Phase Field Methods: Microstructures and Dislocations

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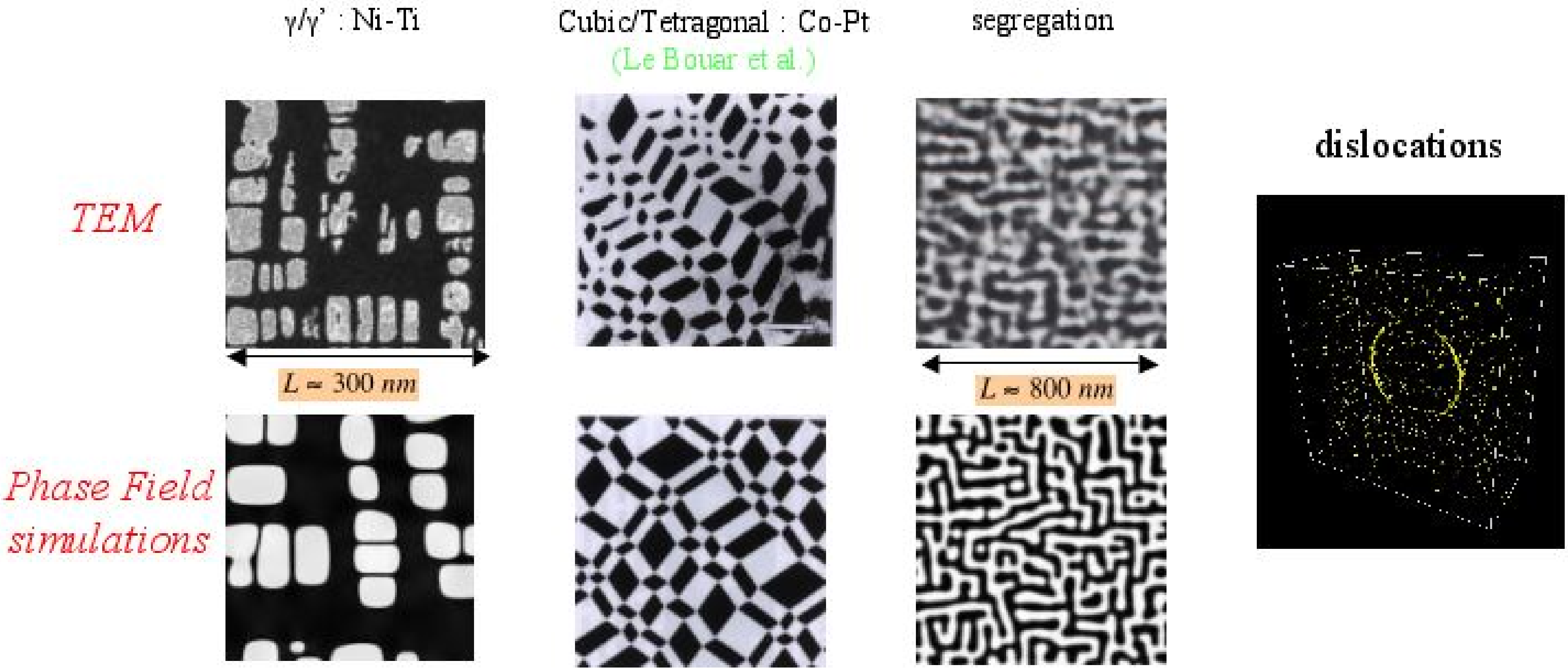
Phase field methods → study microstructures during phase transformations



Introduction of dislocations to study:

- Influence of dislocations on precipitation *(Heterogeneous precipitation)*
- Influence of precipitation on dislocations *(Alloy hardening)*

• Ex: Ginzburg-Landau free energy for a 2-phase separation

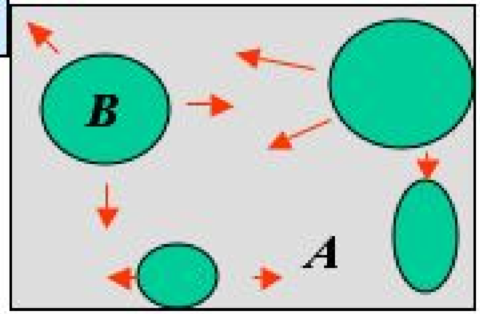
$$F_{chemical} = \int d^3r \left\{ -\frac{\mu}{2}\phi(r)^2 + \frac{\gamma}{4}\phi(r)^4 + \frac{\lambda}{2}\|\nabla\phi(r)\|^2 \right\}$$

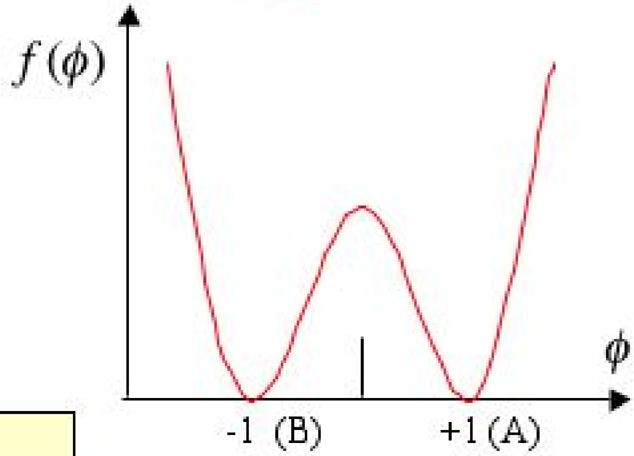
$$\phi(r) = c(r) - \bar{c}$$

→ Short range interactions

→ Fluctuations smaller than d are averaged out *(coarse-graining)*

→ *choice of the lenght scale d*





• Elastic energy in coherent systems:

field $\phi_p(r)$ → *eigenstrain* $\varepsilon^0_{ij}(r) = \varepsilon^0_{ij}(p)\,\phi_p(r)$

→ *elastic energy* $E_{strain} = \frac{1}{2}\int \lambda_{ijkl}\,\{\varepsilon_{ij}(r) - \varepsilon^0_{ij}(r)\}\,\{\varepsilon_{kl}(r) - \varepsilon^0_{kl}(r)\}$

Vegard law: $\varepsilon^0_{ij} = \lambda\,\delta_{ij}$

Tetragonal precipitates: $\varepsilon^0_{xx} = \frac{a - a_0}{a_0}$

$\varepsilon^0_{yy} = \frac{a - a_0}{a_0}$

$\varepsilon^0_{zz} = \frac{c - a_0}{a_0}$

Elastic equilibrium → $\varepsilon_{ij}(r)$ *such that* E_{strain} *minimum*

→ $E_{strain} = \frac{V}{2}\sum_{p,q}\sum_{k} B_{p,q}(k)\,\phi_p(k)\,\phi_q(k)^*$

→ $B_{p,q}(k) = \lambda_{ijkl}\,\varepsilon^0_{ij}(p)\,\varepsilon^0_{kl}(q) - k_i\,\sigma^0_{ij}(p)\,\Omega_{jl}(\vec{k})\,\sigma^0_{lk}(q)\,k_k$

$\Omega^{-1}_{ij}(k) = \lambda_{imjl}\,k_m\,k_l$

$\sigma^0_{ij}(p) = \lambda_{ijkl}\,\varepsilon^0_{kl}(p)$

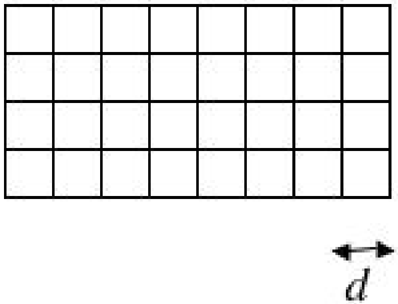
$\|k\| \le \frac{2\pi}{d}$

Kinetics equations

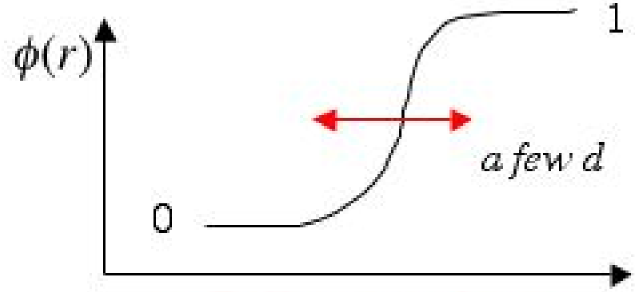
conserved : $$\frac{\partial \phi(r)}{\partial t} = \Gamma \nabla^2 \frac{\partial (F_{chemical} + E_{strain})}{\partial \phi(r)}$$

non − conserved : $$\frac{\partial \phi(r)}{\partial t} = -\Gamma \frac{\partial (F_{chemical} + E_{strain})}{\partial \phi(r)}$$

Simulations



grid spacing "d"
$\phi(r)$ continuous
→



« Diffuse interface »

$$E_{strain} = \frac{V}{2} \sum_{p,q} \sum_{k} B_{p,q}(k)\, \phi_p(k)\, \phi_q(k)^*$$

$$F_{chemical} = \int d^3 r \left\{ -\frac{\mu}{2}\phi(r)^2 + \frac{\gamma}{4}\phi(r)^4 + \frac{\lambda}{2}\left\| \nabla \phi(r) \right\|^2 \right\}$$

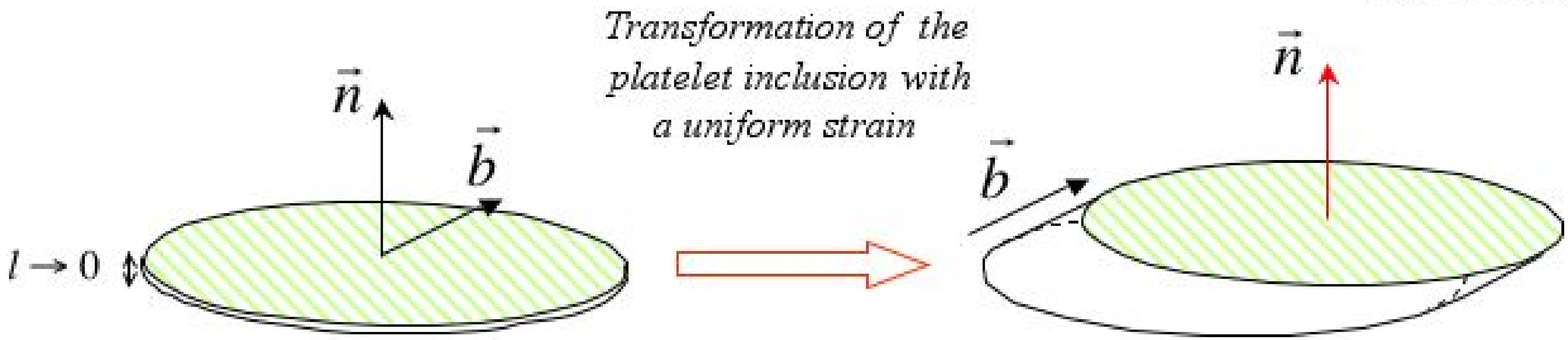
$$\frac{\partial}{\partial x} \rightarrow \phi(x+d) - \phi(x)$$

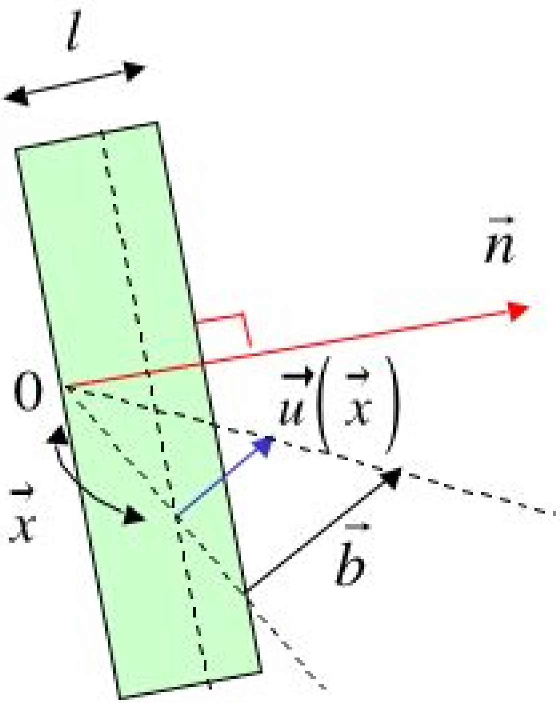
$$\sum_{k} \rightarrow \sum_{k} \quad \text{with } \| k \| \leq \frac{2\pi}{d}$$

How to introduce dislocations (1) ?

⇨ Via an analogy between Volterra procedure and a phase transformation

(Nabarro, 1951)





$$u_i(\vec{x}) = b_i \frac{\vec{x} \cdot \vec{n}}{l}$$

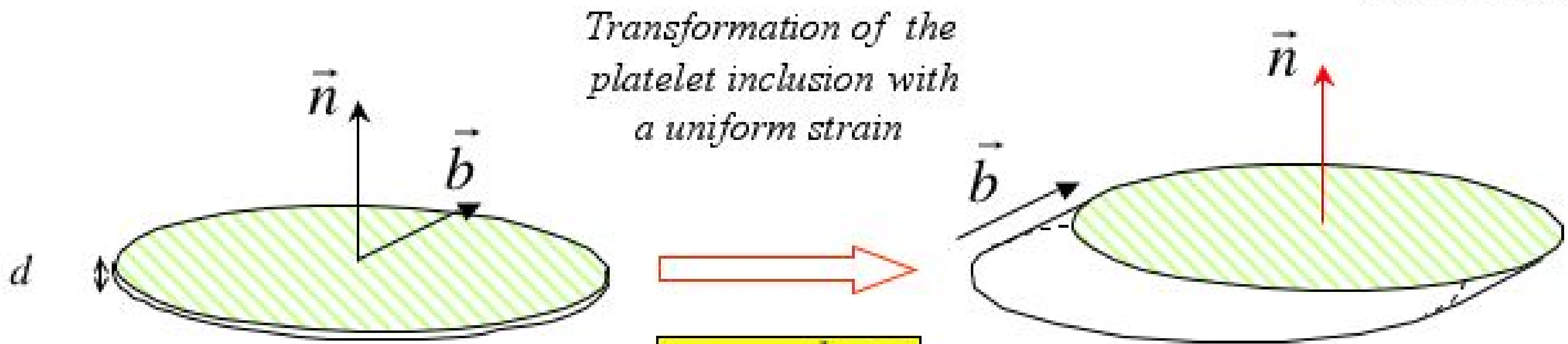
$$\frac{\partial u_i}{\partial x_j} = \frac{b_i n_j}{l}$$

$$\varepsilon_{ij}^0 = \frac{1}{l} \frac{b_i n_j + b_j n_i}{2}$$

How to introduce dislocations (2) ?

⇒ Via an analogy between Volterra procedure and a phase transformation

(Nabarro, 1951)



$$\varepsilon^0_{ij} = \frac{b_i\, n_j}{d}$$

⇒ Dislocations are introduced in a phase field code as extra phases

⇒ In FCC, 1 phase for each slip system characterized by :

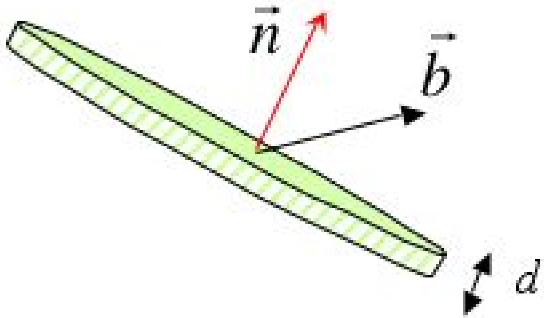
$$\underbrace{\varepsilon^0_{ij}(r)}_{} = \frac{b_i n_j}{d}\underbrace{\theta(r)}_{}$$

(see also A. Khachaturyan et al., and L.Q. Chen, 2001)

Stress-free strain ⟺ *Plastic strain* *along loop surfaces*

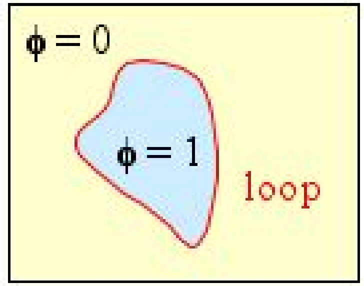
Dislocation field (= ..., -1,0,1,...)

$$\varepsilon^0_{ij}(r) = \sum_p \frac{b_i^{(p)}\, n_j^{(q)}}{d}\, \phi_p(r)$$



Glide system p

$$\phi_p(r) = 1 \quad \textit{if} \quad \textit{dislocation of type p has glided once over r}$$
$$= 0 \quad \textit{if} \quad \textit{not}$$



Glide plane

Elastic coupling

$$E_{strain} = \frac{V}{2}\sum_{p,q}\sum_k B_{pq}(k)\,\phi_p(k)\,\phi_q(k)^* + \frac{V}{2}\sum_p\sum_k B_{p,conc}(k)\,\phi_p(k)\,c(k)^*$$

$$B_{pq}(k) = \lambda_{ijkl}\,\varepsilon_{ij}^{0(p)}\,\varepsilon_{kl}^{0(q)} - k_i\,\sigma_{ij}^{0(p)}\,\Omega_{jl}(k)\,\sigma_{lk}^{0(q)}\,k_k$$

$$\Omega^{-1}_{ij}(k) = \lambda_{imjl}\,k_m\,k_l$$

$$\varepsilon_{ij}^{0(p)} = \frac{b_i^{(p)}\,n_j^{(p)}}{d} \qquad \sigma_{ij}^{0(p)} = \lambda_{ijkl}\,\varepsilon_{kl}^{0(p)}$$

$$\varepsilon^0_{ij}(conc) = \lambda\,\delta_{ij} \qquad \sigma^0_{ij}(conc) = \lambda_{ijkl}\,\varepsilon^0_{kl}(conc)$$

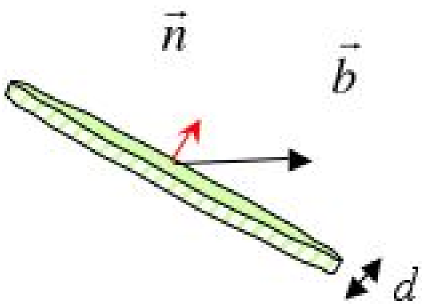
Equivalence « platelet inclusion - dislocation loop »

General:

$$u_i(\mathbf{r}) = \bar{\varepsilon}_{ij} r_j + \sum_{\mathbf{K}\neq 0} -iG_{im}(\mathbf{K})\sigma^0_{mn}(\mathbf{K})K_n \exp i\mathbf{K}\mathbf{r}$$

if $\varepsilon^0_{ij} = \dfrac{b_i n_j}{d}$ and $V \to \infty$:

$$u_i(\mathbf{r}) = -i\lambda_{mnkl}\frac{b_k n_l}{d}\sum_{\mathbf{K}\neq 0} G_{im}(\mathbf{K})\theta(\mathbf{K})K_n \exp i\mathbf{K}\mathbf{r}$$



$$\theta(\mathbf{K}) = \frac{1}{V}\int_V d^3r\, \theta(\mathbf{K}) \exp -i\mathbf{K}\mathbf{r} \to \frac{d}{V}\int_S dS \exp -i\mathbf{K}\mathbf{r}$$

Result:

$$u_i(\mathbf{r}) = -i\lambda_{mnkl}\frac{b_k n_l}{V}\int_S dS' \sum_{\mathbf{K}\neq 0} G_{im}(\mathbf{K})K_n \exp i\mathbf{K}(\mathbf{r}-\mathbf{r}')$$

$$= \lambda_{mnkl} b_k n_l \int_S dS' \frac{\partial}{\partial r'_n} G_{im}(\mathbf{r}-\mathbf{r}')$$ **Burgers eq.:**

with $G_{im}(\mathbf{r}) = \int \frac{d^3k}{(2pi)^3} G_{im}(\mathbf{K}) \exp i\mathbf{K}\mathbf{r}$

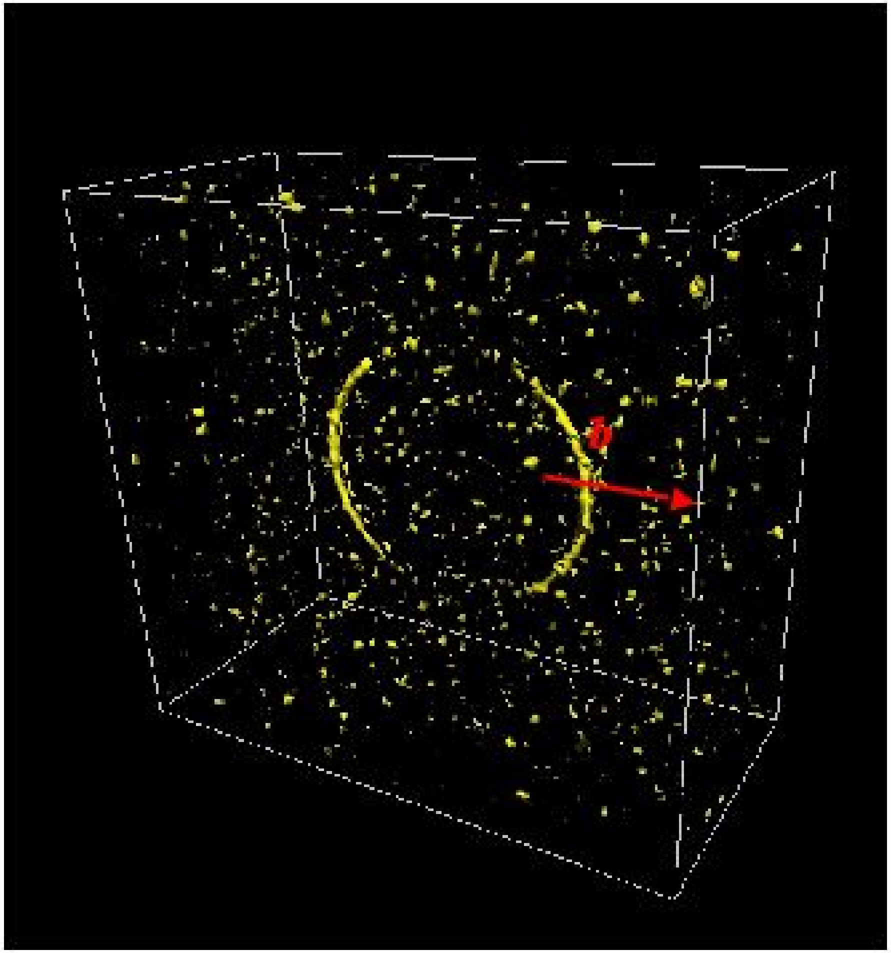
Application to heterogeneous precipitation

A static slip dislocation in a binary alloy with lattice parameter mismatch

Cahn-Hilliard dynamics for the conc. field :

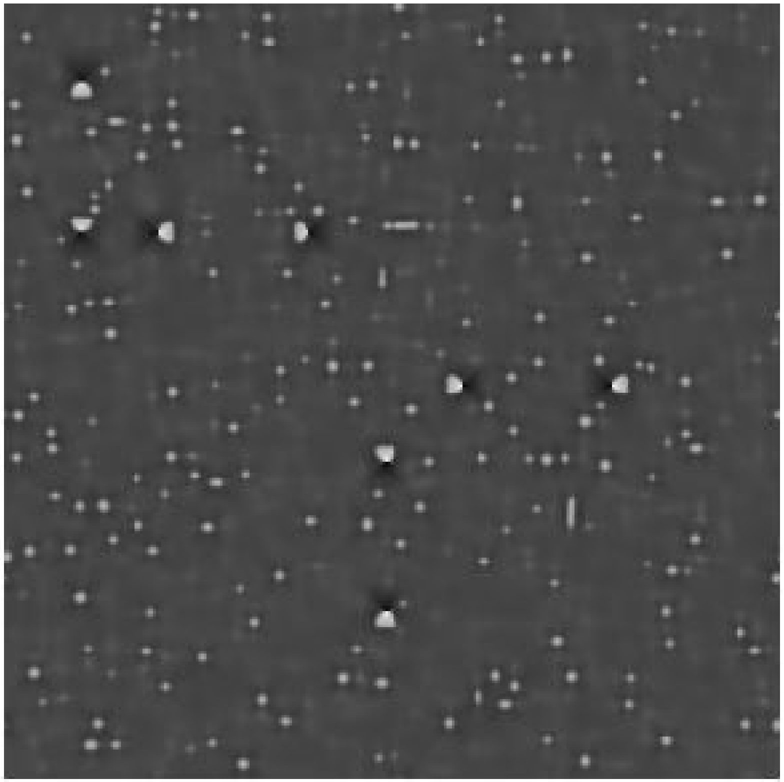
$$\frac{\partial c(r)}{\partial t} = \Gamma \; \nabla \cdot c(r) \left\{1 - c(r)\right\} \nabla \frac{\partial \left(E_{strain} + F_{chemical}\right)}{\partial c(r)}$$

Precipitation of the phase with smallest lattice parameter in the compression region of the edge parts of the slip loop



System size: 512 x 512

System size: 512 x 512
Static edge dislocation loops
Precipitation with lattice parameter mismatch



$t = 50$

$t = 4000$

Dislocation dynamics: 1st method

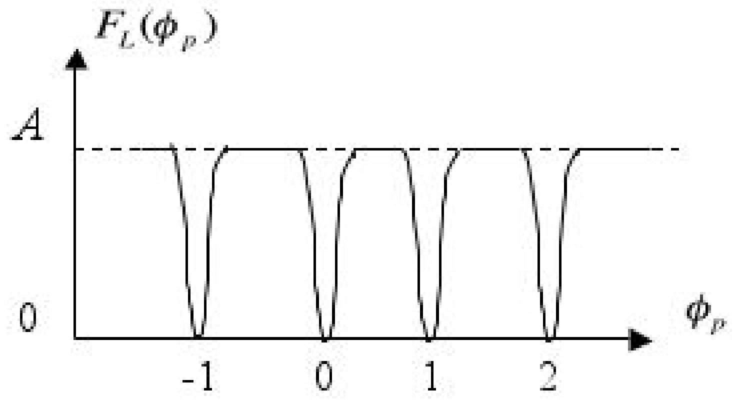
Phase Field spirit: continuous dynamics on $\phi_p(r) \rightarrow$ diffuse dislocation cores

Ginzburg-Landau energy:

$$E_{GL} = A \sum_p \int d^3r \sum_n \left(1 - e^{-\frac{(\phi_p(r)-n)^2}{2\sigma^2}}\right) + \frac{\lambda}{2} \left\| n_p \wedge \nabla \phi_p(r) \right\|^2$$

Localize the field on integers (Gauss wells)

finite core size a few "d"



$$\phi_p(r) = 1,\ 2, 3 \ldots\ldots -1, -2 \ldots$$

Kinetics:

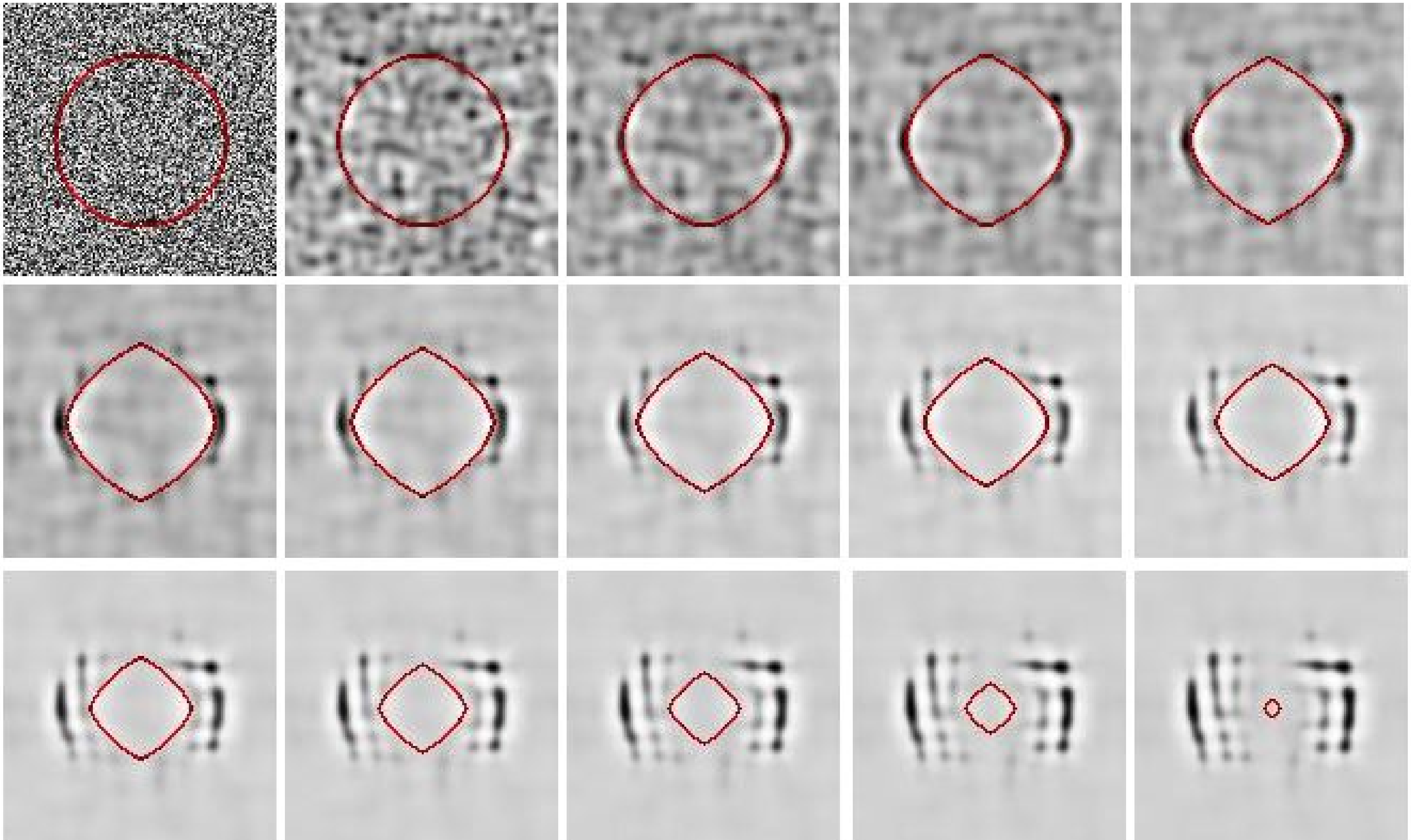
$$\frac{\partial \phi_p(n)}{\partial t} = -\Gamma \frac{\partial (E_{strain} + E_{GL})}{\partial \phi_p(n)}$$

$$-\frac{\partial (E_{strain} + \ldots)}{\partial \phi_p(n)} = \sum_k \sum_q B_{qp}(k)\, e^{ik.n}\, \phi_q(k) \quad \rightarrow \quad \| k \| \leq \frac{2\pi}{d}$$

$$= d^3 \left\langle \sigma_{ij}(r) \right\rangle \varepsilon^0_{ij}(p) \quad \rightarrow \quad \textit{Peach-Khoeler force}$$

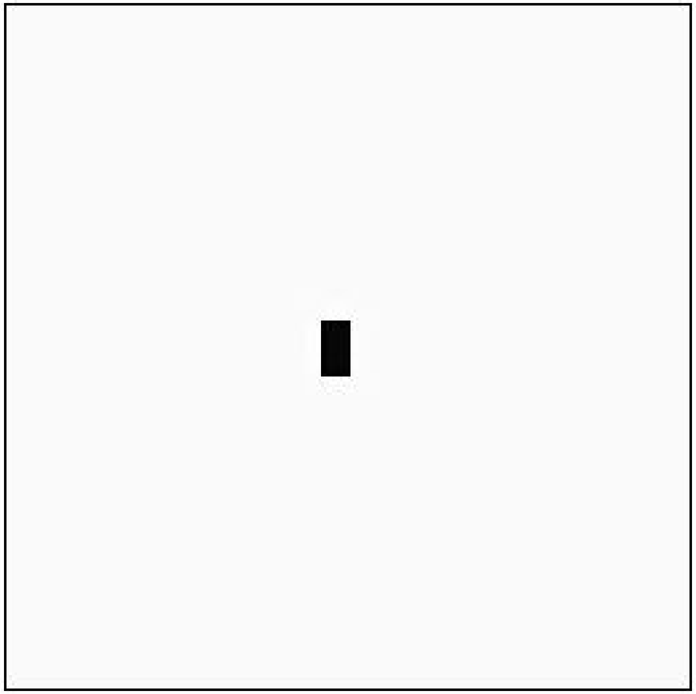
Dislocations Dynamics

Shrinking of a shear loop during phase separation



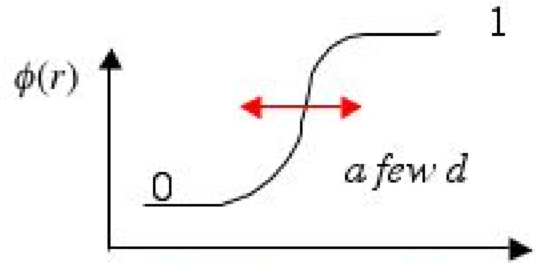
Dislocations Dynamics

Dislocation multiplications: Frank-Read source



Problem:

- grid spacing "d" ($\|k\| \leq \frac{\pi}{d}$): *only one characteristic length* !!!
- mesoscopic scale: $d \propto nm \propto 10\ b$
- size of any heterogeneity: *a few d*
- dislocation core: $l > 50\ b$!!!!
- maximum stress near dislocation: $\sigma \approx \frac{\mu}{2\pi}\frac{b}{l} << \frac{\mu}{2\pi}$



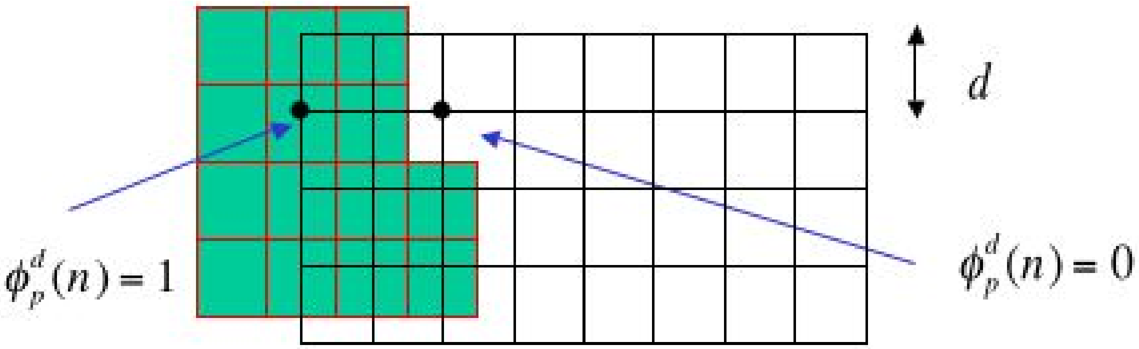
« Diffuse interface »

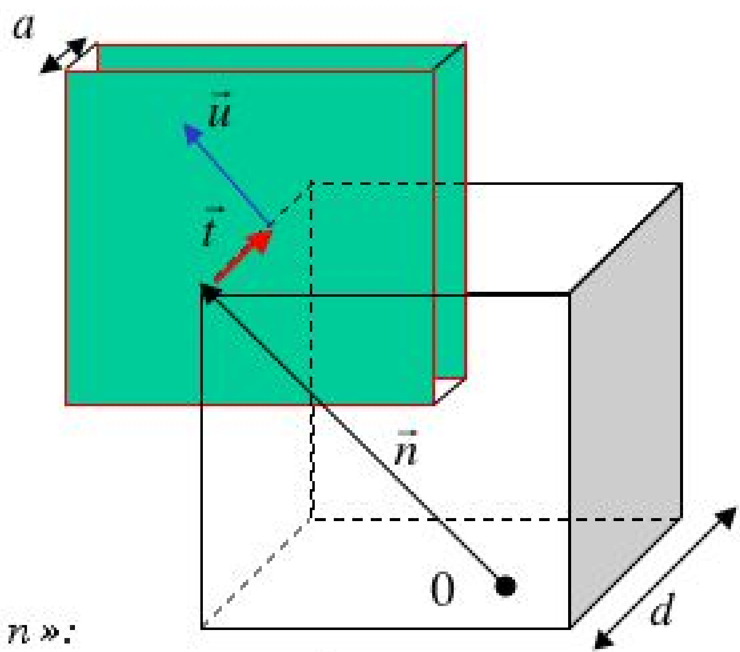
→ ***Weak short range interactions between dislocations***

→ *need to introduce another length scale… ..*

loopons

→ decompose $\phi_p(r)$ into a superposition of elementary loops: "loopons"





$\vec{r} = \vec{n} + \vec{t} + \vec{u}$

$\vec{n}$ = position of cube $d \times d \times d$

$\vec{t}$ = center of loopon in cube " n"

$\phi_p^d(n)$ → defined only on the grid points

$S_p(r - r_n)$ → Shape function of loopon of type « p » in cube « n »:

$$\phi_p(r) = \sum_n \phi_p^d(n)\, S_p(r - r_n) \longrightarrow \phi_p(k) = \phi_p^d(k)\, S_p(k)$$

$$S_p(k) = \frac{1}{d^3}\int_V d^3r\, S_p(r)\, e^{-ik.r} = \frac{a}{d}\,\frac{\sin(k_x d/2)}{k_x d/2}\,\frac{\sin(k_y d/2)}{k_y d/2}\,\frac{\sin(k_z a/2)}{k_z a/2}\, e^{-ik_z \frac{d}{2}}$$

$$\phi_p^d(k) = \frac{1}{N}\sum_n \phi_p(n) e^{-ik.n} \longrightarrow \phi_p^d(k+K) = \phi_p^d(k) \qquad K = \frac{2\pi}{d}(h\,k\,l)$$

$$E_{strain} = \frac{V}{2} \sum_{p,q} \sum_{k \in ZB} \left\{ \sum_{K} B_{pq}(k+K)\, e^{-i(k+K).(t_p - t_q)}\, S_p(k+K)\, S_q(k+K)^* \right\} \phi_p^d(k)\, \phi_q^d(k)^*$$

Usual form:

$$E_{strain} = \frac{V}{2} \sum_{p,q} \sum_{k \in ZB} B_{pq}^{dec}(k)\; \phi_p^d(k)\, \phi_q^d(k)^*$$

With new « B(k) »

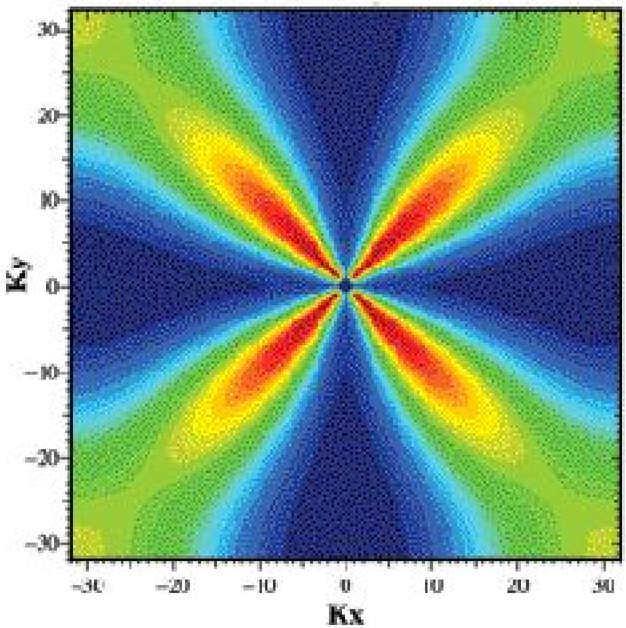
$$B_{pq}^{dec}(k) = \sum_{K} B_{pq}(k+K)\; e^{-i(k+K).(t_p - t_q)}\, S_p(k+K)\, S_q(k+K)^*$$

$$K \leq K_{max} \rightarrow 2^{nd} \text{ characteristic length: } \quad a \propto K_{max}^{-1}$$

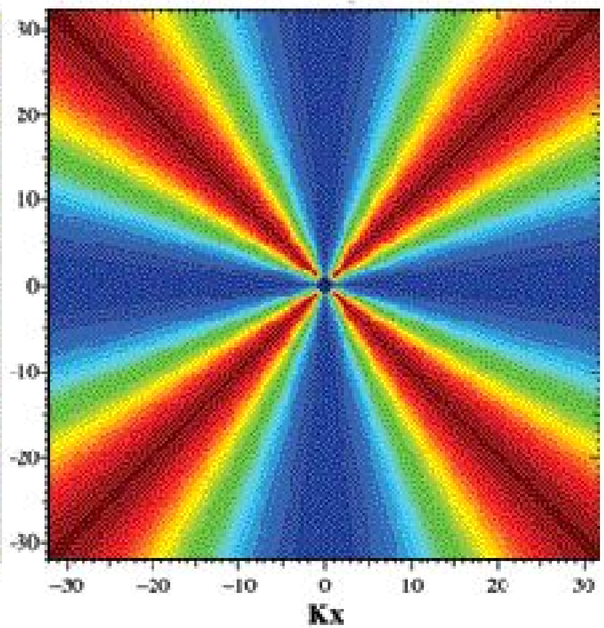
→ *New length scale for dislocation cores, independent of grid spacing « d »*

→ *Typically:* $\| K_{max} \| \propto \frac{2\pi}{b} \;:\; \| b \| / d = \frac{1}{10} \Rightarrow \| K_{max} \| \propto \frac{2\pi}{d} \times 10$

Two length scales: d *and* K_{max}^{-1}

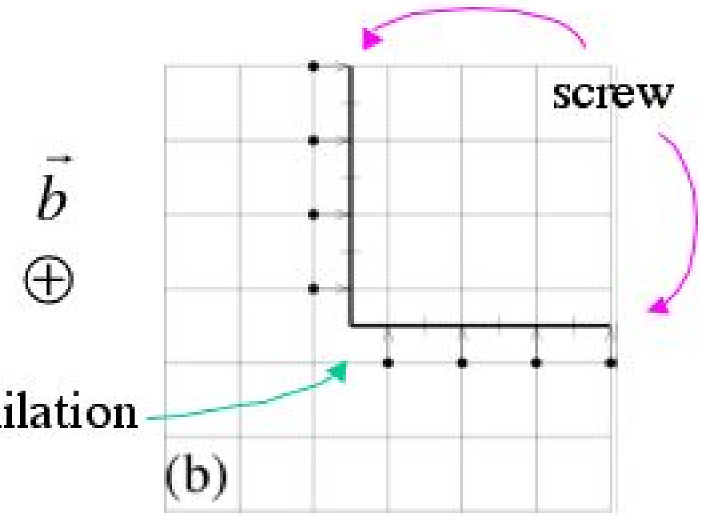


Only d



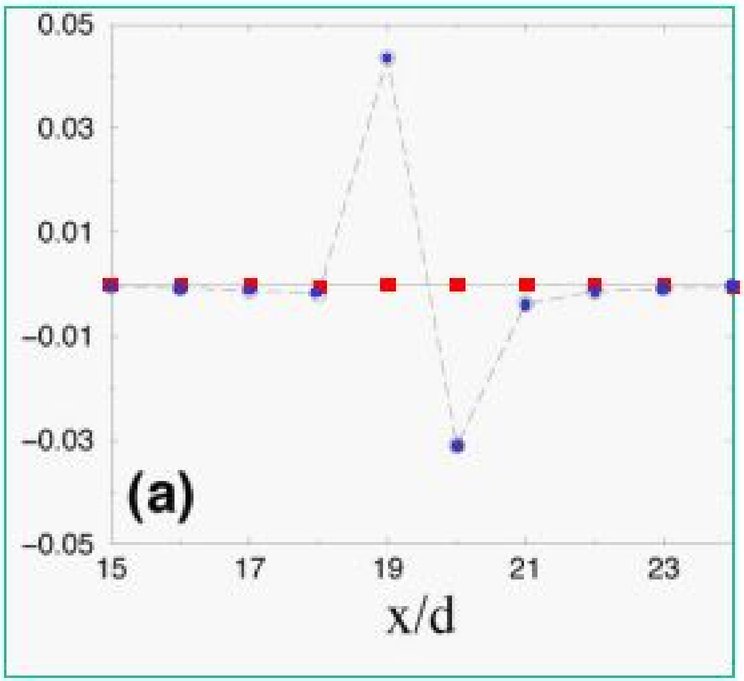
Improvements of the discrete approach

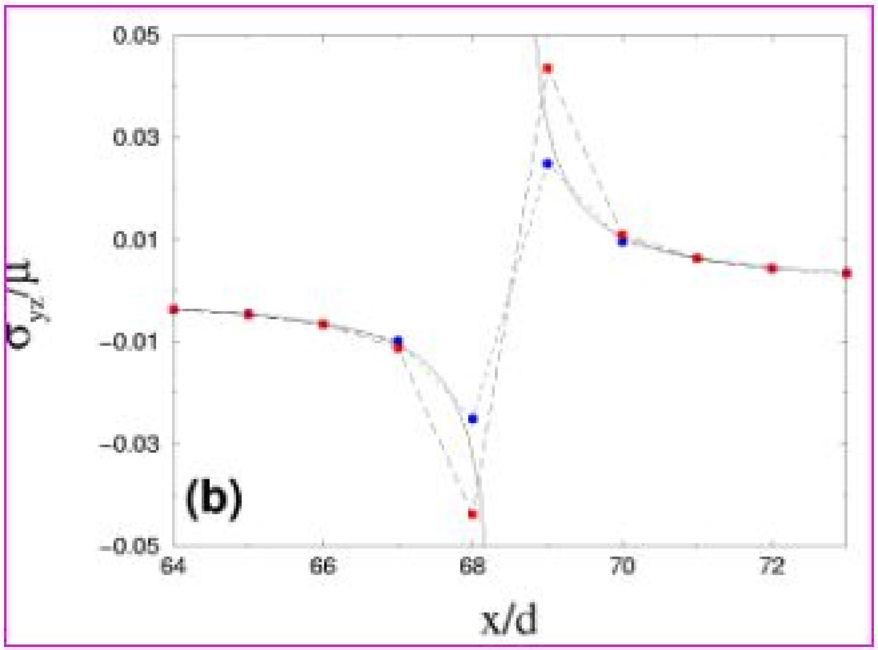
$C_{11} = 170, \quad C_{12} = 70, \quad C_{44} = 50 \quad (units: 10^9\ Pa)$
$d = 10b \approx 3nm$
$5 \times 5 \times 5$ *Brillouin zones* $\rightarrow$ *cores* $\approx b$



Case # 1: $\| K_{\max} \| = \dfrac{\pi}{d}$

Case # 2: $\| K_{\max} \| = \dfrac{5\pi}{d}$





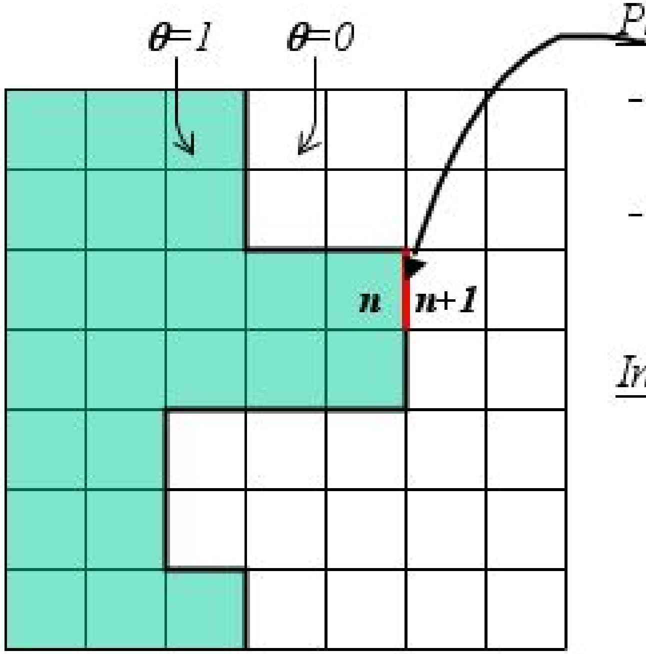
Discrete dislocation dynamics

⇒ We use :

$$-\frac{\partial(E_{strain})}{\partial\phi_p(n)} = \sum_k \sum_q B_{qp}(k)\, e^{ik.n}\, \phi_q(k) = d^3 \langle \sigma_{ij}(r) \rangle \frac{b_i^{(p)} n_j^{(p)}}{d}$$

Resolved Shear Stress on slip system

(including the self-stress of the dislocations)



Philosophy of the algorithm :

- *RSS on segment in X direction :* $F_n^+ = -\frac{1}{2}\left(\frac{\delta E_{strain}}{\delta\theta(n)} + \frac{\delta E_{strain}}{\delta\theta(n+1)}\right)$

- *Move the segment propor. to F*

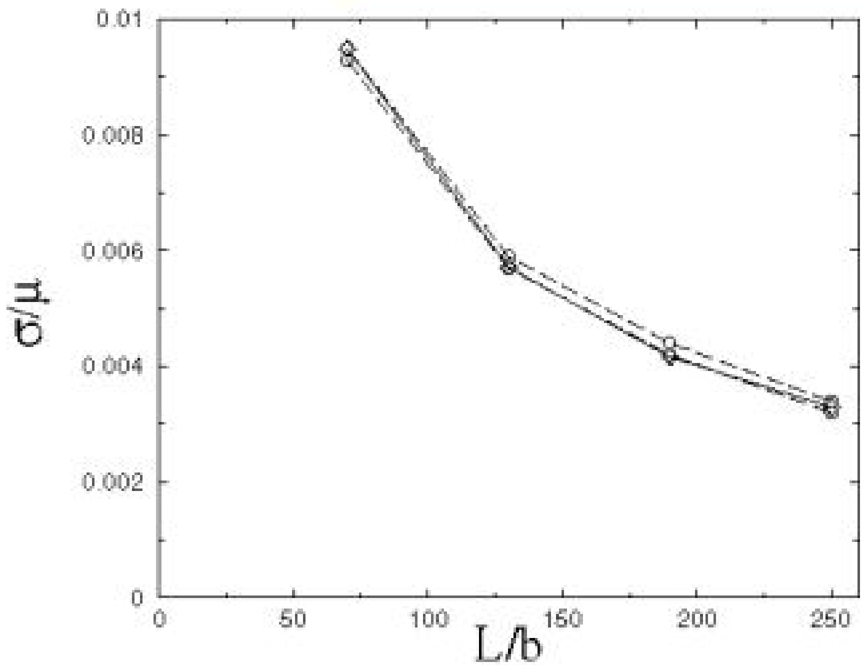
In terms of fields : $\frac{\partial\theta(n)}{\partial t} = M\sqrt{\left(\tilde{F}_x^- + \tilde{F}_x^+\right)^2 + \left(\tilde{F}_y^- + \tilde{F}_y^+\right)^2}$

where $\tilde{F}_x^+ = \left|(\theta_{n+1} - \theta_n)F_n^+\right| \times H\left[(\theta_{n+1} - \theta_n)F_n^+\right]$

and θ *is updated when* $\delta\theta$ *reaches 1*

⇒ Frank-Read stress in agreement with elasticity with $R_{core} = b$

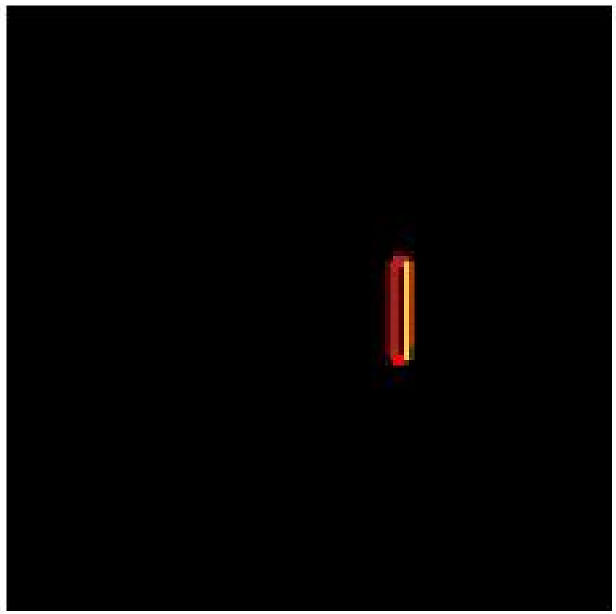
Activation stress of a Frank Read source, initially of edge character



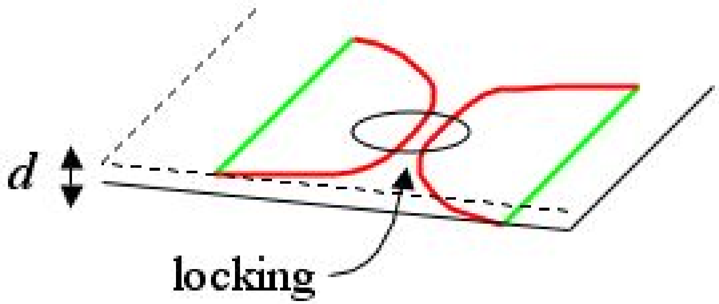
○ Simulation

◇ Elastic model: $$\frac{\sigma}{\mu} = \frac{1 - 3/2\,\nu}{2\pi(1-\nu)}\,\frac{b}{L}\left(\ln\left(\frac{L}{b}\right) + 1\right)$$

- *Simulation box: 128 x 128 x 128*
- *Isotropic medium:* $C_{11}=170$ $C_{12}=70$ $C_{44}=50$ *(unit:Gpa)*
- *glide system: <100>(001)*
- *b/d = 0.1*



Test of short range interaction:
two FR sources in parallel glide planes

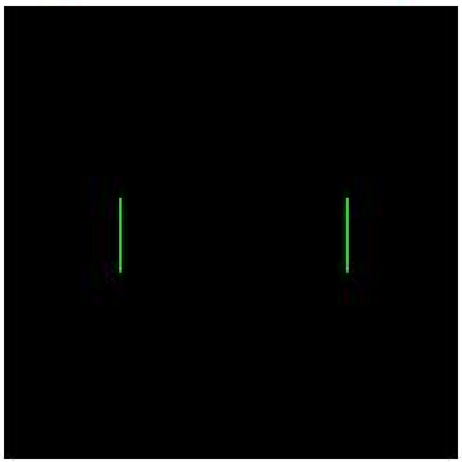


$$\sigma_{unlock} = \frac{\mu}{8\pi(1-\nu)}\frac{b}{d} \quad \textit{if edge}$$

$$\sigma_{unlock} = \frac{\mu}{4\pi}\frac{b}{d} \quad \textit{if screw}$$

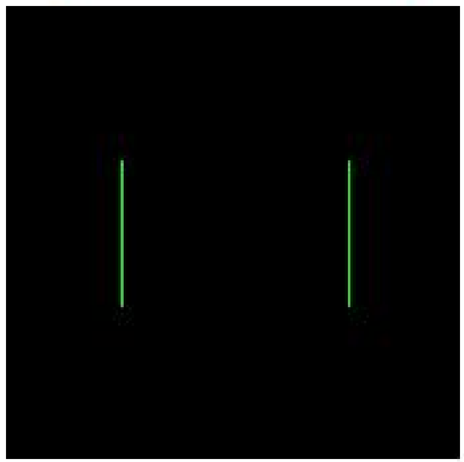
edge : $\sigma_{unlock} / \mu = 5.7\ 10^{-3}$

$\sigma_{ext} / \mu = 5\ 10^{-3}$

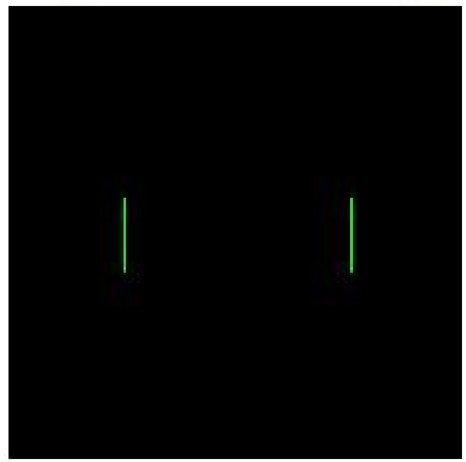


screw : $\sigma_{unlock} / \mu = 8.0\ 10^{-3}$

$\sigma_{ext} / \mu = 5\ 10^{-3}$



$\sigma_{ext} / \mu = 9\ 10^{-3}$

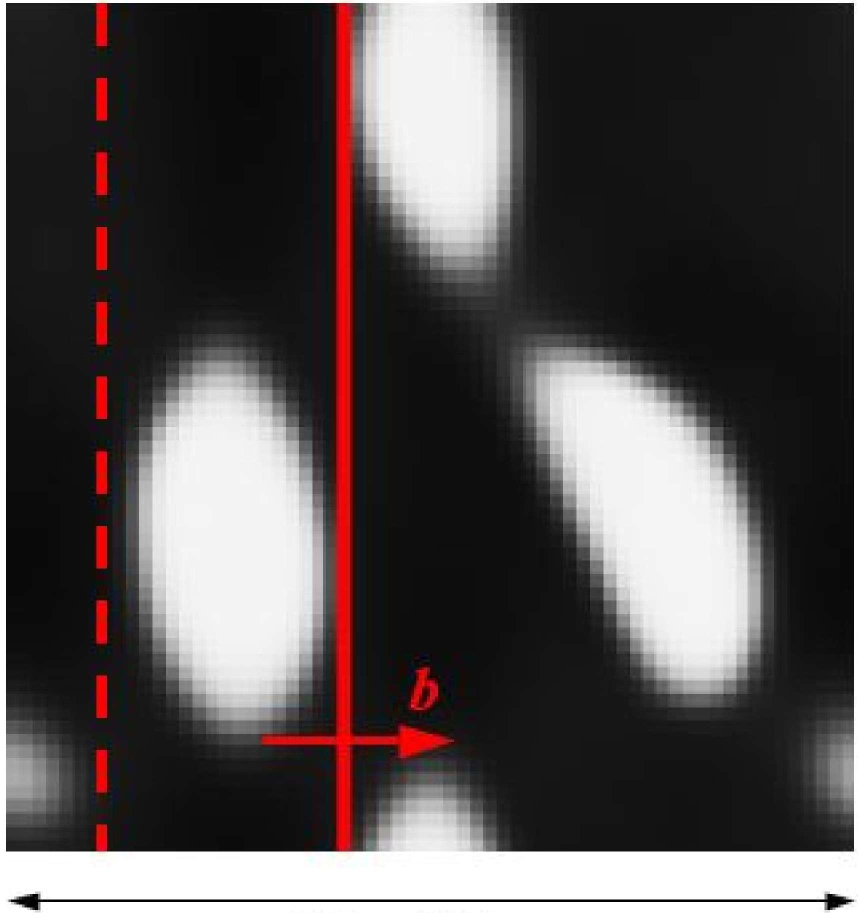


<u>*Application to Alloy Hardening (1)*</u>

Consider a binary alloy with
a lattice parameter mismatch (2%)

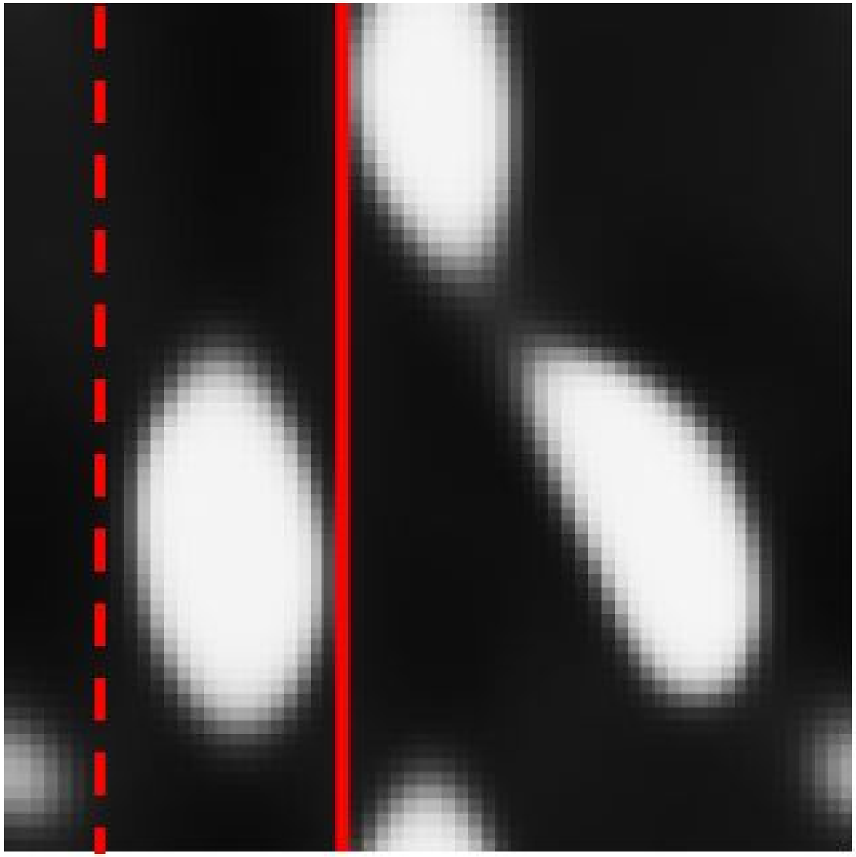
Step 1 : Let the microstructure evolve
in absence of any dislocation.

Step 2 : Place a slip loop which creates
2 edge dislocations.
Use 'Frank-Read trick' to
annihilate one of the dislocations.

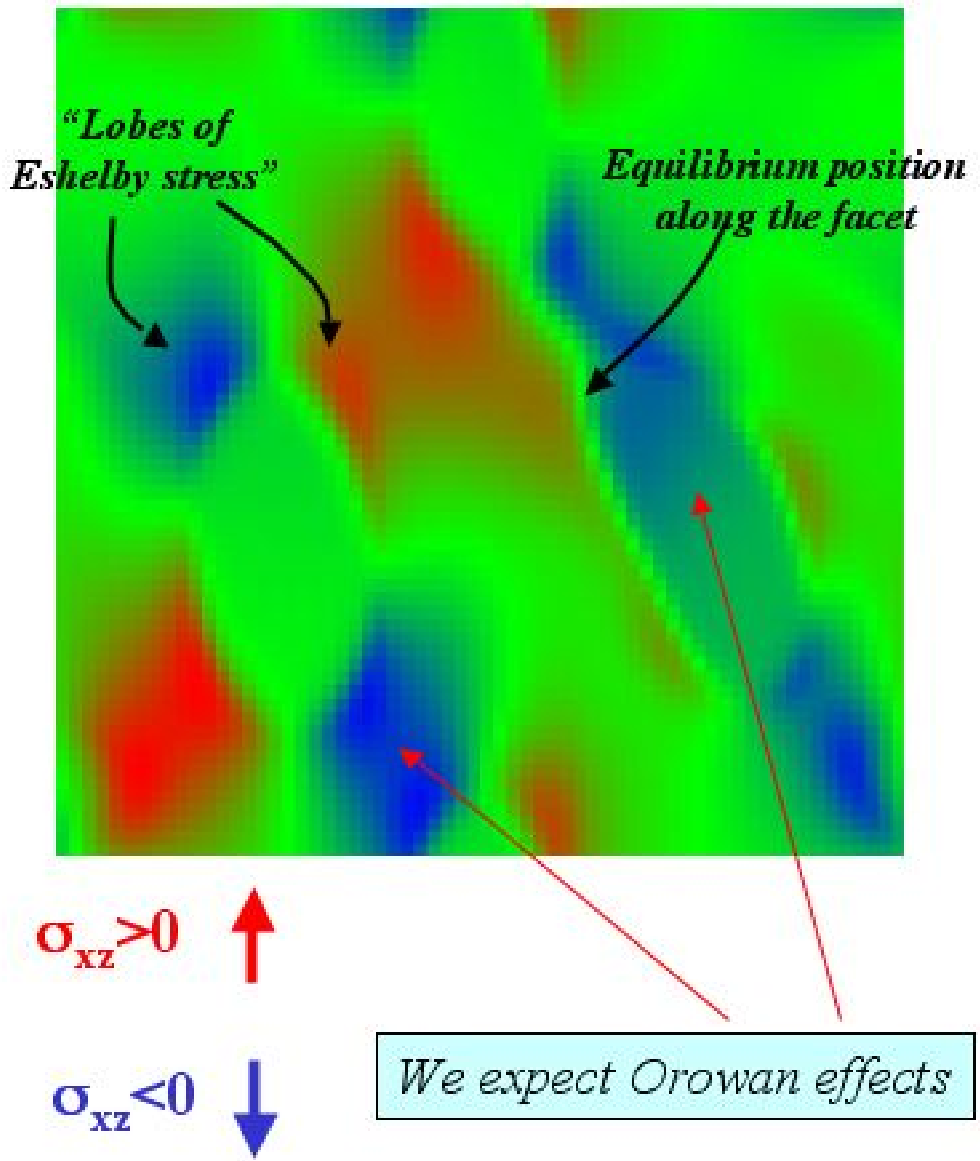


64d = 0,16 µm
(cell dim. = 64x64x64, d=10b,
periodic boundary cond.
anisotropic elasticity)

Microstructure

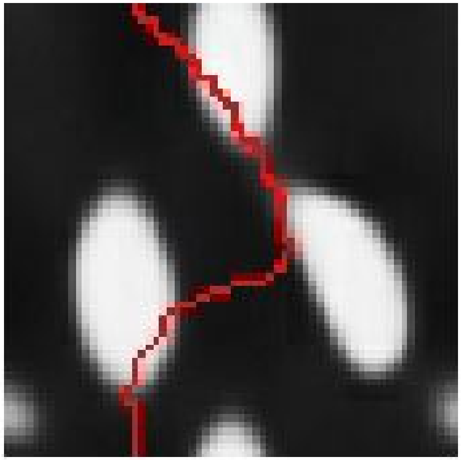


RSS (σ_{xz}) due to the microstructure

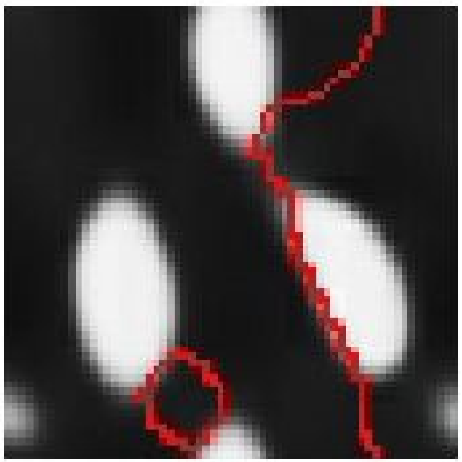


Step 1: $\sigma/C_{44} = 0$; let the dislocation equilibrate.

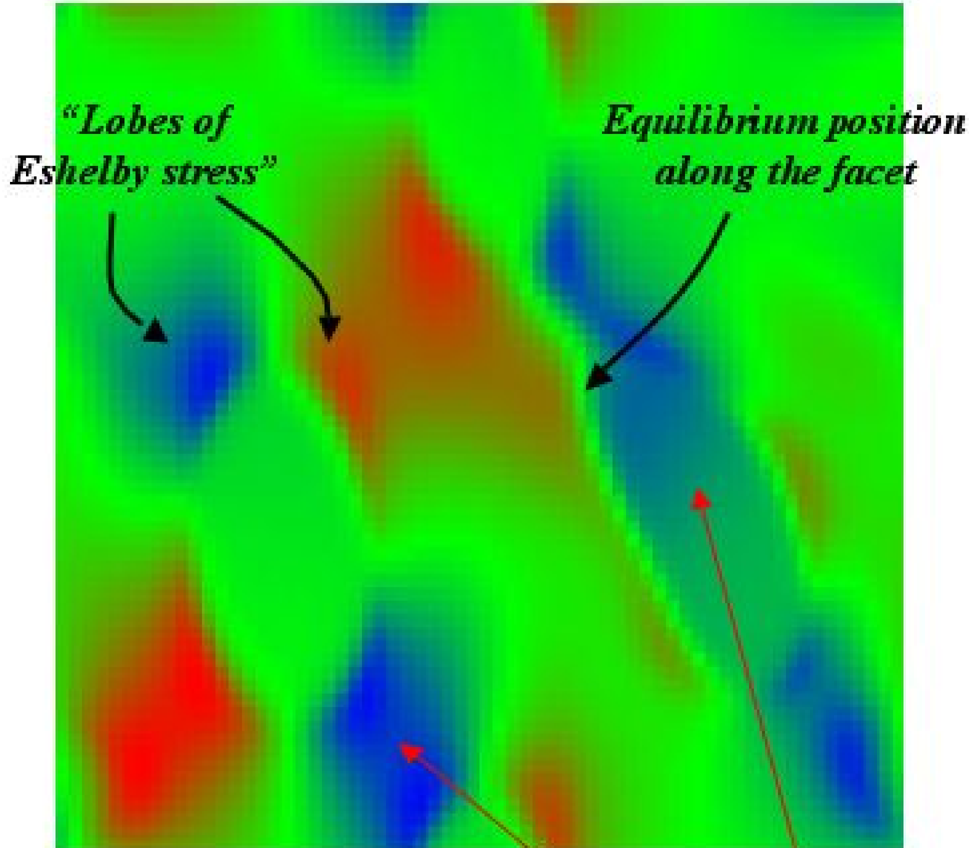
$\sigma/C_{44} = 2\,10^{-3}$



$\sigma/C_{44} = 2.7\,10^{-3}$



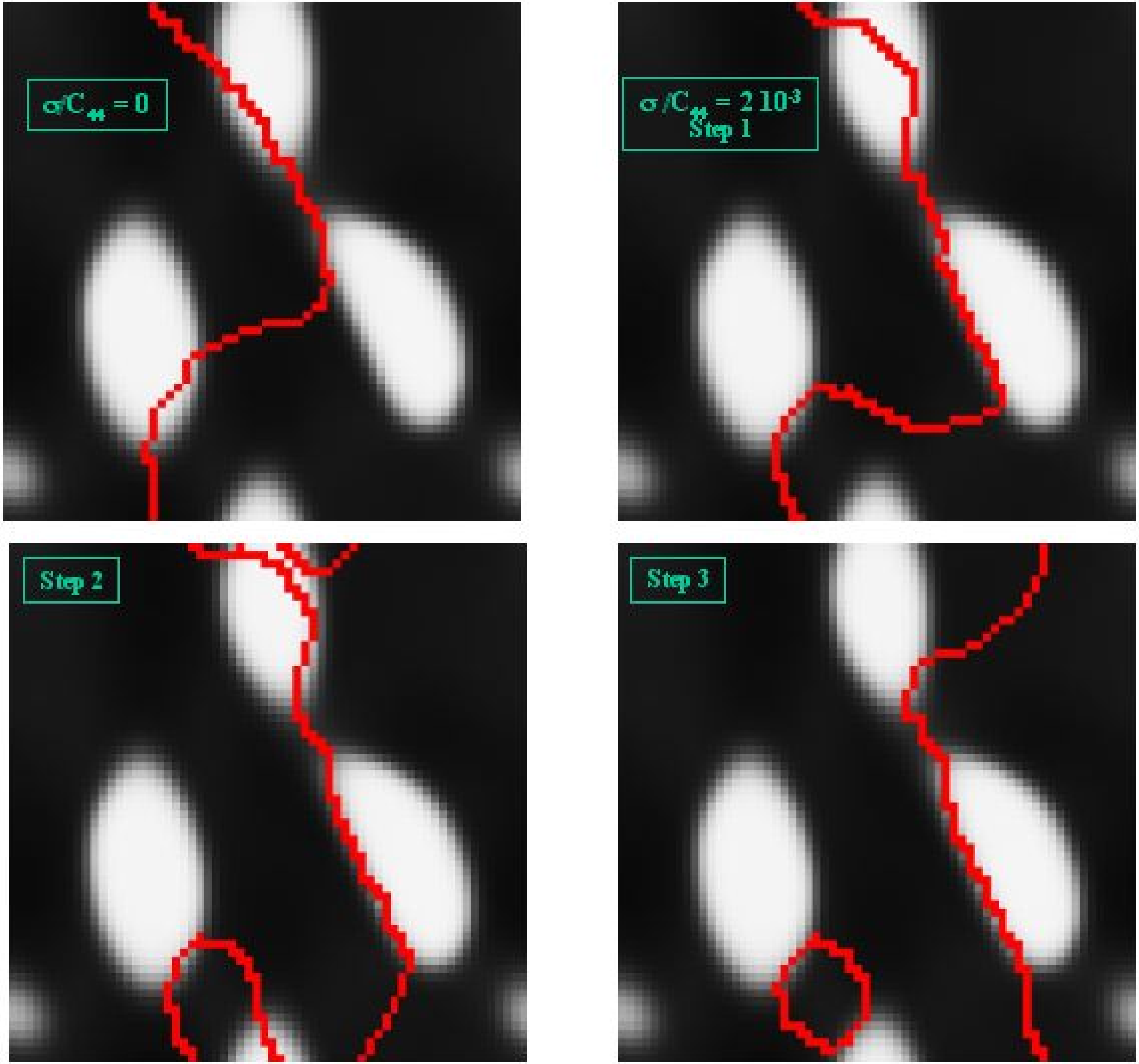
RSS (σ_{xz}) due to the microstructure

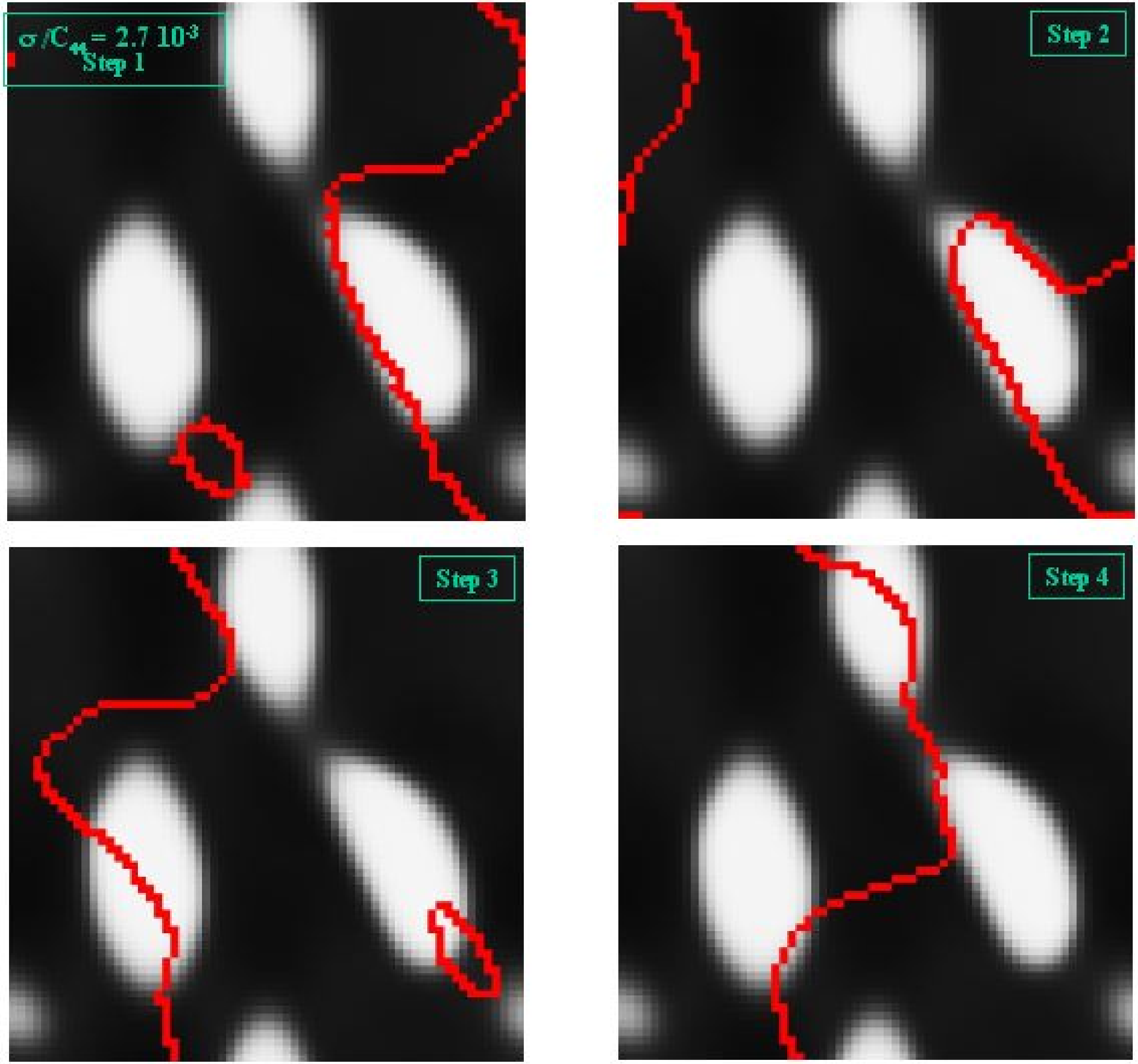


$\sigma_{xz}>0$ ↑

$\sigma_{xz}<0$ ↓

We expect Orowan effects


$\sigma/C_{44} = 0$
$\sigma/C_{44} = 2\ 10^{-3}$
Step 1
Step 2
Step 3


σ /C44 = 2.7 10-3
Step 1
Step 2
Step 3
Step 4

Application to Alloy Hardening (2)

Consider a FCC binary alloy with a lattice parameter mismatch (0.014)

Step 1: Let the microstructure evolve (up to late stage) in absence of any dislocation.

Step 2 : Place a slip loop $<\bar{1}01>\ (111)$

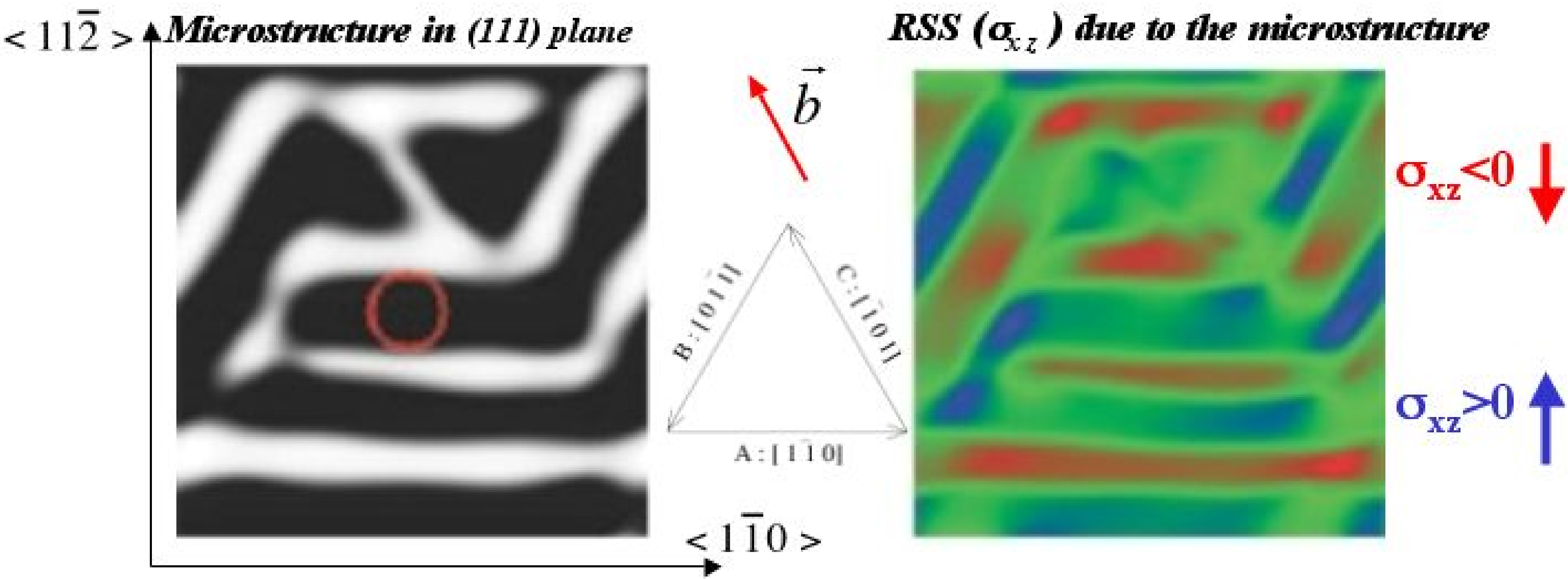
Anisotropic medium: $C_{11} = 102$ $C_{12} = 70$ $C_{44} = 50$ *(unit: Gpa)*

Interfacial energy: $50\ mJ.m^{-2}$

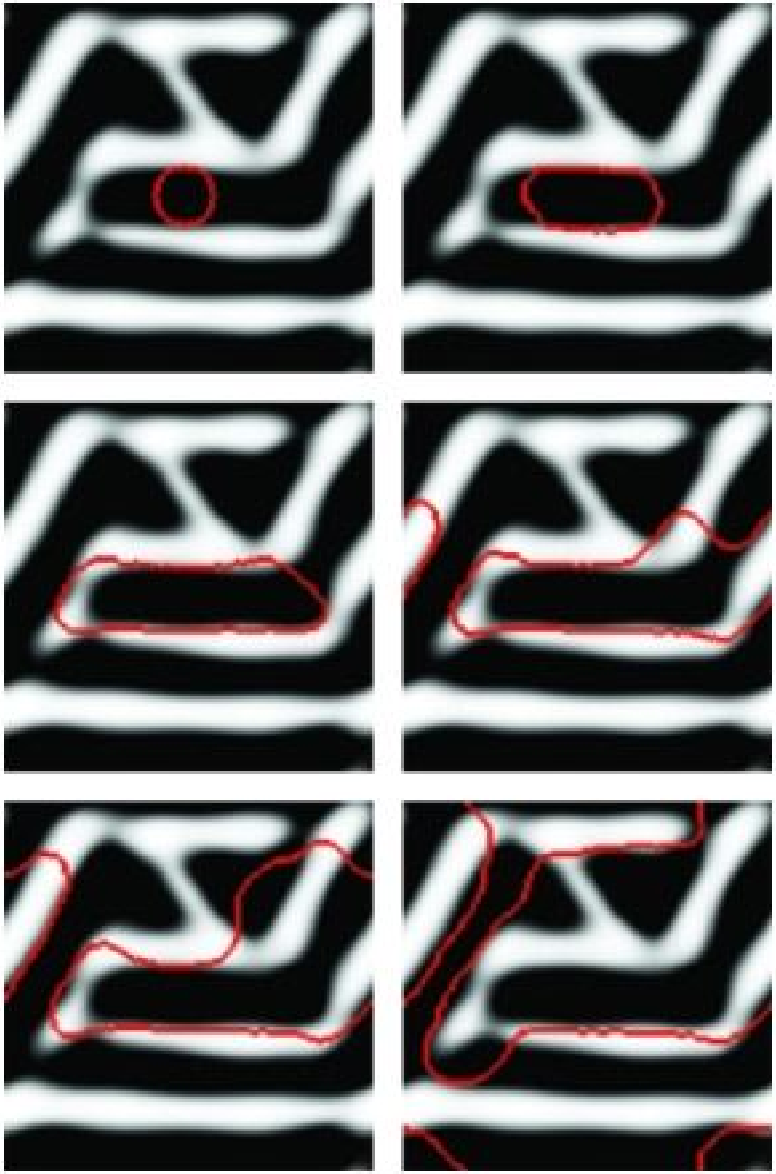
Grid spacing: $d = 5\ nm$

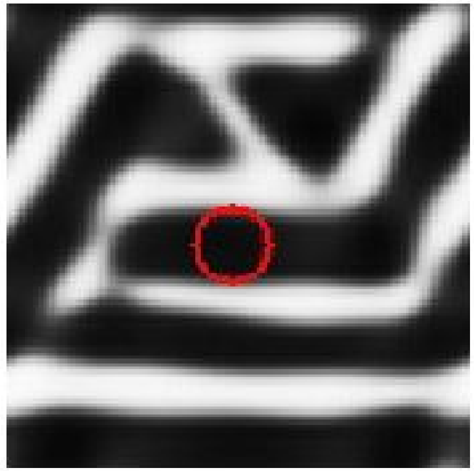
Burger's vector: $b/d = 0.1$

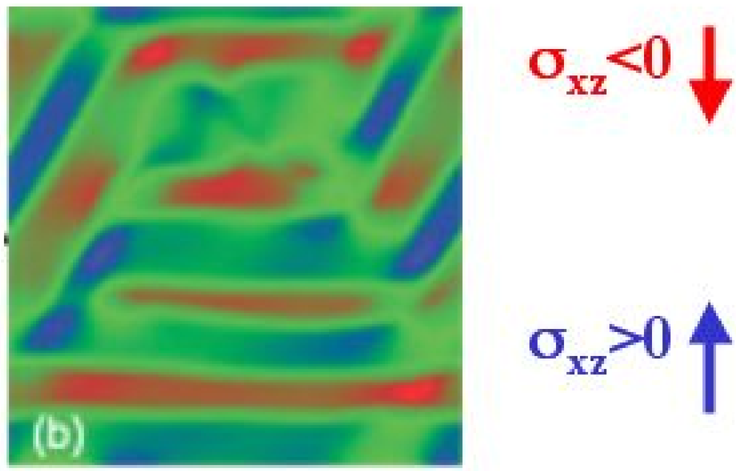
Simulation box: $128 \times 128 \times 128$ $(128\ d = 0{,}64\ \mu m)$



$$\textit{applied stress} \quad \sigma = 2.45\ 10^{-3}\, C_{44}$$







Application to Alloy Hardening (3)

Consider a FCC binary alloy with a lattice parameter mismatch (0.014)

Step 1: *Let the microstructure evolve (up to late stage)* in absence of any dislocation.

Step 2 : *Place a slip loop* $\langle 1\bar{1}0 \rangle$ (111)

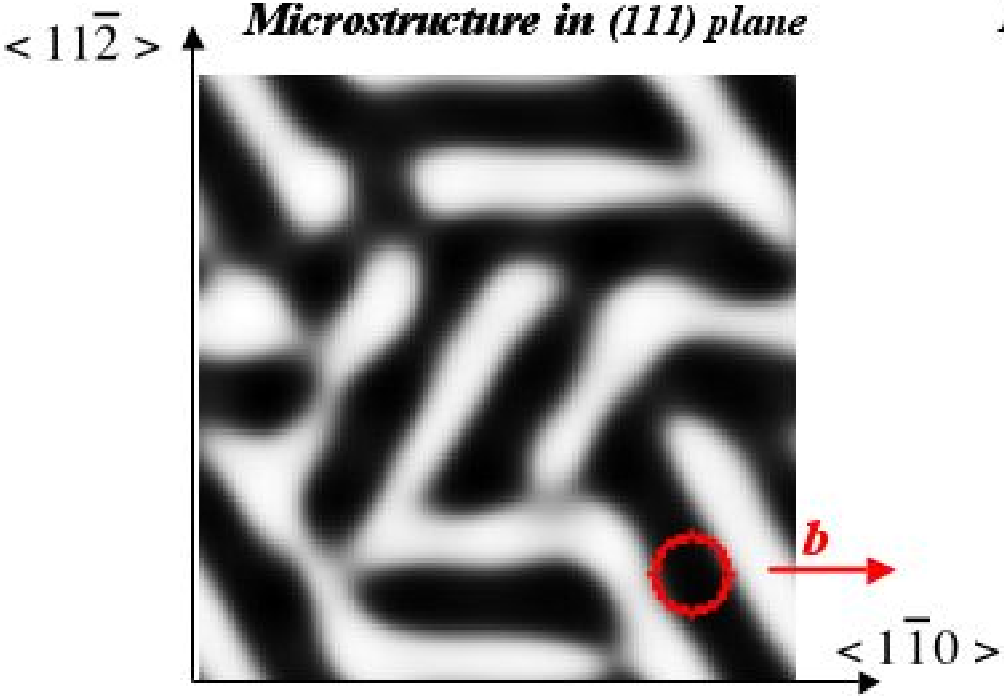
Anisotropic medium: $C_{11} = 102$ $C_{12} = 70$ $C_{44} = 50$ (unit: Gpa)

Grid spacing: $d = 5$ nm

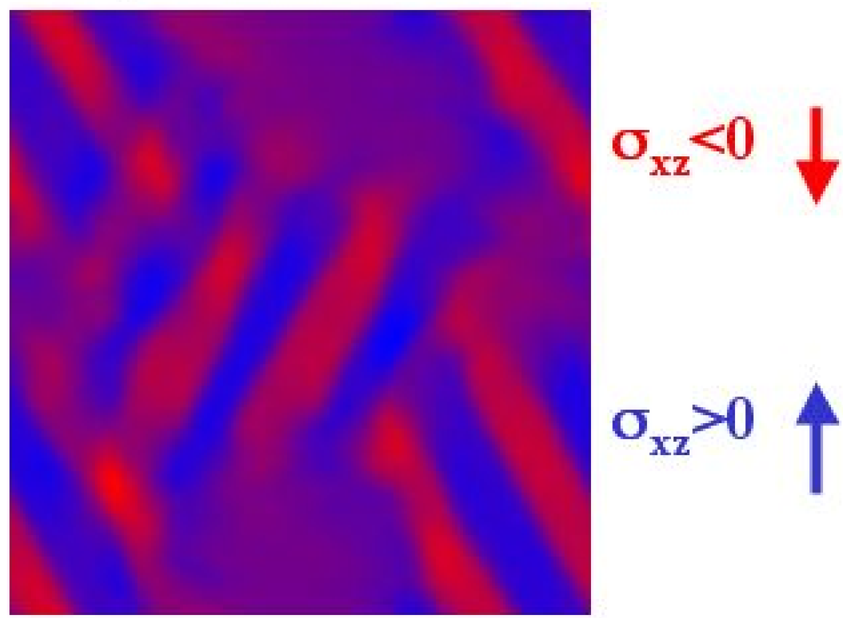
Burger's vector: $b/d = 0.1$

Simulation box: 128 x 128 x 128 (128 d = 0,64 µm)

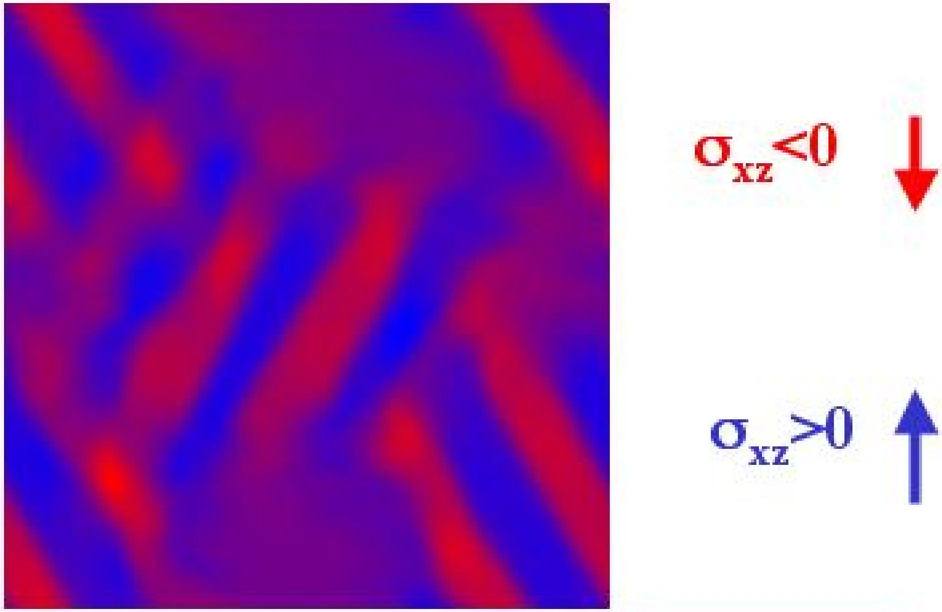
Microstructure in (111) plane



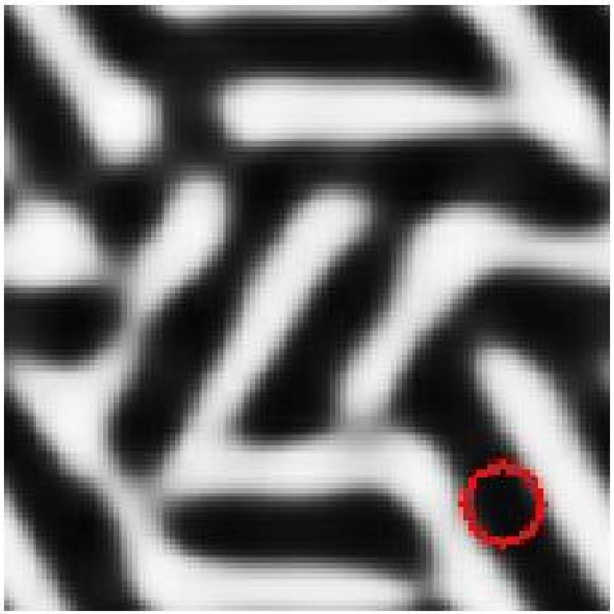
RSS (σ_{xz}) due to the microstructure



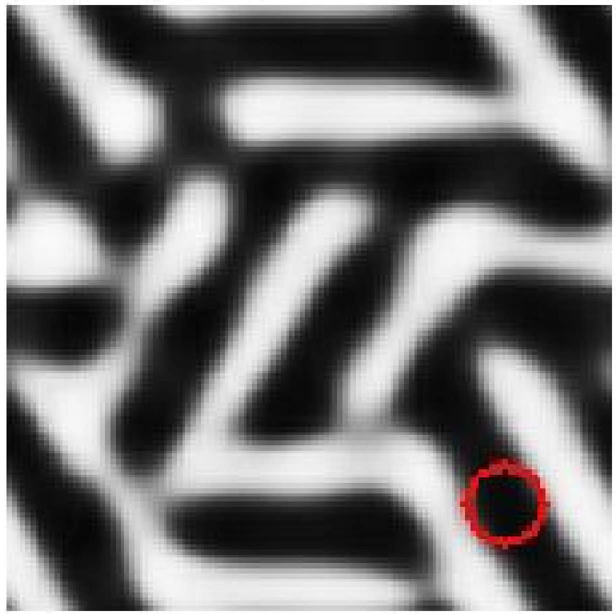
RSS (σ_{xz}) due to the microstructure



$\sigma/C_{44} = 0.8\ 10^{-2}$



$\sigma/C_{44} = 10^{-2}$



Conclusion

Phase transformation and microstructures:

- Growth laws with lattice mismatch
- Complexe morphologies
- Phase Field may be fitted to a specific system (Ni-Ti, Al-Zr)

Dislocations and plasticity:

- Same formalism for microstructures and dislocations
- Rôle of dislocations on coarsening (and vice-versa)
- Two length scales: d (> nm) and b (Å): realistic dislocation cores
- Short range interactions correct
- May be used for small (or thin) precipitates