合金材料の結晶粒界と強度特性

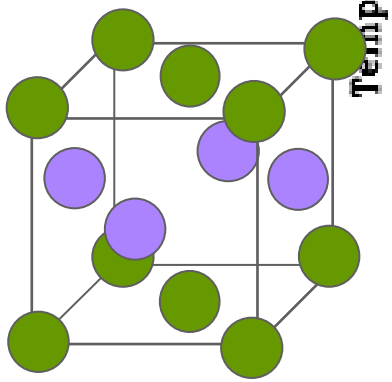
北海道大学 大学院工学研究院

材料科学部門　材料数理学研究室

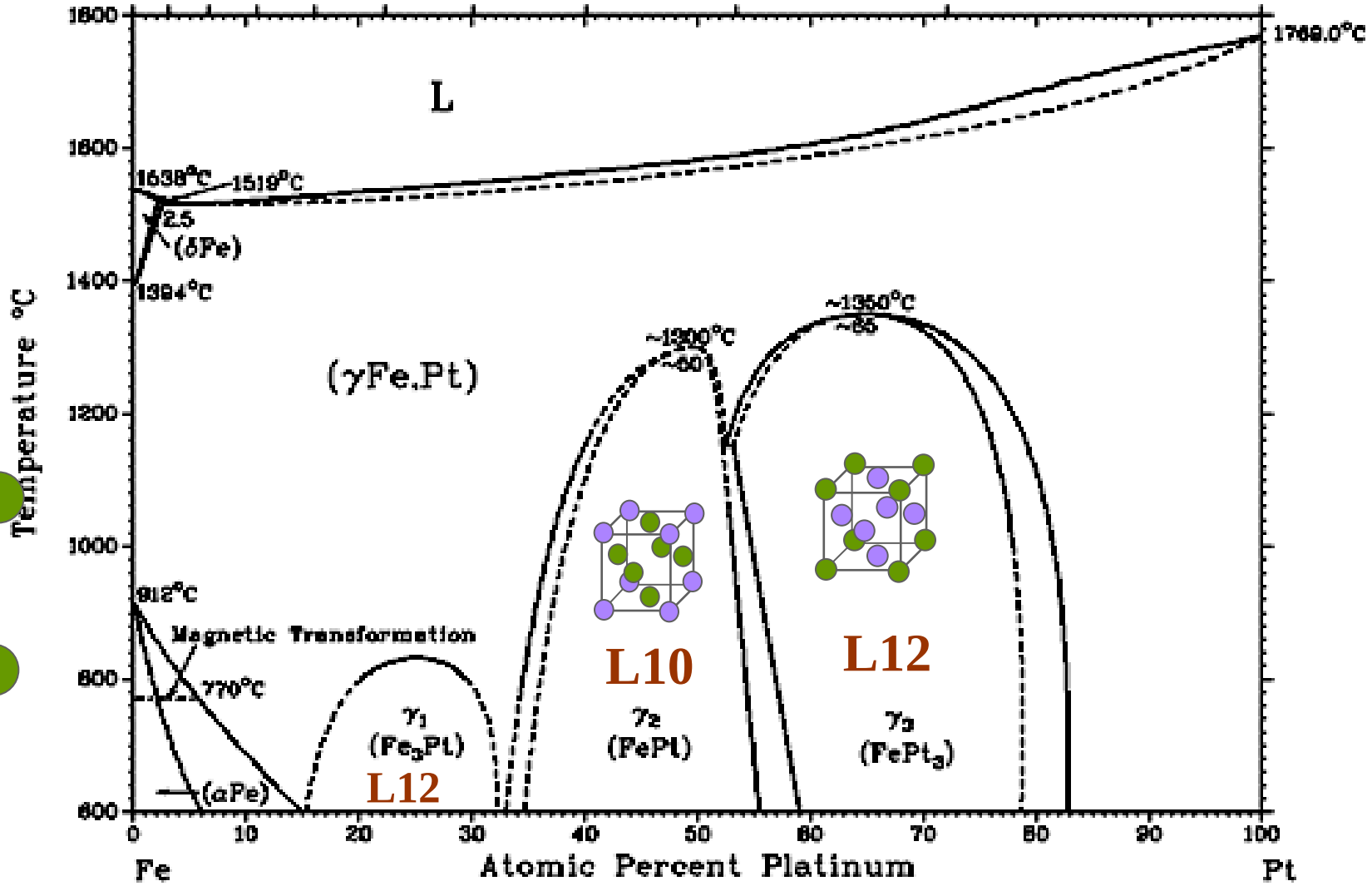
毛 利哲雄

Background Phase Diagram

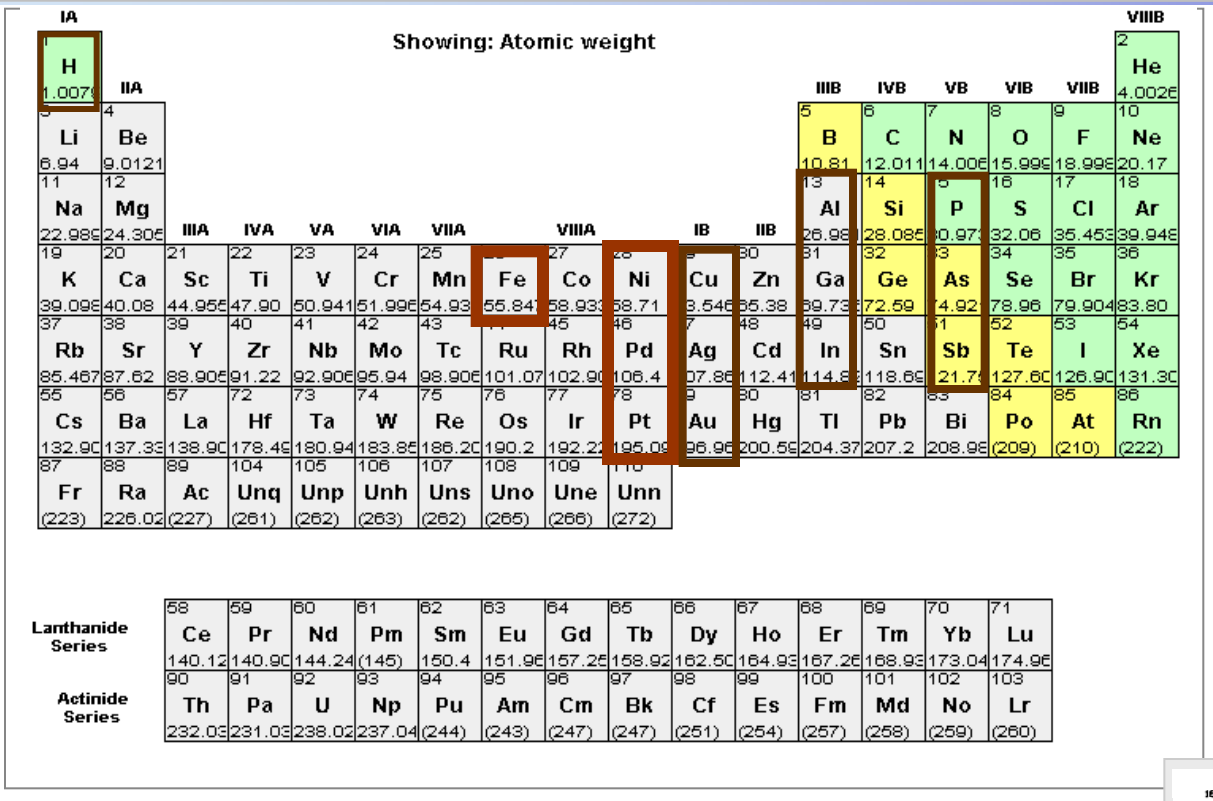
Fe-Pt

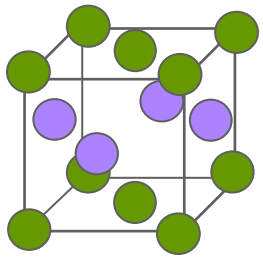


L10



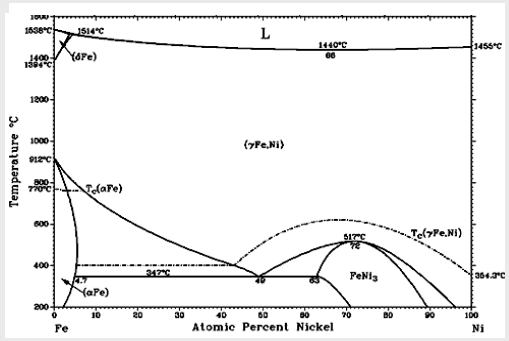
Background



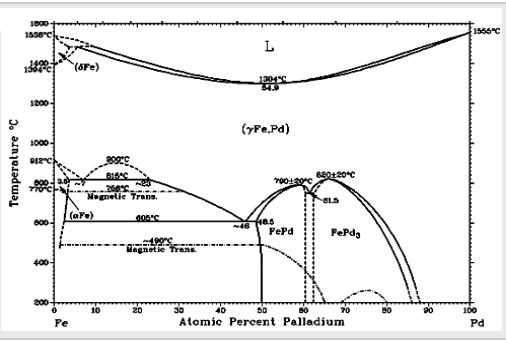


Mechanical property

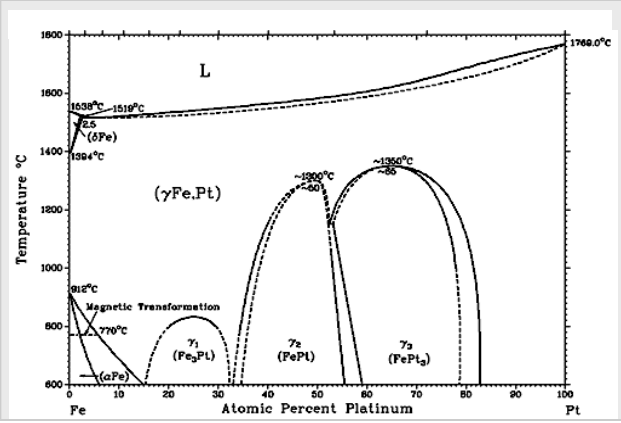
High density magnetic recording media



Fe-Ni



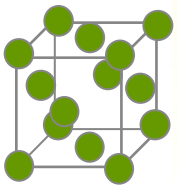
Fe-Pd

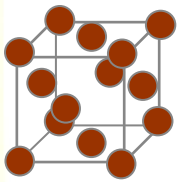


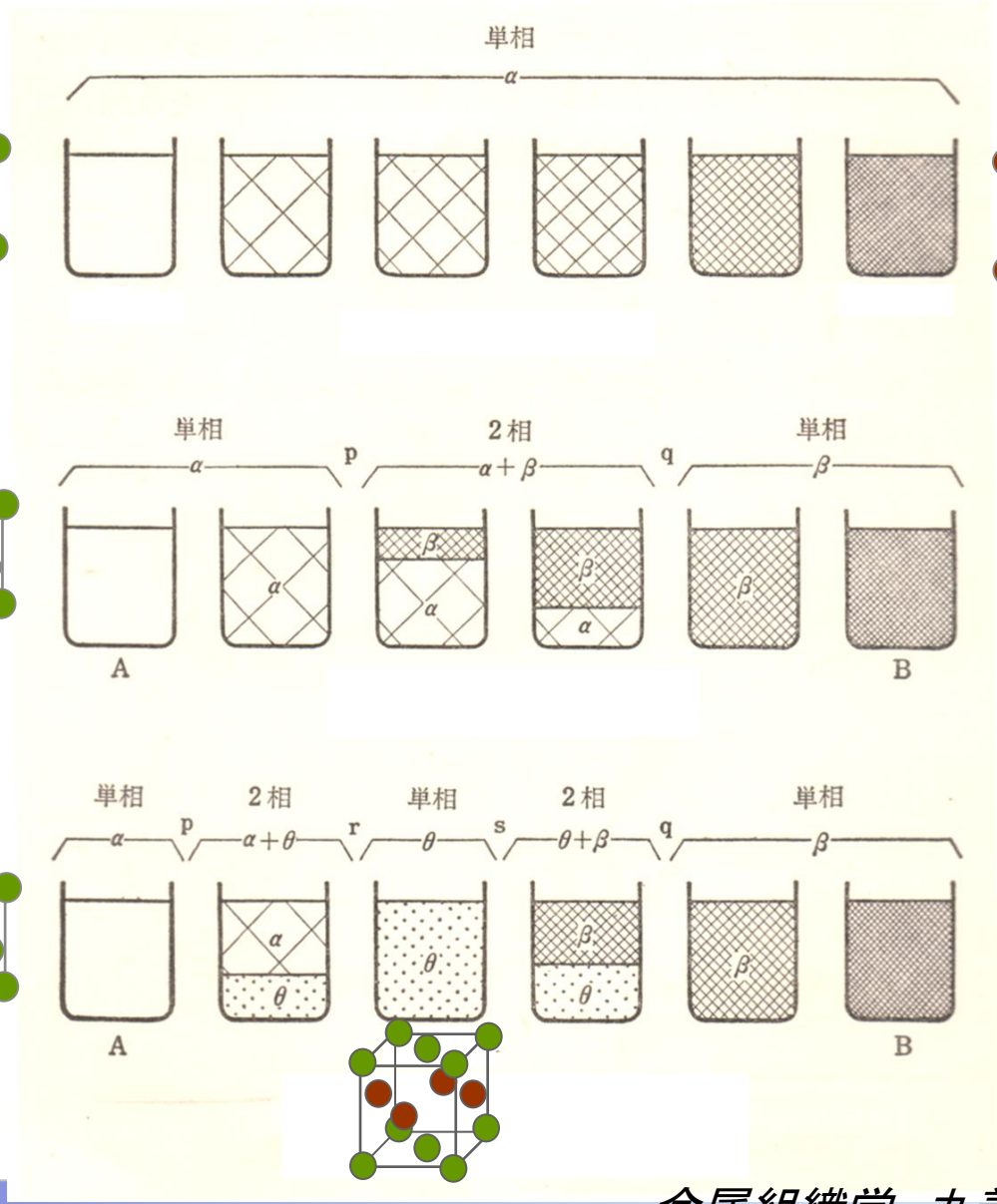
Fe-Pt

Basic concept

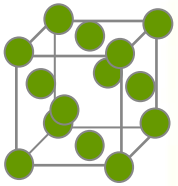
固溶体
Solid Solution

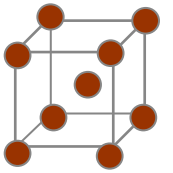






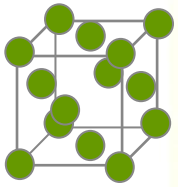
相分離
Phase separation

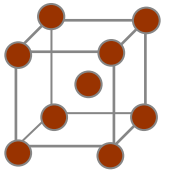




固溶限　Solubility limit

中間相
Intermediate phase

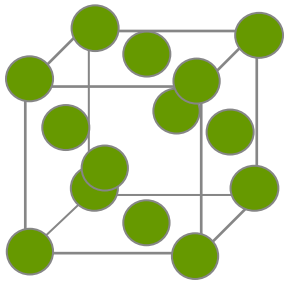


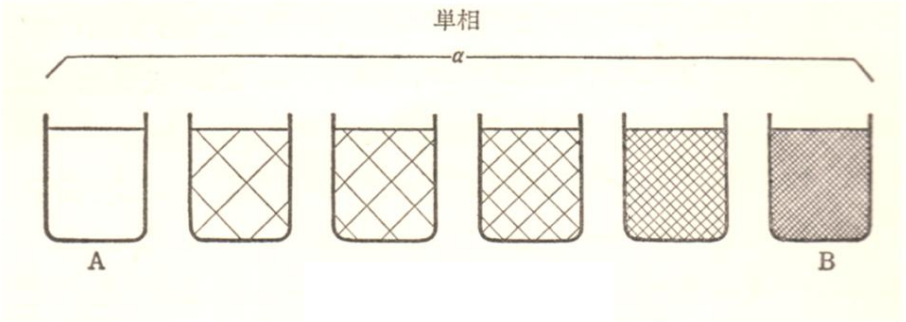


Ordered phase　規則相

金属組織学　丸善 (1972)

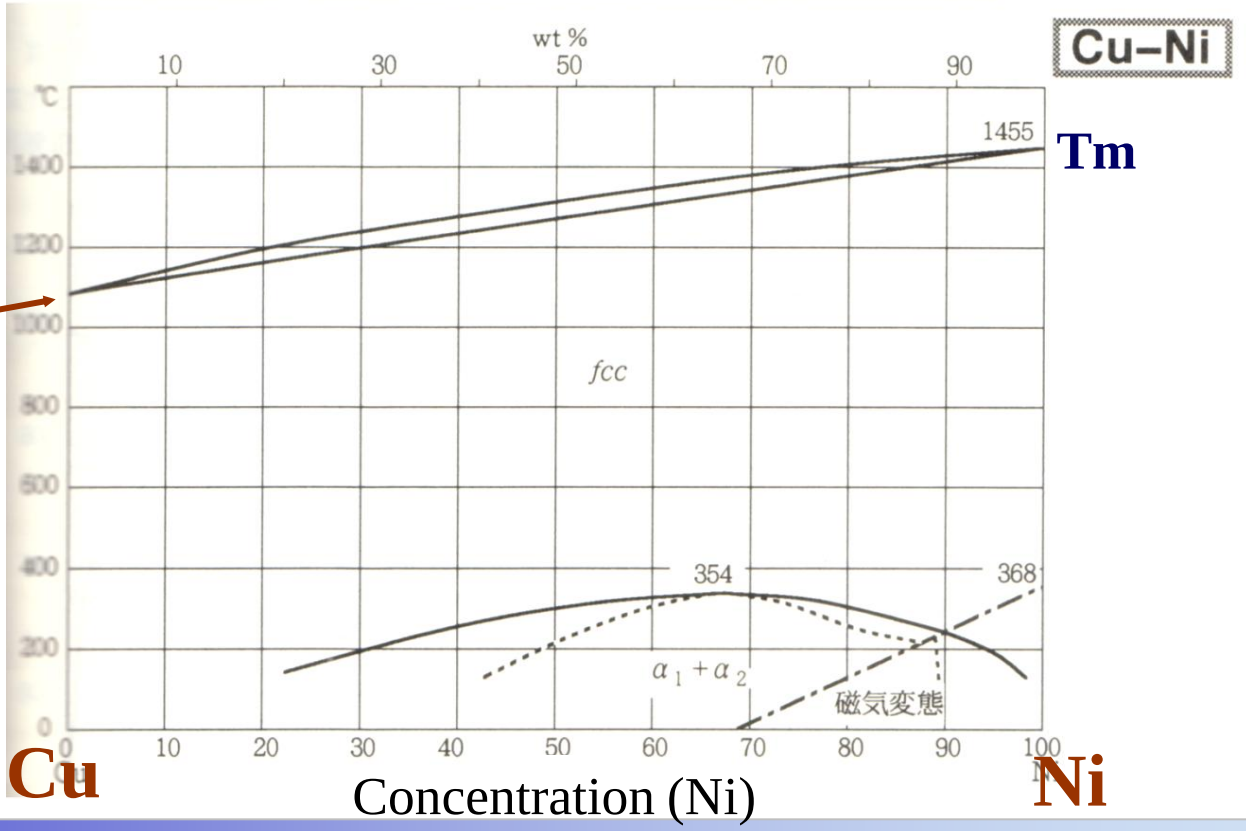
solid solution type alloy　固溶体型合金





Phase Diagram

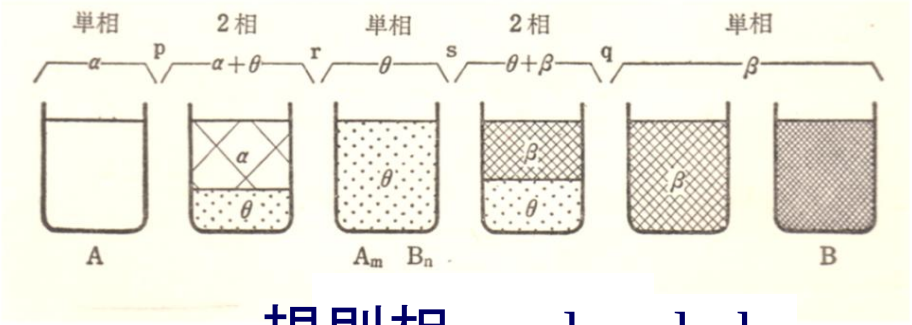
融点
melting point



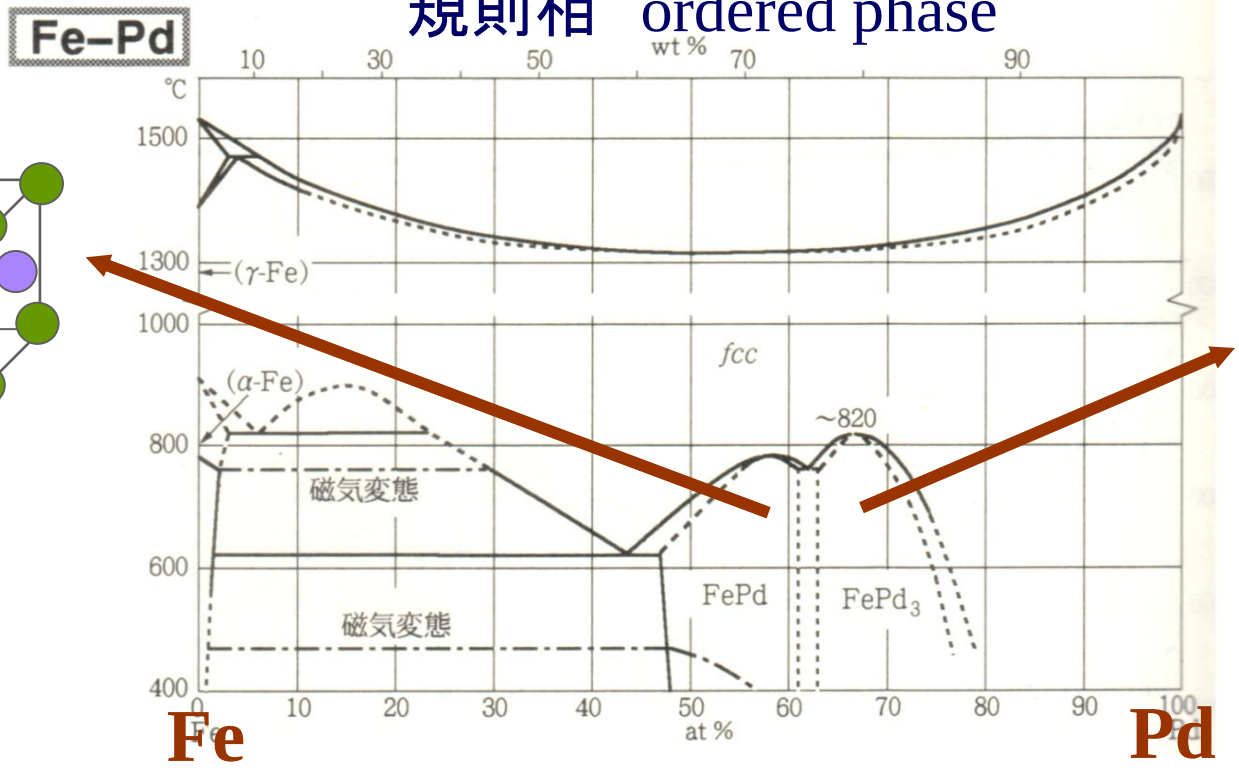
intermediate phase　中間相型

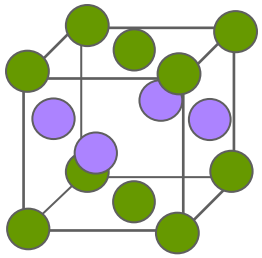
強度･靭性の付与

機能の付与

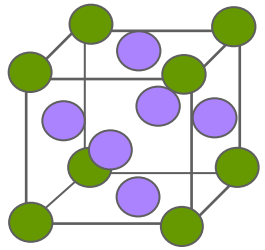


規則相　ordered phase





L10



L12

Theoretical Procedure　First-principles calc.

- Total energy calculation at the ground state: FLAPW
- Cluster Expansion Method (CEM)

$$\Delta E\left(V(r),\{\xi_i\}\right)=\sum_j v_j\left(V(r)\right)\cdot\xi_j^m$$

(i; ∘ ∘–∘ △ ◇ ... ; $\xi_i^m=\langle\sigma_1\cdot\sigma_2\cdots\sigma_i\rangle$

$$v_i=\sum_m\left\{\xi_j^m\right\}^{-1}\cdot\Delta E^{(m)}$$

- Cluster Variation Method (CVM)

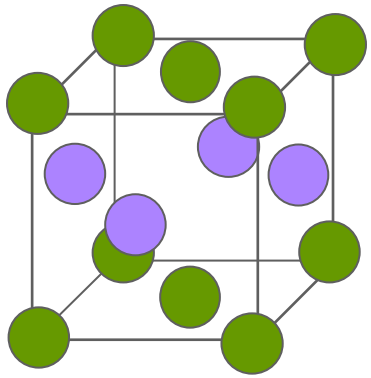
$$S=k_B\cdot\ln\frac{\prod_{i,j}\left\{Ny_{ij}!\right\}^6\cdot\left\{N!\right\}}{\prod_i\left\{Nx_i!\right\}^5\cdot\prod_{i,j,k,l}\left\{Nw_{ijkl}!\right\}^2}\qquad x_i,y_{ij},(z_{ijk}),w_{ijkl}\ \rightarrow\ \{\xi_i\}$$

$$g\left(T,V(r),\{\xi_i\}\right)=E\left(V(r),\{\xi_i\}\right)-T\cdot S\left(\{\xi_i\}\right)$$

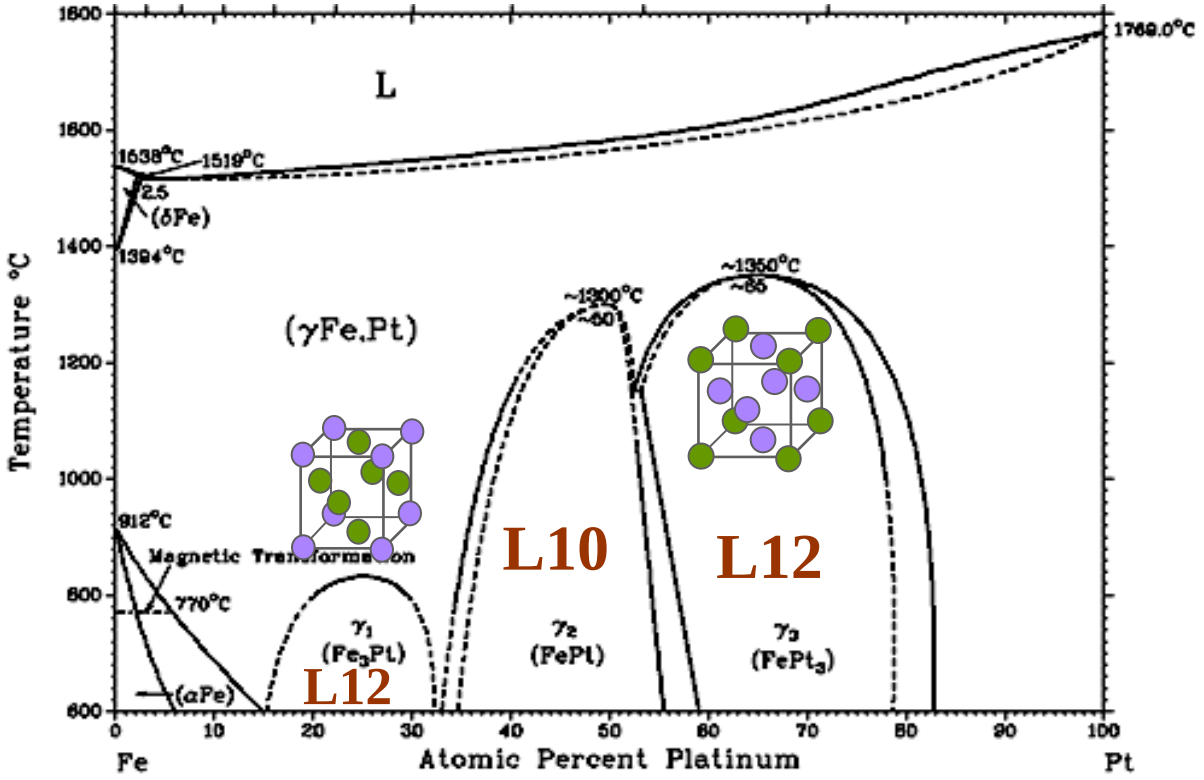
Background Fe-Pt L10

First-principles calculation of phase stability and

$L1_0$-disorder phase equilibria for **Fe-Pt** system



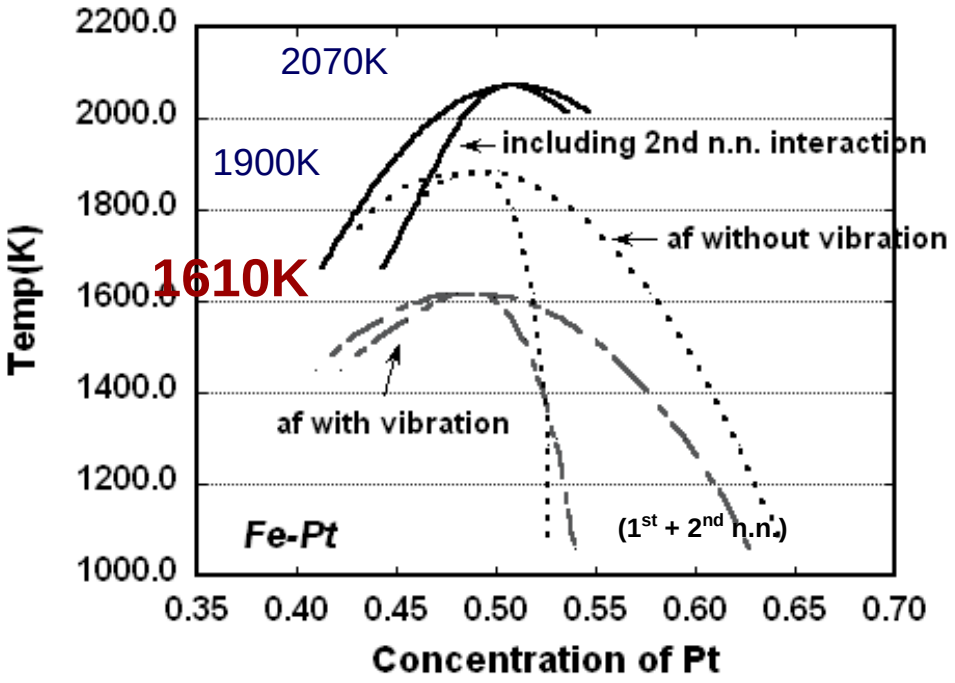
L10



Phase Diagram

L10-disorder

Fe-Pt



Exp. 1600K

26, 78

Fe, Pt

J. Alloys and Compounds (2004)

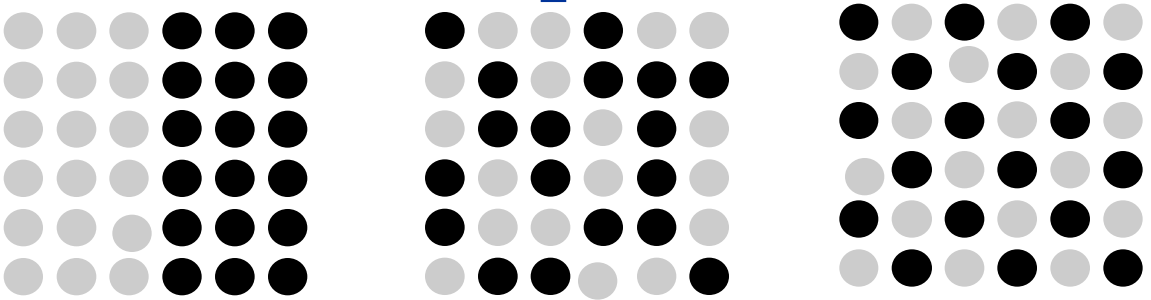
Entropy and Cluster Variation Method (CVM)

Bragg-Williams approx.

$$S = k_B \cdot \ln \frac{N!}{\prod_i \{Nx_i!\}} = -k_B \left(x \ln x + (1-x) \ln(1-x) \right), \; F = F(x)$$

Local atomic configuration ?

$\nu_2 < 0$ $\nu_2 = 0$ $\nu_2 > 0$



$y_{AA} = y_{BB} = 0.5$ $y_{AA} = y_{BB} = y_{AB}$. $y_{AB} = 1.0$

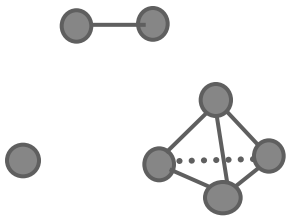
50%

$$F = F(x_i, y_{ij})$$

$$F = F(x_i, y_{ij}, z_{ijk} \cdots)$$

CVM

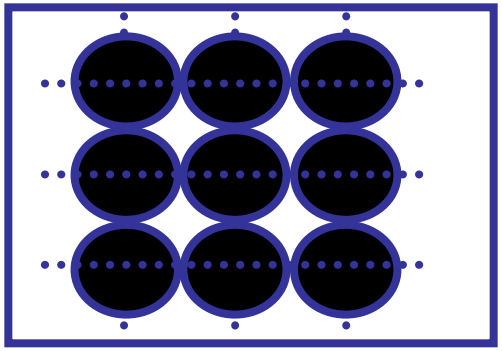
$$S = k_B \cdot \ln \frac{\prod_{i,j} \{Ny_{ij}!\}^6 \cdot \{N!\}}{\prod_i \{Nx_i!\}^5 \cdot \prod_{i,j,k,l} \{Nw_{ijkl}!\}^2}$$



Phase Field Method

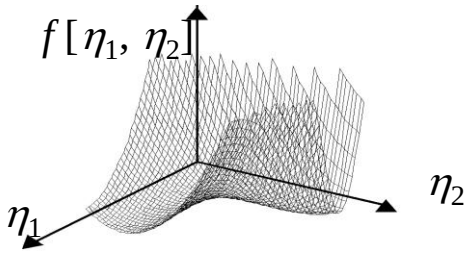
$$F_{chem} = \int \left(f\left[\{\eta_i\}\right] + \sum_{i=1} \kappa_i \left(\nabla \eta_i\right)^2 \right) \cdot dV$$

Microstructure

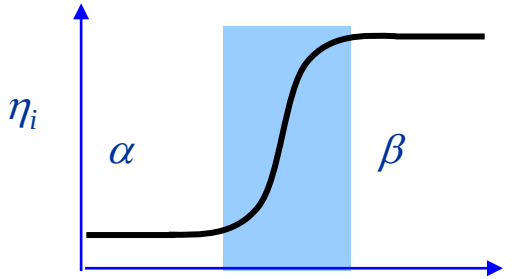


Free energy of microstructure

$\eta_i(\mathbf{r})$: *field variable*



Free energy of homogeneous system



interface

Time evolution of $\eta_i(\mathbf{r})$

Conserved
C

$$\frac{\partial \eta_i}{\partial t} = -\nabla \left(-M \nabla \frac{\delta F_{chem}}{\delta \eta_i}\right)$$

Non-Conserved
LRO

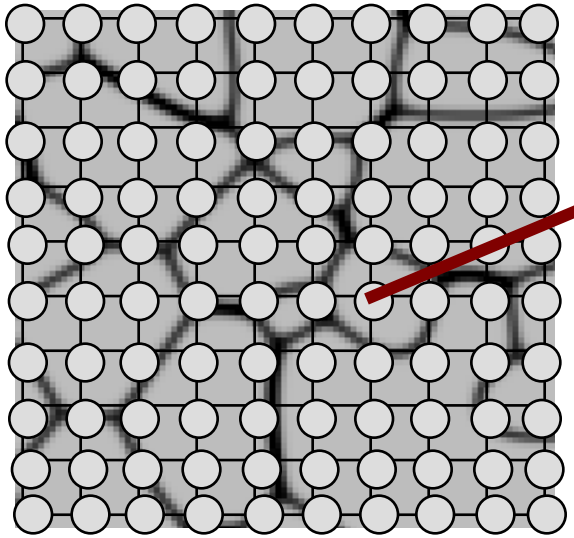
$$\frac{\partial \eta_i}{\partial t} = -\sum_j L_{ij} \frac{\delta F_{chem}}{\delta \eta_j}$$

κ_i : gradient energy coefficient,
M : mobility
L_{ij} : relaxation constant.

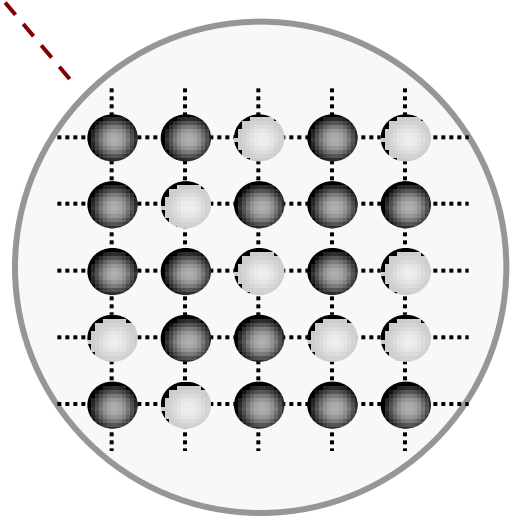
Hybrid Model

1:1

$$\frac{\partial \xi_i}{\partial t} = -L_i \left\{ \frac{\partial f_{\mathrm{CVM}}}{\partial \xi_i} - \kappa_i \nabla^2 \xi_i \right\}$$



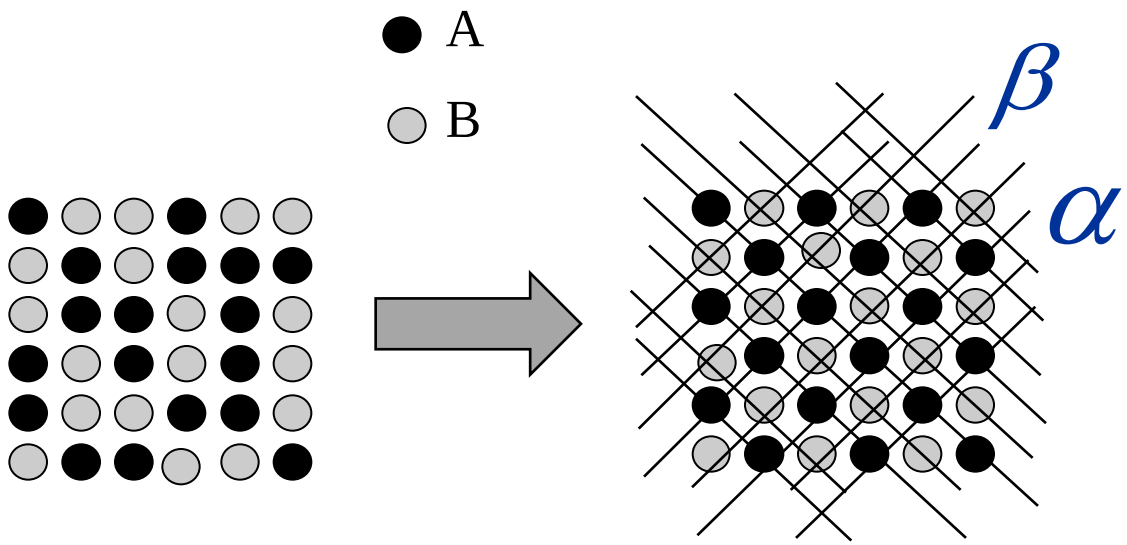
Microstructure
PFM



Atomistic
CVM

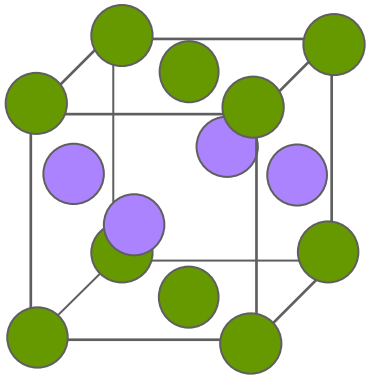
Multi-scale

Long Range Order parameter

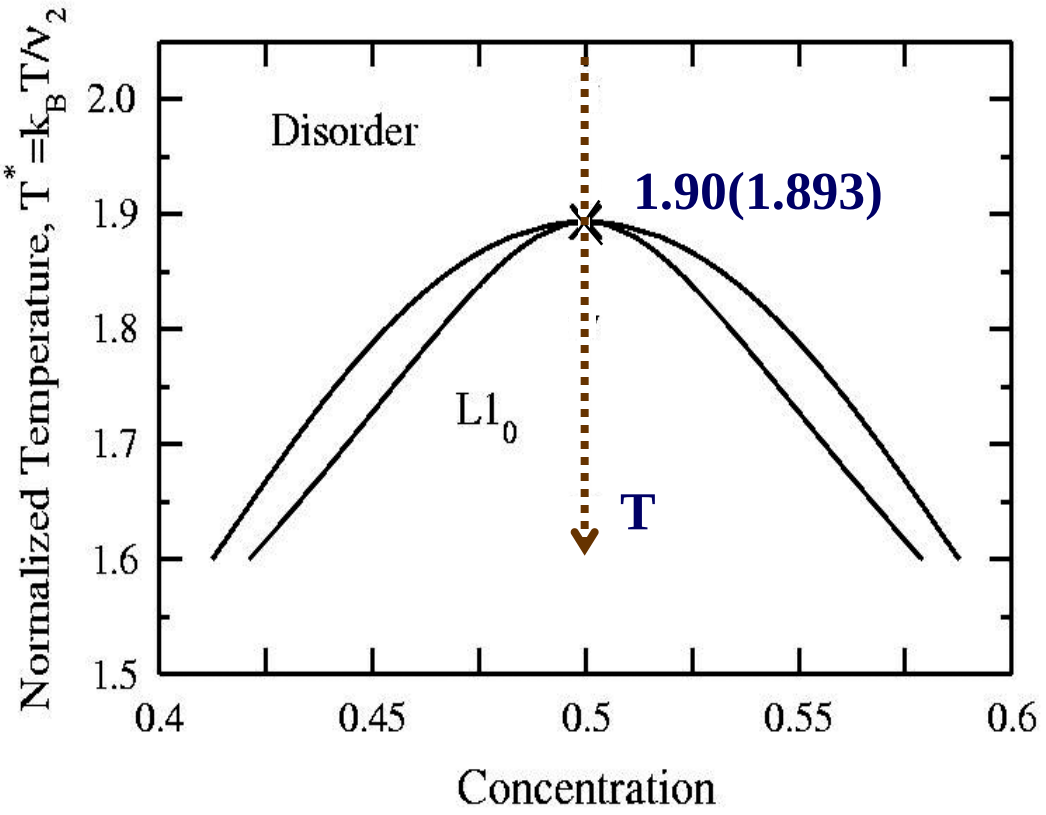


LRO $\eta = x_A^{\alpha} - x_A^{\beta}$

Preliminary calculation

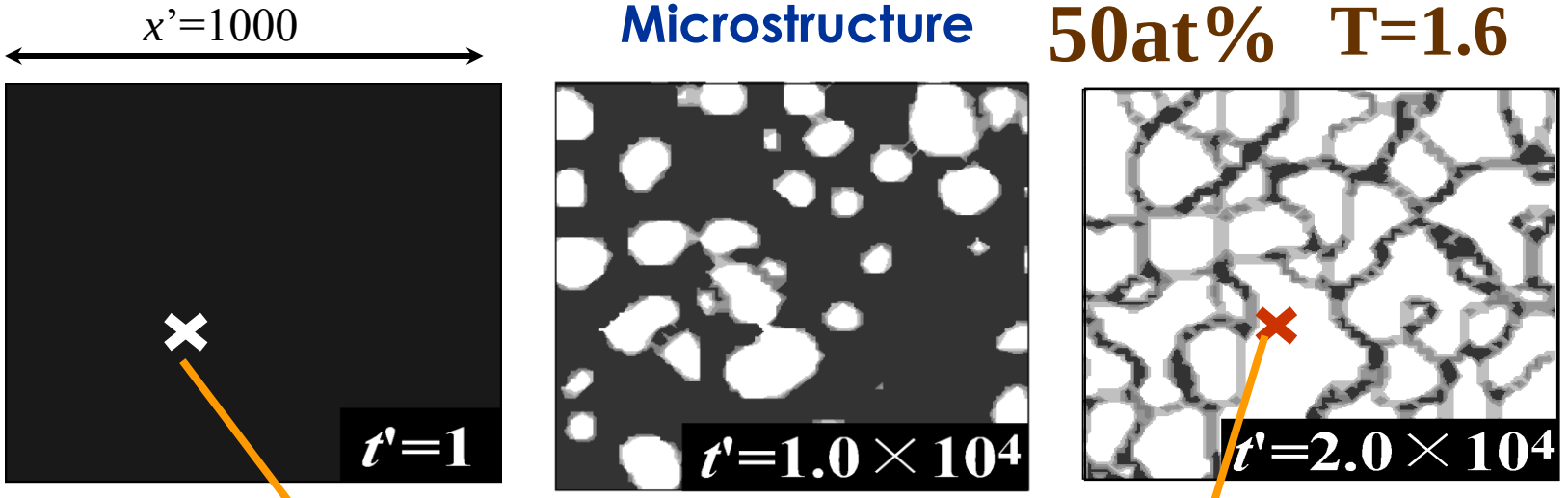


L10



v_2 ; n.n. effective pair interaction energy

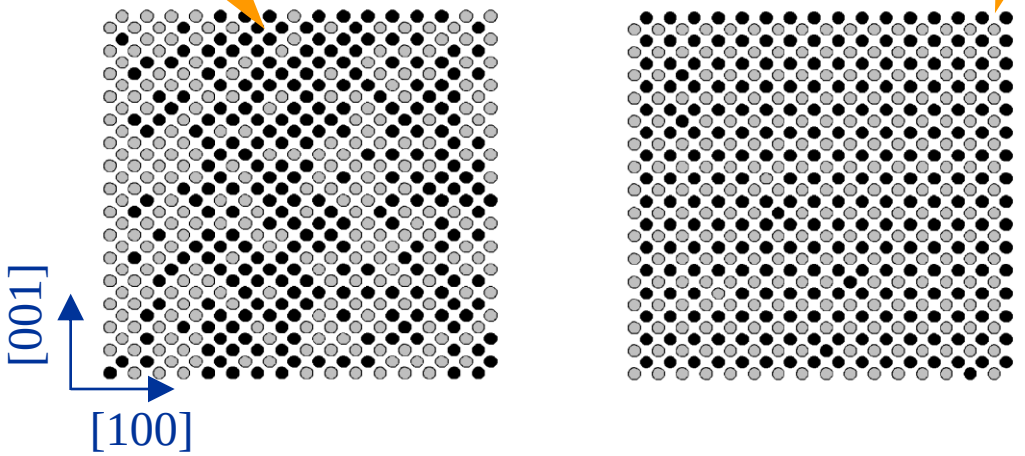
Simultaneous calculations for Multi-scales

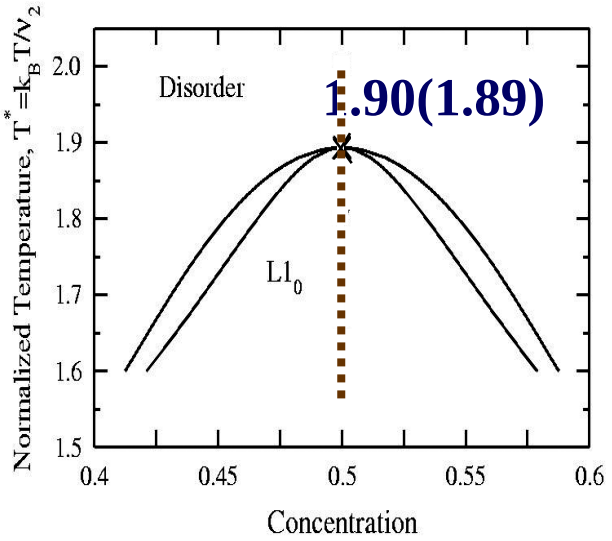


120x120x120 fcc algorithm; Williams

$$\sum_i |\{\xi\}_{in} - \{\xi\}_{out}| < 0.01$$

Atomistic

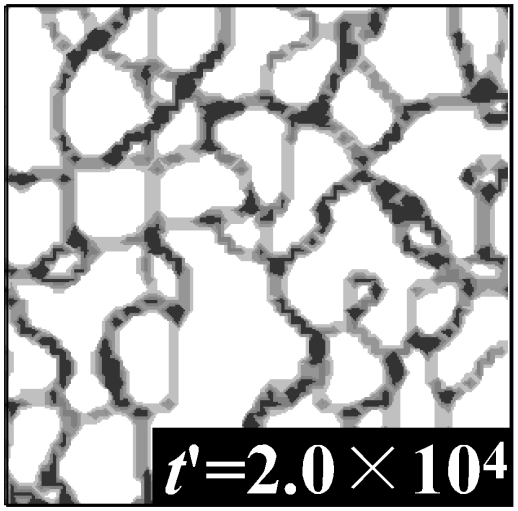




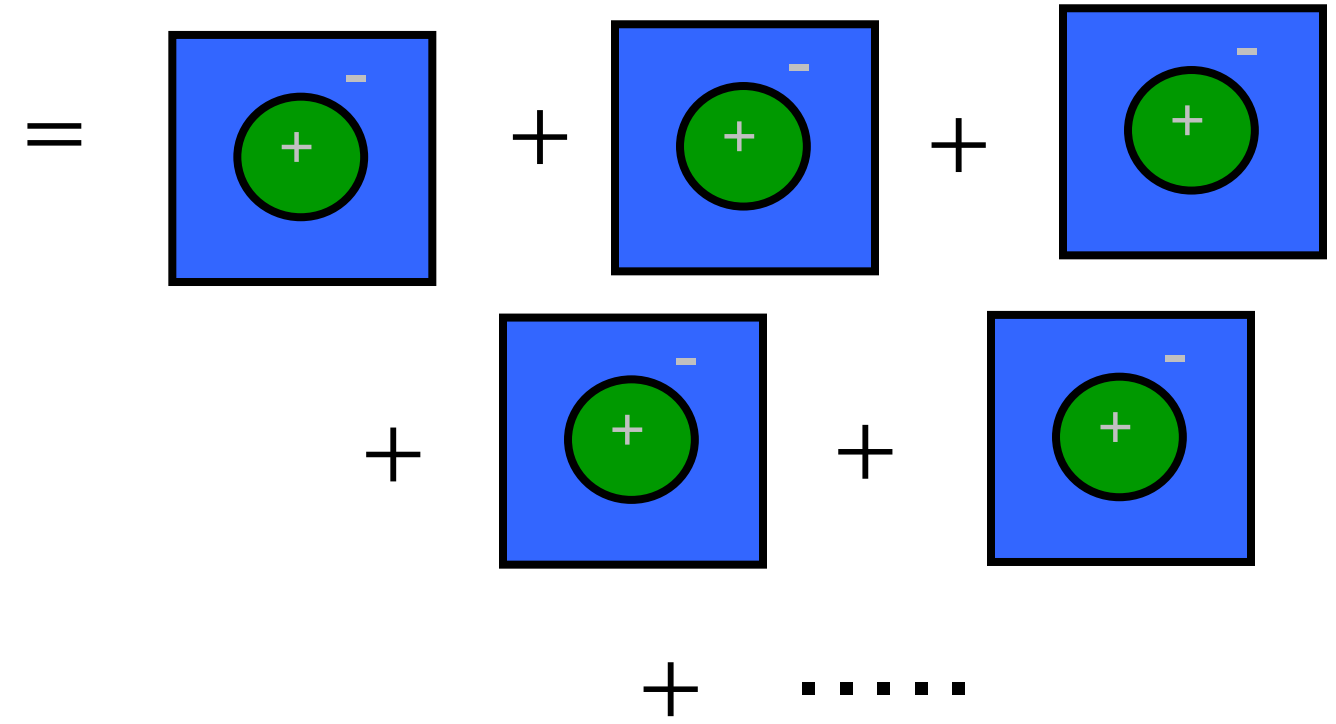
M. Ohno Ph.D Thesis Hokkaido Univ. (2004)

Multi-scale Analysis -Hybridized Model-

Elementary processes

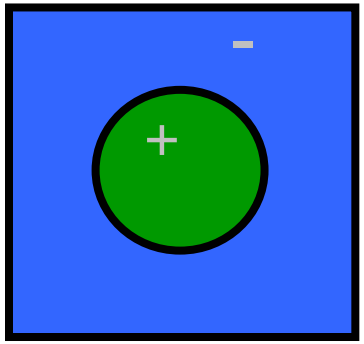


Circle shaped APB

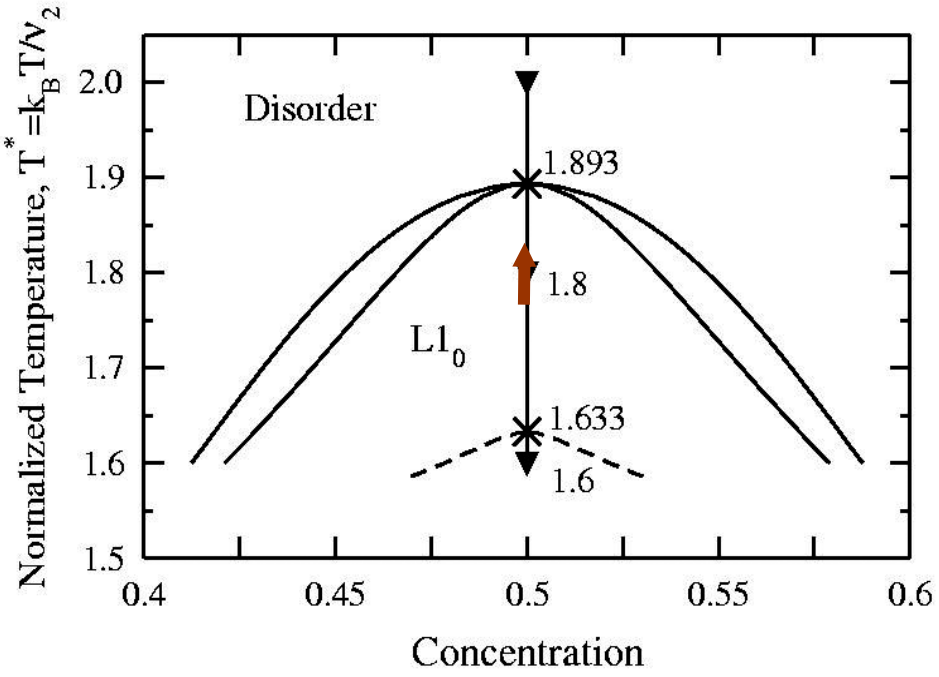


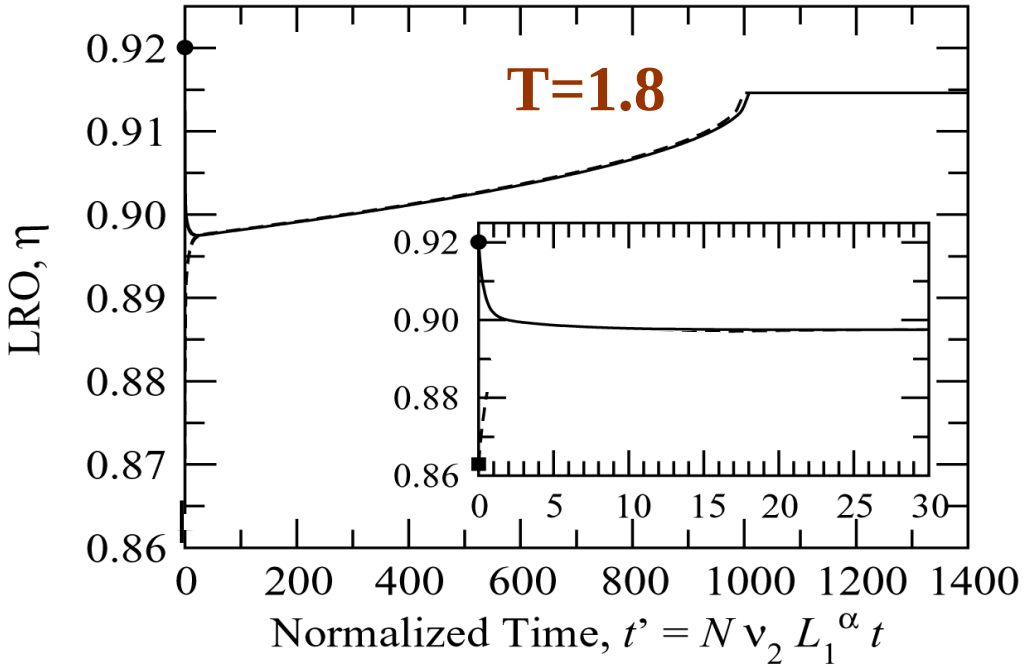
Philosophical Magazine(2003)

Kinetics of a Circle Shaped APB



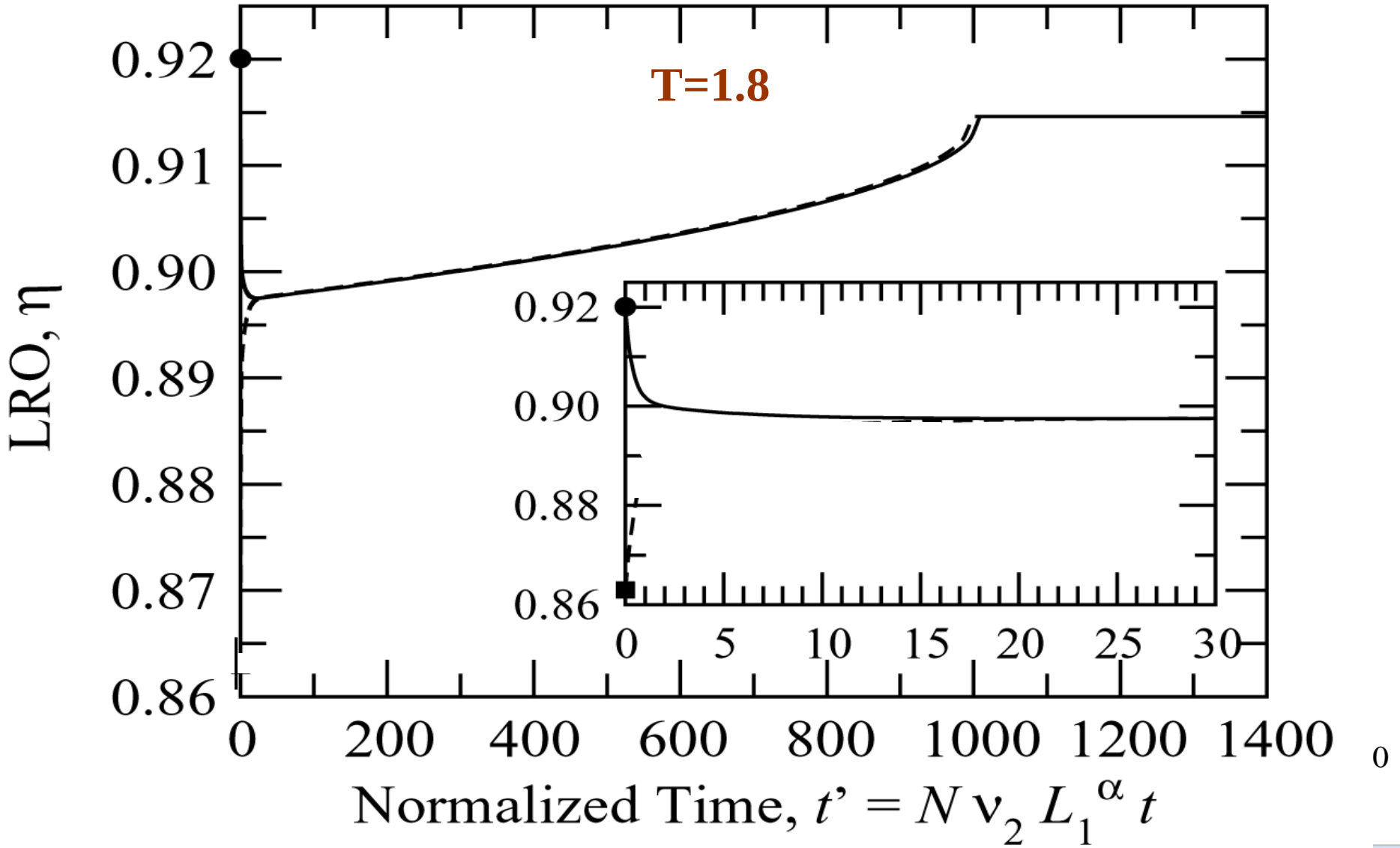
T=1.75 → 1.8





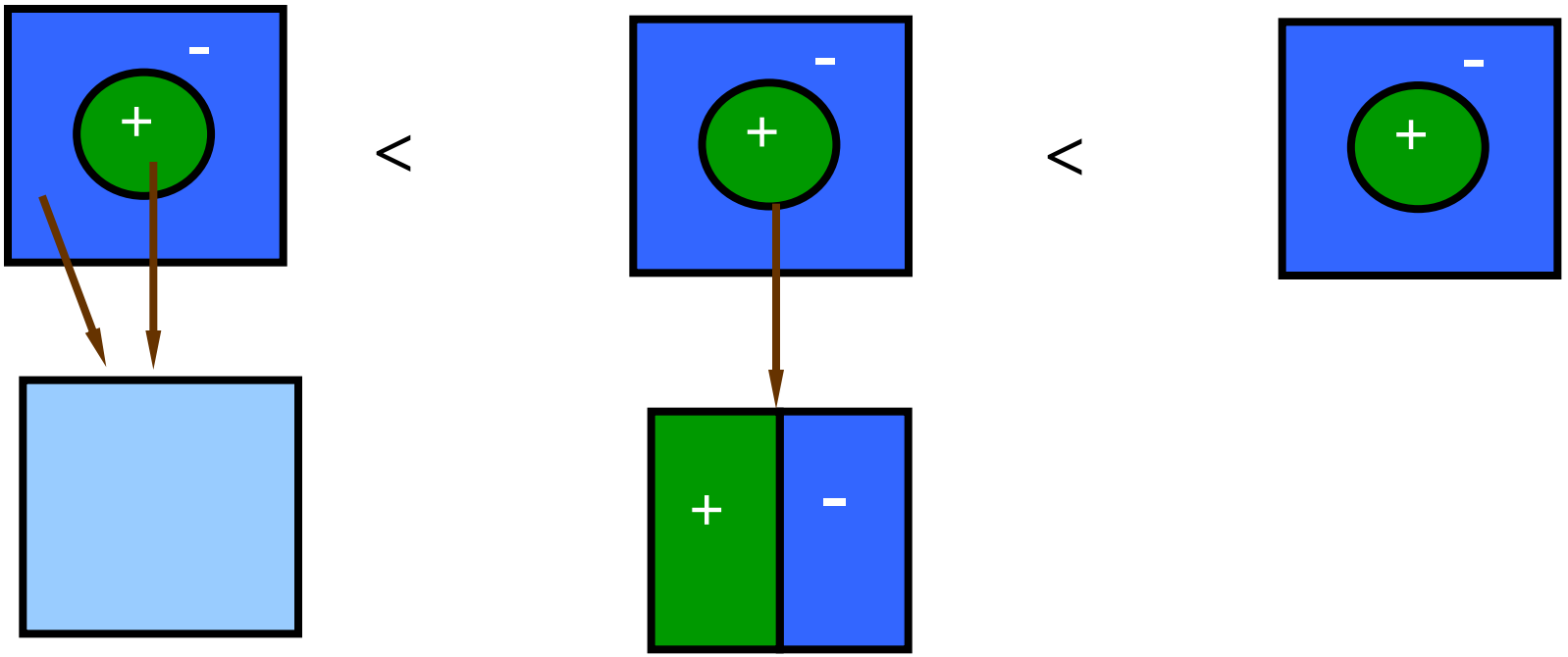
Philosophical Magazine(2003)

Kinetics of a circle shaped APB



Philosophical Magazine(2003)

Elementary process



1. <u>inside/outside</u> APB

homogeneous

$\tau_u = 1 \sim 3$

diffusion

2. <u>at</u> APB

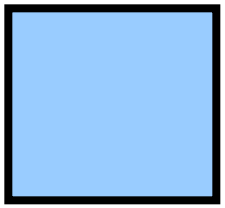
line-shaped APB

3. <u>movement</u> of APB

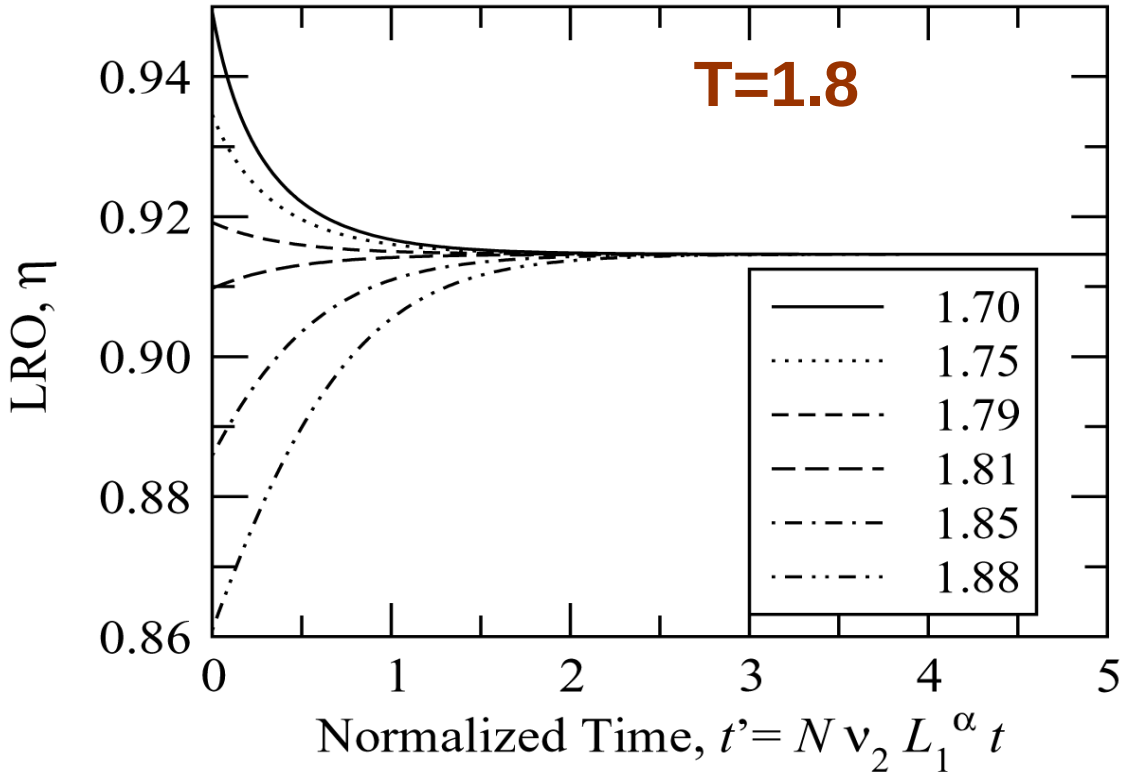
$\tau_u > 100$

Philosophical Magazine(2003)

kinetics of a Uniform System



$$\frac{\partial \xi_i}{\partial t} = -L_i\left(\frac{\partial f_{CVM}[\{\xi_i\}]}{\partial \xi_i} - \kappa_i \nabla^2 \xi_i\right)$$



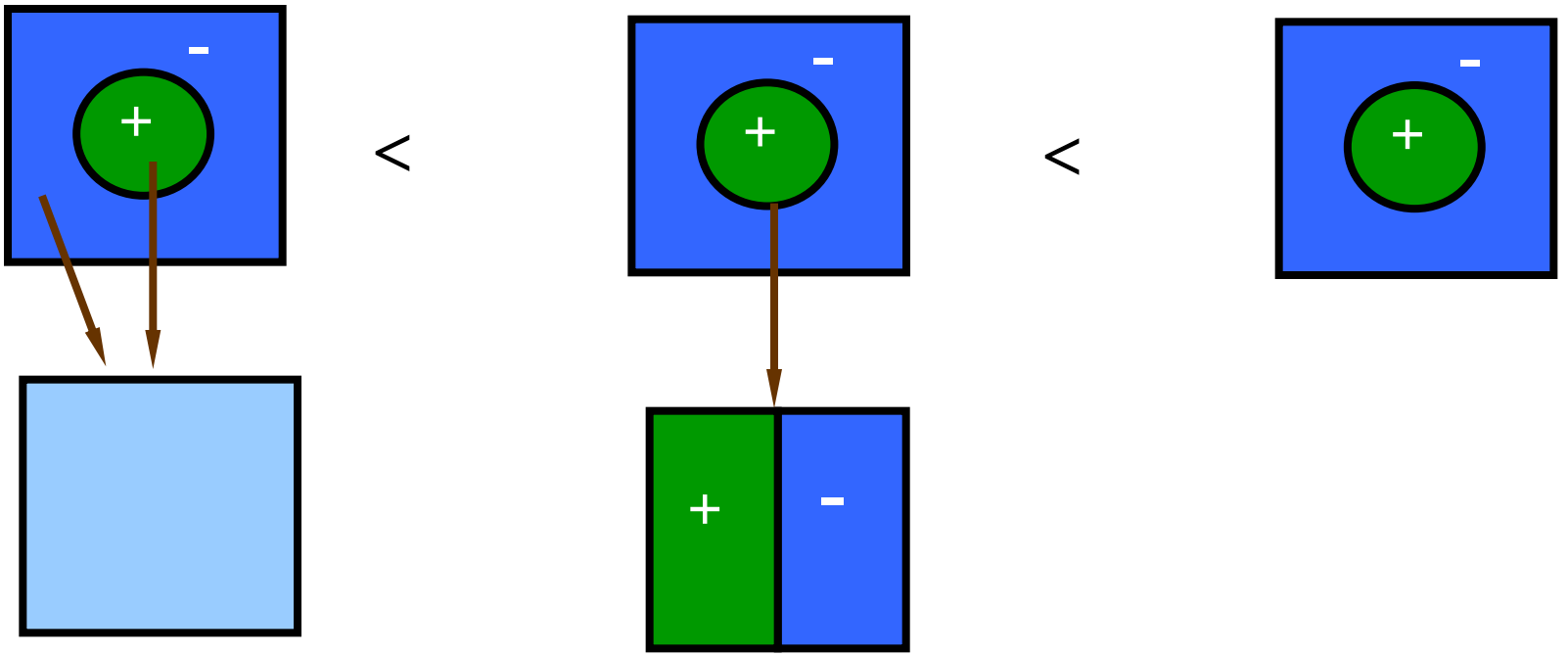
η_e

$$\eta(t) = a \cdot \exp\left(-\frac{t}{\tau_u}\right) + \eta_e$$

$\tau_u = 1 \sim 3$

Philosophical Magazine(2003)

Elementary process



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line-shaped APB

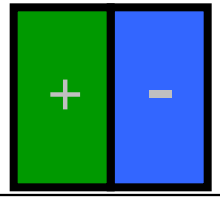
3. <u>movement</u> of APB

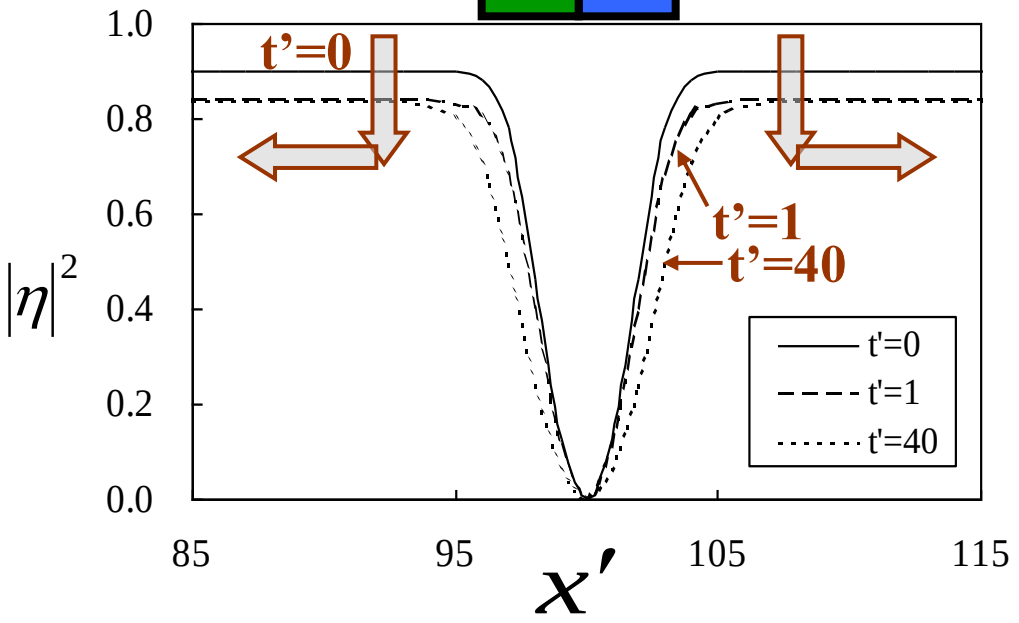
$\tau_u > 100$

Philosophical Magazine(2003)

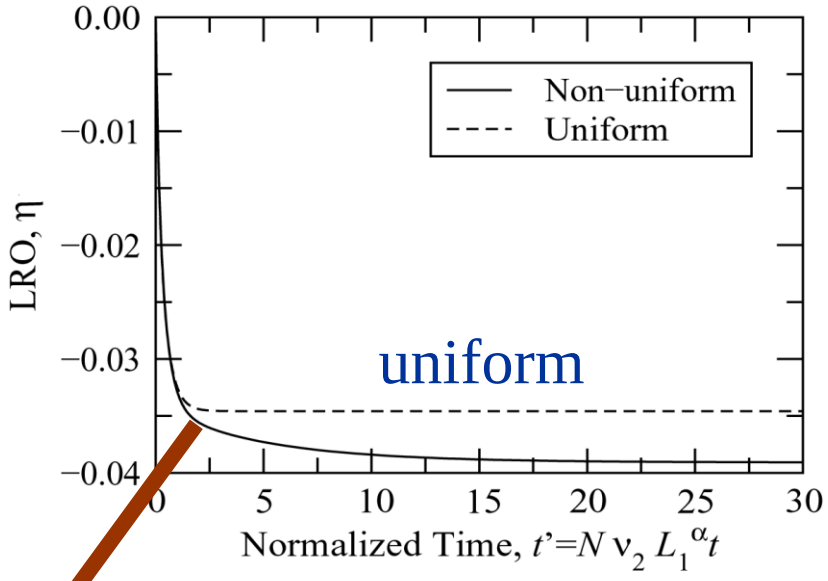
Kinetics of a line-shaped APB

T=1.7 ⟶ 1.8





Wetting



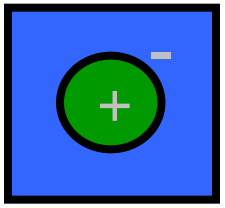
$$\eta(t) = a_f \exp\left(-\frac{t}{\tau_f}\right) + a_s \cdot \exp\left(-\frac{t}{\tau_s}\right) + \eta_e$$

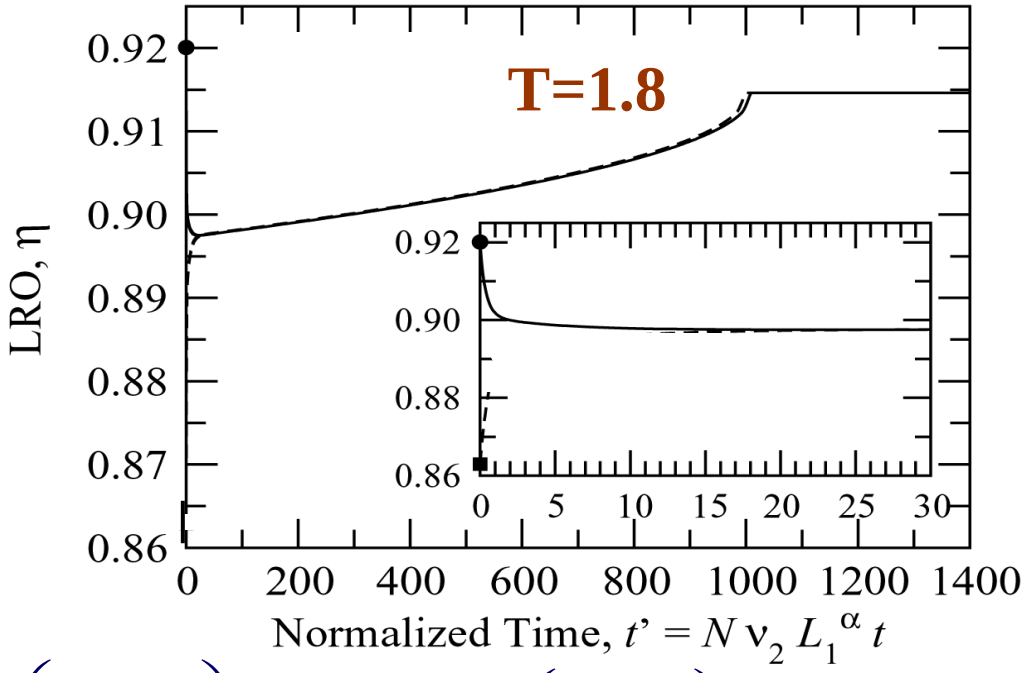
$\tau_f = 1 \sim 3$ $\tau_s = 10 \sim 30$

$$x' = x \cdot \sqrt{(N \cdot \nu_2)/(2\kappa_1^{\alpha})}$$

Philosophical Magazine(2003)

Hybrid model and multi scale calc.





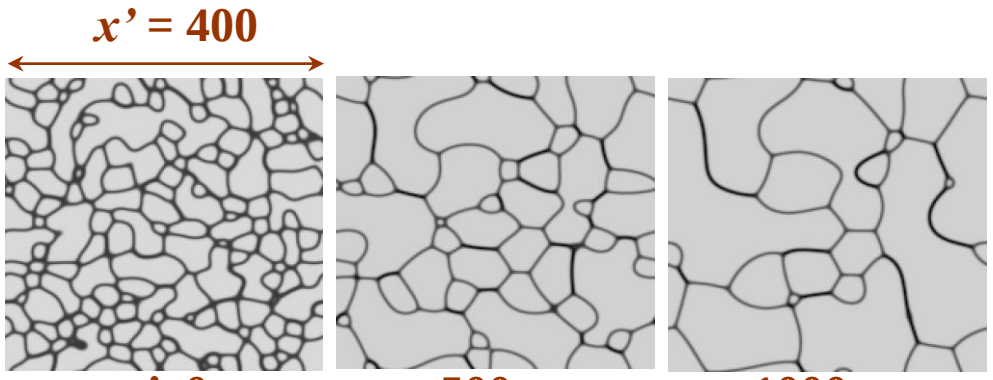
$$\eta(t) = a_f \exp\left(-\frac{t}{\tau_f}\right) + a_s \cdot \exp\left(-\frac{t}{\tau_s}\right) + \eta_{APB}(t) + \eta_e$$

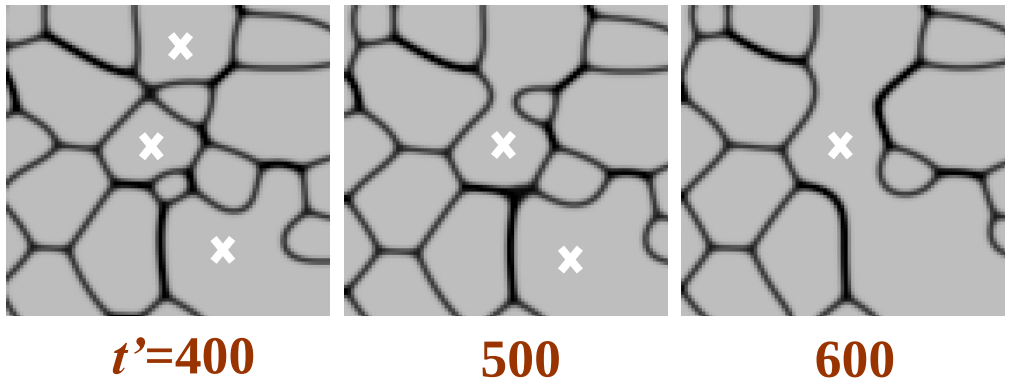
atomistic **wetting** **motion**

τ_f =1~3 τ_s =10~30 τ >100

Philosophical Magazine(2003)

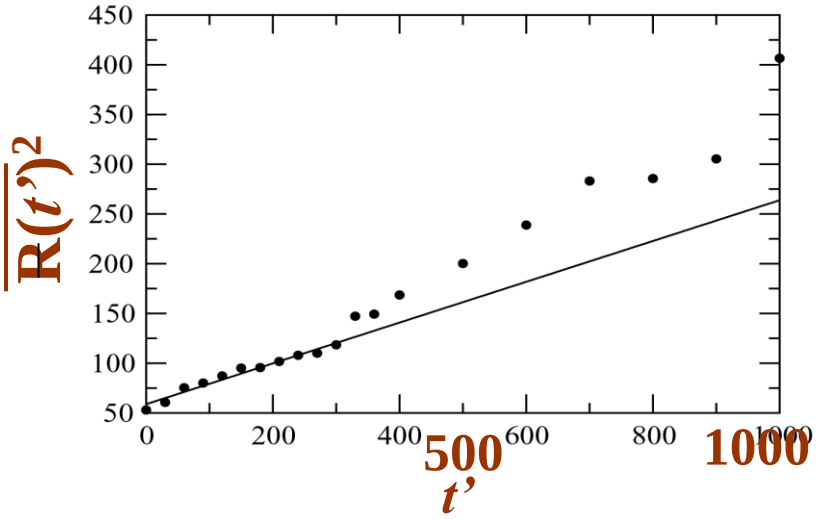
Coarsening Process





Coalescence

T=1.8



Curvature driven growth

$$V_{APB} = 2\kappa L \cdot H$$

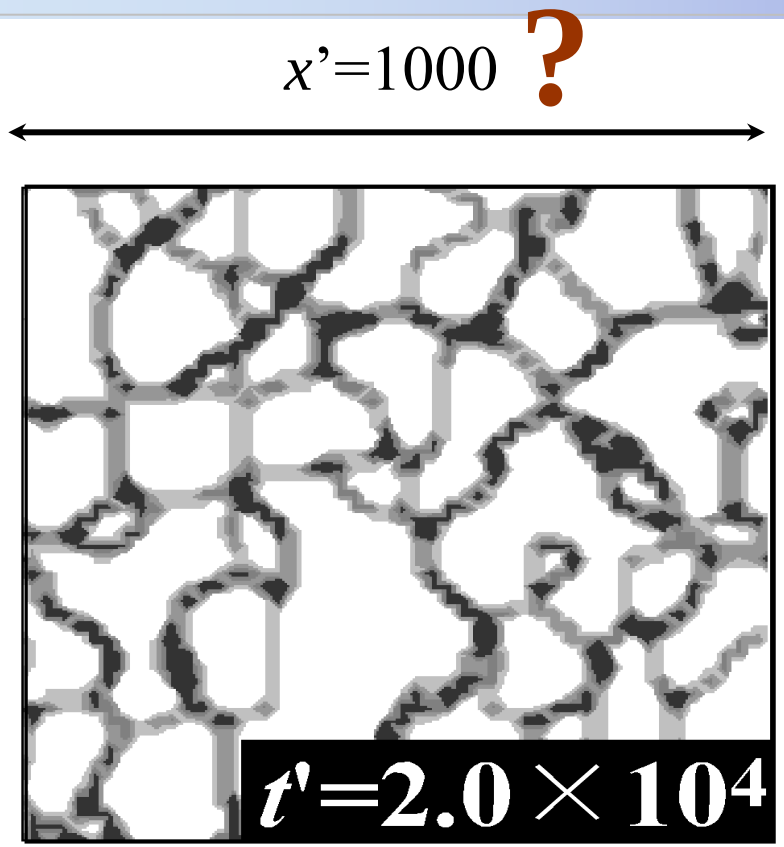
$$\langle R(t)\rangle^2 - \langle R(0)\rangle^2 = b \cdot t$$

H; local mean curvature

$$\frac{\partial \xi_i}{\partial t} = -L_i\left(\frac{\partial f_{CVM}[\{\xi_i\}]}{\partial \xi_i} - \kappa_i \nabla^2 \xi_i\right)$$

Philosophical Magazine(2003)

Scale?



$$x' = x \cdot \sqrt{\left(N \cdot \nu_2\right) / \left(2\kappa_1^{\alpha}\right)}$$

Spatial scale

Crystallographic orientation

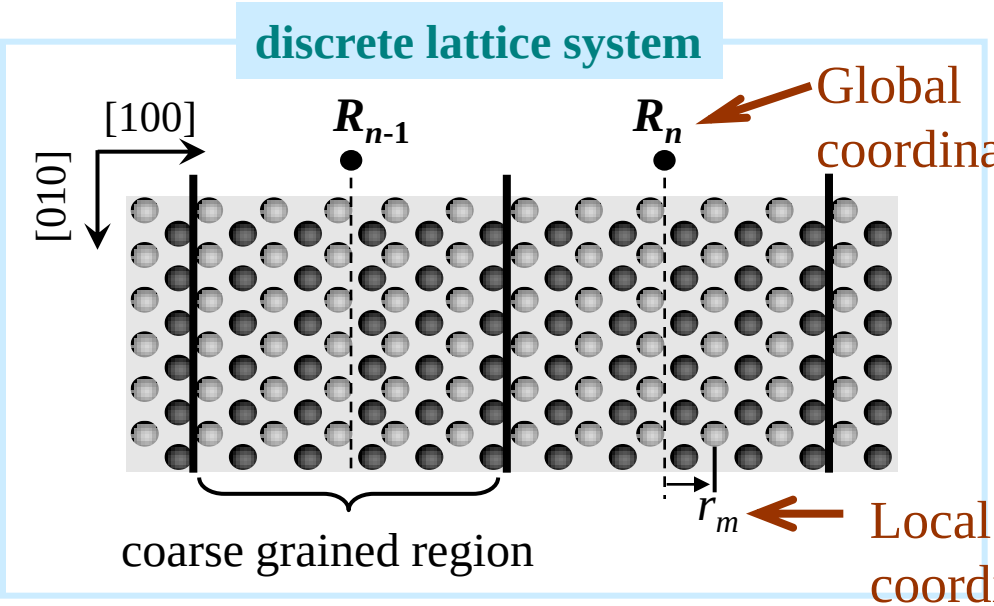
ν_2: **Pair interaction energy**

κ_i : **gradient energy coeff.**

Atomistic model of APB

M. Ohno Ph.D Thesis Hokkaido Univ. (2004)

Coarse Graining



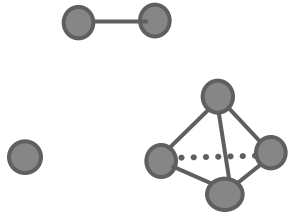
cells

R_n; Global coordinate

r_m; Local coordinate

$p_l = R_n + r_m$;atomic plane

$\phi_s(R_n + r_m + h(a))$;cluster probability



$$F = \sum_l f_{CVM}(p_l) = \sum_{n,m} f_{CVM}\left[\{\phi_s(R_n + r_m + h(a))\}\right]$$

$$\phi_s(R_n + r_m + h(a)) \cong \phi_s(R_n) + (r_m + h(a)) \cdot \nabla\phi_s(R_n) + \frac{1}{2}(r_m + h(a))^2 \cdot \nabla^2\phi_s(R_n)$$

$$F \cong \sum_{n,m} f_{CVM}\left(r_m + h(a), \{\phi_s(R_n)\}, \{\nabla\phi_s(R_n)\}, \{\nabla^2\phi_s(R_n)\}\right)$$

M. Ohno Ph.D Thesis Hokkaido Univ. (2004)

Coarse Graining [2]

$$F \cong \sum_{n,m} f_{CVM}\left(r_m + h(a), \{\phi_s(R_n)\}, \{\nabla\phi_s(R_n)\}, \{\nabla^2\phi_s(R_n)\}\right)$$

$$f_{CVM}\left(r_m + h(a), \{\phi_s(R_n)\}, \quad 0, \quad 0\right)$$

$$F \cong \sum_n \left\{ \sum_m f_{CVM}\left(\{\phi_s(R_n)\}\right) + \sum_{m,s} \left.\frac{\partial f_{CVM}}{\partial(\nabla\phi_s)}\right|_0 (\nabla\phi_s) + \sum_{m,s} \left.\frac{\partial f_{CVM}}{\partial(\nabla^2\phi_s)}\right|_0 (\nabla^2\phi_s) + \frac{1}{2}\sum_{m,s,s'} \left.\frac{\partial^2 f_{CVM}}{\partial(\nabla\phi_s)\partial(\nabla\phi_{s'})}\right|_0 (\nabla\phi_s)(\nabla\phi_{s'}) \right\}$$

homogeneous state

$$= \sum_n \left\{ \sum_m f_{CVM}\left(\{\phi_s(R_n)\}\right) + \sum_{s,m} C_{1,s}(r_m, a, \{J\})\cdot(\nabla\phi_s) + \sum_{m,s} C_{2,s}(r_m, a, \{J\})\cdot(\nabla^2\phi_s) + \sum_{m,s} C_{3,s}(r_m, a, \{J\})(\nabla\phi_s)^2 \right\}$$

$$F = \frac{1}{L}\int \left\{ \sum_m f_{CVM}\left(\{\phi_s(R_l)\}\right) + \sum_{s,m} C_{1,s}(r_m, a, \{J\})\cdot(\nabla\phi_s) + \sum_{m,s} C_{2,s}(r_m, a, \{J\})\cdot(\nabla^2\phi_s) + \sum_{m,s} C_{3,s}(r_m, a, \{J\})(\nabla\phi_s)^2 \right\} dx$$

M. Ohno Ph.D Thesis Hokkaido Univ. (2004)

Coarse Graining [3]

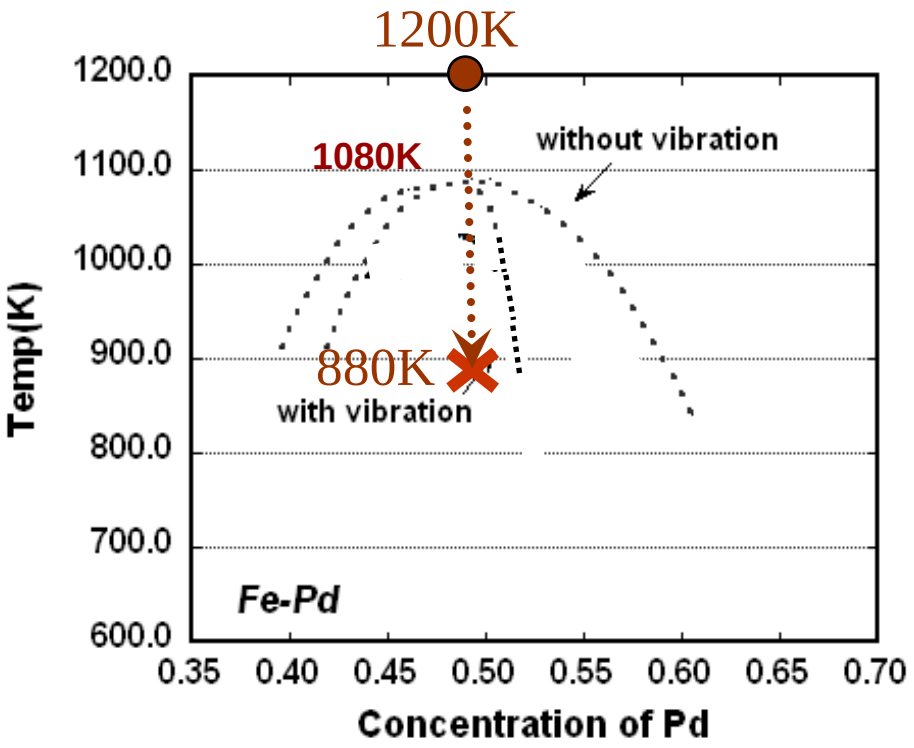
Ginzburg-Landau type

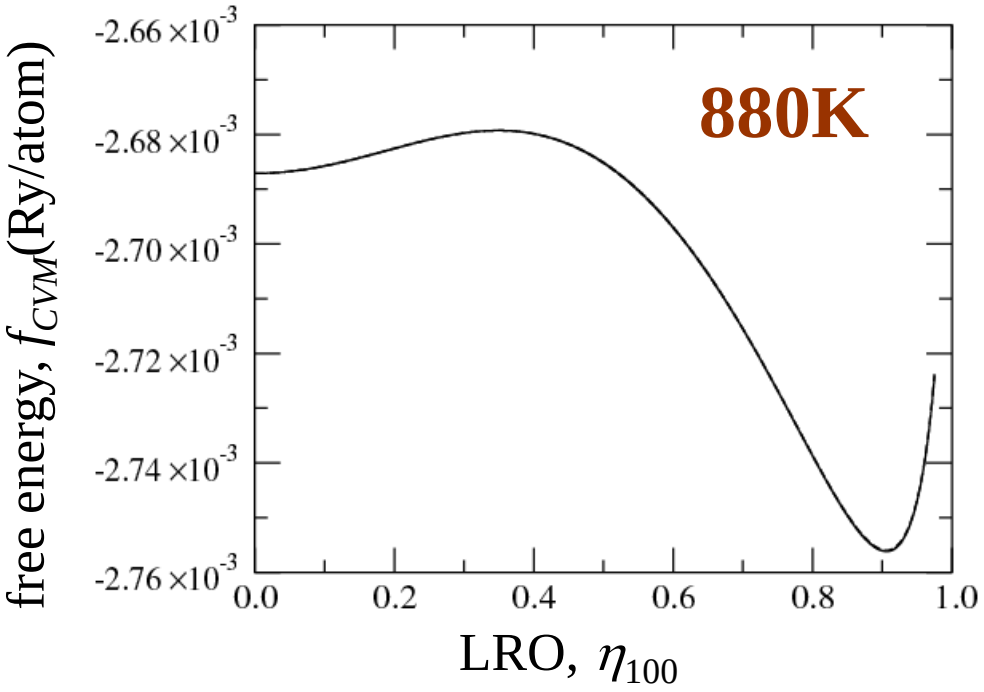
$$F = \frac{1}{L}\int \left[N' \cdot f_{CVM}\left[\{\phi_s\}\right] + \sum_{s,s'} \kappa_{s,s'} \left(\nabla \phi_s\right)\left(\nabla \phi_{s'}\right) \right] \cdot dx$$

$$\kappa_{s,s'} = N \cdot k_B \cdot T \cdot \sum_{J} V_{s,s'}\left(r_m, a, \{J\}\right)$$

M. Ohno Ph.D Thesis Hokkaido Univ. (2004)

Free energy -LRO profile





Fe-Pd

——— lattice constant is optimized
- - - - - - - - lattice constant is fixed at a_{dis}

f_{dis} = –2.687 (mRy/atom)
f_{ord} = –2.756 (mRy/atom)
$\Delta f(f_{dis}-f_{ord})$ = 0.069 (mRy/atom)

J. Phase Equil. and Diffusion, (2006)

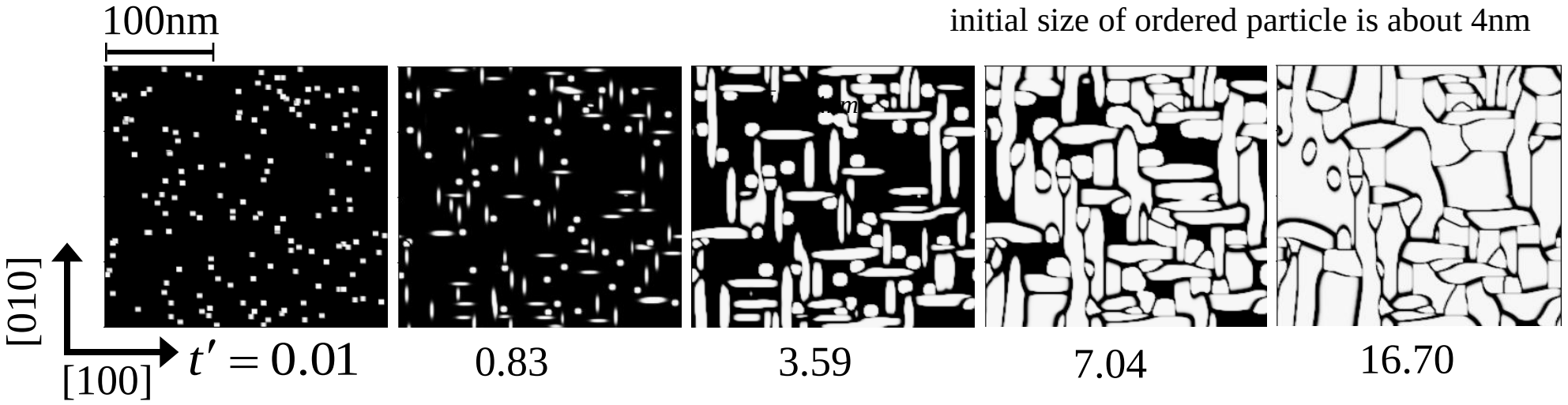
First principles Microstructural Calculation

Fe-Pd **disorder – $L1_0$ at c=0.5**

$\bar{d}_{in} \approx 4nm$

T=1200K→ 880K

initial size of ordered particle is about 4nm



$\left|v_{2,2}/v_{2,1}\right| \approx 0.1$ T-O approximation

$t' = N \cdot L \cdot \Delta f \cdot t$ PFM+PPM

J. Phase Equil. and Diffusion, (2006)

背景

科学技術基本計画

ライフサイエンス、情報通信、
環境、ナノテク・材料

マテリアル

構造用材料

鉄鋼材料

高温耐熱合金

Fe,Ni,Cr,Co,Mo

高比強度軽金属合金

Ti,Al,Mg

ナノ材料

機能性材料

磁性、半導体物性、光物性

強度の高精度設計

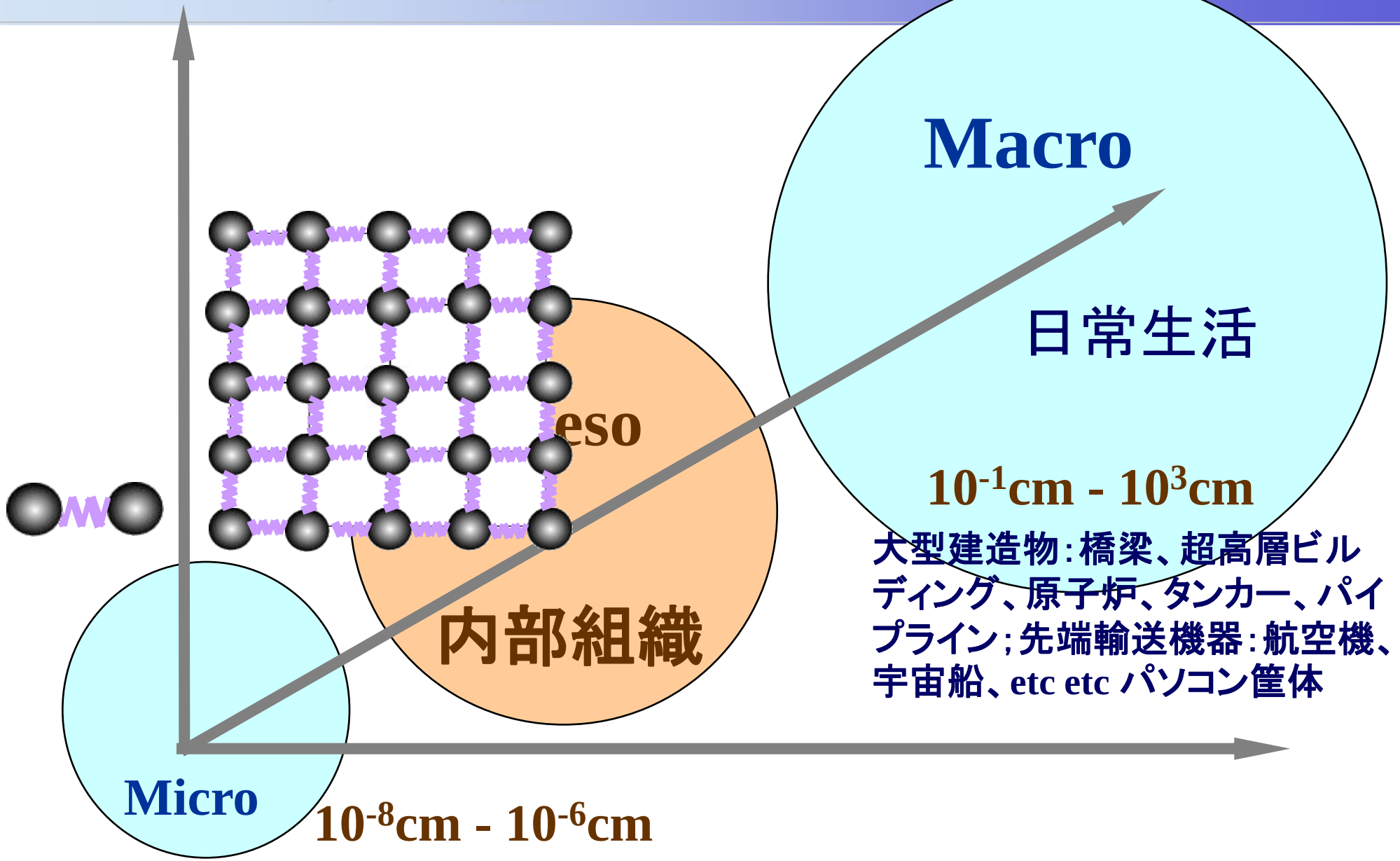
エネルギー問題
経済効果

強度

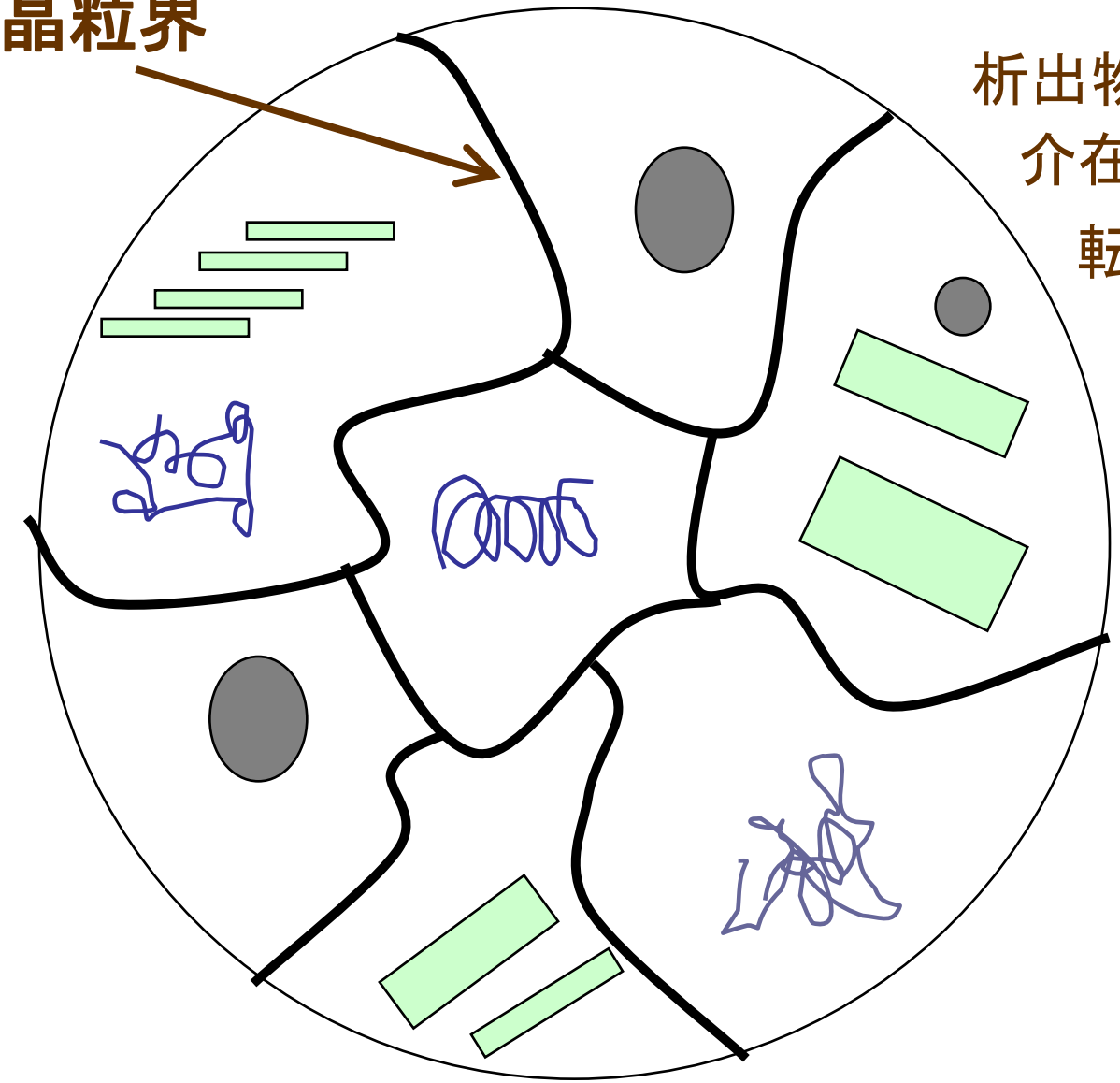
強度の本質
強度の科学

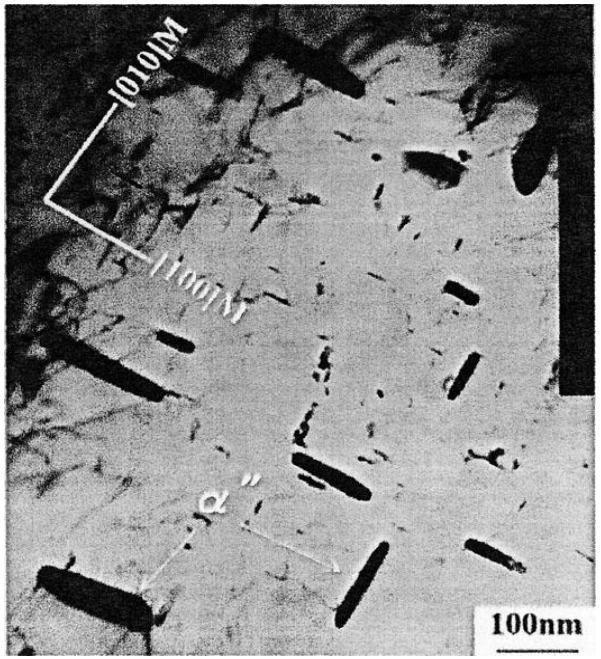
大型建造物：橋梁、超高層ビルディング、原子炉、タンカー、パイプライン；先端輸送機器：航空機、宇宙船、etc etc パソコン筐体

マルチスケール性

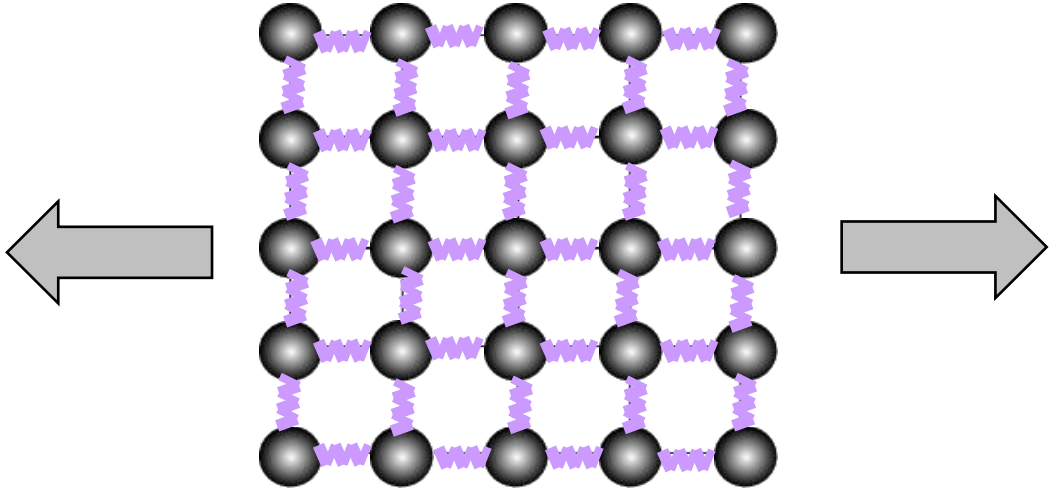

Macro
日常生活
10^{-1}cm - 10^{3}cm
大型建造物：橋梁、超高層ビルディング、原子炉、タンカー、パイプライン；先端輸送機器：航空機、宇宙船、etc etc パソコン筐体
eso
内部組織
Micro
10^{-8}cm - 10^{-6}cm

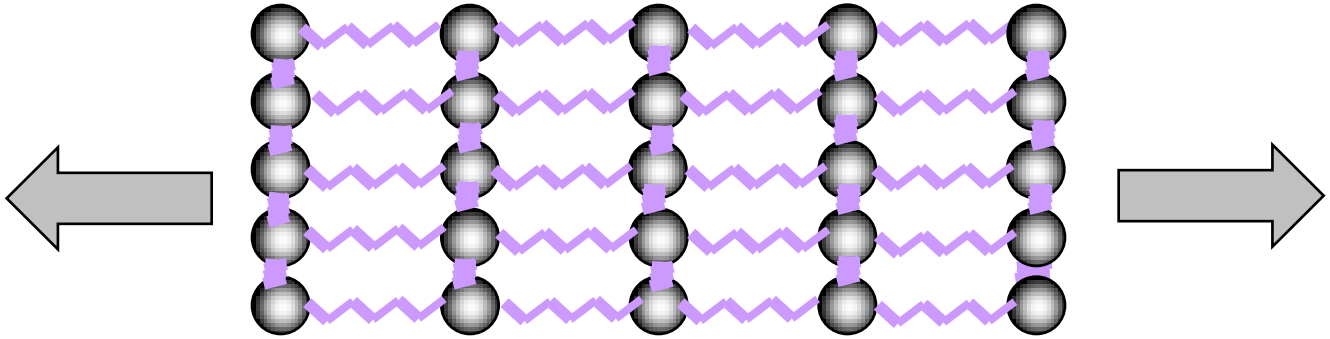
内部組織



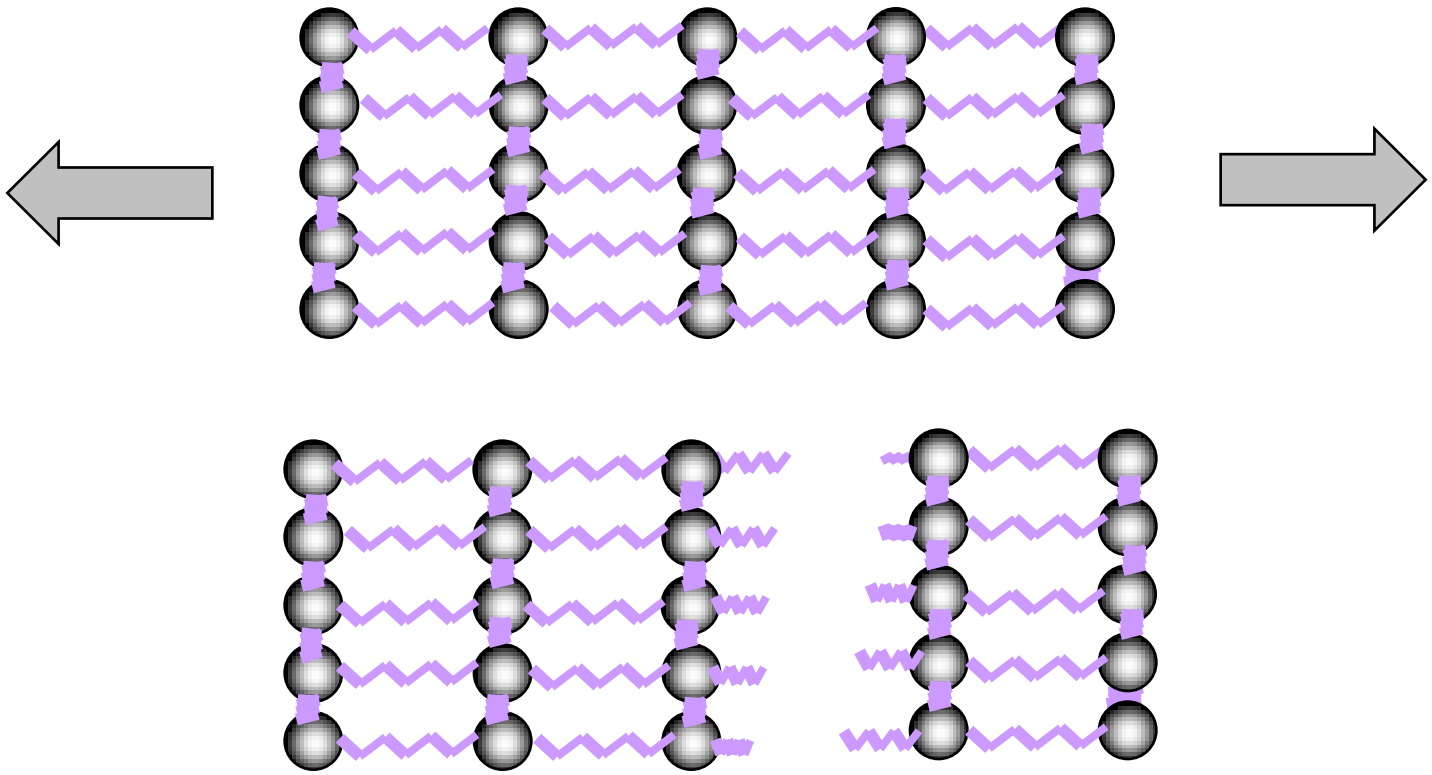


変形過程（弾性変形）



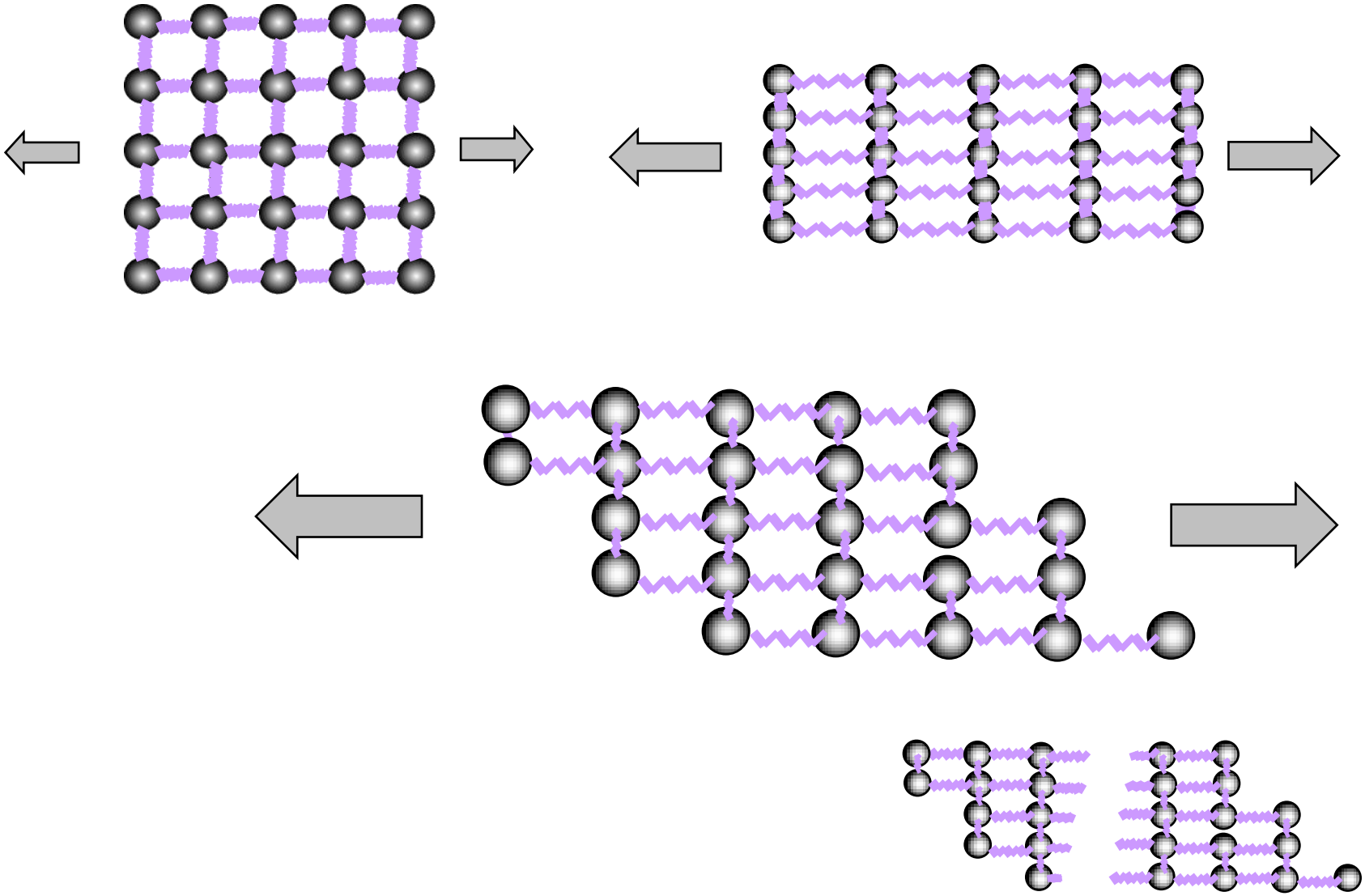


変形過程

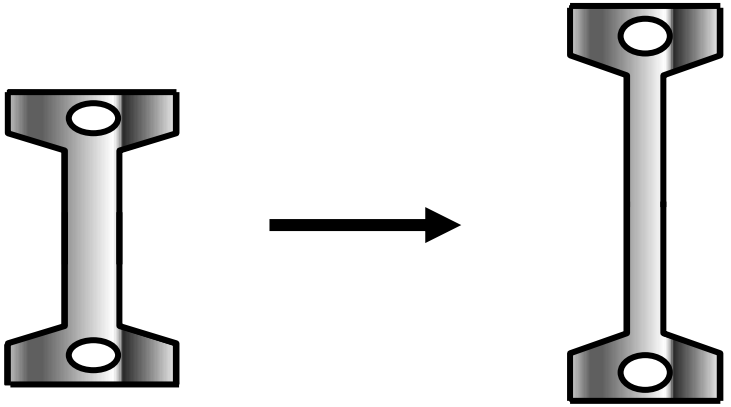


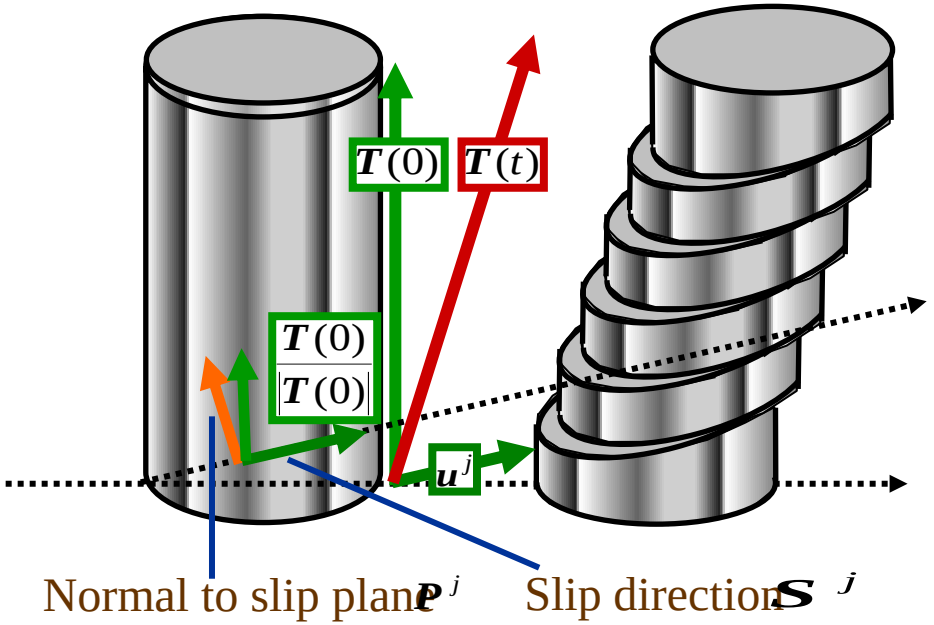
破壊

塑性変形

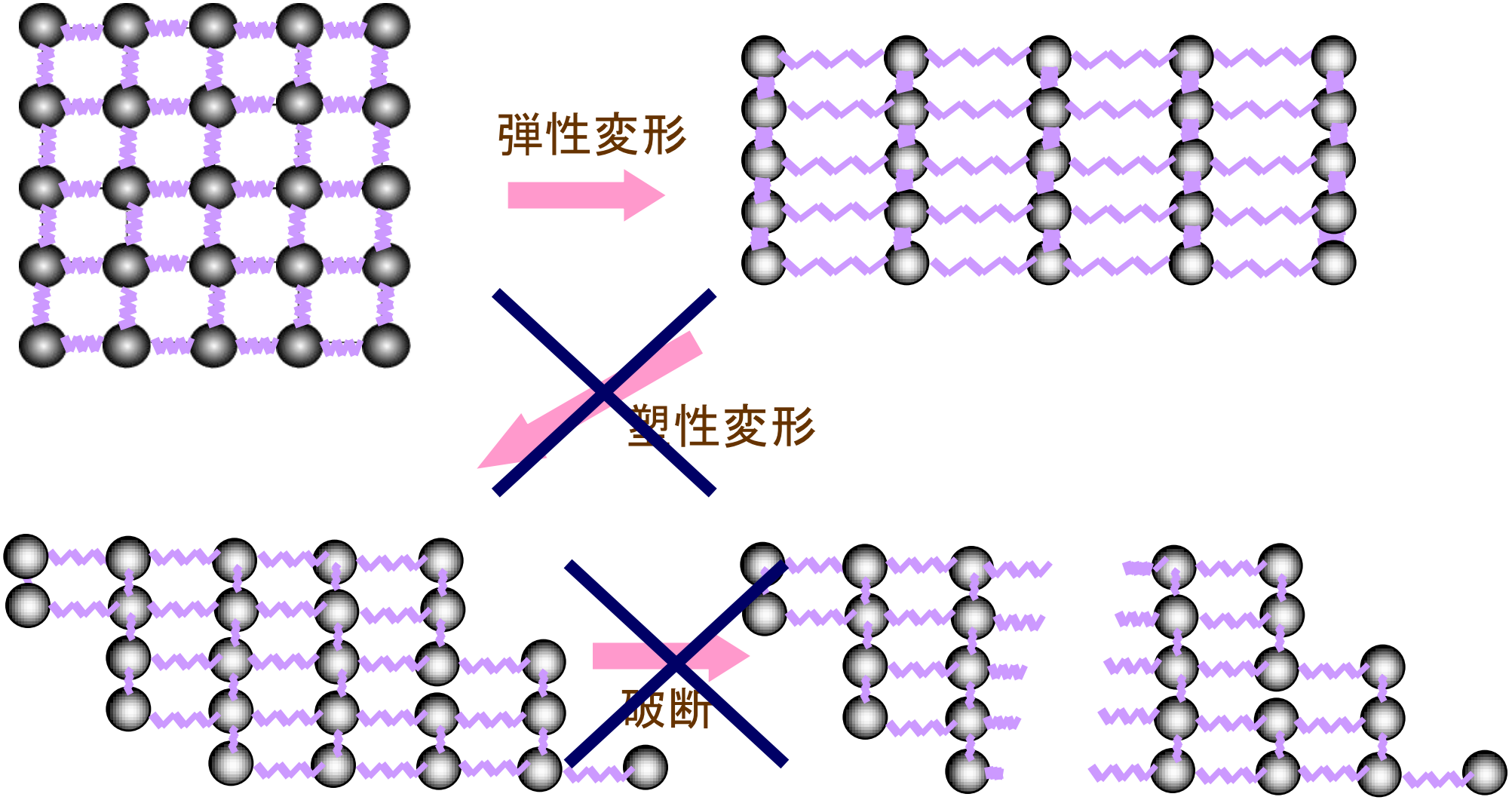


塑性変形

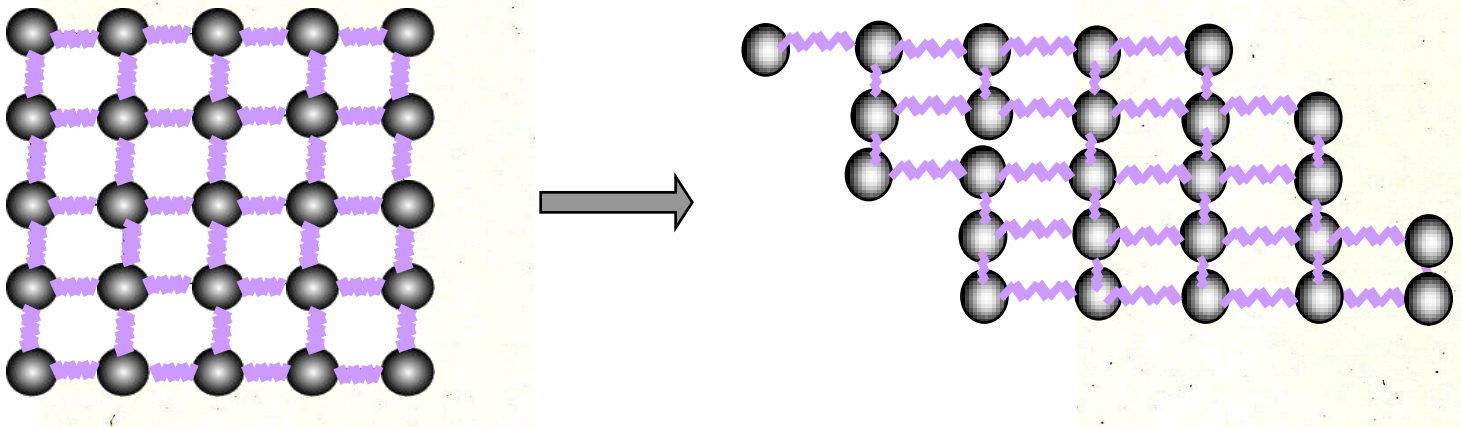


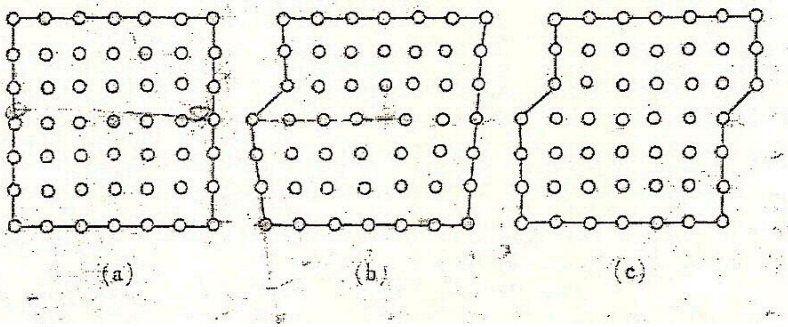


合金材料の変形挙動



塑性変形





“しわ“の伝播

金属物理学序論　コロナ社　（1971）

転位運動と変形

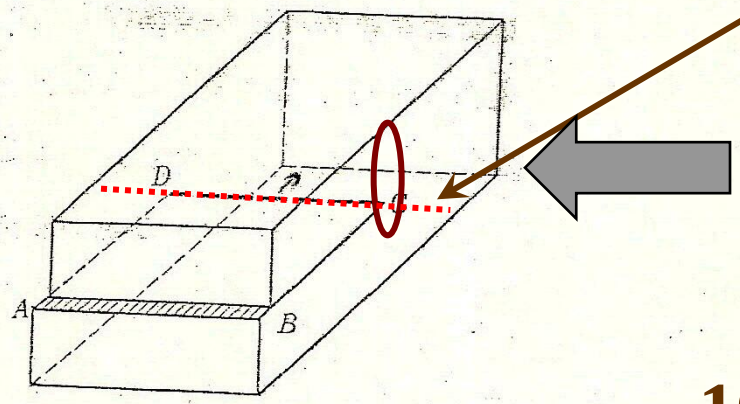


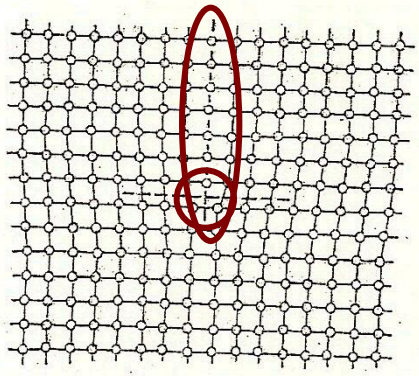
図 8·6　刃状転位によるすべり変形

転位線 dislocation

変形＝転位線の運動

$10^6 cm/cm^3 \rightarrow 10^{12} cm/cm^3$

地球の赤道周囲の250倍!



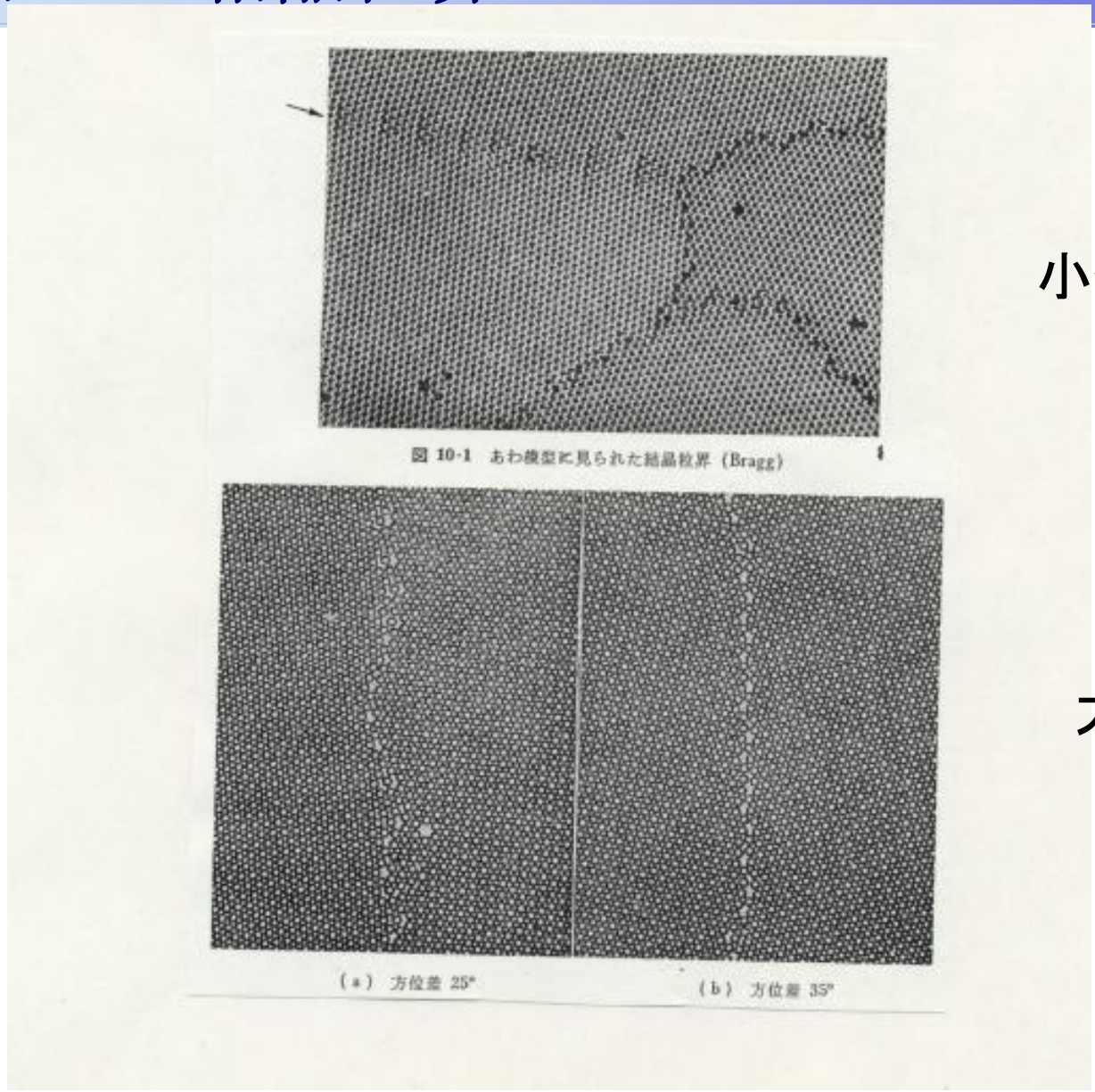
強度設計

転位運動の制御

内部組織（障害物ex　析出物）

金属物理学序論　コロナ社　（1971）

泡モデルと結晶粒界



小傾角粒界

大角粒界

結晶粒界

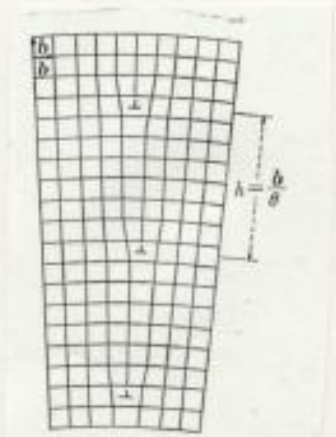


図 10·9 対称性の小傾角境界 (Read) θ: 傾きの角

対称小傾角粒界

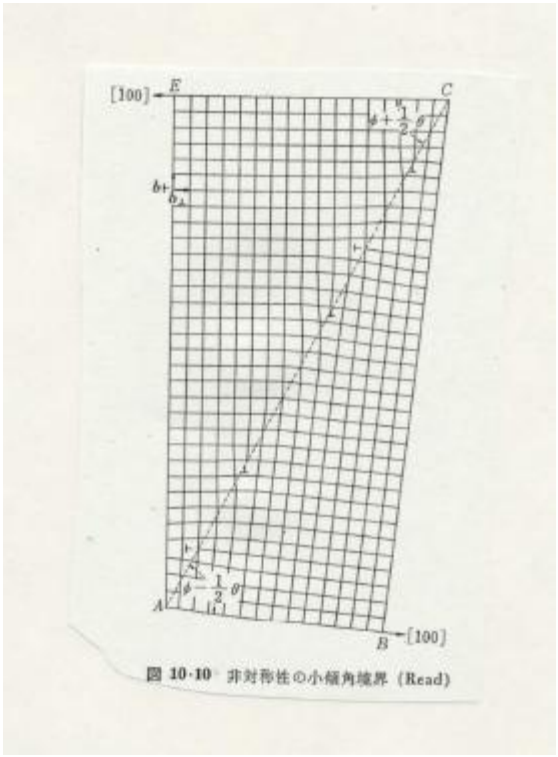


図 10·10 非対称性の小傾角境界 (Read)

非対称小傾角粒界

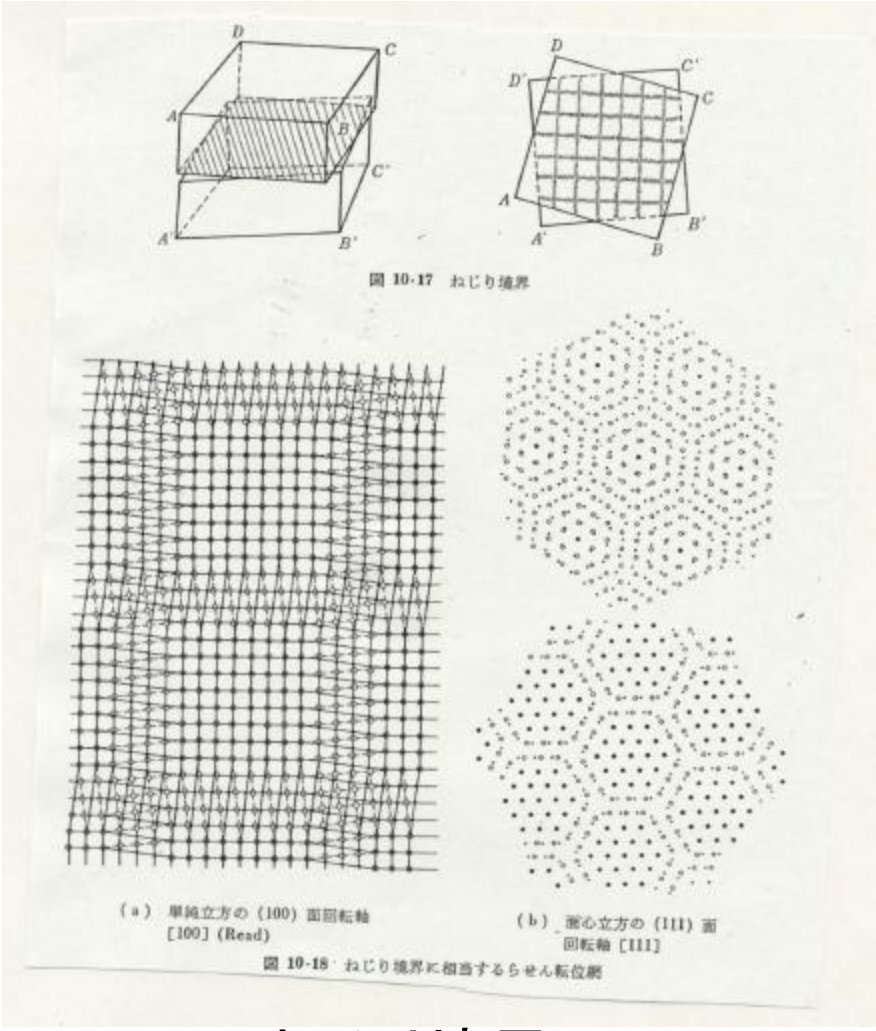


図 10·17 ねじり境界

(a) 単純立方の (100) 面回転軸 [100] (Read)

(b) 面心立方の (111) 面回転軸 [111]

図 10·18 ねじり境界に相当するらせん転位網

ねじり境界

金属物理学序論 コロナ社 (1971)

Plasticity within dislocation theory

１．単一転位の挙動

Single dislocation behavior

２．単一転位の複数障害物場での挙動

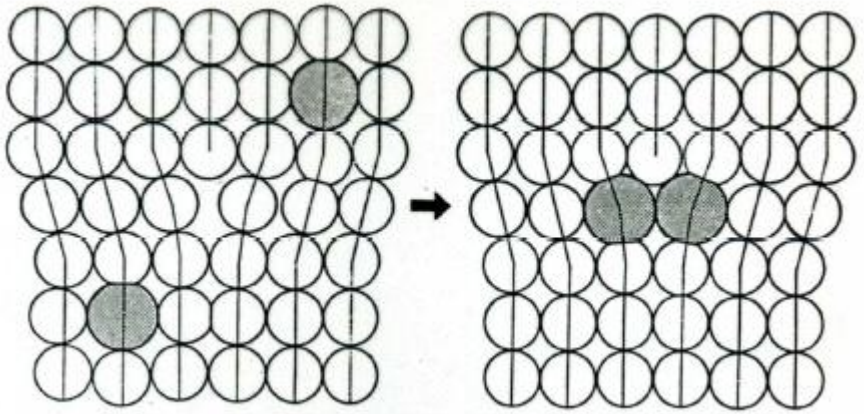
Single dislocation behavior in the obstacle field

３．多数転位の（複数障害物場での）挙動

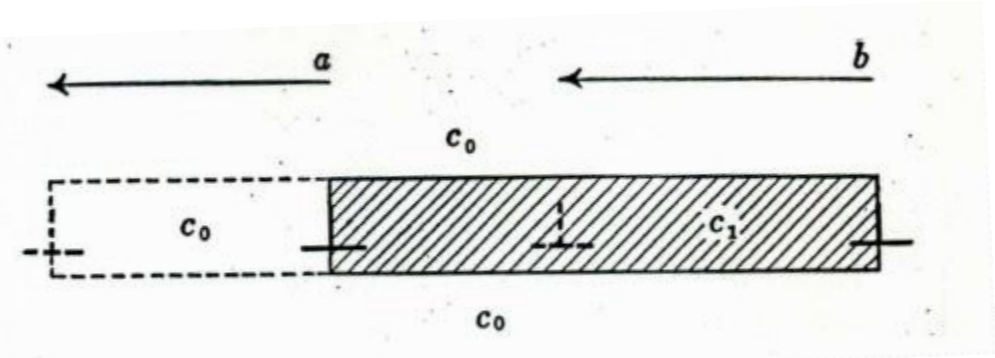
Many-body behavior of dislocations

単一転位の挙動 (Elementary Interaction process)[1]

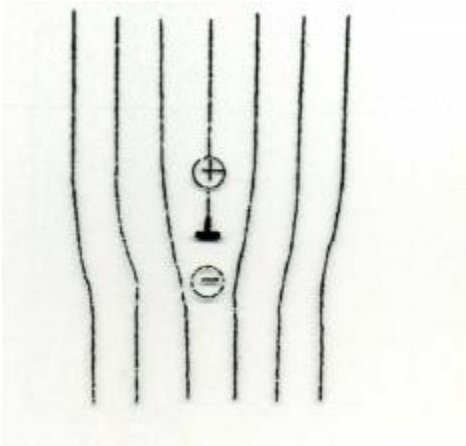
Elastic Interaction



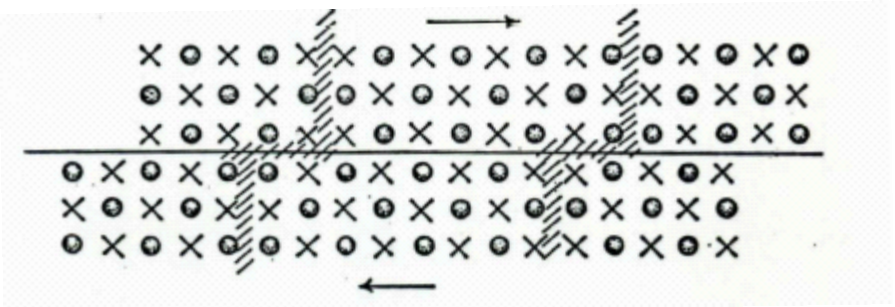
Chemical Interaction



Electric Interaction



Geometrical Interaction



Plasticity within dislocation theory

１．単一転位の挙動

Single dislocation behavior

２．単一転位の複数障害物場での挙動

Single dislocation behavior in the obstacle field

３．多数転位の（複数障害物場での）挙動

Many-body behavior of dislocations

単一転位の複数障害物場での挙動
Single dislocation behavior in the obstacle field

N_i **Number of *i*-th type obstacle**

f_i **Elementary interaction force with *i*-th type obstacle**

$$\tau = \sum N_i \cdot f_i \quad ?$$

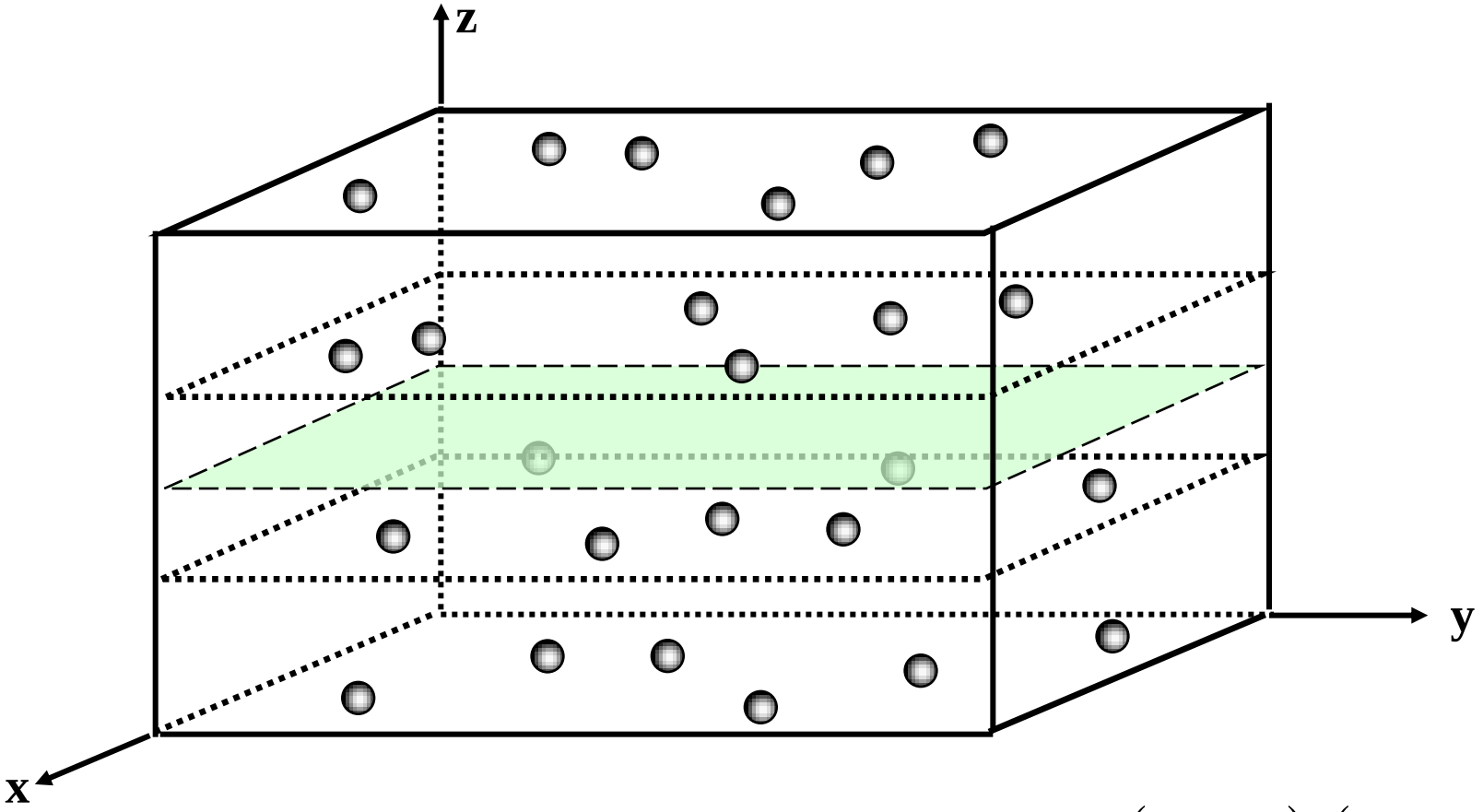
$$\tau = f\left(\Gamma, w, C, \text{distributi on}\right)$$

Γ **Line tension**

w **width of an obstacle**

C **concentration of an obstacle**

Single dislocation behavior



100 x 300 x 4

$$stress(x,y,z) = \frac{(y-y_s)\cdot(z-z_w)}{\left\{(x-x_s)^2+(y-y_s)^2+(z-z_s)^2+C\right\}^{5/2}}$$

String model of a dislocation

$$m\frac{\partial^2 y}{\partial t^2}+B\frac{\partial y}{\partial t}+\Gamma\frac{\partial^2 y}{\partial x^2}+\tau_{eff}\cdot b=0$$

m ;mass of a dislocation

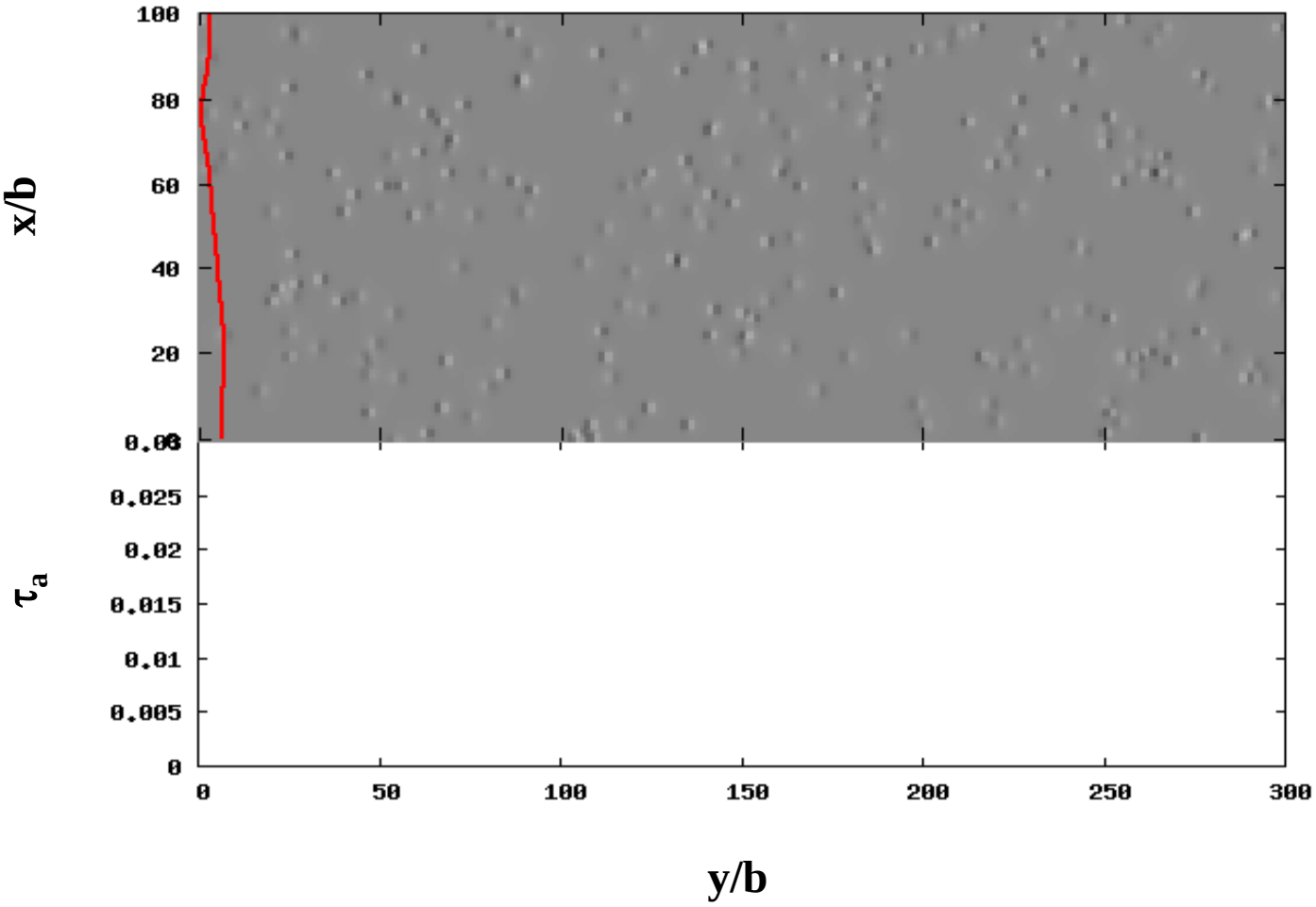
B ;damping

Γ ;line tension

τ_{eff} ;effective stress on a disloc.

$$\tau_{eff}=\tau_{appl.}-\tau_{\text{int.}}$$

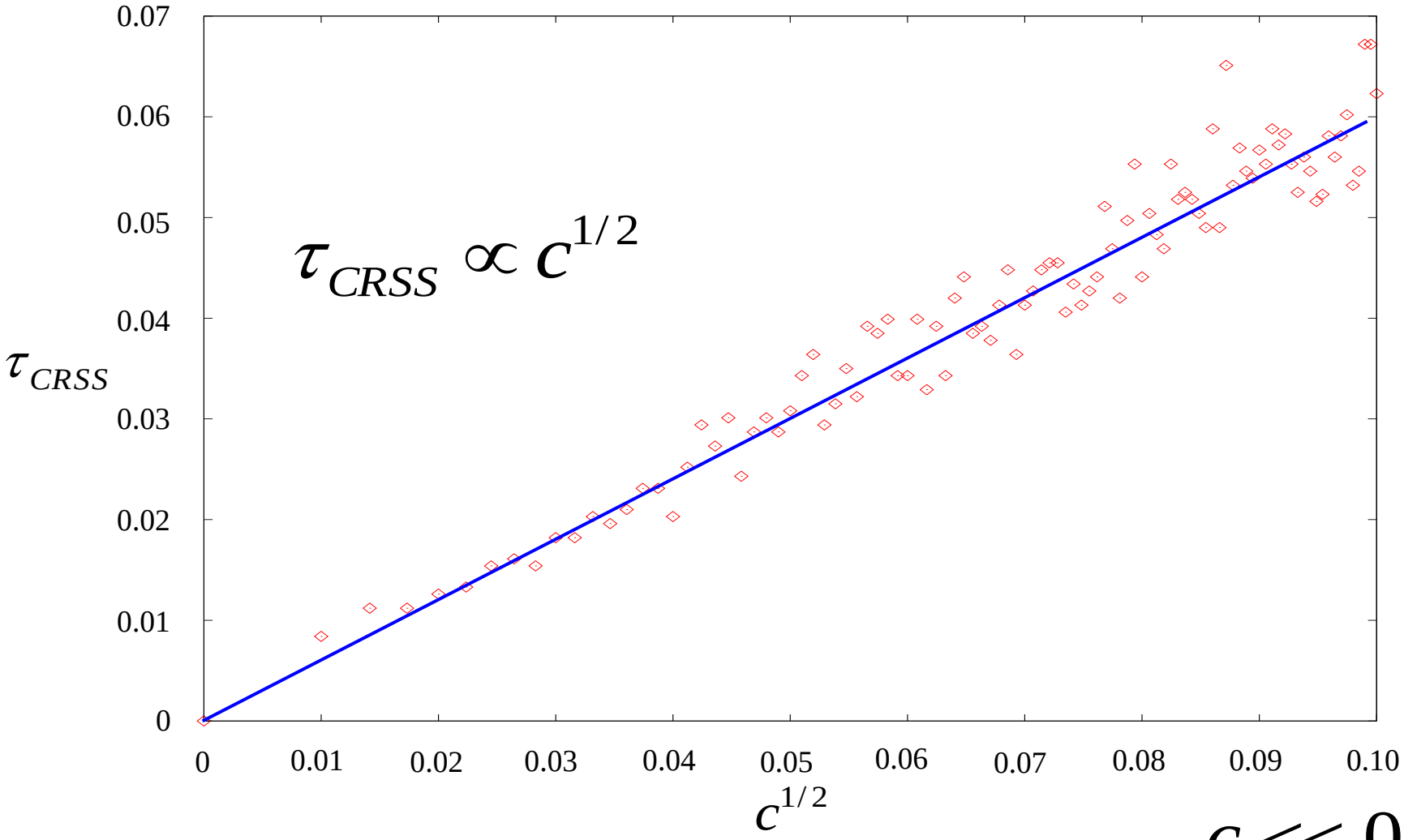
外部応力と転位の安定平衡位置



濃度c＝0.2 %

M. Fukushi BE Thesis Hokkaido U. (2007)

Friedel Regime



$c << 0.01$

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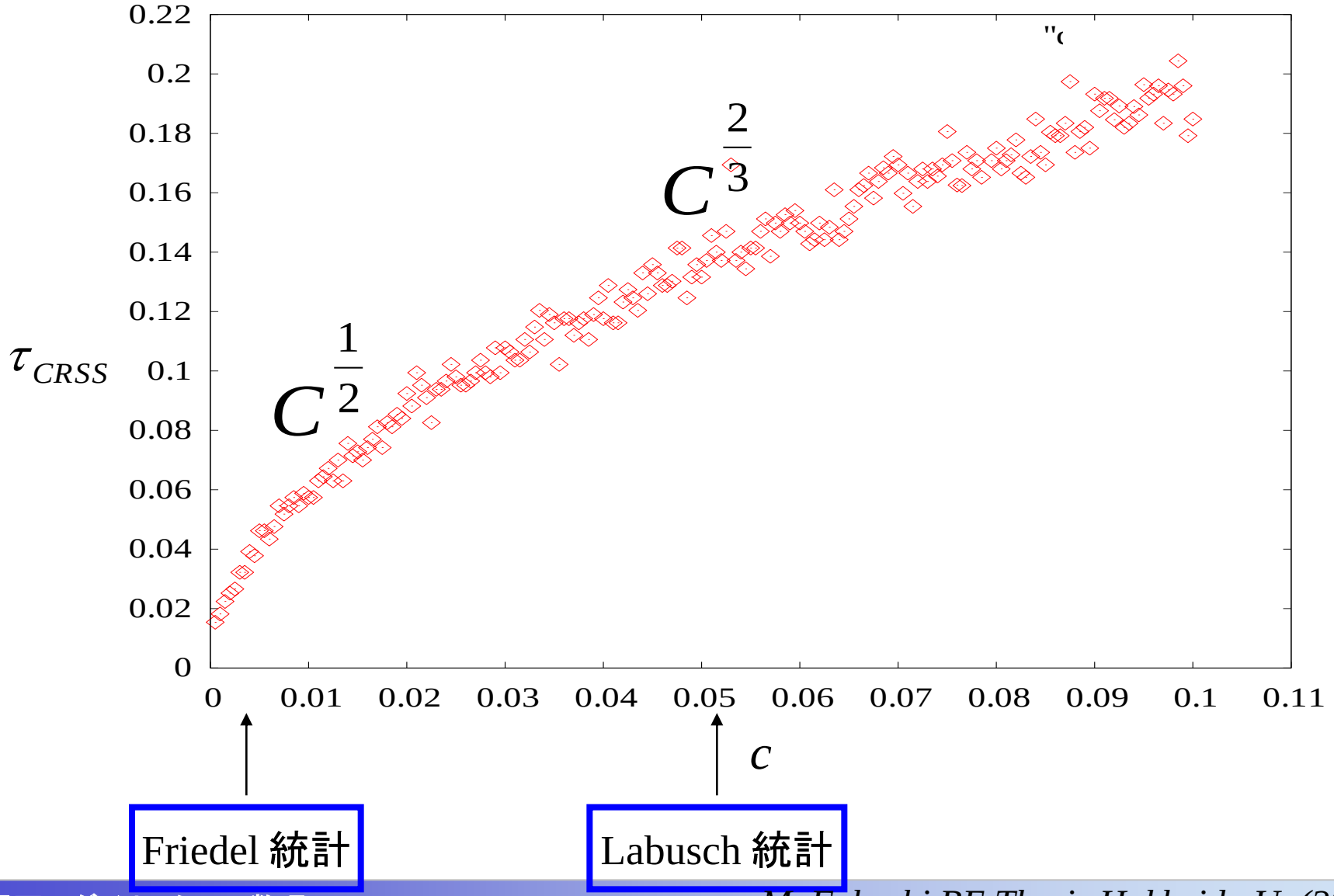
Other Regimes



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Plasticity within dislocation theory

１．単一転位の挙動

Single dislocation behavior

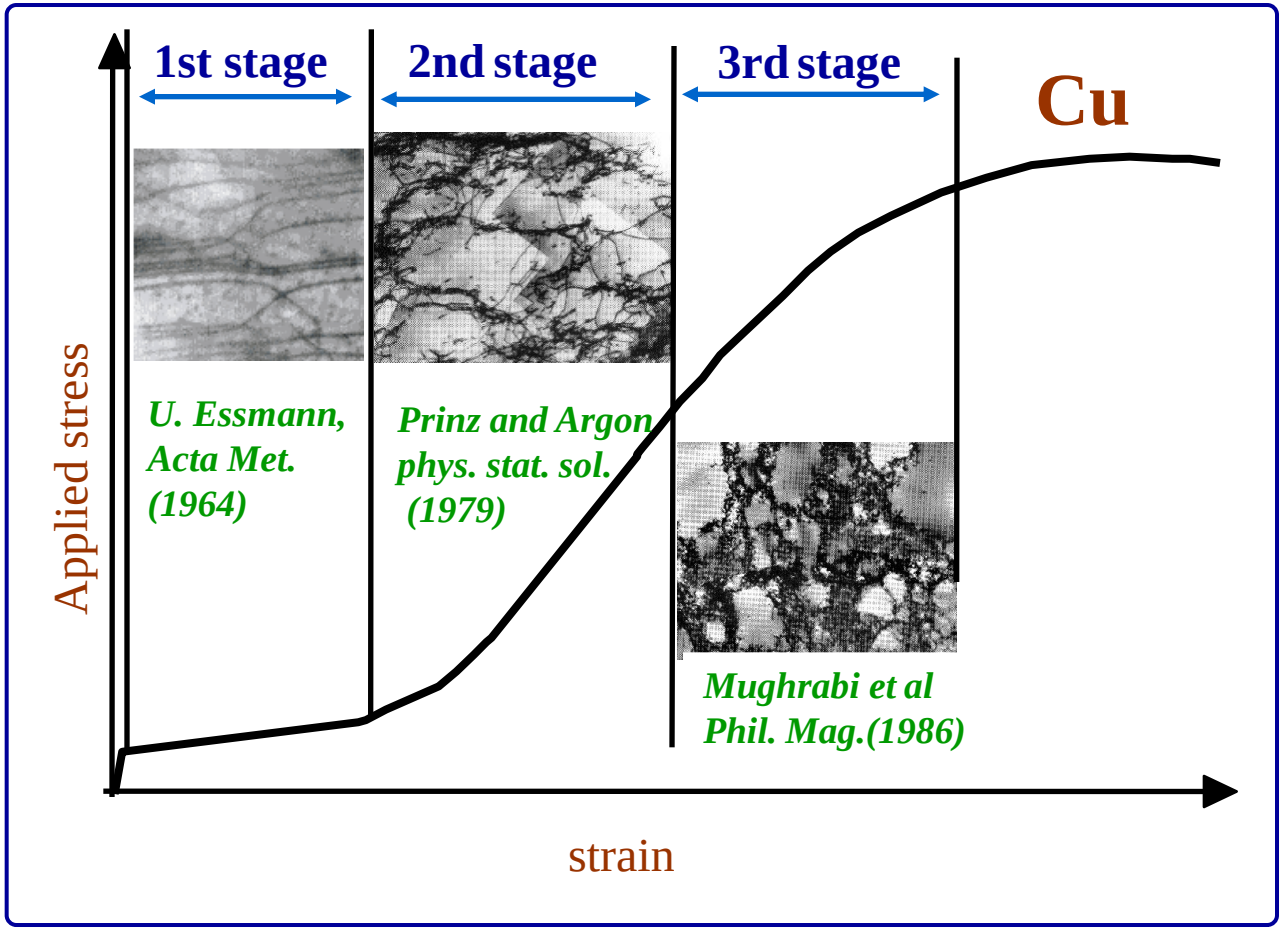
２．単一転位の複数障害物場での挙動

Single dislocation behavior in the obstacle field

３．多数転位の（複数障害物場での）挙動

Many-body behavior of dislocations

Actual situations



Dislocation reactions
Multiplication,
Dynamic recovery,
Immobilization/
mobilization of
mobile/immobile
dislocations
tangling

Heterogeneous distribution of dislocations

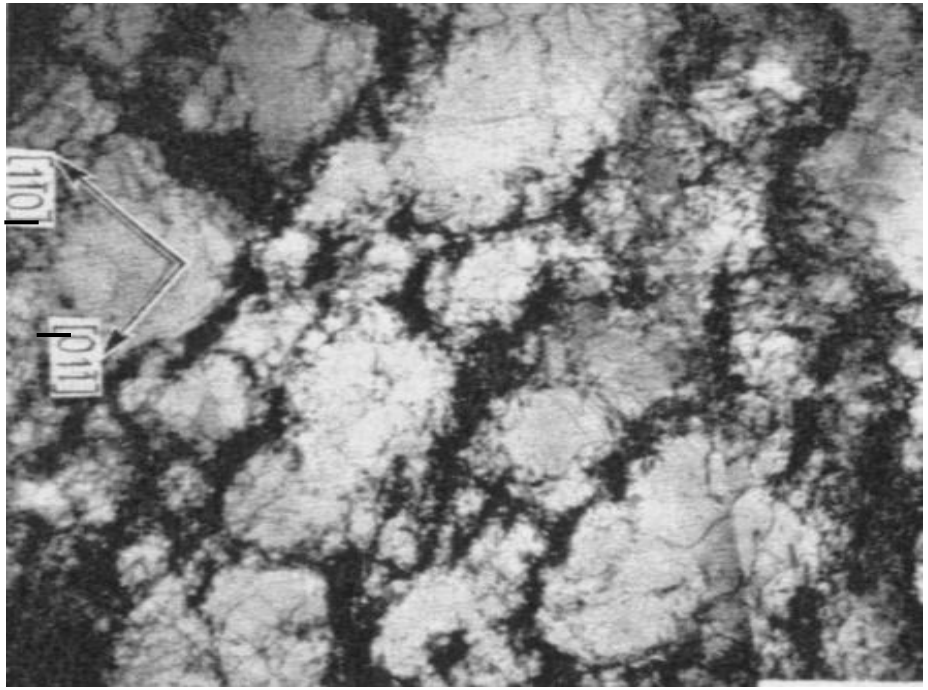
Example : Formation process of Persistent Slip Bands(PSBs)
C. Shiller and D. Walgraef: Acta Metall. 36, 3 (1988)

Reaction-Diffusion equation

Fatigue

T. Shoji Ph.D Thesis Hokkaido U. (2003)

Objective

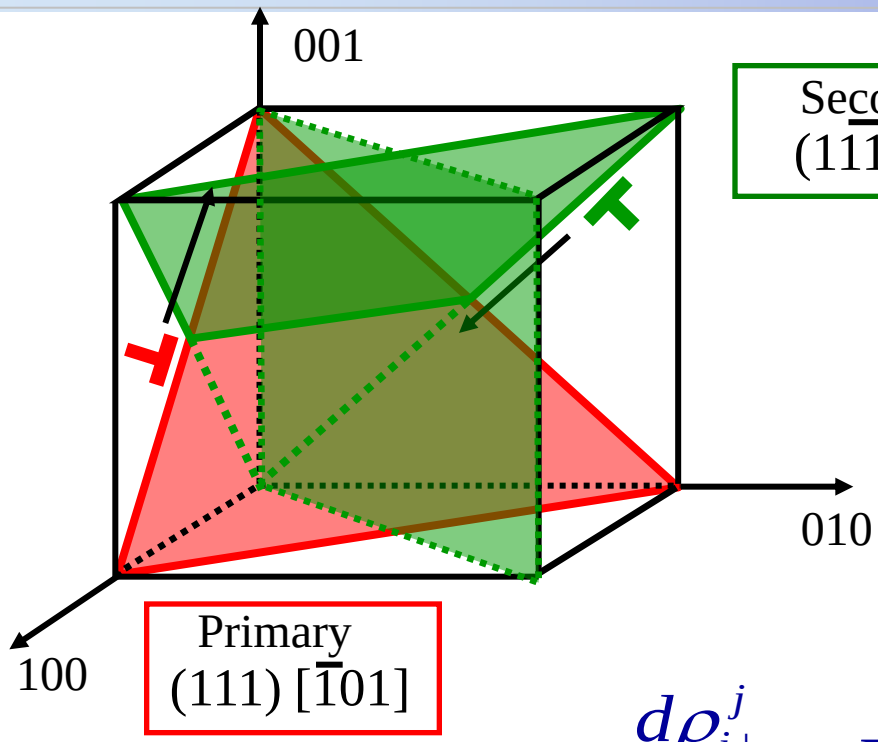


U. Essman : phys. stat.sol. (1963)

Calculation of a *S-S* curve under Constant Strain Rate Tensile Test

- Three stages of S-S curve
- dislocation microstructure
- **Energetic origin of dislocation structural formation**

Slip systems and evolution equations (R-D)



$\rho_{n\pm}^{j}$

- j: j-th slip system : $j = (p, s)$
- $n\pm$: Sign of Burgers vector
- n: immobile(i), mobile(m) : $n = (i, m)$

$$\frac{d\rho_{i\pm}^{j}}{dt} = D_i \nabla^2 \rho_{i\pm}^{j} + f_{i\pm}^{j}(\rho_{i\pm}^{j}, \rho_{m\pm}^{j}, \rho_{i\pm}^{k}, \rho_{m\pm}^{k})$$

Conservative motion of dislocation　　Reaction

$$\frac{d\rho_{m\pm}^{j}}{dt} = D_m \nabla_x^{\,2} \rho_{m\pm}^{j} \mp v_{m\pm}^{j} \nabla_x \rho_{m\pm}^{j} + f_{m\pm}^{j}(\rho_{i\pm}^{j}, \rho_{m\pm}^{j}, \rho_{i\pm}^{k}, \rho_{m\pm}^{k})$$

Glide motion

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R-D equation and Reaction terms

Mobile and Immobile

$$f^{j}_{n\pm}(\rho^{j}_{n\pm},\rho^{k}_{n\pm}) = f^{j}_{intra}(\rho^{j}_{n\pm}) + \sum_{k} f^{jk}_{inter}(\rho^{j}_{n\pm},\rho^{k}_{n\pm})$$

Intra slip system

Inter slip system

$$f^{j}_{intra}(\rho^{j}_{n\pm}) = f^{j}_{conservative}(\rho^{j}_{n\pm}) + f^{j}_{non-conservative}(\rho^{j}_{n\pm})$$

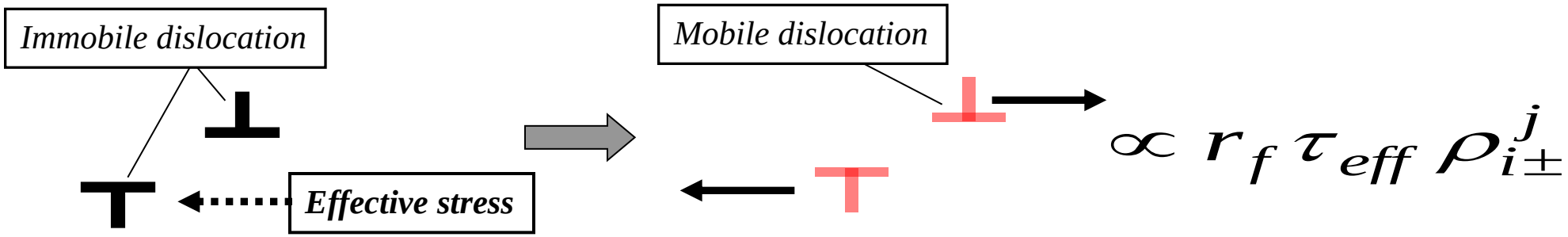
Conservative reaction

Non-conservative reaction

Reactions: Intra slip system; conservative

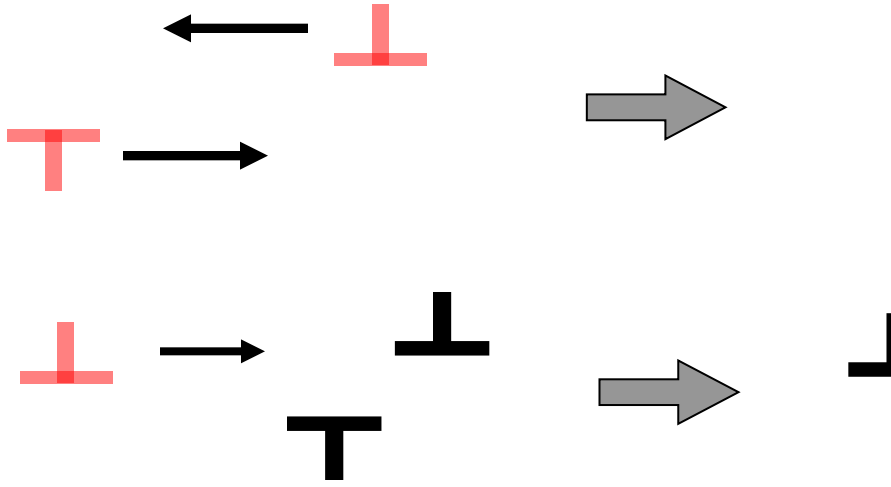
$$f^{j}_{intra}(\rho^{j}_{n\pm}) = f^{j}_{conservative}(\rho^{j}_{n\pm}) + f^{j}_{non-conservative}(\rho^{j}_{n\pm})$$

1. Mobilization



$$\propto r_f \tau_{eff} \rho^{j}_{i\pm}$$

2. Immobilization ; Dipolization・Multi-polization



$$\propto r_d v^{j}_{m} \rho^{j}_{m+} \cdot \rho^{j}_{m-}$$

$$\propto r_p v^{j}_{m} \rho^{j}_{m\pm} \cdot \rho^{j}_{i+} \cdot \rho^{j}_{i-}$$

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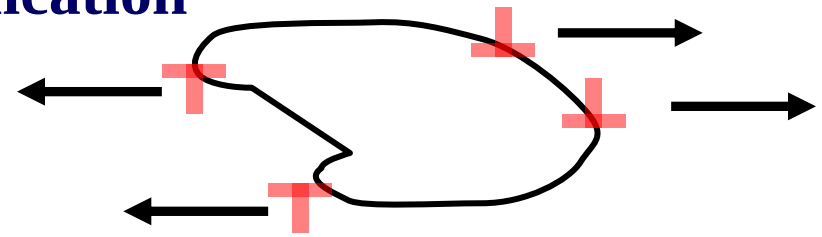
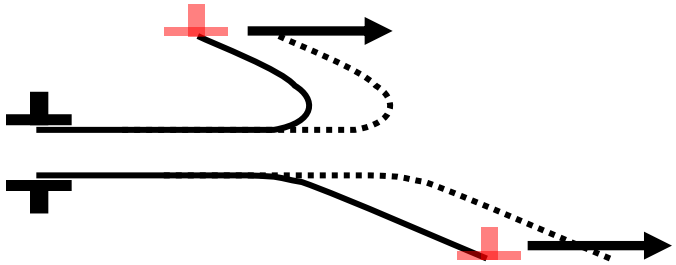
Reactions: Intra slip system; non-conservative

$$f^{j}_{intra}(\rho^{j}_{n\pm}) = f^{j}_{conservative}(\rho^{j}_{n\pm}) + f^{j}_{non-conservative}(\rho^{j}_{n\pm})$$

3. Multiplication

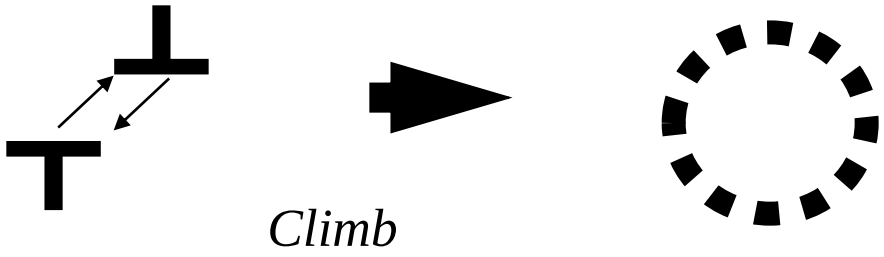


$$\propto r_{mm} v^{j}_{m} \rho^{j}_{m\pm}$$



$$\propto r_{im} v^{j}_{m} \rho^{j}_{m\pm} \cdot \rho^{j}_{i\pm}$$

4. Recovery

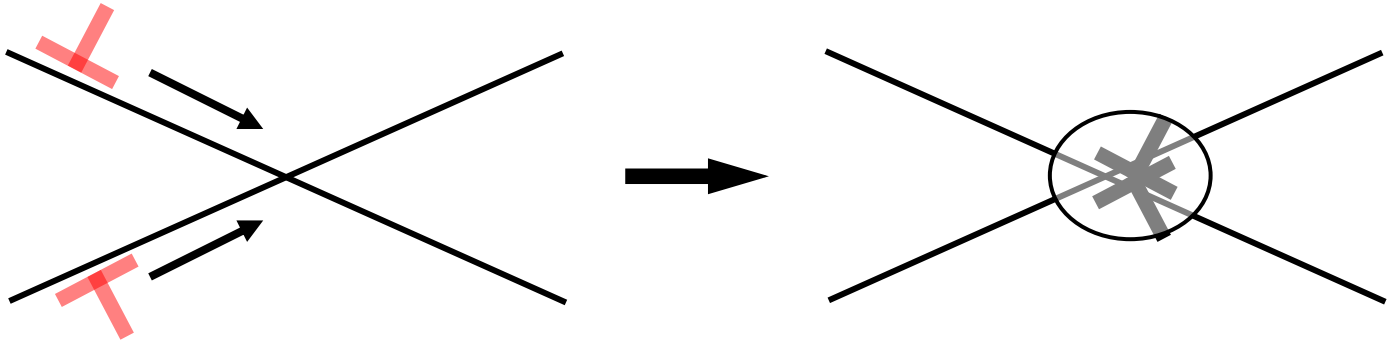


$$\propto r_{r} v_{i} \rho^{j}_{i+} \cdot \rho^{j}_{i-}$$

Reactions: Inter slip system

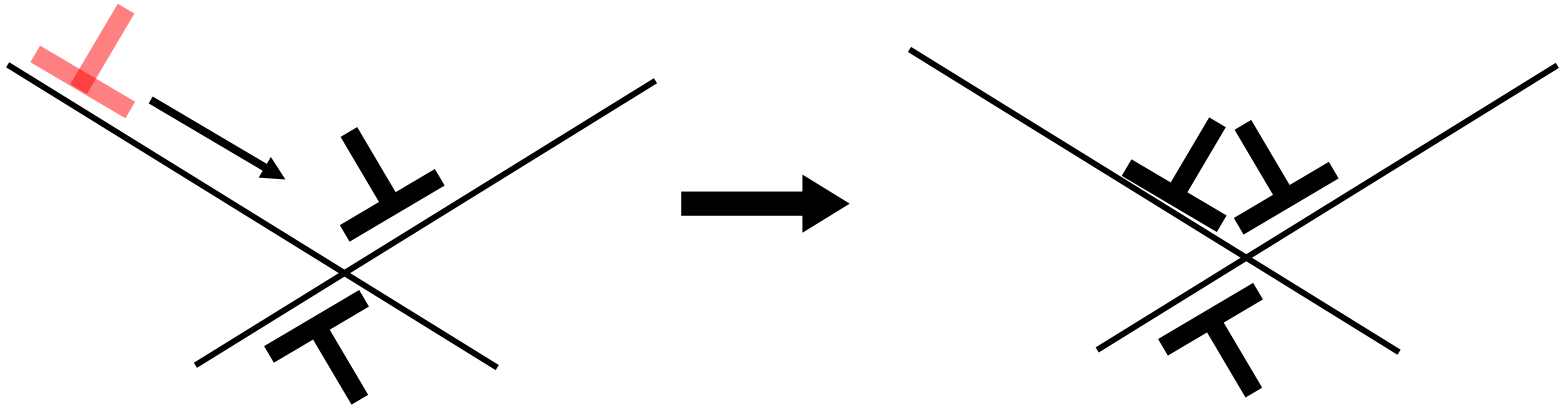
Lomer-Cottrell lock formation

$$\propto r_{LC} v_m^{jk} \rho_{m\pm}^{j} \cdot \rho_{m\mp}^{k} \quad (j,k = p,s \quad j \neq k)$$



Tangling of dislocations

$$\propto r_t v_m^{j} \rho_m^{j} \cdot \left(\rho_i^{k}\right)^2 (j,k = p,s \quad j \neq k)$$



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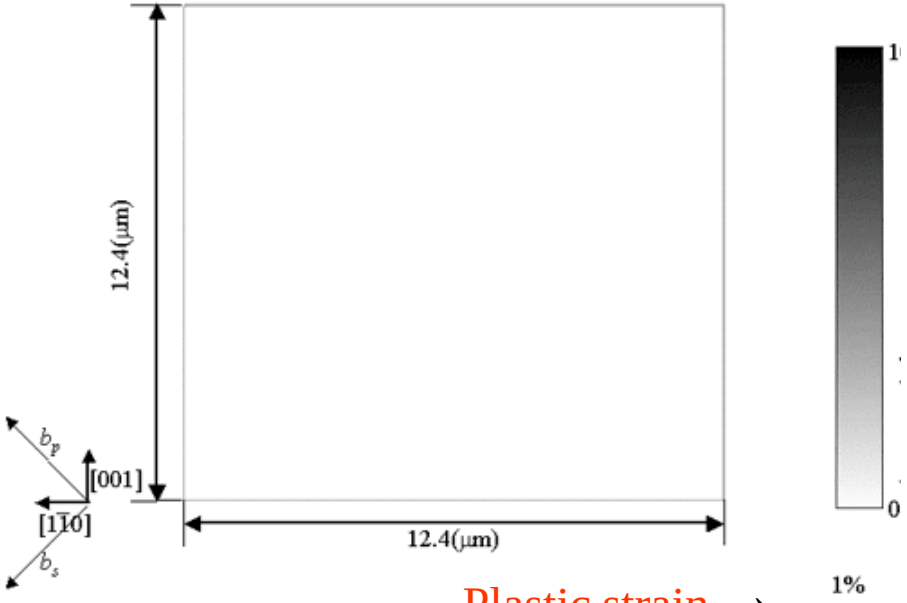
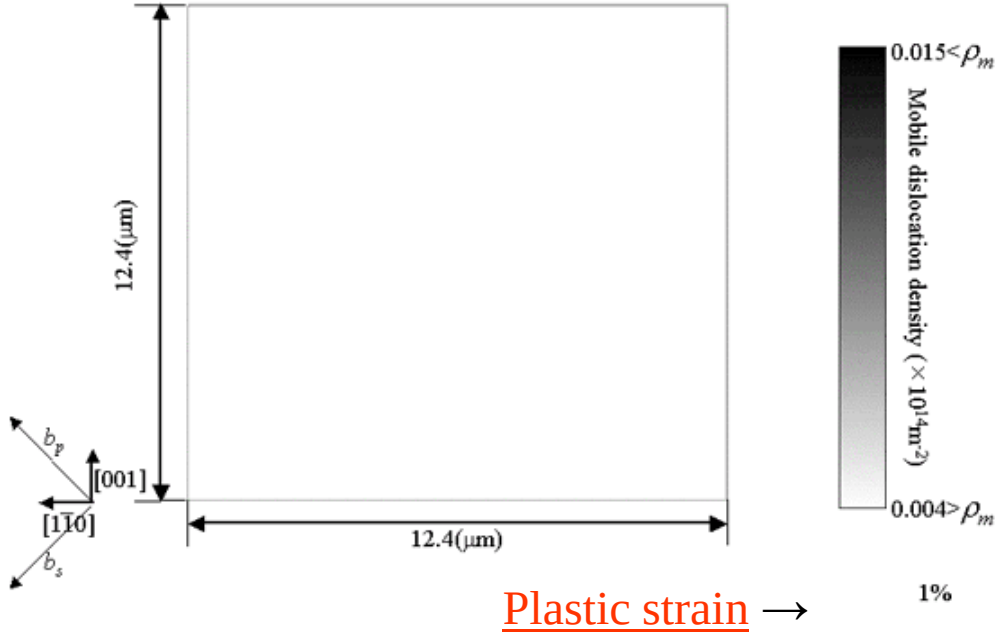
Evolution of dislocation structures

Immobile dislocation



Plastic strain →

Mobile dislocation



Plastic strain →

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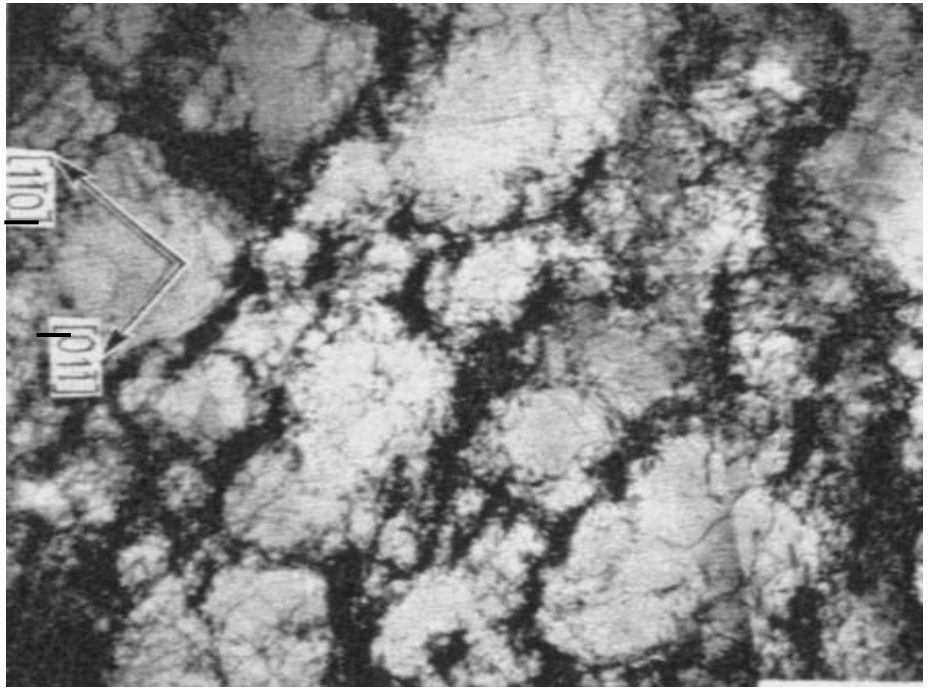
Objective



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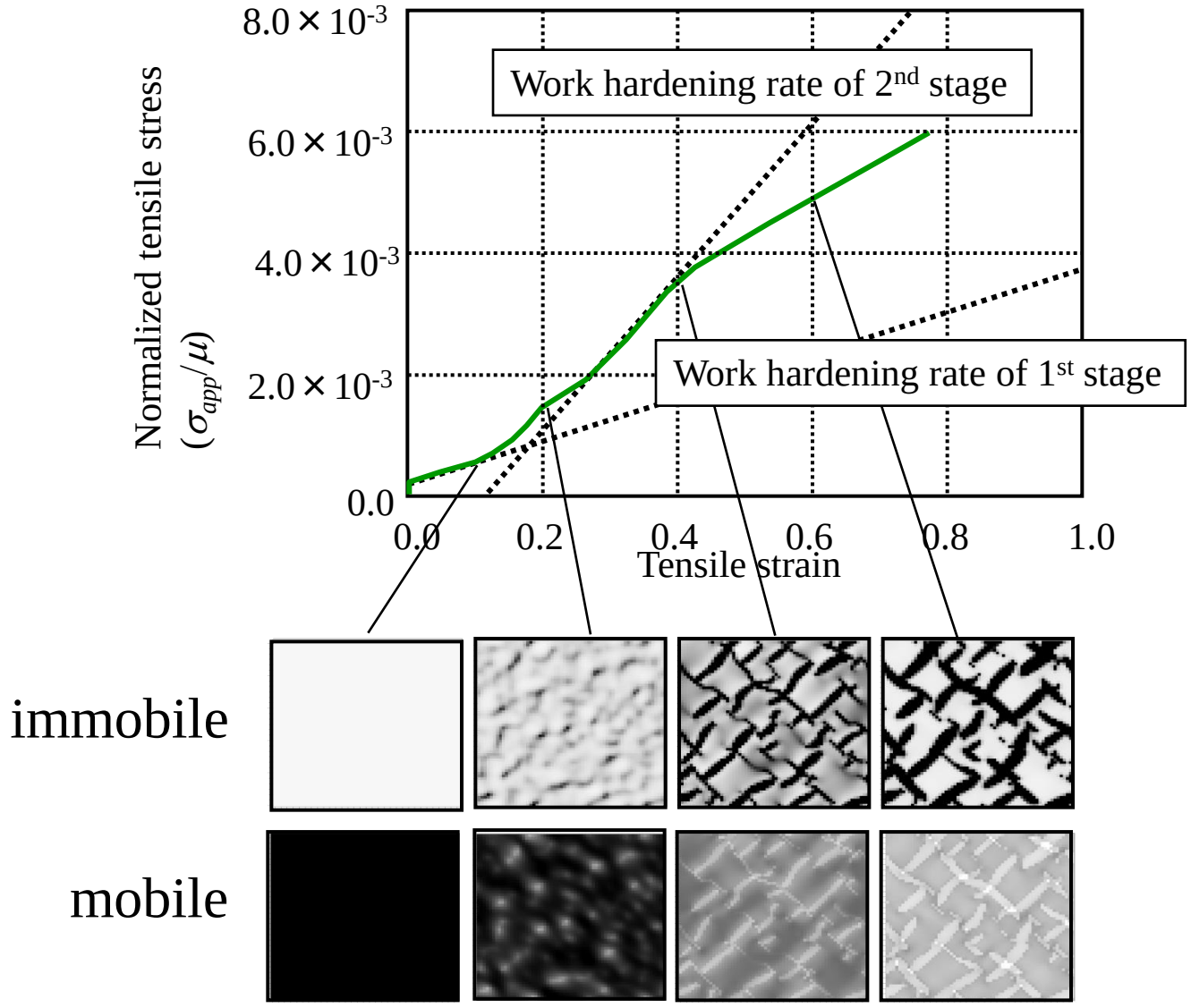
T. Shoji Ph.D Thesis Hokkaido U. (2003)

Stress-Strain Curve and Dislocation structure



T. Shoji Ph.D Thesis Hokkaido U. (2003)

変形の非平衡熱力学 **Non-equilibrium** Statistical Thermodynamics

弾性変形 (Elastic deformation）　外力下での系の静的平衡状態

Static equililbrium of a system under the applied stress

塑性変形 (Plastic deformation ）

降伏強度　(yielding), クリープ強度 (creep), 超塑性 (super plasticity)

etc.

転位密度(dislocation density),　内部組織　(microstructure) etc

外力下での系の状態の時間的変化　　非平衡状態

Time evolution process of a microstructure under the applied stress

原理？

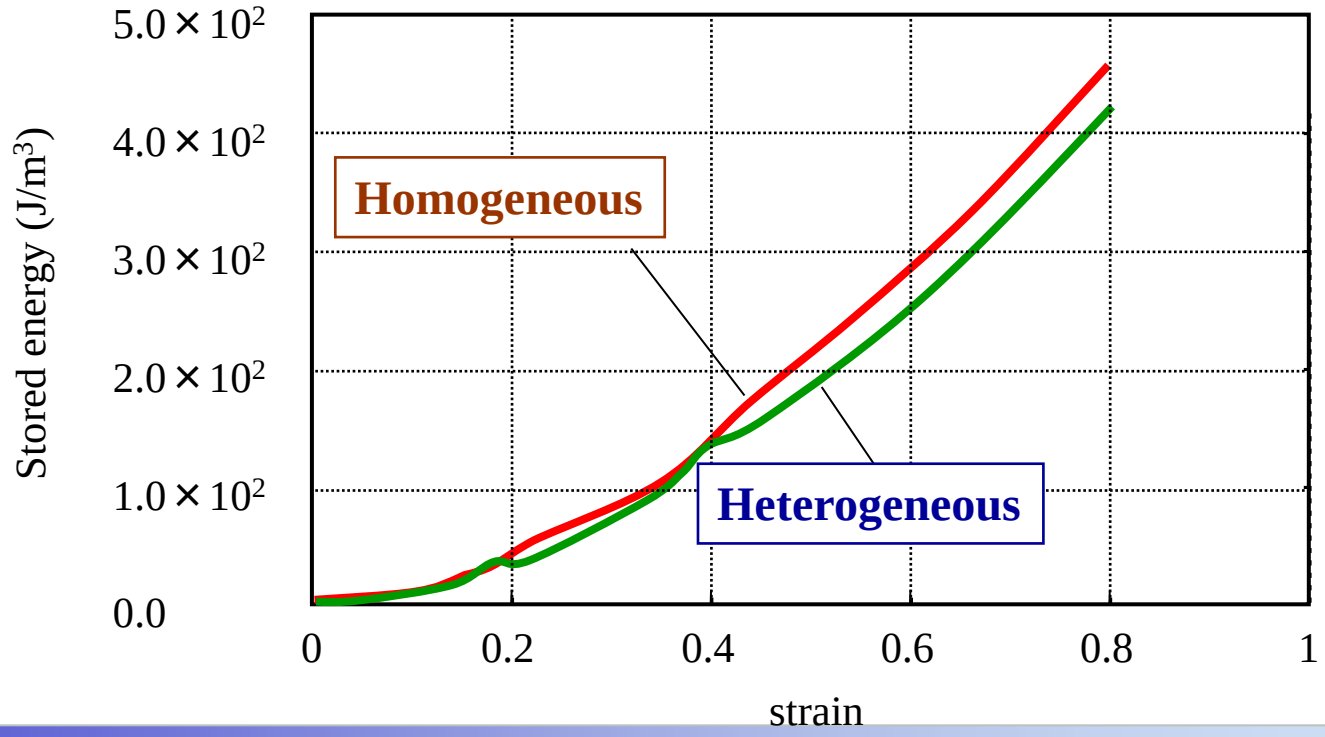
静止転位

Internal energy due to stored dislocations

Line energy of dislocation per unit length

$$e_{line}(\rho(\mathbf{x})) \approx \mu b^2 \frac{1-\upsilon/2}{4\pi(1-\upsilon)} \ln\left(\frac{1}{b(\rho(\mathbf{x}))^{1/2}}\right)$$

- Homogeneous distribution $E_{store}^{homo} = \langle\rho\rangle e_{line}(\langle\rho\rangle)$
- Heterogeneous distribution $E_{store}^{hetero} = \frac{1}{\Omega}\int_{\Omega} E_{store}^{local}(\rho(\mathbf{x}))d\mathbf{x} = \frac{1}{\Omega}\int_{\Omega} \rho(\mathbf{x}) e_{line}(\rho(\mathbf{x}))d\mathbf{x}$



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転位運動と変形

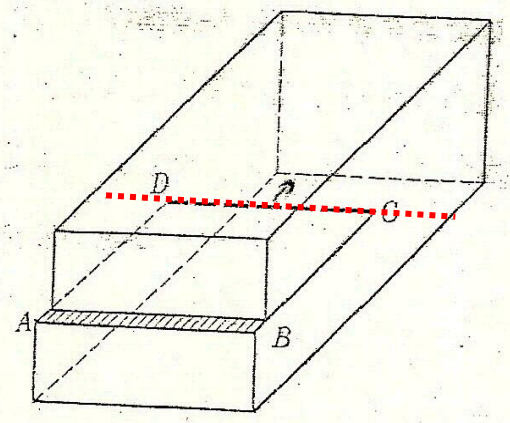
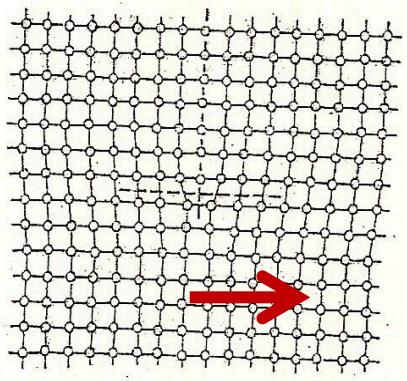


図 8·6　刃状転位によるすべり変形



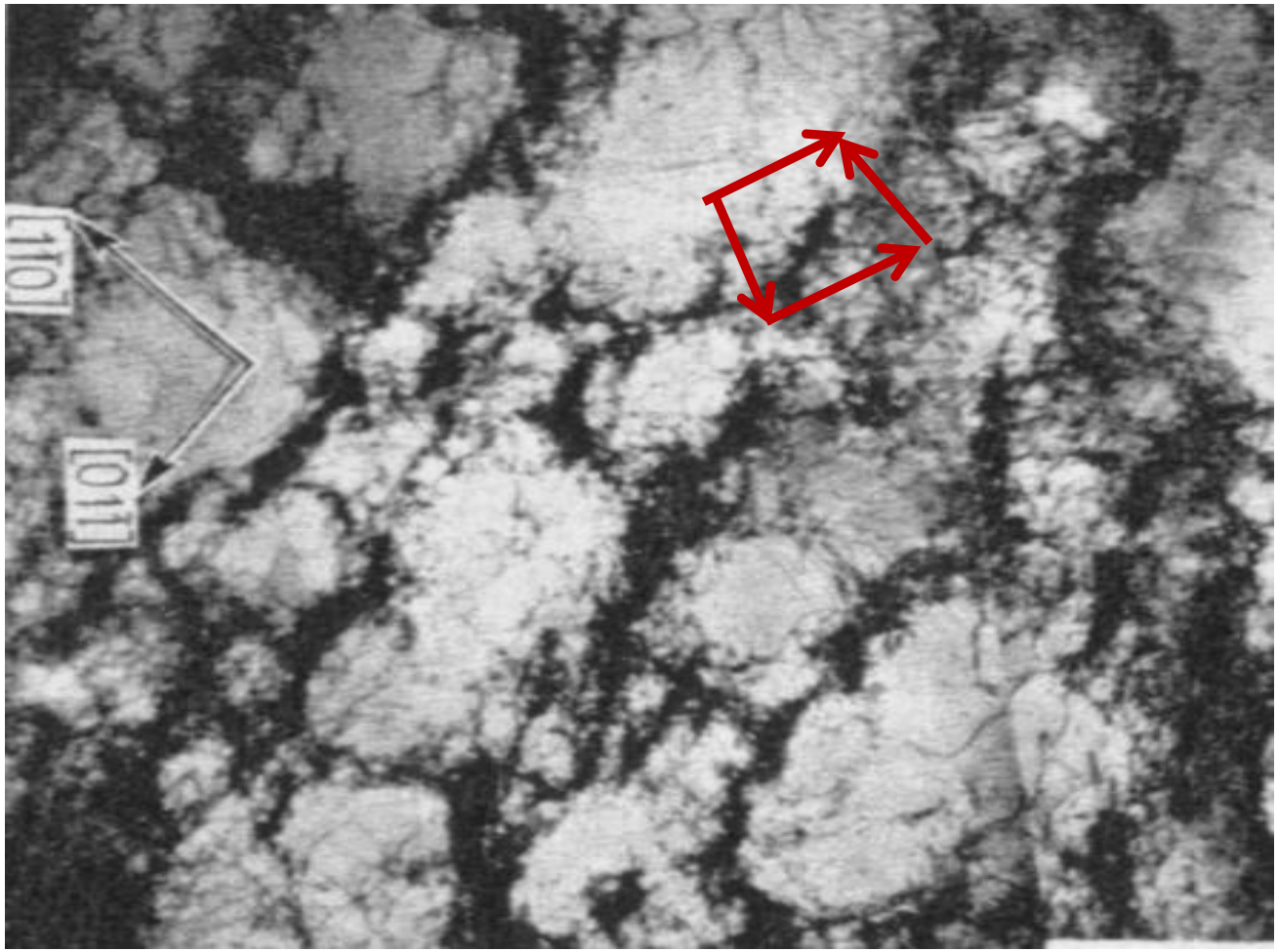
b

(a)　(b)

Burgers vector

多数転位の挙動 Many-body behavior of dislocations

静止転位（static dislocation） $\sum_i |\mathbf{b}_i|^2 = minimum$



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etc.

転位密度(dislocation density),　内部組織　(microstructure) etc

外力下での系の状態の時間的変化　　非平衡状態

Time evolution process of a microstructure under the applied stress

原理？

静止転位　　動転位??　　転位密度-応力??

保存則 Conservation law

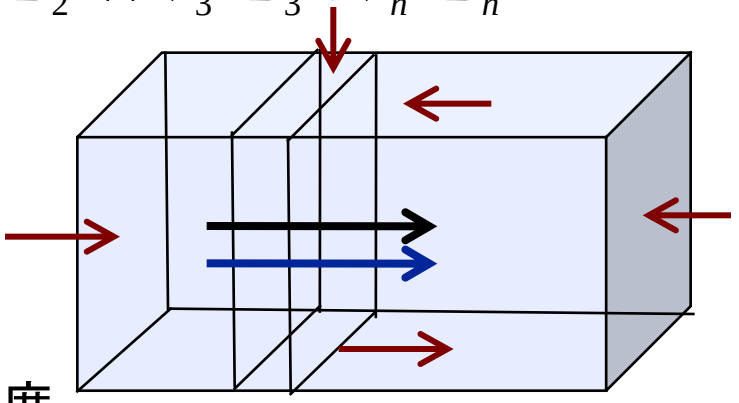
$$\frac{\partial n}{\partial t} = -\nabla \cdot \mathbf{J}_n + \Gamma \cdot \nu_n$$

$$\frac{\partial u}{\partial t} = -\nabla \cdot \mathbf{J}_u$$

$$\frac{\partial s}{\partial t} \neq -\nabla \cdot \mathbf{J}_s \qquad \dot{s} = \frac{\partial s}{\partial t} + \nabla \cdot \mathbf{J}_s$$

エントロピー生成速度
(entropy production rate)

$$\nu_1 \cdot B_1 + \nu_2 \cdot B_2 \leftrightarrow \nu_3 \cdot B_3 + \nu_n \cdot B_n$$



$$\rho \frac{du}{dt} = -\nabla \cdot \mathbf{J}_u + \sigma_{ij} \cdot \frac{\partial w_i}{\partial x_j}$$

熱エネルギー (thermal energy)

力学的エネルギー (mechanical energy)

n 粒子数 (number of species)

u 内部エネルギー(internal energy)

Γ 反応速度 (reaction rate)

ρ 密度(density)

σ_{ij} 応力 (stress)

w_i 速度(component of the velocity)

Energy conservation

$$\rho \frac{du}{dt} = -\nabla \mathbf{J}_u + \sigma_{ij} \cdot \frac{\partial w_i}{\partial x_j}$$

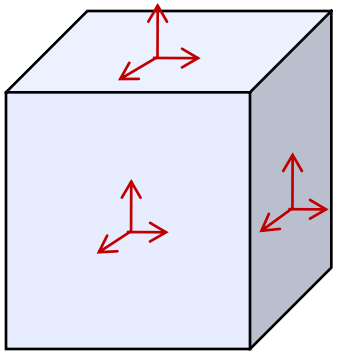
$$\frac{du}{dt} = -p \cdot \frac{\partial v}{\partial t} + \frac{1}{\rho} \sigma'_{ij} \cdot \frac{\partial w_i}{\partial x_j} - \frac{1}{\rho} \nabla \mathbf{J}_u$$

$$\frac{\partial w_i}{\partial x_j} = \dot{\varepsilon}_{ij} + \omega_{ij} \qquad \dot{\varepsilon}_{ij} = \frac{1}{2}\left\{\left(\frac{\partial w_i}{\partial x_j}\right) + \left(\frac{\partial w_j}{\partial x_i}\right)\right\} \qquad \omega_{ij} = \frac{1}{2}\left\{\left(\frac{\partial w_i}{\partial x_j}\right) - \left(\frac{\partial w_j}{\partial x_i}\right)\right\}$$

$$\frac{du}{dt} = -p \cdot \frac{\partial v}{\partial t} + \frac{1}{\rho} \sigma'_{ij} \cdot \dot{\varepsilon}_{ij} - \frac{1}{\rho} \nabla \mathbf{J}_u$$

w_i 速度(component of the velocity)

$$\sigma_{ij} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$$



ρ 密度(density)

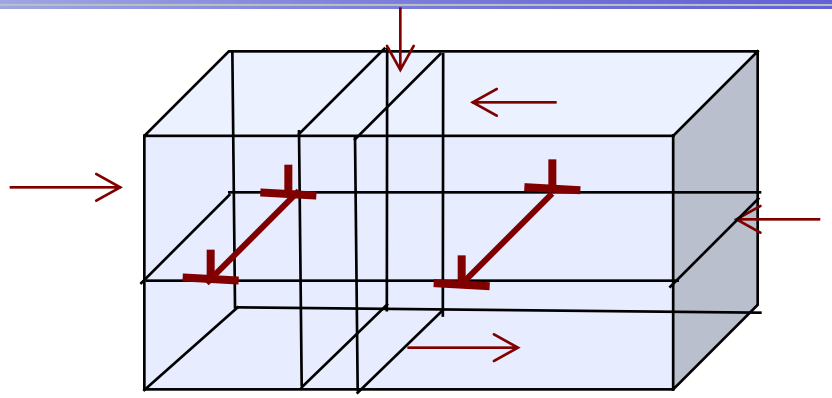
$\mathbf{J}_u$ 熱流束(component of the heat flux)

Local equilibrium and energy conservation

$$du = T \cdot ds - p \cdot dv + \lambda \cdot dN_d$$

N_d 転位密度 (dislocation density)

$$\lambda = \frac{\partial u}{\partial N_d}$$



$$\frac{du}{dt} = T \cdot \frac{\partial s}{\partial t} - p \cdot \frac{\partial v}{\partial t} + \lambda \cdot \frac{\partial N}{\partial t}$$

$$\sigma_{ij} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$$

$$\frac{du}{dt} = -p \cdot \frac{\partial v}{\partial t} + \frac{1}{\rho} \sigma'_{ij} \cdot \dot{\varepsilon}_{ij} - \frac{1}{\rho} \nabla \mathbf{J}_u$$

$$\mathbf{J}_s = \frac{1}{T} \mathbf{J}_u$$

$$\dot{s} = \frac{\partial s}{\partial t} + \nabla \cdot \mathbf{J}_s = \mathbf{J}_u \cdot \nabla \left(\frac{1}{T} \right) + \frac{1}{T} \left(\sigma_{ij} \cdot \dot{\varepsilon}_{ij} - \rho \cdot \lambda \cdot \frac{\partial N}{\partial t} \right)$$

K. Nishioka et al., (1978)

Entropy Production Rate

$$\dot{s} = \frac{\partial s}{\partial t} + \nabla \cdot \mathbf{J}_s = \mathbf{J}_u \cdot \nabla\left(\frac{1}{T}\right) + \frac{1}{T}\left(\sigma_{ij} \cdot \dot{\varepsilon}_{ij} - \rho \cdot \lambda \cdot \frac{\partial N}{\partial t}\right) = \frac{1}{T}\left(\tau \cdot \dot{\varepsilon} - \rho \cdot \lambda \cdot \frac{\partial N}{\partial t}\right)$$

$$\tau_{app} = \tau_{eff} + \tau_i + \tau_h$$

$$\dot{\varepsilon} = N_m \cdot \bar{v} \cdot b$$

$$\tau_h \cdot N_m \cdot \bar{v} \cdot b = \rho \cdot \lambda \cdot \frac{\partial N_m}{\partial t}$$

$$\bar{v} = k \cdot \tau_{eff}^{2/3}$$

$$\tau_i = C \cdot \sqrt{N_m}$$

τ_{app} 付加応力(applied stress)

τ_{eff} 有効応力(effective stress)。

τ_i 動転位の相互作用応力 (interaction stress)

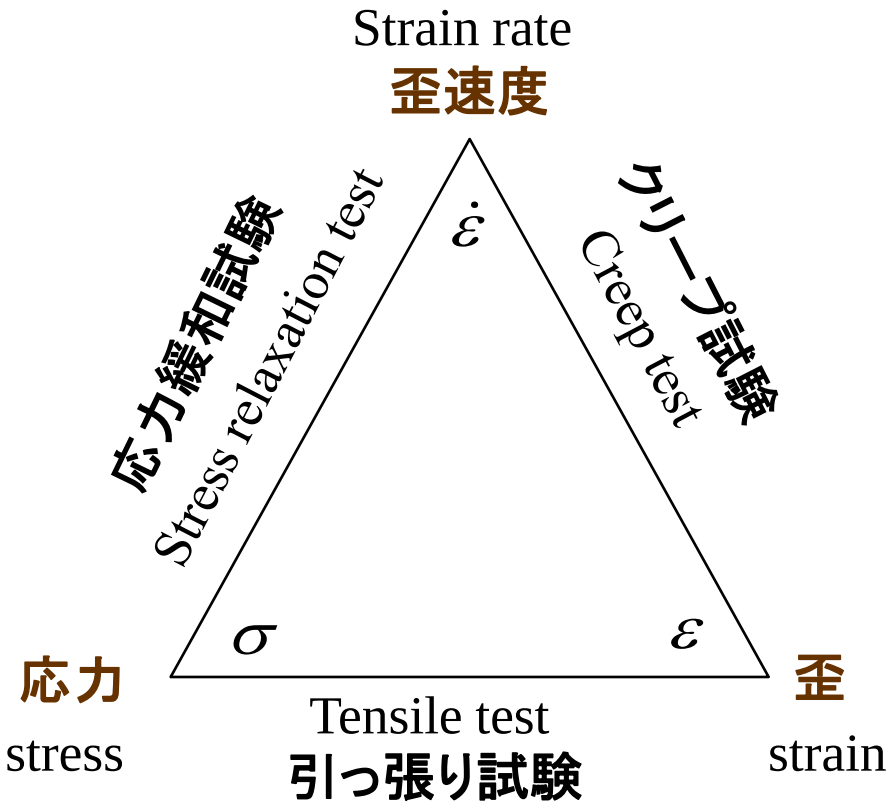
τ_h 加工硬化(work hardening)

$$\dot{s} = \frac{1}{T} \cdot \left\{ \left(\frac{\dot{\varepsilon}}{k \cdot b}\right)^{2/3} \cdot N_m^{-2/3} + C \cdot N_m^{1/2} \right\} = f\left(N_m\right)$$

$$\dot{s} = \left(\tau_{eff} + \tau_i\right) \cdot \dot{\varepsilon} = \tau\left(N\right) \cdot \dot{\varepsilon}$$

$$\left.\frac{\partial \dot{s}}{\partial N}\right|_{\dot{\varepsilon}} \propto \left.\frac{\partial \tau}{\partial N}\right|_{\dot{\varepsilon}}$$

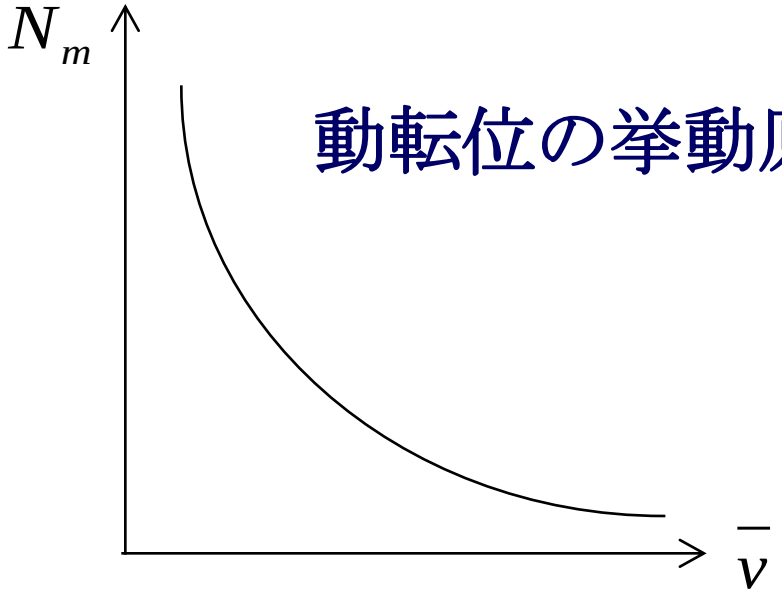
塑性変形の原理 (principle of deformation)



変形応力が一定の条件下では変形速度を最大とするように運動転位の密度が決定される。

$$\dot{s} = (\tau_{eff} + \tau_i)\cdot\dot{\varepsilon} = \tau(N)\cdot\dot{\varepsilon}$$

$$\left.\frac{\partial \dot{s}}{\partial N}\right|_{\dot{\varepsilon}} \propto \left.\frac{\partial \tau}{\partial N}\right|_{\dot{\varepsilon}}$$

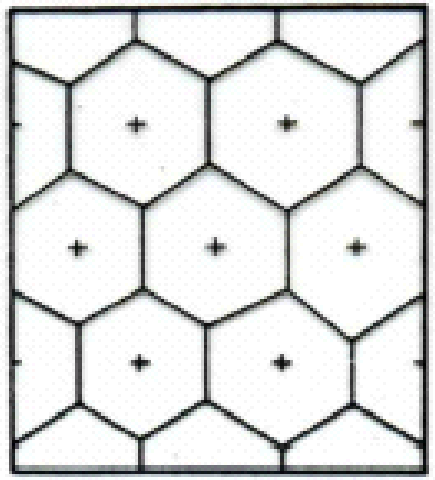


動転位の挙動原理

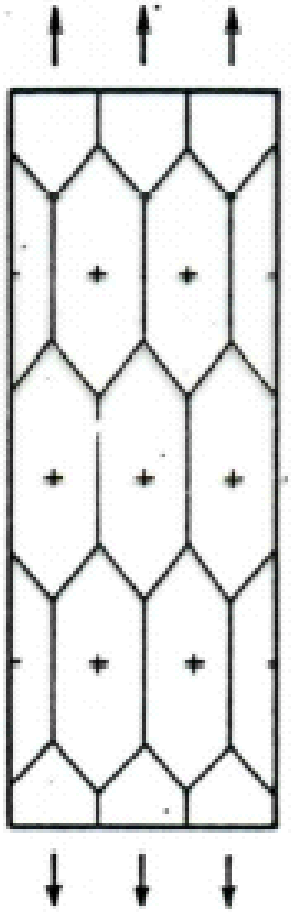
ひずみ速度一定条件下では（ある変形速度が与えられたとき）、運動転位の密度は、そのひずみ速度を保つのに必要な変形応力が最小となるように決まる。

K. Sumino (1971)

超塑性 (Superplasticity)



(a)



(b)

数ミクロン程度の微細結晶粒

高温変形

異常に大きな破断伸び

Non-equilibrium

Statistical Thermodynamics

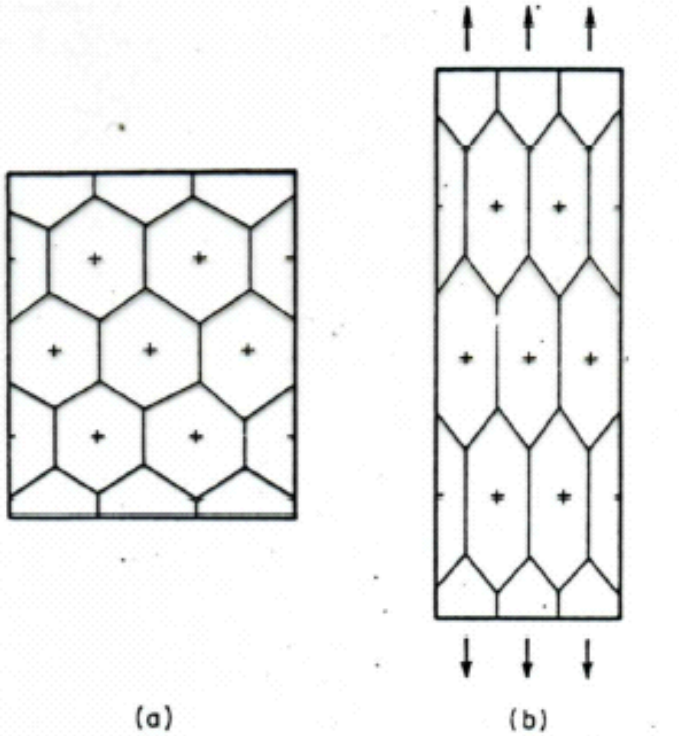
Refined grain

High temperature

Abnormal deformation

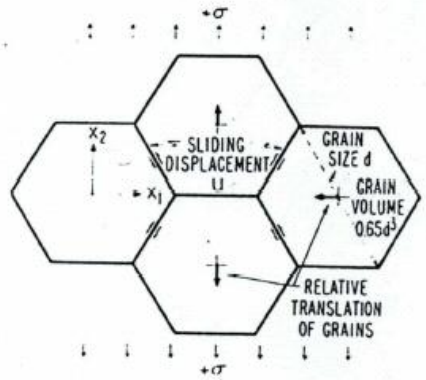
粒界すべり(超塑性)の**非平衡**統計熱力学

超塑性 (Super plasticity)

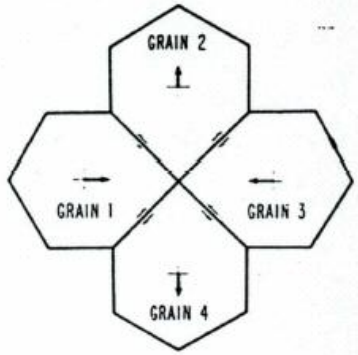


DIFFUSION-ACCOMMODATED FLOW AND SUPERPLASTICITY*

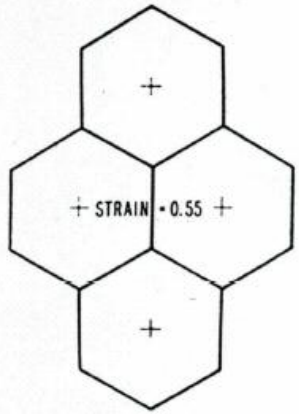
M. F. ASHBY† and R. A. VERRALL†



(a) INITIAL STATE



(b) INTERMEDIATE STATE



(c) FINAL STATE

超塑性 (Super plasticity)

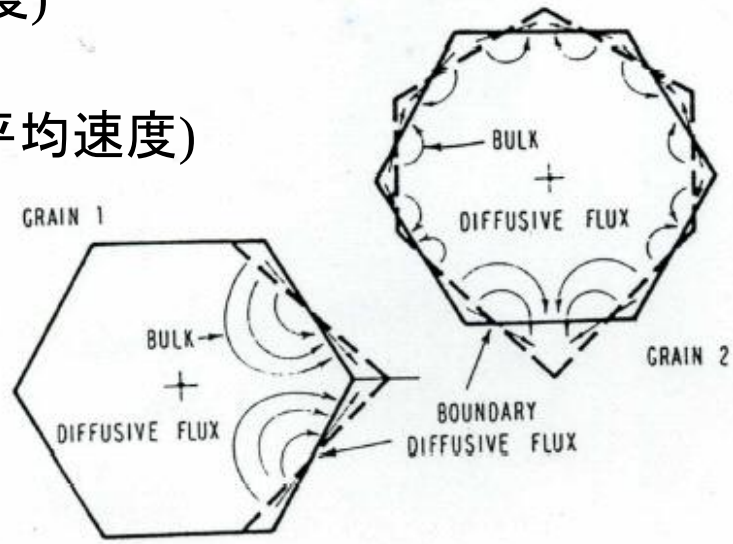
Slip deformation（すべり変形）

Strain rate(歪速度) $\dot{\varepsilon} = N_m \cdot \bar{v} \cdot b$

N_m Mobile dislocation density (可動転位密度)

$\bar{v}$ Average dislocation velocity (可動転位の平均速度)

b Burgers vector (バーガースベクトル)



Super plasticity (超塑性)

Strain rate(歪速度) $\dot{\varepsilon} = N_g \cdot \bar{\omega} \cdot \varepsilon_0$

N_g Rotational grain density (可動結晶粒密度)

$\bar{\omega}$ Average rotational velocity (可動粒の平均回転速度)

ε_0 回転の素過程の歪への寄与

Hall-Petch relation 1

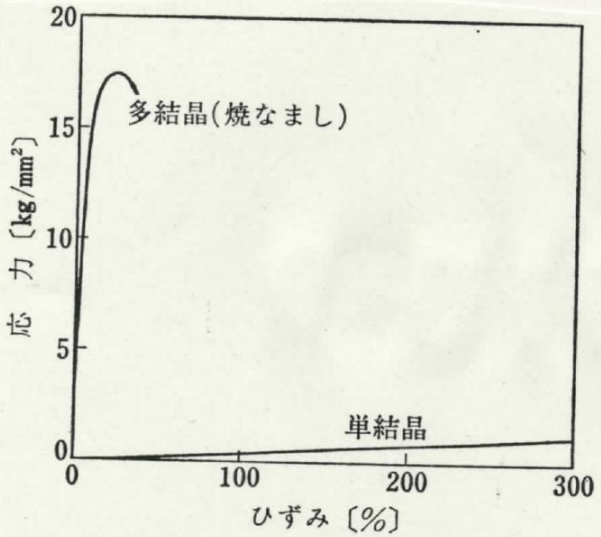


図 8・37　Zn の応力-ひずみ線図

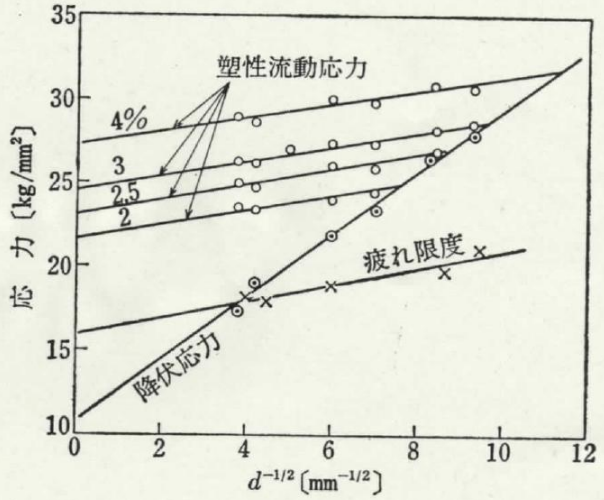


図 8・38　軟鋼（0.11%C）の機械的性質と結晶粒径 d との関係

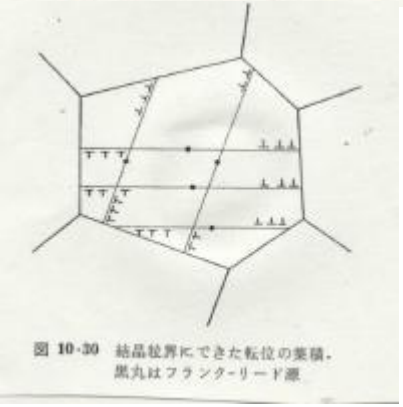


図 10・20　結晶粒界にできた転位の集積．黒丸はフランク-リード源

Hall-Petch relation 2

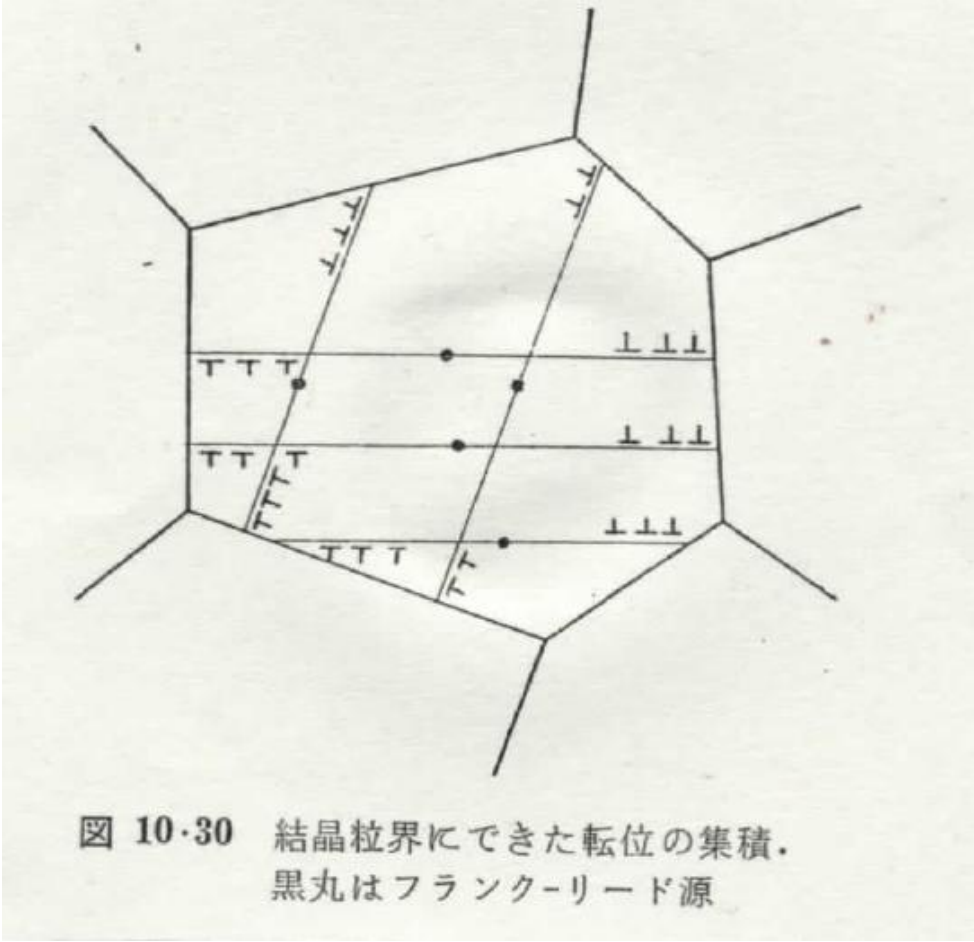


図 10·30 結晶粒界にできた転位の集積．
黒丸はフランクーリード源

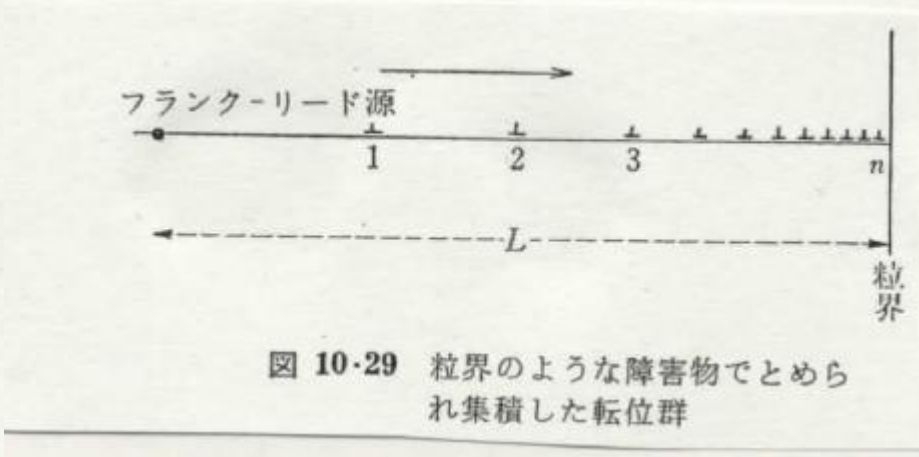
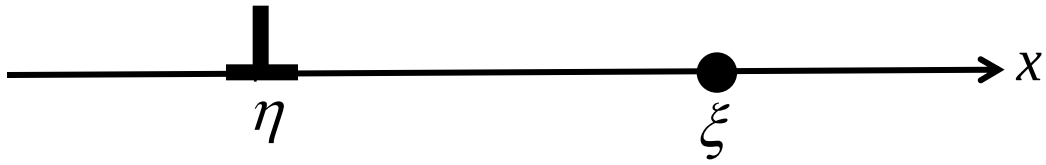


図 10·29 粒界のような障害物でとめられ集積した転位群

Hall-Petch relation 3

$$\tau(\xi) = \frac{A}{\xi - \eta}$$



$$\tau(\xi) = A\int \frac{D(x)}{\xi - x}dx$$

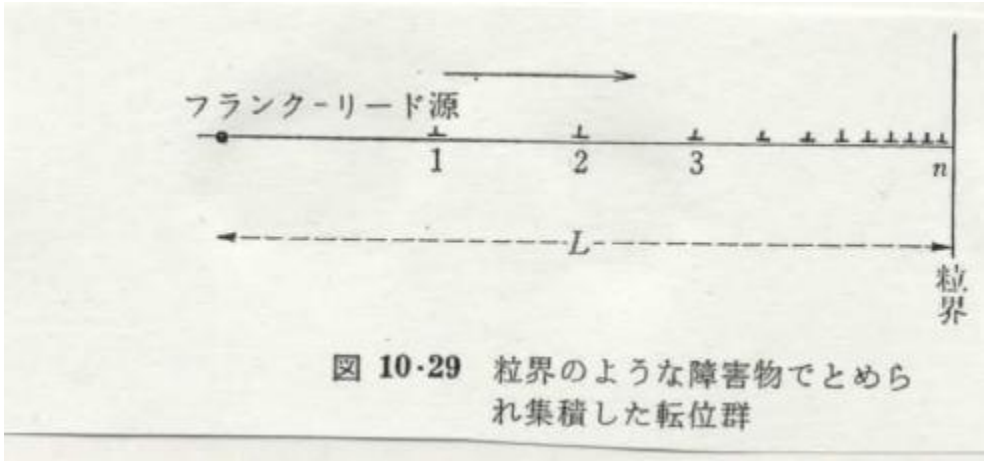


図 10·29 粒界のような障害物でとめられ集積した転位群

$$\tau(\xi) + \tau_a(\xi) = 0$$

$$\tau(\xi) + \tau_a(\xi) = \tau_f$$

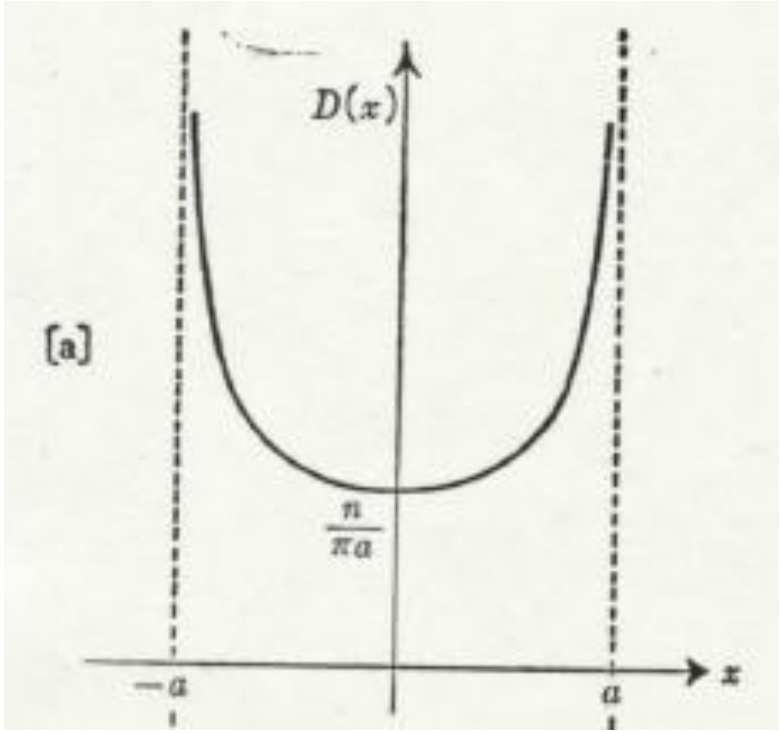
$$\tau_f - \tau_a(\xi) = A\int \frac{D(x)}{\xi - x}dx$$

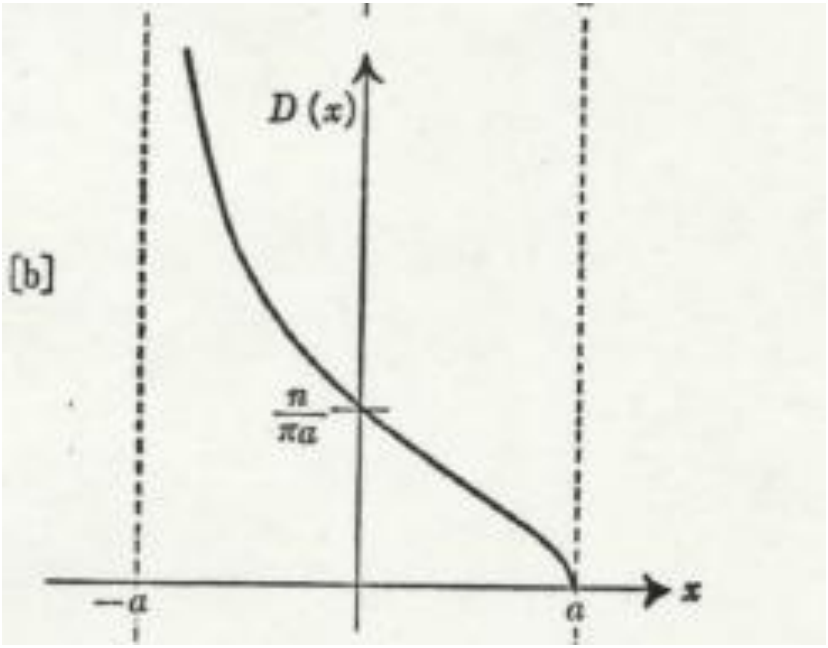
$$\int_{-a}^{+a} D(x)\cdot dx = n$$

Hall-Petch relation 4

$$\tau_a(\xi) = \tau_f = 0$$

$$\tau_a(\xi) = \text{constant}$$



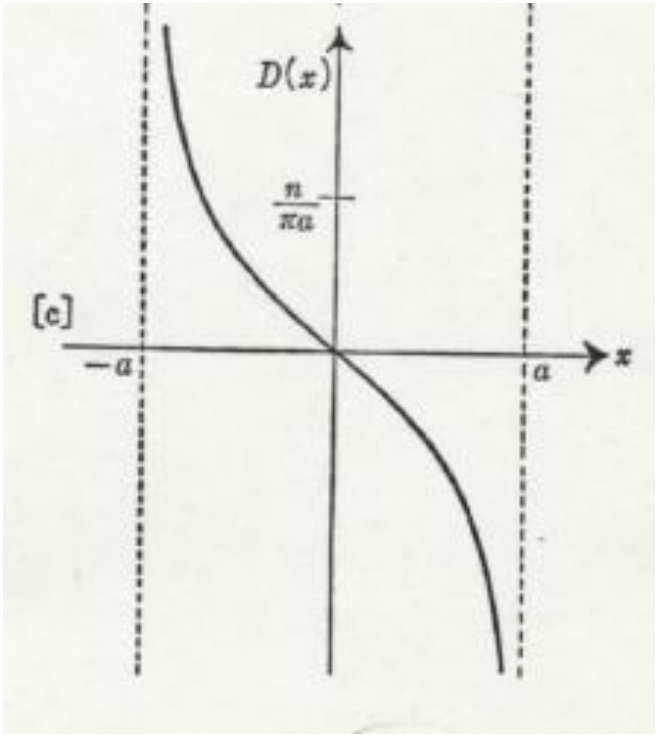


$$D(x) = \frac{n}{\pi} \cdot \frac{1}{\left(a^2 - x^2\right)^{1/2}}$$

$$D(x) = \frac{n}{\pi} \cdot \left(\frac{a-x}{a+x}\right)^{1/2}$$

Hall-Petch relation 5

$$\int_{-a}^{+a} D(x)\cdot dx = 0$$



$$D(x) = -\frac{(\tau_a - \tau_f)}{\pi A}\cdot\frac{x}{(a^2 - x^2)^{1/2}}$$

$$f(\delta) = A\int_{-a}^{+a}\frac{D(x)}{(a+\delta)-x}dx + \tau_a$$

$$f(\delta) = -\frac{\tau_a - \tau_f}{\pi}\int_0^{\pi}\frac{\cos\theta}{\left(1+\frac{\delta}{a}\right)-\cos\theta}d\theta + \tau_a$$

$$= (\tau_a - \tau_f)\left[-1+\frac{\delta + a}{\sqrt{2\delta a + \delta^2}}\right] + \tau_a$$

$$= (\tau_a - \tau_f)\frac{1}{\sqrt{2}}\sqrt{\frac{a}{\delta}} + \tau_f \qquad \delta \ll a$$

金属物理学序論　コロナ社　（1971）

Hall-Petch relation 6

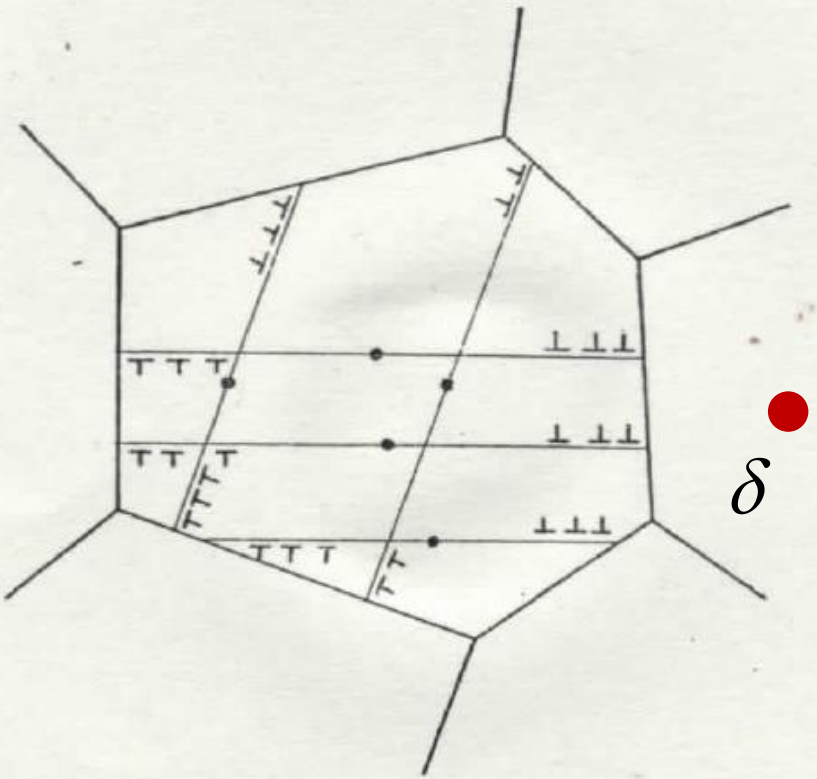


図 10·30 結晶粒界にできた転位の集積．黒丸はフランクーリード源

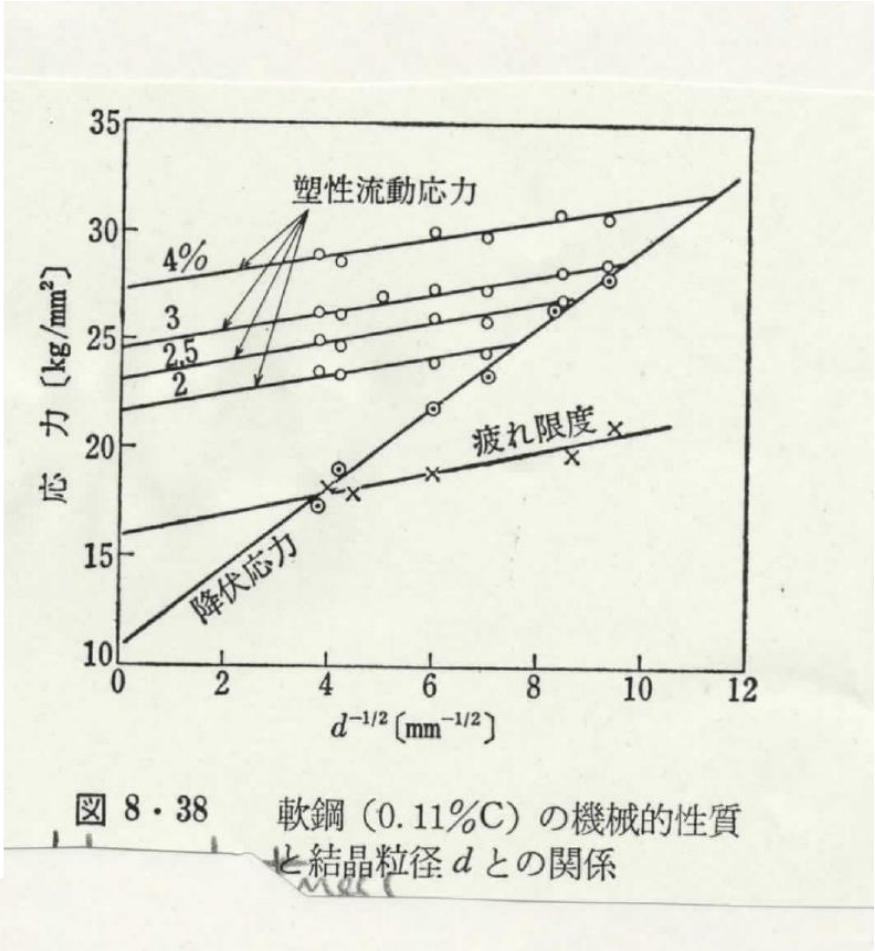


図 8・38 軟鋼（0.11%C）の機械的性質と結晶粒径 d との関係

$$\tau_a = \tau_f + (\tau_c - \tau_f)\sqrt{\delta}\cdot d^{-1/2}$$

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