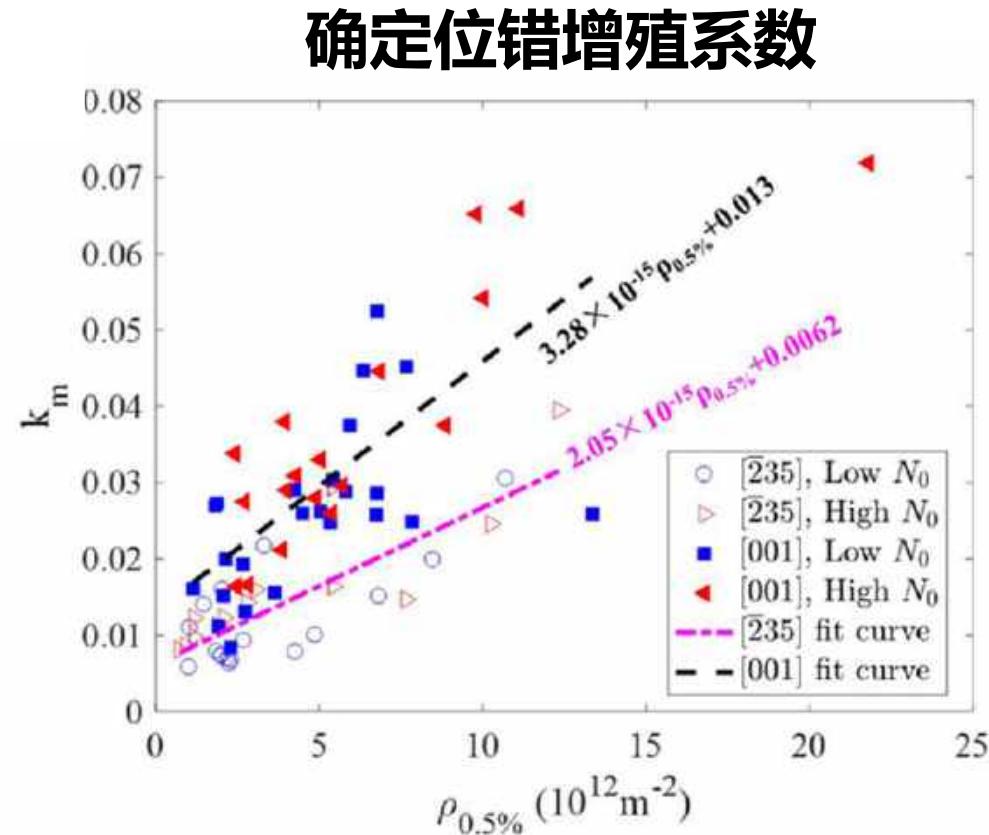
关键：确定位错密度演化
确定位错速度

4.3 基于DDD的连续介质力学模型

确定位错密度演化方程参数

$$\frac{d\rho}{d\gamma^p} = \frac{1}{bl_{fr}} - \frac{y_a\rho}{b},$$

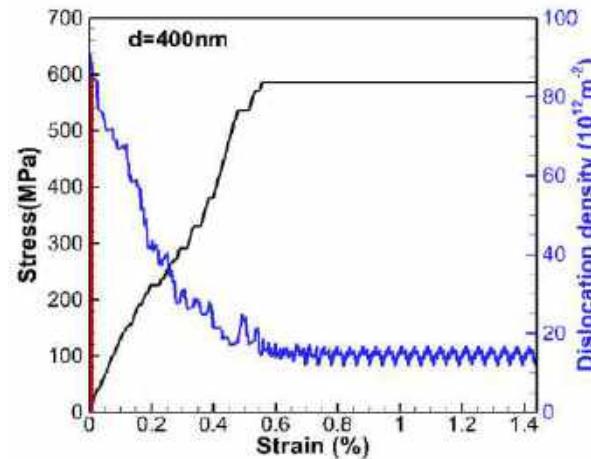
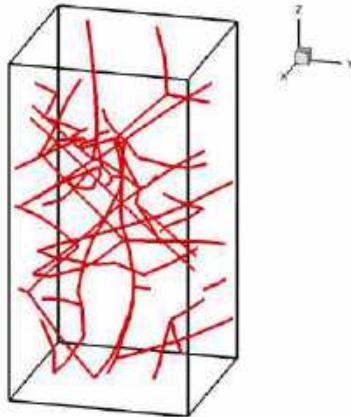
$$l_{fr} = \frac{1}{k_m \sqrt{\rho}}$$



YN Cui et al., Scripta Mater. 2018

4.3 基于DDD的连续介质力学模型

建立新的位错密度演化方程



块体材料

$$\frac{d\rho_{bulk}}{d\gamma} = \frac{1}{b\lambda_{FR}} - \frac{y}{b}\rho$$

表面湮灭

$$\frac{d\rho_{surf}}{d\gamma} = -\frac{2\cos^2(\beta/2)}{bd}$$

单臂源

$$\frac{d\rho_{SAS}}{d\gamma} = \frac{1}{2b\bar{\lambda}}$$

$$\frac{d\rho}{d\gamma} = \frac{1}{2b\bar{\lambda}} - \frac{2\cos^2(\beta/2)}{bd} + \frac{k_f\sqrt{\rho}}{b} - \frac{y}{b}\rho$$

小尺寸起主导作用

4.3 基于DDD的连续介质力学模型

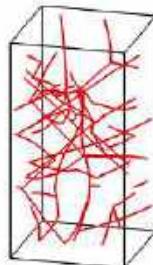
确定位错速度



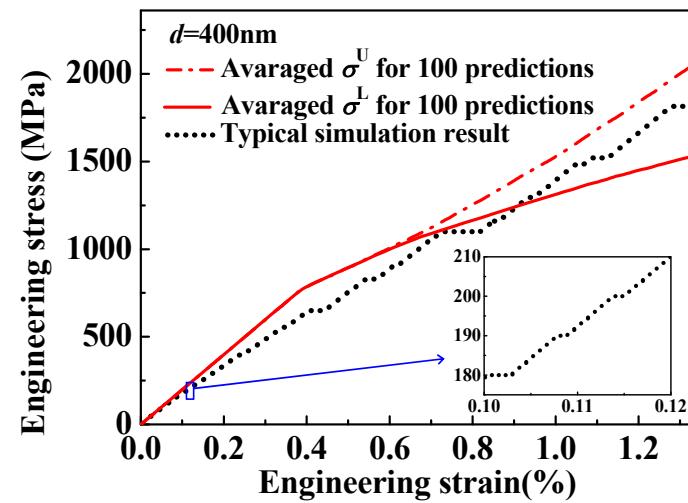
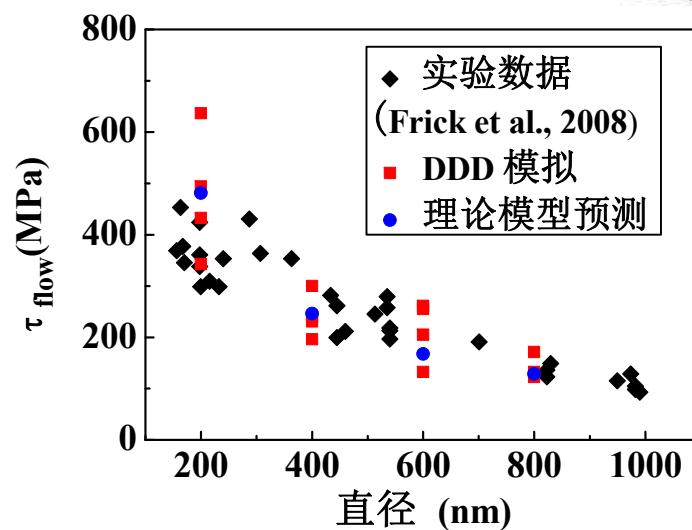
$$v = f (\tau_{app} - \tau)$$

确定位错运动阻力方程

$$\tau = \tau_0 + \alpha \mu b \sqrt{\rho} + \frac{k \mu b}{\lambda}$$



$$\tau = \tau_0 + \alpha \mu b \sqrt{\rho_{mobile}} + \frac{k_s \mu}{\lambda / b} + \alpha' \cdot \mu b d \rho_{trapped}$$

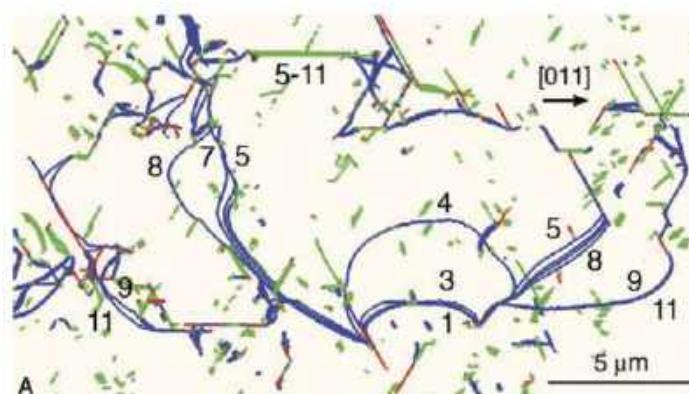


4.3 基于DDD的连续介质力学模型

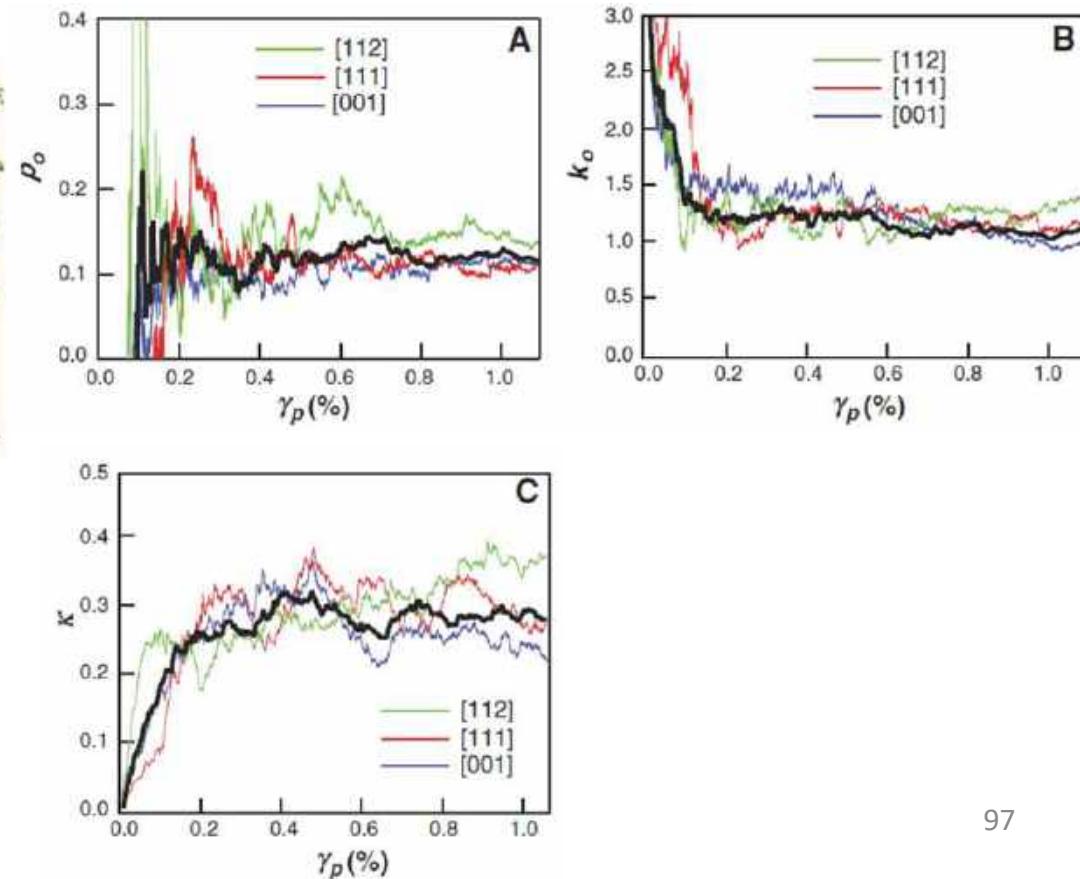
Taylor硬化模型

$$\frac{1}{L^i} = \frac{\tau_c^i}{\mu b K_{hkl}}, \text{ with}$$

$$\tau_c^i = \mu b \sqrt{\sum_j a_{ij} \rho^j}$$



$$K_{hkl} = \left[\frac{n(1 + \kappa)^{3/2}}{p_0 k_0 \sqrt{a}(n - 1 - \kappa)} \right]$$



Devincre et al. Science, 2006

5 应用举例

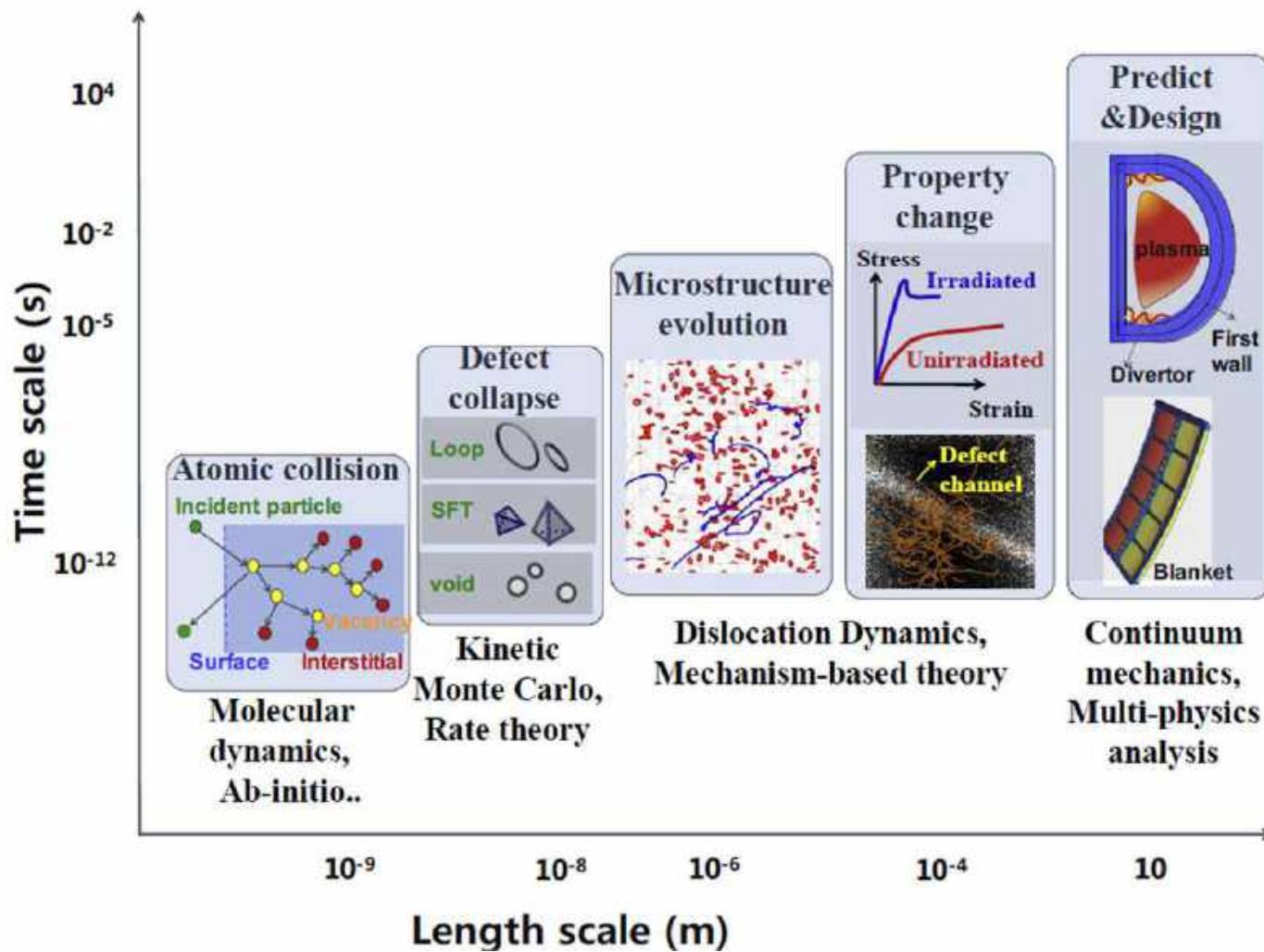
5.1 强辐照损伤力学计算方法建立

5.2 强辐照损伤力学问题研究

5.1 强辐照损伤力学计算方法建立



5.1 强辐照损伤力学计算方法建立

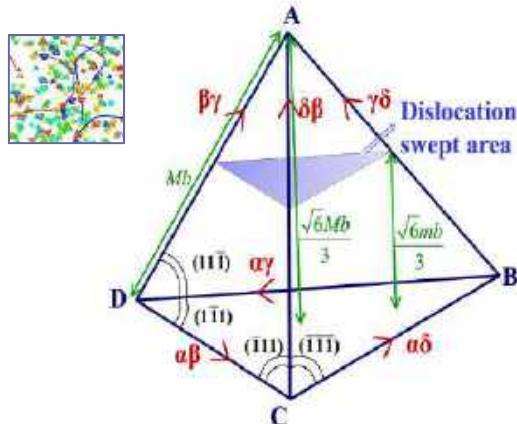


5.1 强辐照损伤力学计算方法建立

(1) 全离散计算

FCC: SFTs (low stacking fault energy)

Silcox-Hirsch mechanism



Atomistic-informed failure mechanism

$\frac{m}{M}$ {
 ≤0.5, probability p_1 to be cut by m/M
 >0.5, probability p_2 to be restored;
 $(1-p_1-p_2)$ probability to be sheared by b ;
 If $M < M_c$, SFT is destroyed.

Y. N. Osetsky et al., Philos. Mag. 2006

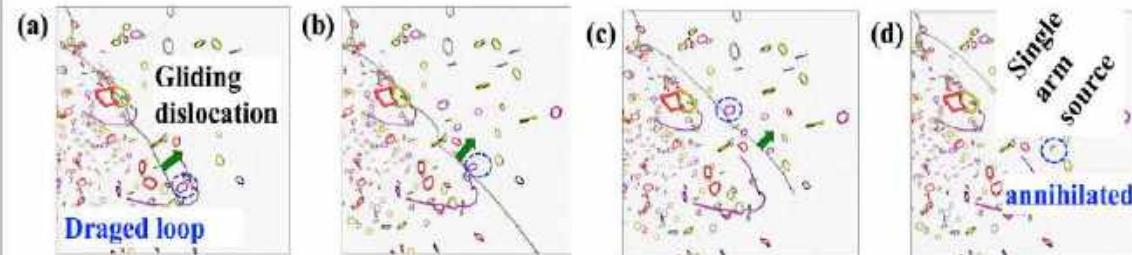


BCC: Interstitial loops

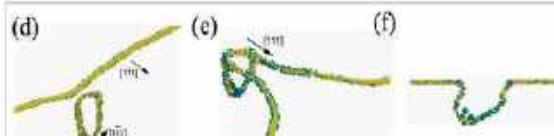
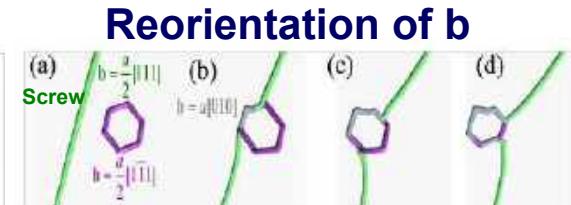
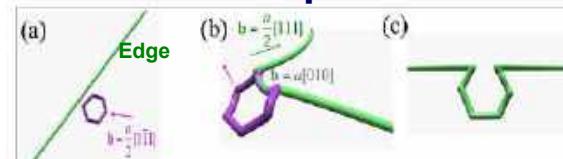


Directly and naturally described by DDD

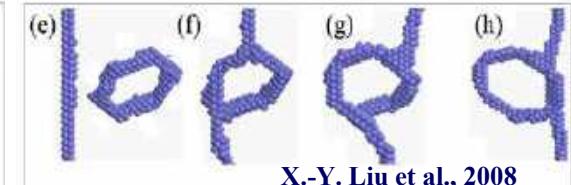
> Elastic drag: b_{loop} belongs to dislocation slip plane



> Junction formation
Absorption

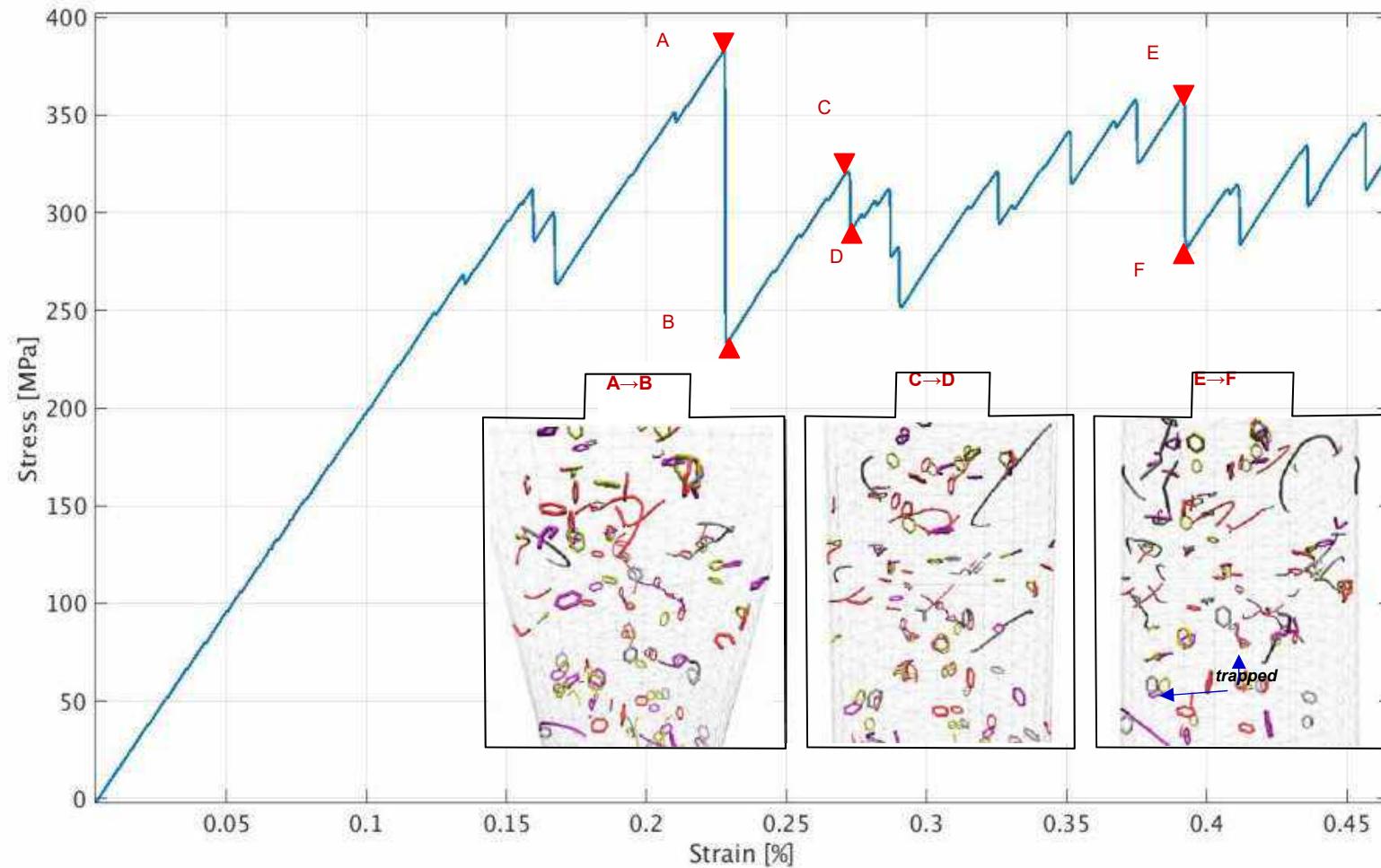


D. J. Bacon et al., 2006



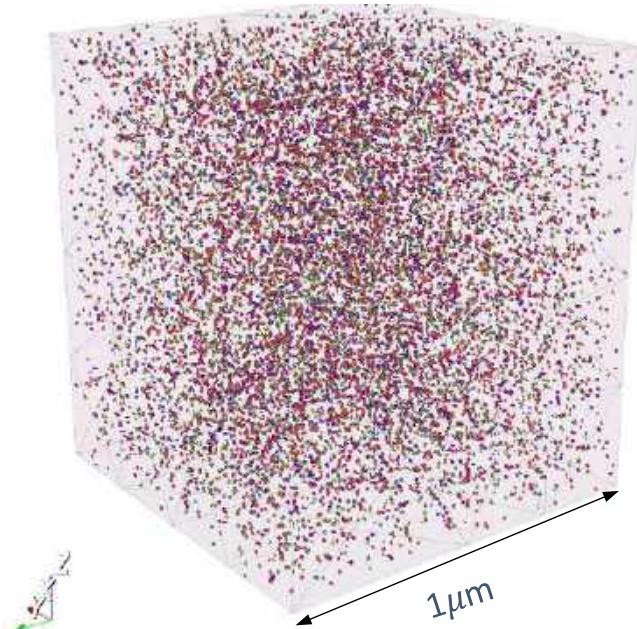
X.-Y. Liu et al., 2008

5.1 强辐照损伤力学计算方法建立

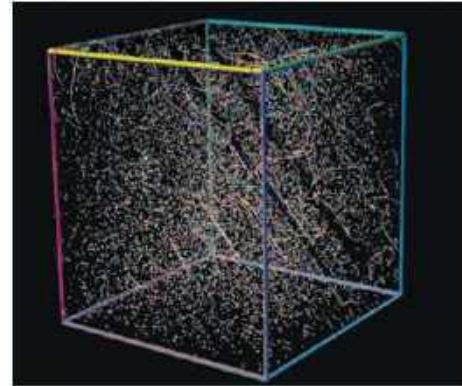


5.1 强辐照损伤力学计算方法建立

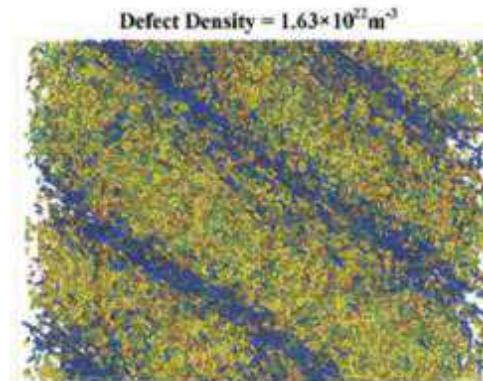
High irradiation defect density
 $10^{21} \sim 10^{23} \text{ m}^{-3}$



$10^{22} \text{ m}^{-3}, N=10^5$



TD de la Rubia et al. nature, 2000



A. Arsenlis et al. Acta Mater. 60, 2012

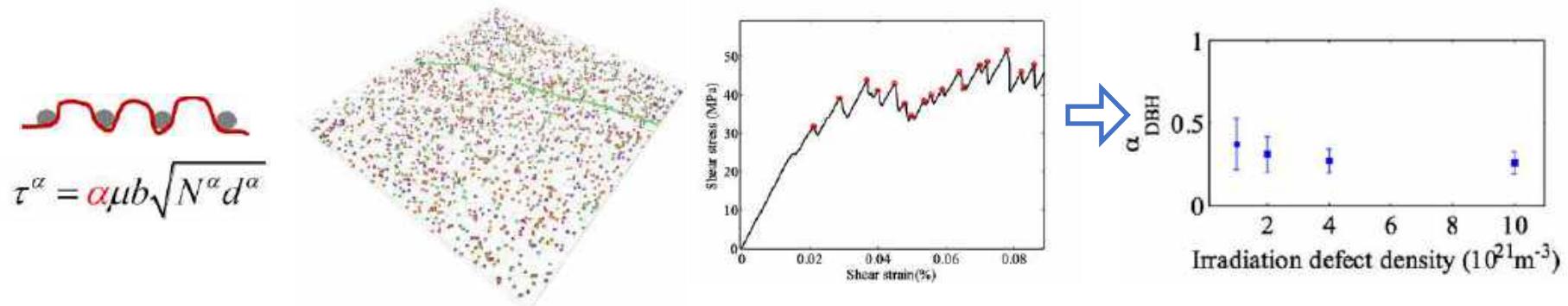
Very expansive calculation!

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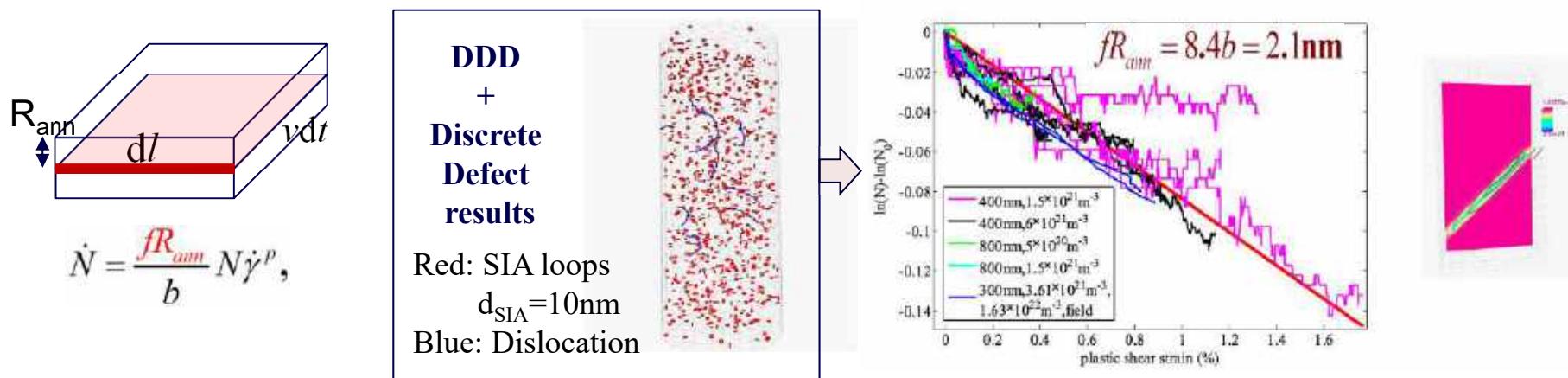
5.1 强辐照损伤力学计算方法建立

(2) 连续化理论

- Resistance stress induced by defects:

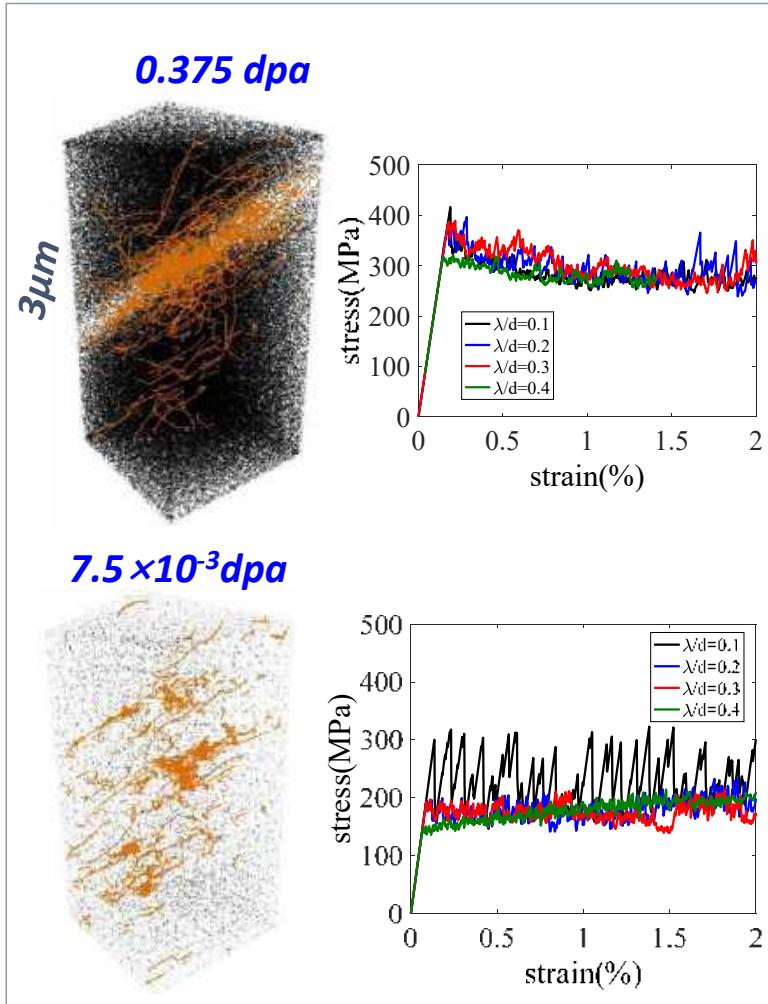


- Irradiation defect kinetics equation:

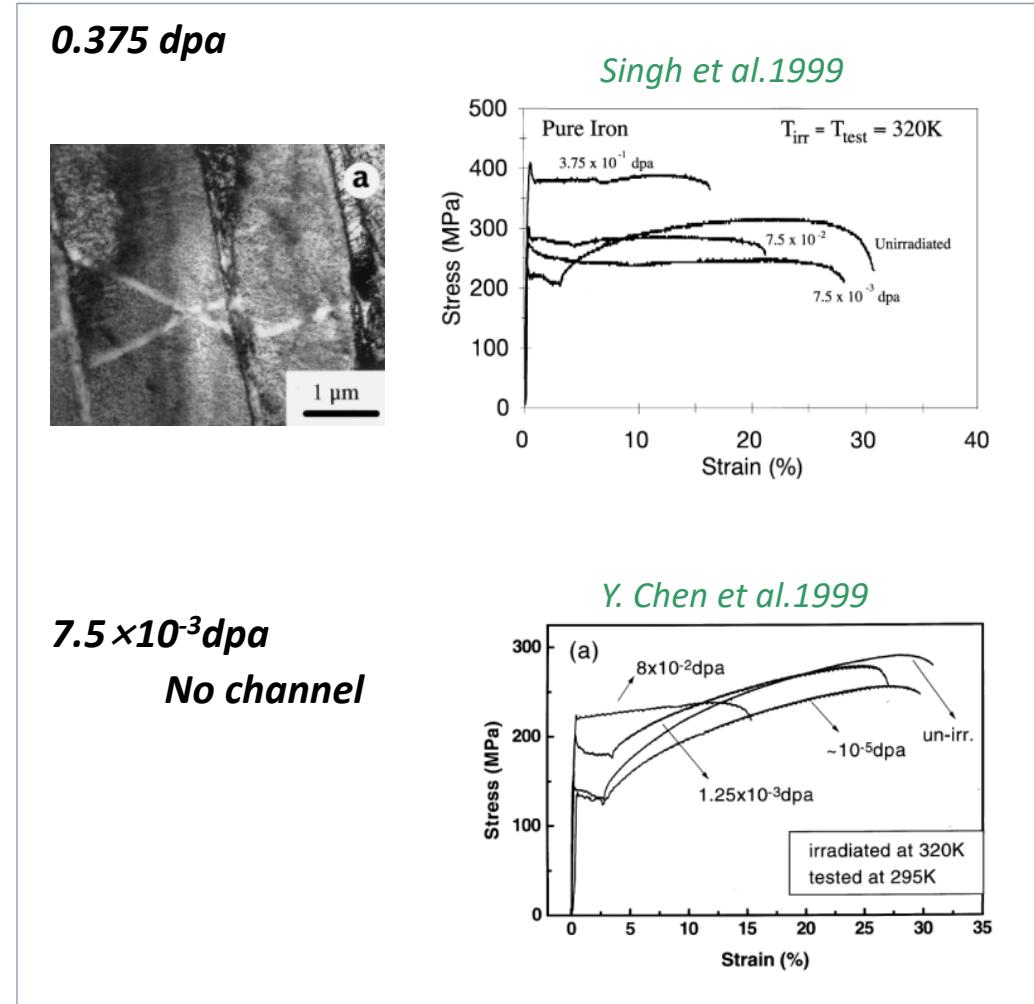


5.1 强辐照损伤力学计算方法建立

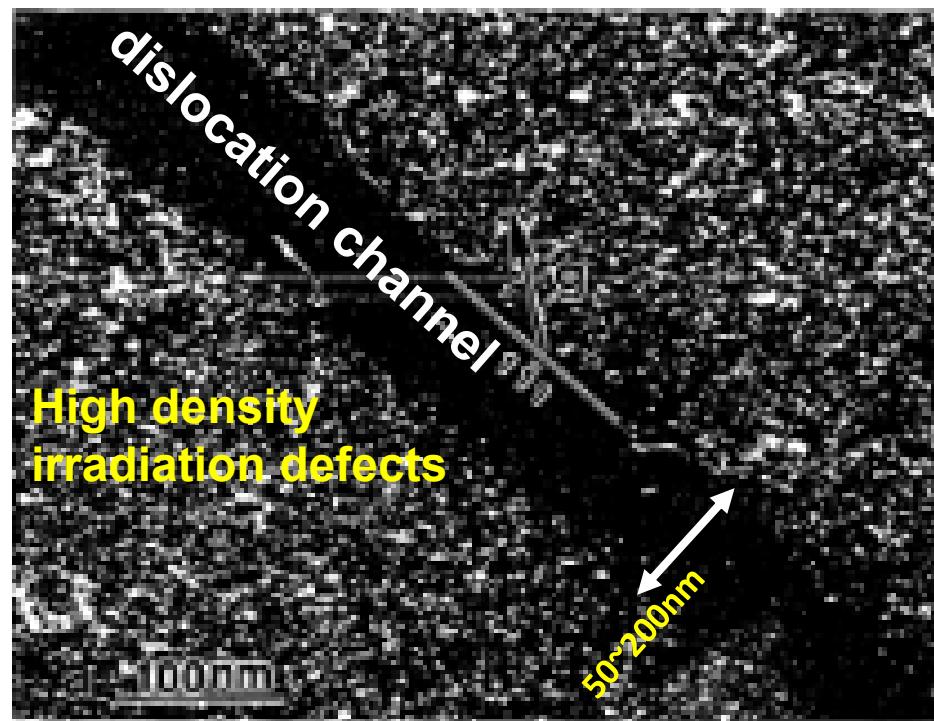
Simulations



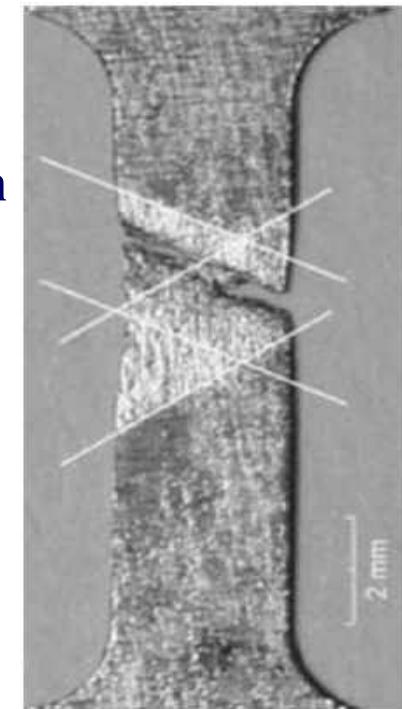
Experiments



5.2 塑性失稳诱发辐照脆化



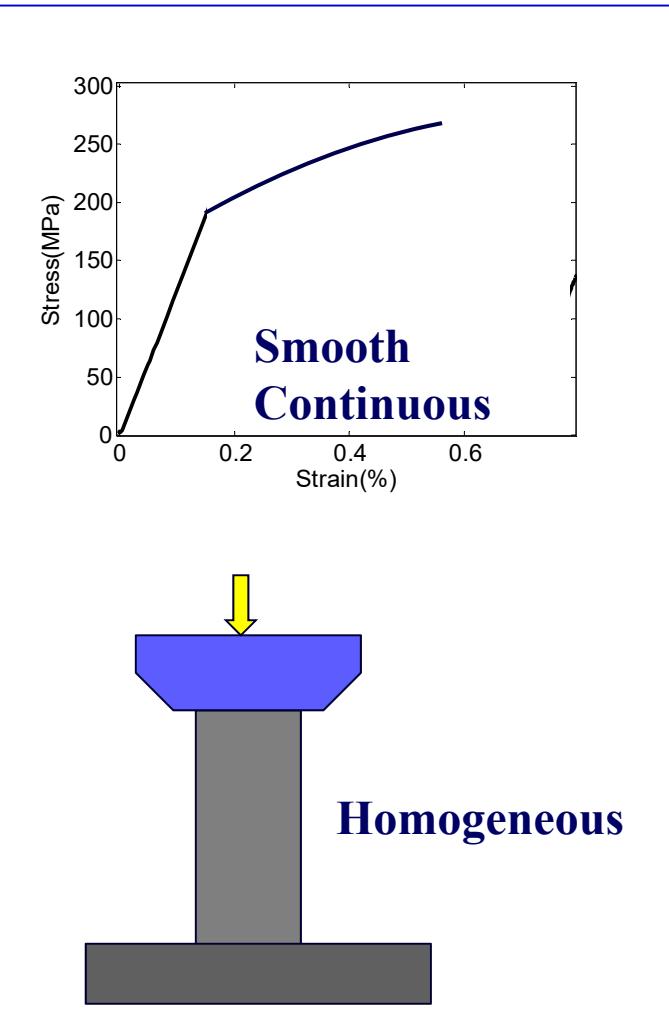
Promote
crack initiation



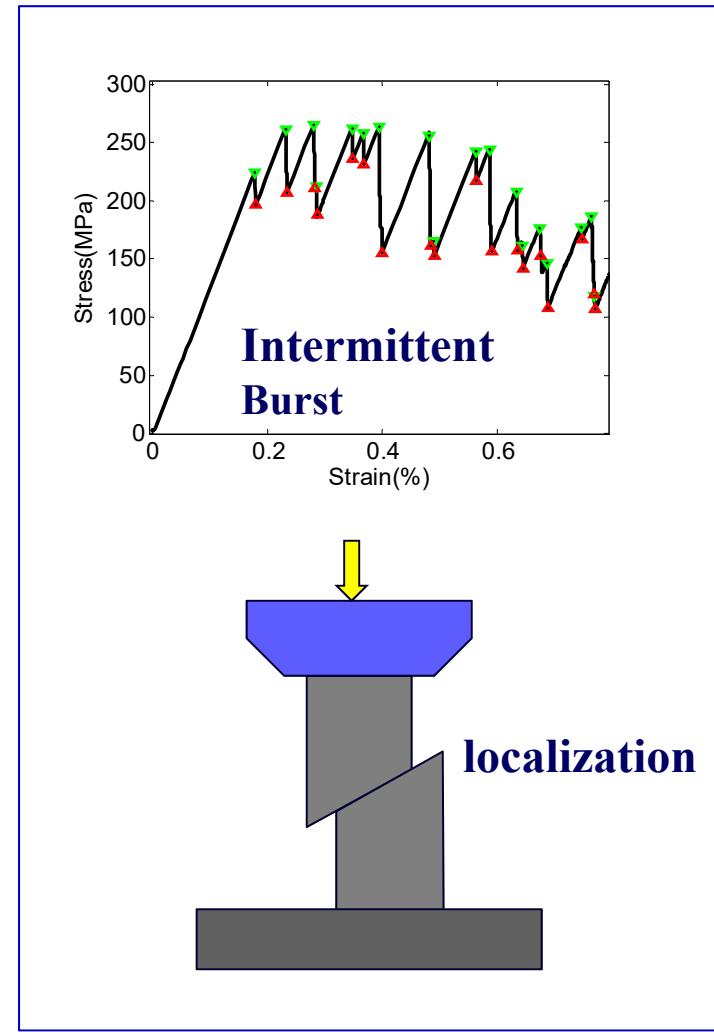
J. of ASTM Int. 2008

5.2 什么是塑性失稳

We hope

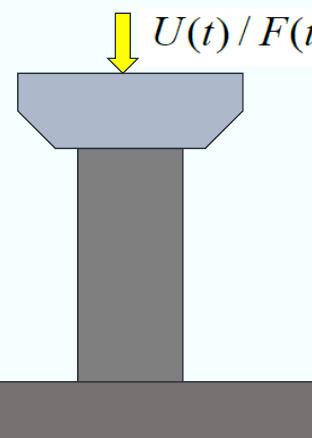
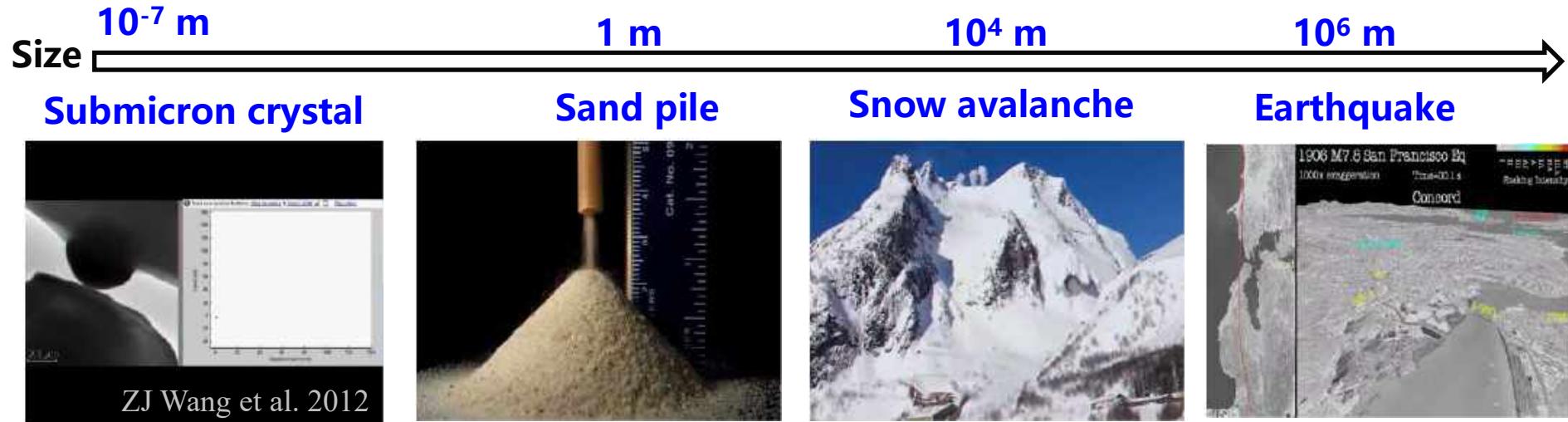


We get

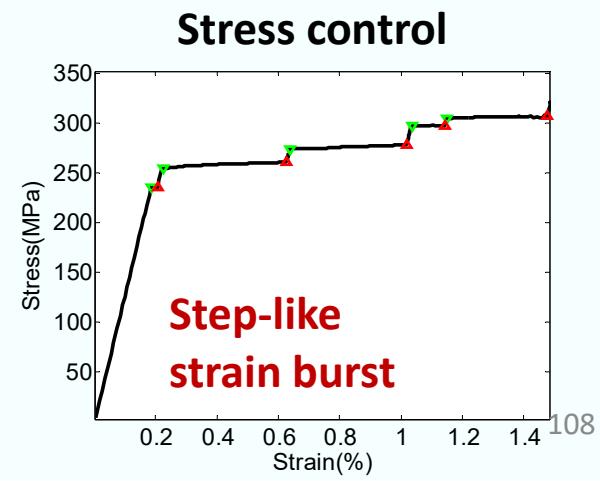
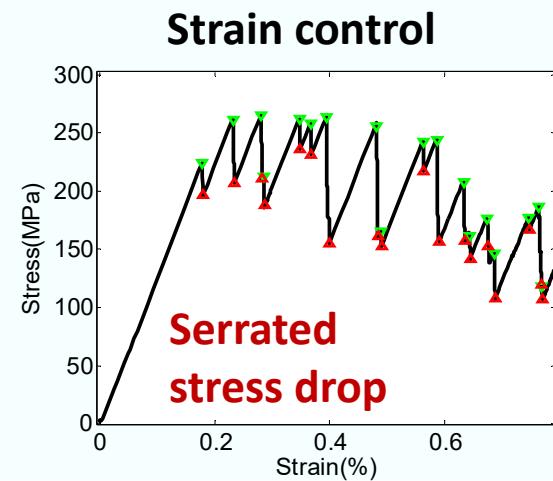


塑性失稳——时间尺度

Temporal plastic instability → nanoquake/Avalanche

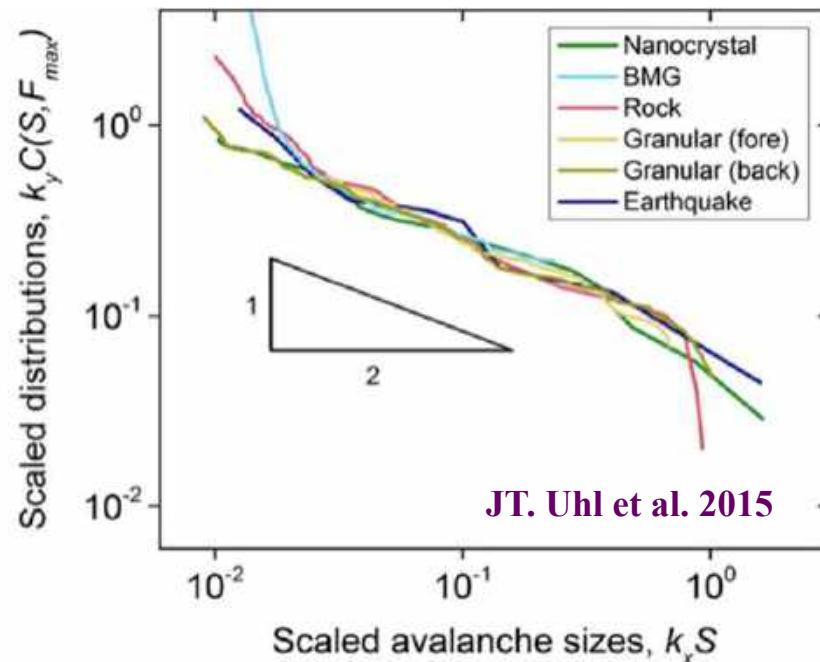


Tsinghua university

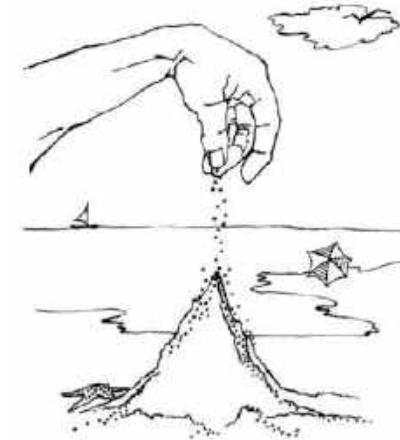


塑性失稳——时间尺度

Universal Quake Statistics



Self-organized criticality



However,
whether SOC tell the whole story?

Some discussions are given in
YN Cui et al. PRL, 2016, 117, 155502

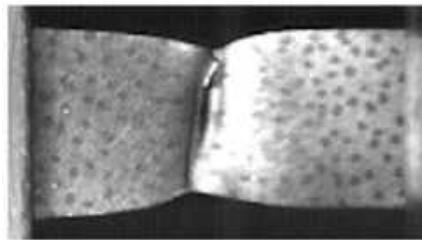
Tsinghua university

Nature is operated by a “blind watchmaker”, so that dynamical system evolves naturally toward a critical state, without fine tuning parameters, with no intrinsic length/time scale.

Bak, Per, et al.1988

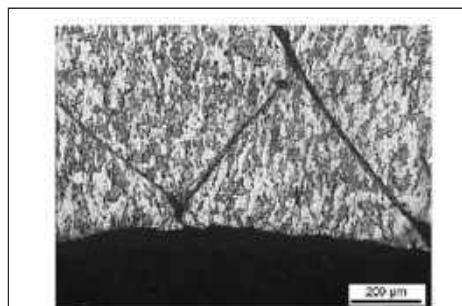
塑性失稳——空间尺度

Necking



S.A. Krishnan et al.
Procedia Engineering 2004

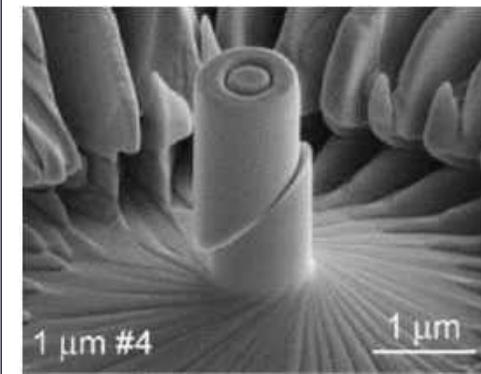
Adiabatic shear bands



Y Yang et al., 2008

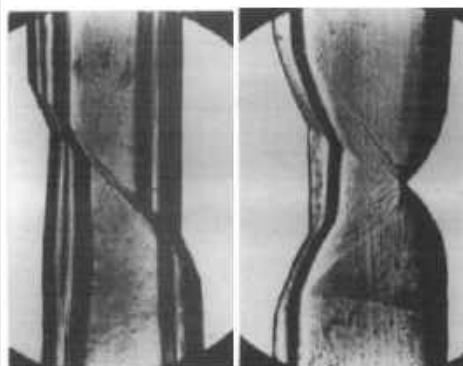
Shear localization

Small size Ni
Size effect



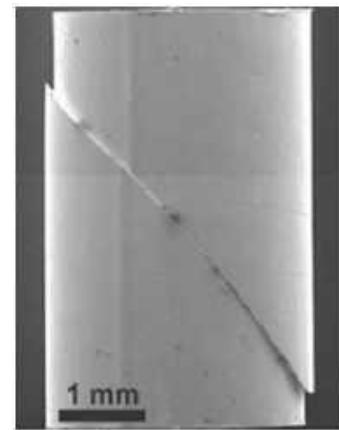
Precipitate
hardening material

coherent carbides Semicohesive carbides

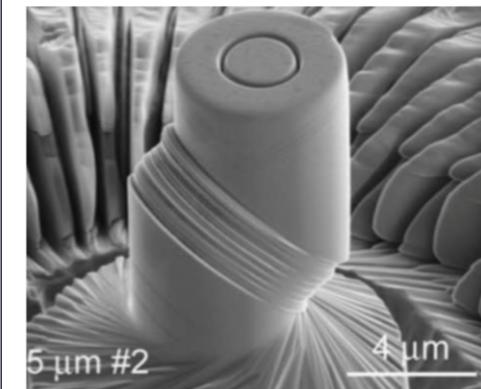


Luft, 1991

Metal glass

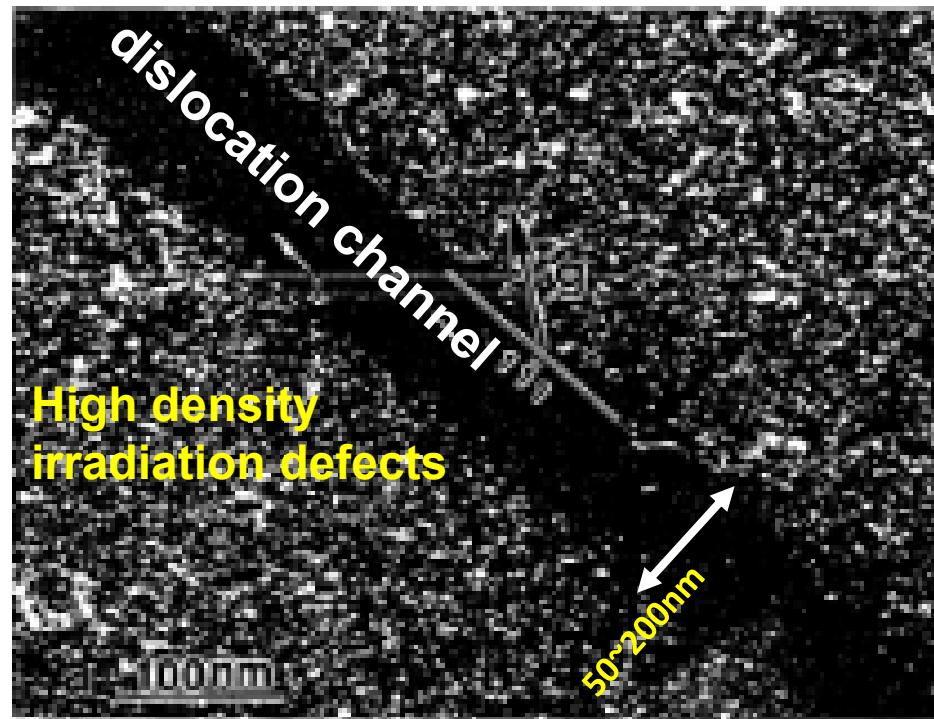


R. Maaß et al., 2015

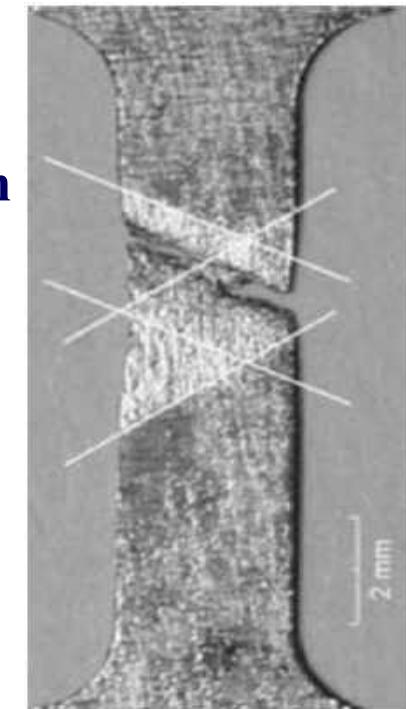


Dimiduk M, Acta Mater. 2005

5.2 塑性失稳诱发辐照脆化



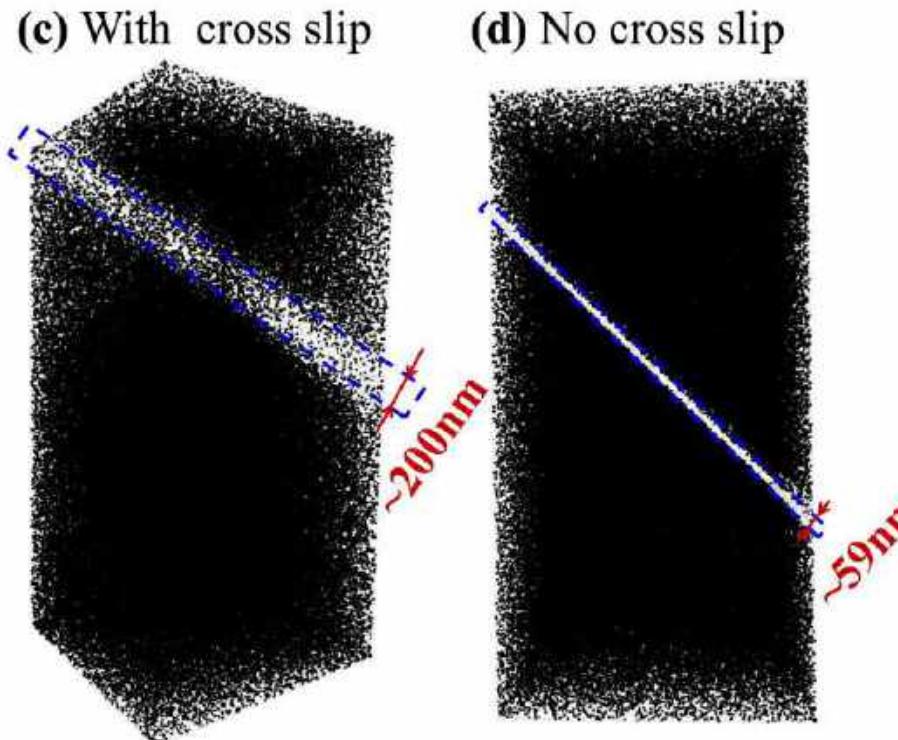
Promote
crack initiation



J. of ASTM Int. 2008

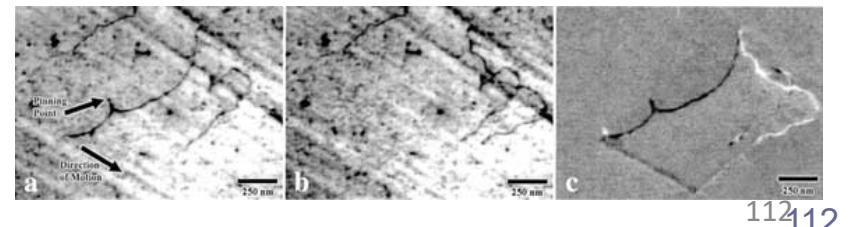
5.2 强辐照损伤力学问题研究

Cross slip widening effect!



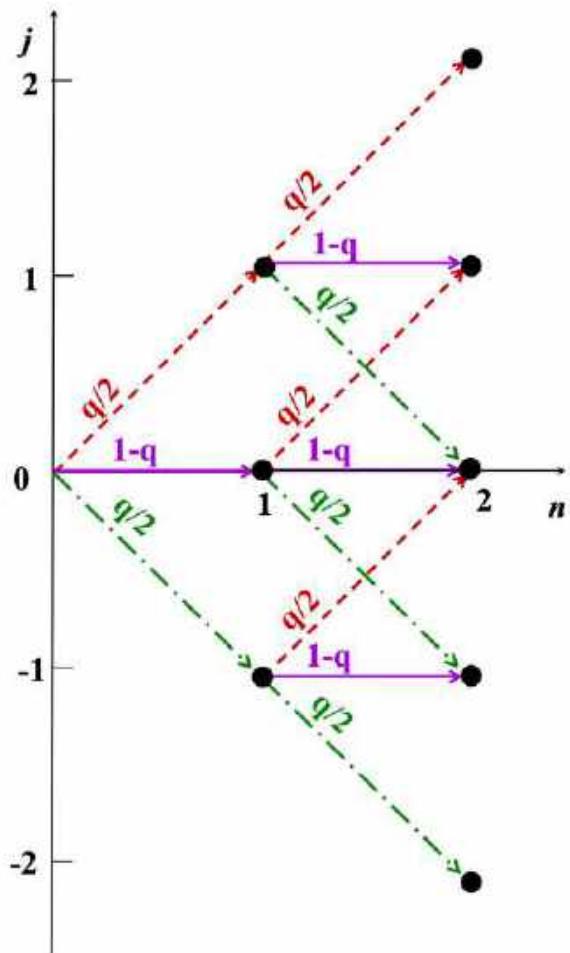
Experimental evidence of cross slip induced widening in bulk sample

J. S. Robach et al. Philos. Mag., 2003



5.2 强辐照损伤力学问题研究

局部化带宽化模型



n is related to sample size
 j is related to channel size
 q is double cross slip possibility

n_+ : upward event number
 n_0 : straight event number
 n_- : downward event number
 $n_+ + n_0 + n_- = n$
 $(+1)^*n_+ + 0^*n_0 + j^*n_- = j$

$$P(n, j, q) = \sum_{\substack{n_+ + n_0 + n_- = n \\ n_+ - n_- = j}} \frac{n!}{n_+! n_0! n_-!} \left(\frac{q}{2}\right)^{n_+} (1-q)^{n_0} \left(\frac{q}{2}\right)^{n_-}$$
$$= \sum_{n_- = \max(-j, 0)}^{n_- \leq (n-j)/2} \frac{n!}{n_-! (j+n_-)! (n-j-2n_-)!} \left(\frac{q}{2}\right)^{j+2n_-} (1-q)^{n-j-2n_-}$$

Cumulative trinomial distribution

YN Cui et al., PRL, 2018

5.2 强辐照损伤力学问题研究

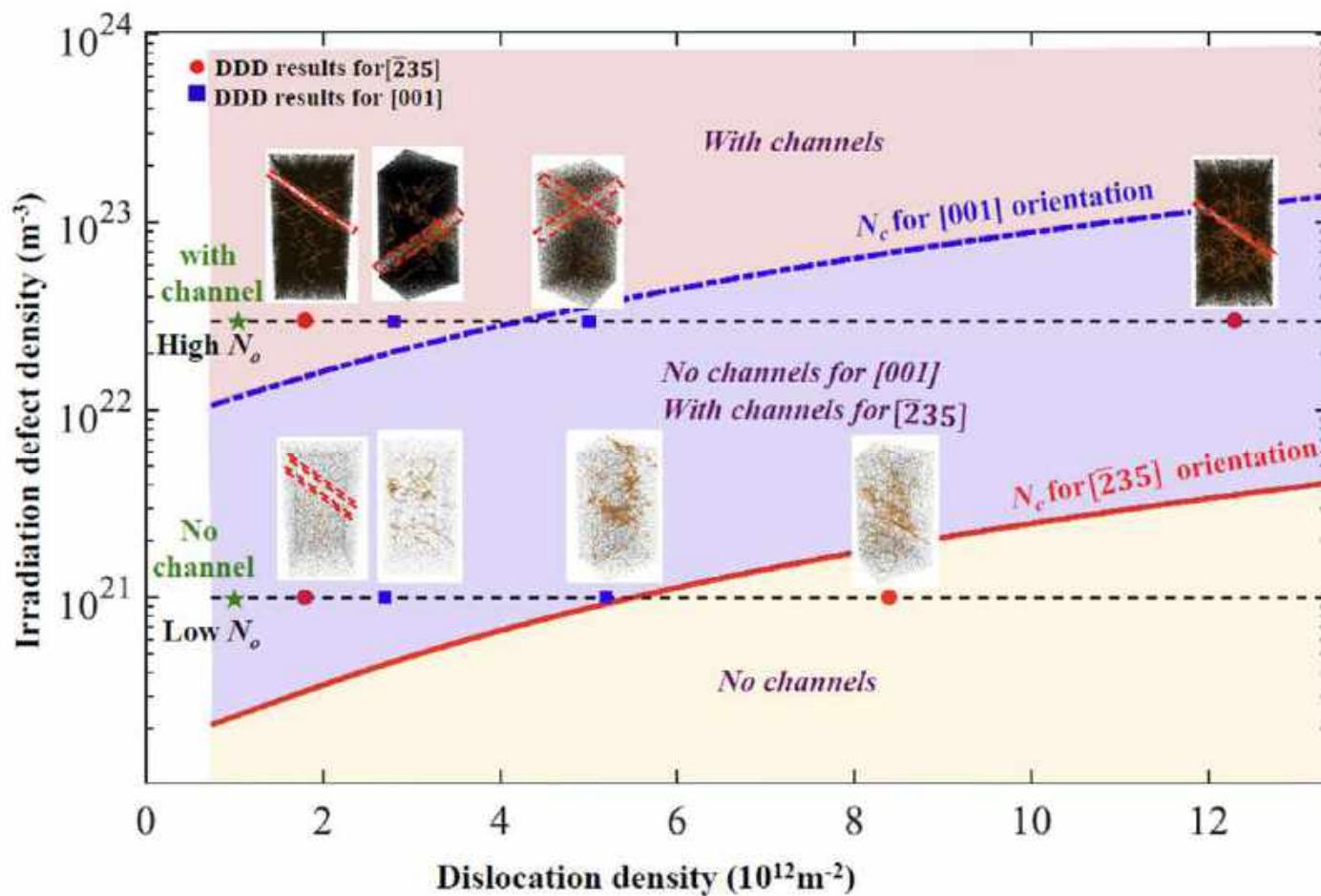
无辐照缺陷通道宽度预测

实验 预测

Case ID	Material	Reported channel width (nm)	Predicted channel width (nm)	Predicted channel width (nm) [81]	Irradiation dose (dpa)	Irradiation defect type	Defect mean size (nm)	Defect density (10^{23} m^{-3})	Grain size (μm)	Reference
1	V	15-85	22-29	18	0.012	DL	1.8	1.1	5-10	[82, 83]
2		25-105	27-36	27	0.12	DL	2.1	1.9	5-10	
3		80-105	30-36	29	0.69	DL	2.1	2.3	5-10	
4	V-4Cr-4Ti	~ 50	66	49	0.5	DL	3.7	1.0	16	[84]
5	Cu	100-250	55	70	0.1	SFT	2.4	4.5	30	[85, 86]
6	Cu-Cr-Zr	50-200	58	77	0.1	SFT	2.5	5.0	30	[85]
7	Mo	60-160	77	61	0.28	DL	3.36	0.2	70	[87]
8	Fe	100-200	105	76	0.79	DL	5	0.6	33	[88]
9	A533B	40	30	25	0.81	DL	1.3	0.65	60	[89]
10	316SS	5-15	38	41	0.17	DL	1.6	1.0	67	[89]
11		10-30	38	77	0.78	DL	1.8	4.0	67	[89]
12	Zr-4	40-75	36	10	0.1	DL	1.8	4.0	13	[89]

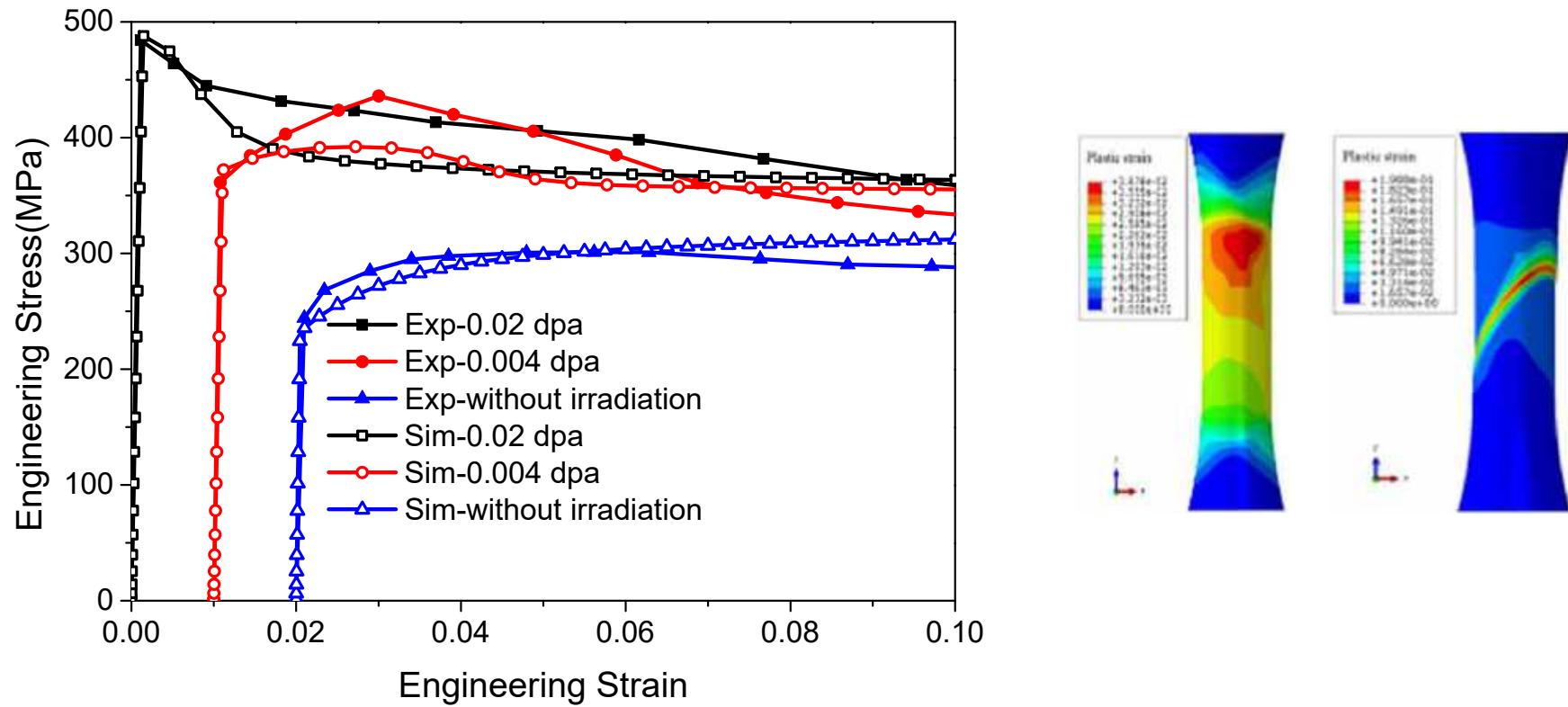
5.2 强辐照损伤力学问题研究

塑性失稳时空演化理论模型



5.2 强辐照损伤力学问题研究

(4) 晶体塑性理论



Unpublished

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6 DDD开源代码介绍

- **Lattice-based** : dislocation lines were discretized into screw and edge segments
(Kubin *et al.*, 1992)
- **Tridis (NuMoDis)**, updated edge-screw simulation, Parallelized, superposition principle
Verdier *et al.* (1998), Shin (2006). Fivel (2012)
<http://www.numodis.fr/tridis/>
- **microMegas**, Periodic boundary conditions + DCM
Devincre, 2012b ; Madec *et al.*, 2004 ;
Lemarchand *et al.*, 2001; Vattré *et al.*, 2012 ; Monnet *et al.*, 2004 ;
http://zig.onera.fr/mm_home_page/
- **MDDP (Multiscale Dislocation Dynamics Plasticity) micro3D**
DD+FEM by superposition principle → shock loading
Yasin *et al.*, 2001 ; Zbib *et al.*, 1998; Rhee *et al.*, 1998
<https://icme.hpc.msstate.edu/mediawiki/index.php/MDDP>
- **PARANOID** (PARAnoid NOdal IBM Dislocation code) Schwarz (1999)
semi-conducting and metallic materials
not currently open to the public

6 DDD开源代码介绍

Modelib--PDD (Parametric Dislocation Dynamics) parametrized cubic splines

Ghoniem *et al.*, 2000; Giacomo Po. 2014 ; Wang *et al* 2006; Han 2003;...

<https://github.com/giacomo-po/MoDELib>

ParaDis (Parallel Dislocation Simulator)

Bulatov and Cai (2006); Arsenlis *et al.* (2007) ; Tang *et al.*, 2006

<http://paradis.stanford.edu/site/about>

<https://ipo.llnl.gov/technologies/paradis>

DDLab : a much simplified version of *ParaDis* able to treat
elementary configurations of moving and interacting dislocations

<http://www.ddlab.com>

6 DDlab入门

A. Arsenlis, Lawrence Livermore National Laboratory (arsenlis1@llnl.gov)
W. Cai, Stanford University (caiwei@stanford.edu)

Target:

1 理解输入输出

2 位错构型演化及力学信息提取

小结

DDD

多微结构

多物理场

多尺度效应

塑性力学+断裂力学+损伤力学+极端环境力学.....

Thank you!

Hope this takes you to a fantastic dislocation world

Yinan Cui (cyn@tsinghua.edu.cn)