Dislocation dynamics: from microscopic models to macroscopic crystal plasticity

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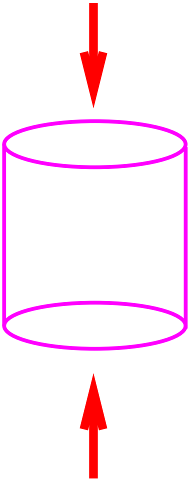
UCLA; February 29, 2012

Physical motivation

Plasticity of metals

compression of a cylinder



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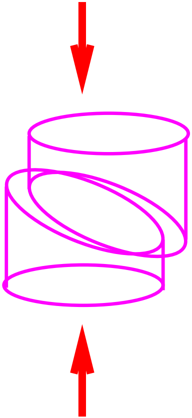
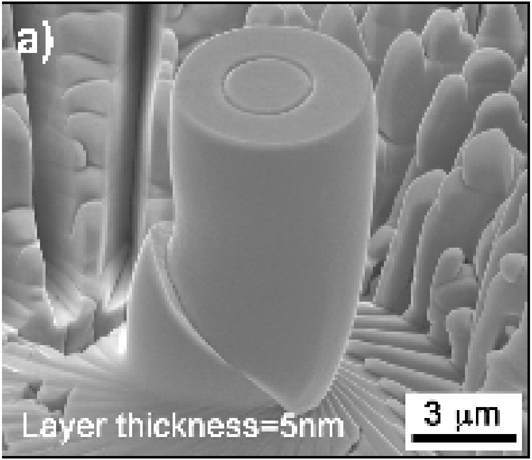
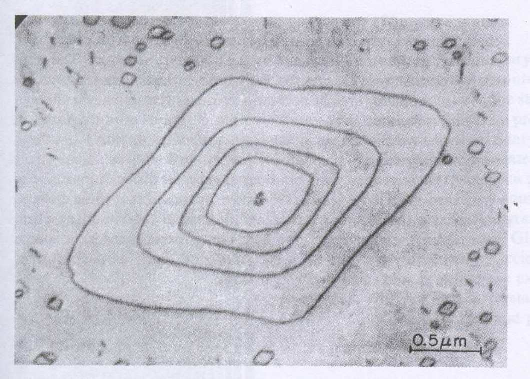


compression of a micro-pillar



Defects in crystal = dislocation loops



Dynamics of loops

Non local, non monotone dynamics

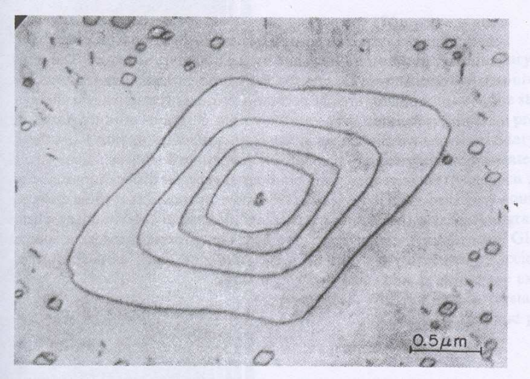
$$u_t = |Du| \ \left(c_0 \star 1_{\{u \geq 0\}}\right) \quad \text{on} \quad \mathbb{R}^N \times (0,T)$$

- "Dynamics of sets"
  (Interior ball)
  [Alvarez, Cardaliaguet, M. (2005)], [Cardaliaguet, Marchi (2006)],
  (Interior cone)
  [Barles, Cardaliaguet, Ley, Monteillet (2009)]

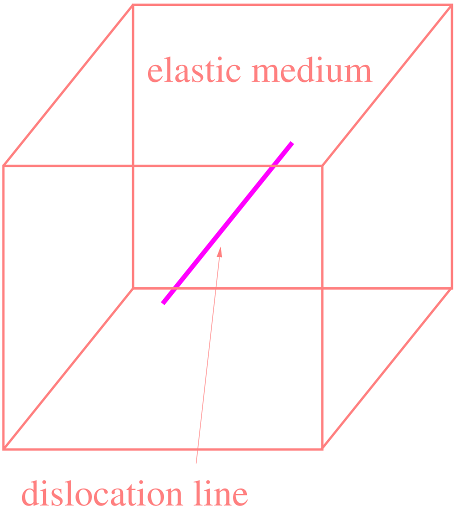
- Level sets
  [Barles, Ley (2006)],
  (Notion of very weak solutions)
  [Barles, Cardaliaguet, Ley, M. (2008)],
  [Barles, Cardaliaguet, Ley, Monteillet (2009)],

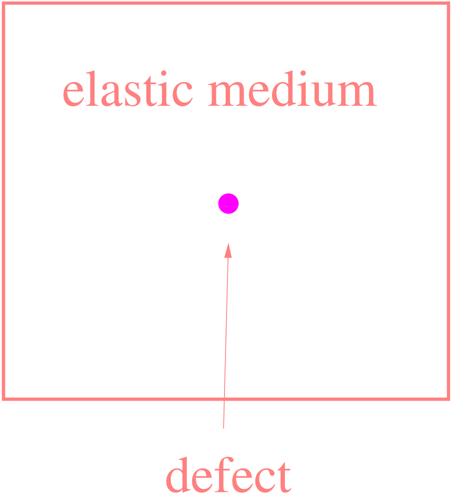
- Numerics : Generalized Fast Marching Method
  [Carlini, Forcadel, M. (2011)]

Dislocations



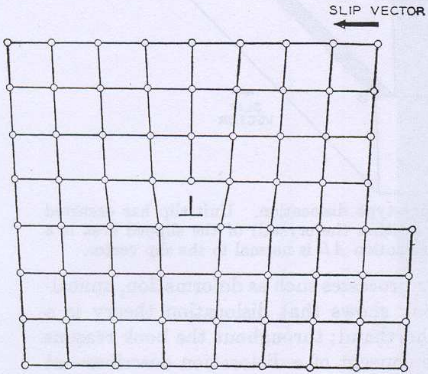
3D continuous model




elastic medium
defect

2D atomic model

(b)



Plan of the talk : Hierarchy of scales

(1) Frenkel-Kontorova (atomic)

$\Downarrow \quad (\varepsilon_1 \to 0)$

(2) Peierls-Nabarro (micro)

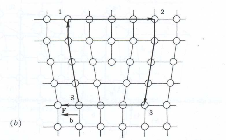
$\Downarrow \quad (\varepsilon_2 \to 0)$

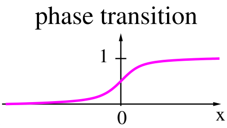
(3) Dynamics of dislocations (meso)

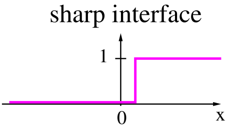
$\Downarrow \quad (\varepsilon_3 \to 0)$

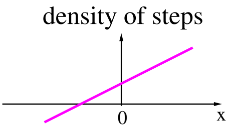
(4) Crystal plasticity (macro)

Hierarchy of scales and models







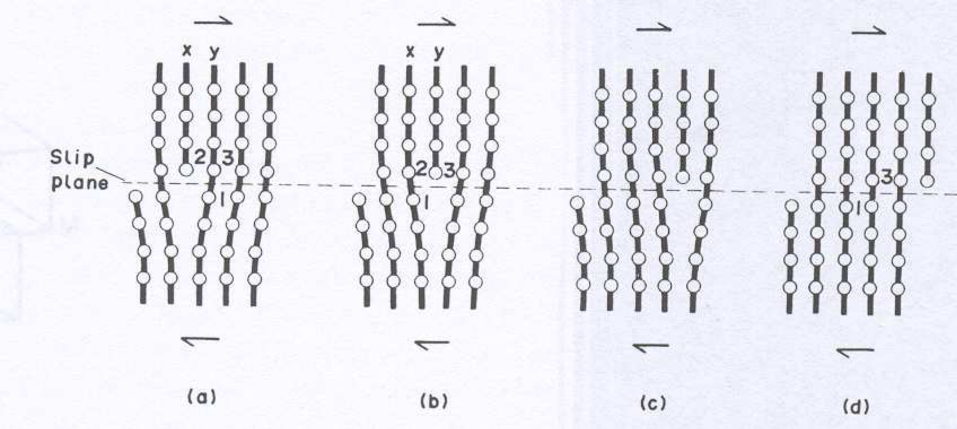


"FK" $\Longrightarrow$ PN $\Longrightarrow$ DD $\Longrightarrow$ Crystal plasticity

2D Frenkel-Kontorova model

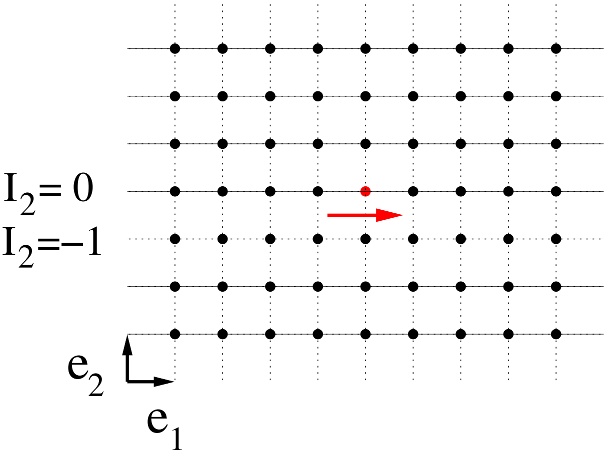
$$(\varepsilon = \varepsilon_1)$$

Motion of a dislocation



2D Frenkel-Kontorova

Points only move on the horizontal axis with $I = (I_1, I_2) \in \mathbb{Z}^2$



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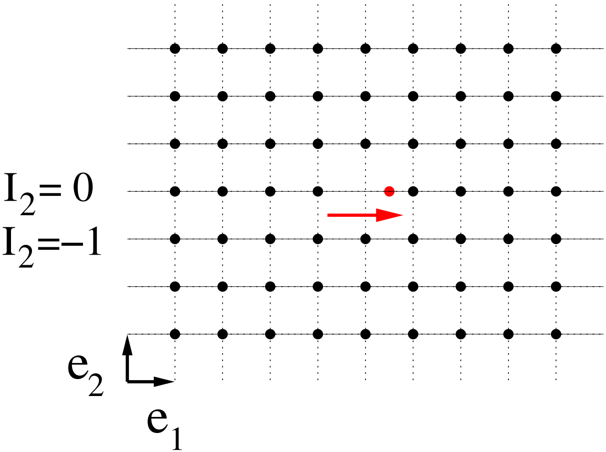
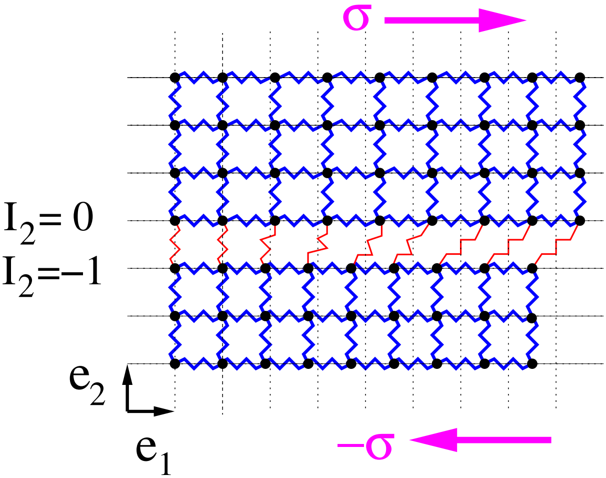
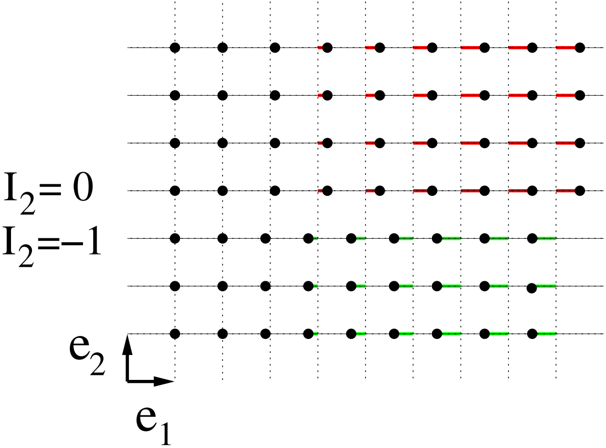


strong springs / weak springs, stress σ

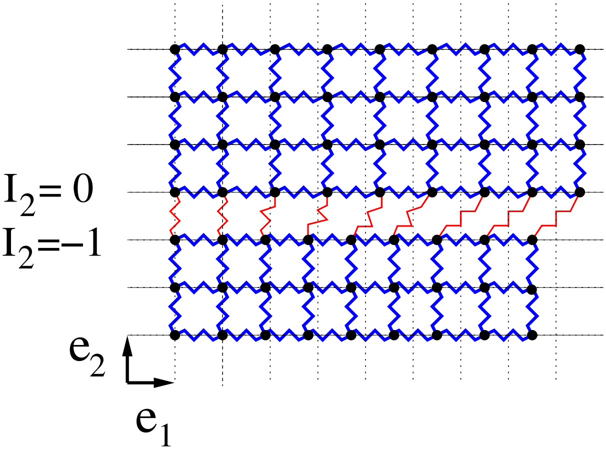


Assumption : antisymmetric horizontal displacement

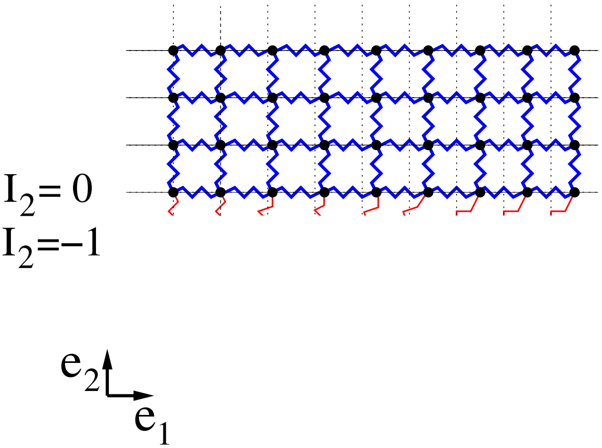
$$U_{(I_1,I_2)} = -U_{(I_1,-I_2-1)}$$



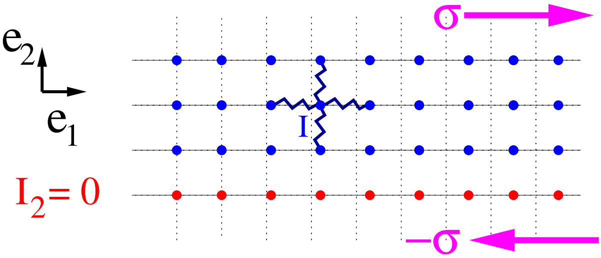
2D Frenkel-Kontorova



Half plane



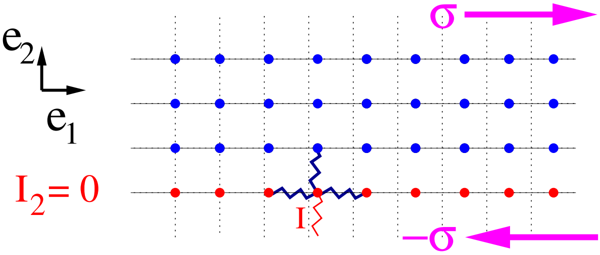
Equilibrium of the blue points



For $I = (I_1, I_2)$ with $I_2 \geq 1$

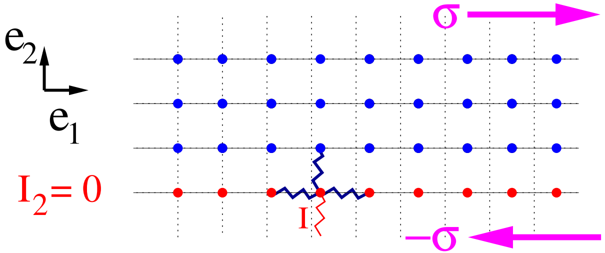
$$\sum_{J \in \mathbb{Z}^2,\ |J-I|=1} (U_J - U_I) = 0$$

(harmonic blue springs)



For $I = (I_1, I_2)$ with $I_2 = 0$

$$\frac{d}{dt}U_I = \qquad -\varepsilon W'(U_I) + \sum_{\substack{J \in \mathbb{Z}^2,\ J_2 \geq 0, \\ |J - I| = 1}} (U_J - U_I)$$



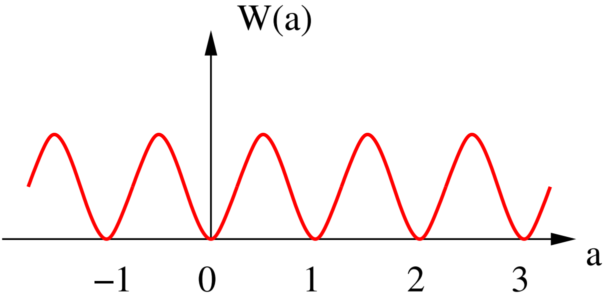
For $I = (I_1, I_2)$ with $I_2 = 0$

$$\frac{d}{dt}U_I = \varepsilon\varepsilon_2\sigma - \varepsilon W'(U_I) + \sum_{\substack{J\in\mathbb{Z}^2,\ J_2\geq 0,\\ |J-I|=1}} (U_J - U_I)$$

The full 2D Frenkel-Kontorova

$$\begin{cases} \displaystyle\sum_{J\in\mathbb{Z}^2,\ |J-I|=1} (U_J - U_I) = 0 & \text{for} \quad I_2 \geq 1 \\ \displaystyle\frac{d}{dt}U_I = \varepsilon\varepsilon_2\sigma - \varepsilon W'(U_I) + \sum_{\substack{J\in\mathbb{Z}^2,\ J_2\geq 0,\\ |J-I|=1}} (U_J - U_I) & \text{for} \quad I_2 = 0 \end{cases} \qquad (1)$$

smooth periodic potential $\quad W(a+1) = W(a)$



W describes the misfit between the two half planes.

Homogenization of 1D FK models

- Fully overdamped FK
  [Forcadel, Imbert, M., (2009)]
- FK with acceleration
  [Forcadel, Imbert, M., (preprint 2010)]
- FK with parabolic rescaling
  [Alibaud, Briani, M. (2010)]

Traveling waves for 1D FK models

- Fully overdamped FK
  [work in progress]

Convergence to the Peierls-Nabarro model

$$(\varepsilon = \varepsilon_1 \to 0)$$

Hyperbolic rescaling

$$u^{\varepsilon}(X,t) = U_{\frac{X}{\varepsilon}}\left(\frac{t}{\varepsilon}\right) \quad \text{for} \quad X = (X_1, X_2) \in (\varepsilon\mathbb{Z}) \times (\varepsilon\mathbb{N})$$

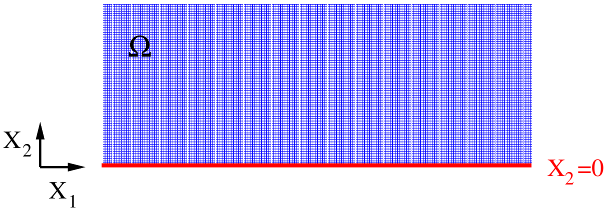
Thm 1 (convergence FK $\to$ PN) [Fino, Ibrahim, M. (2012)]

As $\varepsilon \to 0$, we have

$$u^\varepsilon \to u^0 \quad \text{in} \quad L^\infty_{loc}(\mathbb{R}^2_+ \times [0, +\infty))$$

with u^0 solution of the PN model.

Peierls-Nabarro model



For $u^0(X_1, X_2, t)$:

$$\begin{cases} 0 = \Delta u^0 & \text{on} \quad \Omega = \{X_2 > 0\} \\ u_t^0 = \varepsilon_2 \sigma - W'(u^0) + \dfrac{\partial u^0}{\partial X_2} & \text{for} \quad \partial\Omega = \{X_2 = 0\} \end{cases}$$

Reformulation of the PN model

$$\begin{cases} 0 = \Delta u^0 & \text{on} \quad \Omega \\ u_t^0 = \varepsilon_2 \sigma - W'(u^0) + \dfrac{\partial u^0}{\partial X_2} & \text{on} \quad \partial\Omega \end{cases}$$

Reformulation of the PN model

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$\Longrightarrow \quad v(x,t) := u^0(x,0,t)$ satisfies with $\varepsilon = \varepsilon_2$

$$v_t = \varepsilon\sigma - W'(v) + \Delta^{\frac{1}{2}} v \quad \text{for} \quad x \in \mathbb{R} \tag{2}$$

with the Lévy-Khintchine formula

$$(\Delta^{\frac{1}{2}} w)(x) = \frac{1}{\pi} \int_{\mathbb{R}} \frac{dz}{z^2} \left(w(x+z) - w(x) - z w'(x) 1_{\{|z| \leq 1\}} \right)$$

$$v_t = \varepsilon\sigma - W'(v) + \Delta^{\frac{1}{2}} v$$

Homogenization of PN on $\mathbb{R}^N$: [M., Patrizi (2012)]

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Homogenization of PN on $\mathbb{R}^N$: [M., Patrizi (2012)]

Traveling waves for PN : [Gui, Zhao (2012)]

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Homogenization of PN on $\mathbb{R}^N$: [M., Patrizi (2012)]

Traveling waves for PN : [Gui, Zhao (2012)]

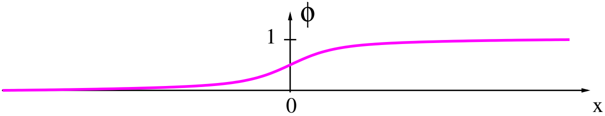
Rescaling to curvature models :

MCM : [Imbert, Souganidis (2009)]
[Caffarelli, Souganidis (2010)]

Variational : [Garroni, Müller (2006)]

The layer solution

[Cabré, Solà-Morales, (2005)]

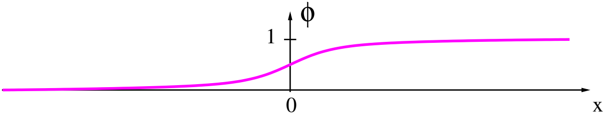


$$\begin{cases} 0 = -W'(\phi) + \Delta^{\frac{1}{2}}\phi \quad \text{on} \quad \mathbb{R} \\ \phi' > 0, \quad \phi(-\infty) = 0, \quad \phi(+\infty) = 1, \quad \phi(0) = \dfrac{1}{2} \end{cases}$$

assuming

$$W''(0) > 0$$

[Cabré, Solà-Morales, (2005)]



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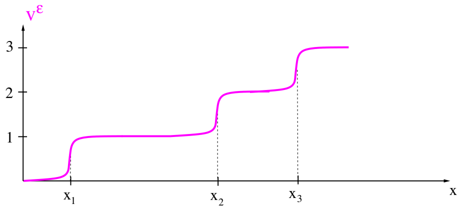
assuming

$$W''(0) = 1$$

Convergence to Dislocation points dynamics

$$(\varepsilon = \varepsilon_2 \to 0)$$

$$v^{\varepsilon}(x,t) = v\left(\frac{x}{\varepsilon}, \frac{t}{\varepsilon^2}\right) \quad \text{for} \quad x \in \mathbb{R}$$



Parabolic rescaling

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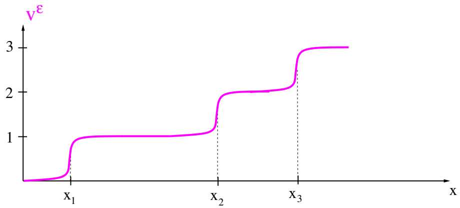


Well-prepared initial data

$$\begin{cases} x_1^0 < x_2^0 < \ldots < x_N^0 \\ \\ v_0^{\varepsilon}(x) = \varepsilon\sigma + \displaystyle\sum_{i=1}^{N} \phi\left(\frac{x - x_i^0}{\varepsilon}\right) \end{cases}$$

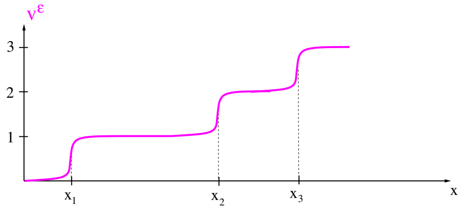
Thm 2 (Convergence PN $\to$ DP) [Gonzalez, M. (2012)]

As $\varepsilon \to 0$, we have

$$v^\varepsilon \to v^0 \quad \text{in} \quad L^1_{loc}(\mathbb{R} \times [0, +\infty))$$

with

$$v^0(x,t) = \sum_{i=1}^{N} H(x - x_i(t)), \qquad (H = \text{Heaviside function})$$



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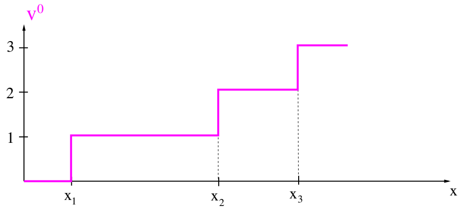


Dislocation points dynamics

$$\left\{\begin{array}{l} \dfrac{dx_i}{dt} = -\gamma \left(\sigma + \displaystyle\sum_{j\neq i} V'(x_i - x_j) \right) \\[2em] x_i(0) = x_i^0 \end{array}\right. \qquad \Bigg| \qquad \text{for} \quad i = 1, \ldots, N$$

with

$$\left\{\begin{array}{l} \gamma = \left(\displaystyle\int_{\mathbb{R}} (\phi')^2 \right)^{-1} \\[2em] V(x) = -\dfrac{1}{\pi} \ln |x| \end{array}\right.$$

$$\left\{\begin{array}{l} \dfrac{dx_i}{dt} = -\left(\sigma + \displaystyle\sum_{j\neq i} V'(x_i - x_j)\right) \\ \\ x_i(0) = x_i^0 \end{array}\right. \qquad \Bigg| \qquad \text{for} \quad i = 1, ..., N$$

with

$$\left\{\begin{array}{l} \gamma = 1 \\ \\ V(x) = -\dfrac{1}{\pi} \ln |x| \end{array}\right.$$

$$\left\{\begin{array}{l} \dfrac{dx_i}{dt} = -\left(\sigma + \displaystyle\sum_{j\neq i} V'(x_i - x_j)\right) \\ \\ x_i(0) = x_i^0 \end{array}\right. \quad \Bigg| \quad \text{for} \quad i = 1, ..., N$$

with

$$\left\{\begin{array}{l} \gamma = 1 \\ \\ V(x) = -\dfrac{1}{\pi}\ln|x| \end{array}\right.$$

$$\phi(x) - H(x) \sim -\frac{1}{\pi x} \quad \text{as} \quad |x| \to +\infty$$

Related results

- Micromagnetic thin films (gradient flow) : [Kurzke (2007)]
- Slow motion for non linear heat equation
  Energy approach : [Bronsard, Kohn (1990)]
  [Kalies, Van der Vorst, Wanner (2001)]
  Invariant manifold : [Car, Pego (1989)]
  [Chen (2004)]
  [Ei (2002)]
  [Fusco, Hale (1989)]

Ansatz

$$\tilde{v}^{\varepsilon}(x,t) = \varepsilon\sigma + \sum_{i=1}^{N} \left\{ \phi\left(\frac{x - x_i(t)}{\varepsilon}\right) \right\}$$

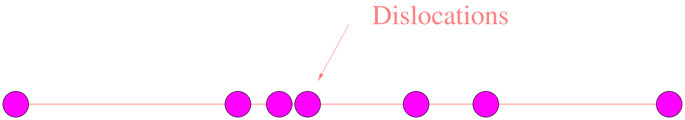
Ansatz

$$\tilde{v}^{\varepsilon}(x,t) = \varepsilon\sigma + \sum_{i=1}^{N} \left\{ \phi\left(\frac{x - x_i(t)}{\varepsilon}\right) - \varepsilon \dot{x}_i(t) \psi\left(\frac{x - x_i(t)}{\varepsilon}\right) \right\}$$

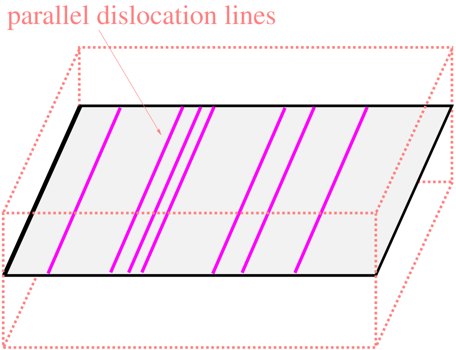
with the corrector ψ solving

$$\Delta^{\frac{1}{2}}\psi - W''(\phi)\psi = \phi' + W''(\phi) - W''(0)$$

Points



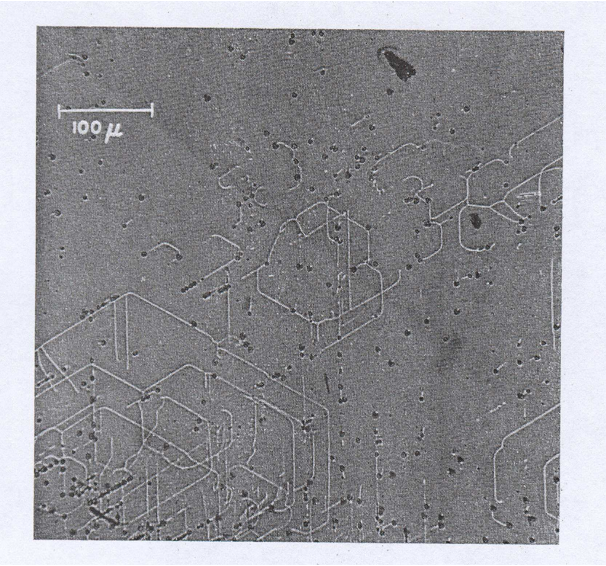
Straight dislocations lines



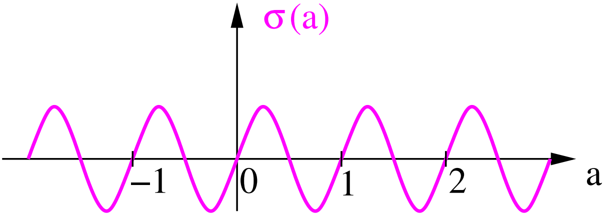
Dislocation dynamics with periodic obstacles

$$(\varepsilon = \varepsilon_3)$$

Precipitates = obstacles

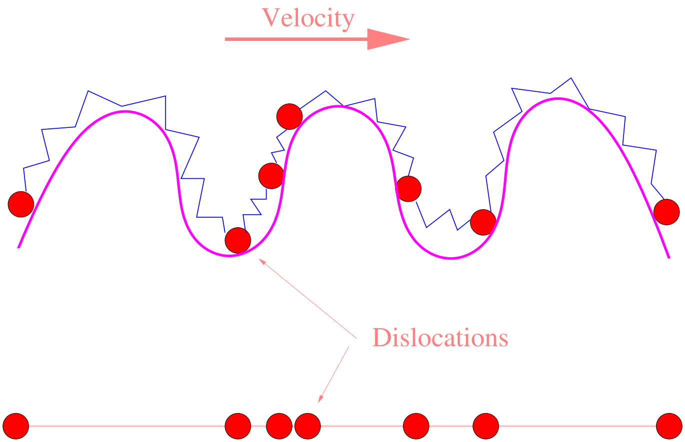


smooth periodic stress $\quad \sigma(a+1) = \sigma(a)$



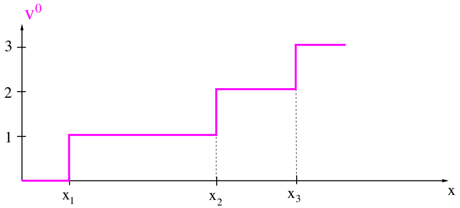
σ describes the obstacles to the motion of dislocations

Dynamics with two-body interactions



$$\begin{cases} N_\varepsilon \quad \text{dislocations} \quad x_1^0 < \dots < x_{N_\varepsilon}^0 \\ \\ \dfrac{dx_i}{dt} = -\left(\sigma(x_i) + \displaystyle\sum_{j \neq i} V'(x_i - x_j) \right) \\ \\ x_i(0) = x_i^0 \end{cases} \qquad (3)$$

$$v^0(x,t) = \sum_{i=1}^{N_\varepsilon} H(x - x_i(t))$$



Convergence to crystal plasticity

$$(\varepsilon = \varepsilon_3 \to 0)$$

Hyperbolic rescaling

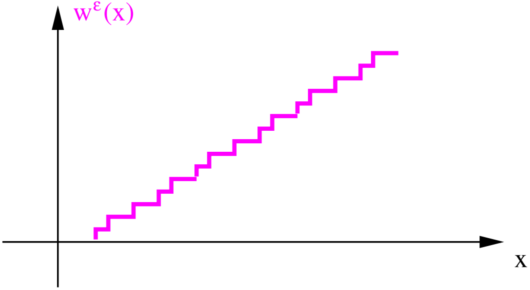
$$w^{\varepsilon}(x,t) = \varepsilon v^0\left(\frac{x}{\varepsilon}, \frac{t}{\varepsilon}\right)$$

Thm 3 (Convergence DD $\to$ CP) [Forcadel, Imbert, M. (2009)]

As $\varepsilon \to 0$, we have

$$w^\varepsilon \to w^0 \quad \text{in} \quad L^\infty_{loc}(\mathbb{R} \times [0, +\infty))$$

where w^0 is a solution to the crystal plasticity model.



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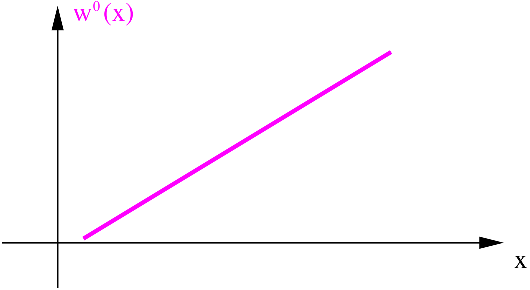

Dynamics for densities of dislocations

Crystal (elasto-visco-) plasticity

$$w_t^0 = \bar{H}(w_x^0, \Delta^{\frac{1}{2}} w^0) \tag{4}$$

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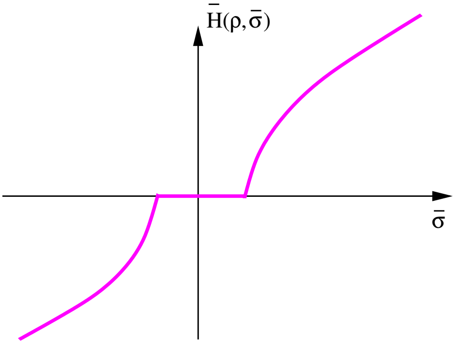
$$w_t^0 = \bar{H}(w_x^0, \Delta^{\frac{1}{2}} w^0) \tag{4}$$

Mechanical interpretation

$$\begin{cases} w^0 & = \text{plastic strain} \\ w_t^0 & = \text{plastic strain velocity} \\ w_x^0 & = \text{density of dislocations} \\ \Delta^{\frac{1}{2}} w^0 & = \text{self-stress created by the density of dislocations} \\ w_t^0 & = \bar{H}(w_x^0, \Delta^{\frac{1}{2}} w^0) \quad \text{is the visco-plastic law} \end{cases}$$

Crystal (elasto-visco-) plasticity

$$w_t^0 = \bar{H}(w_x^0, \Delta^{\frac{1}{2}} w^0)$$



Orowan's law if no mesoscopic obstacles ($\sigma = 0$)

$$\bar{H}(\rho, \bar{\sigma}) = |\rho|\bar{\sigma}$$

$\Longrightarrow$

$$w_t = (\Delta^{\frac{1}{2}} w)|w_x|$$

Study of self-similar solutions
[Biler, Karch, M. (2010)]

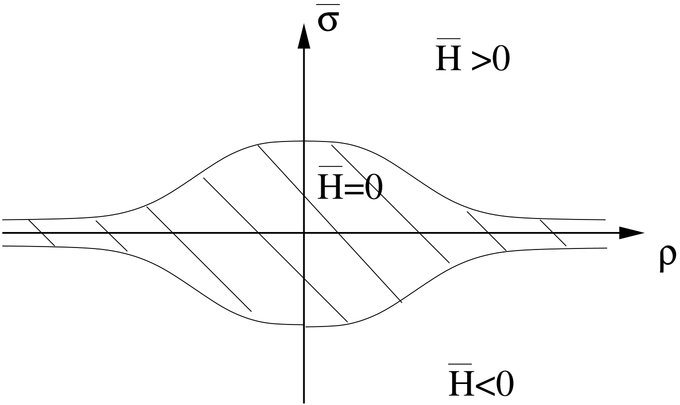
Dynamics for densities of dislocations

Conservation law for $\rho = w_x^0$ and $\bar{\sigma} = \Delta^{\frac{1}{2}} w^0$, $\bar{H}(\rho, \bar{\sigma}) = |\rho|\bar{\sigma}$

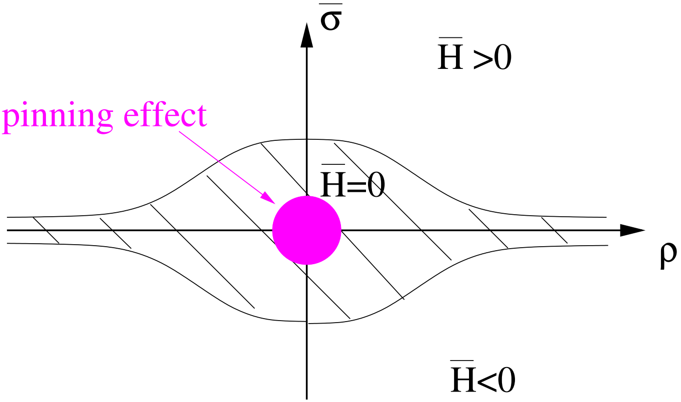
$$\rho_t = -(|\rho|\mathcal{H}\rho)_x \quad \text{with} \quad \mathcal{H} = \text{Hilbert transform}$$

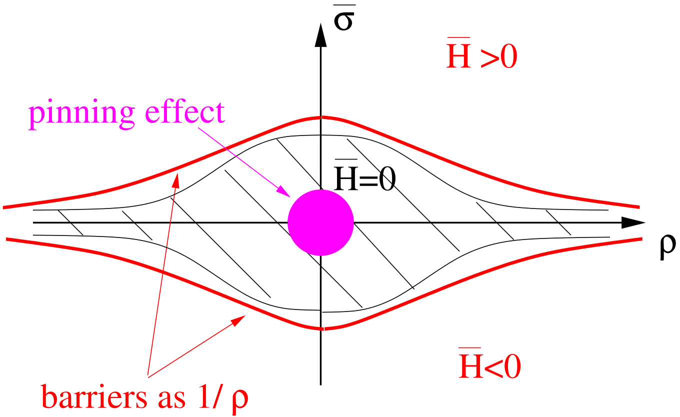
- Quasi-Geostrophic type equation
  [Córdoba, Córdoba, Fontelos (2005)]
- Gradient flow approach with Wasserstein metric
  [Carrillo, Ferreira, Precioso (2011)]
- Fractional porous medium equation
  [Biler, Karch, Imbert (2011)]
  [Caffarelli, Vazquez (2011)]

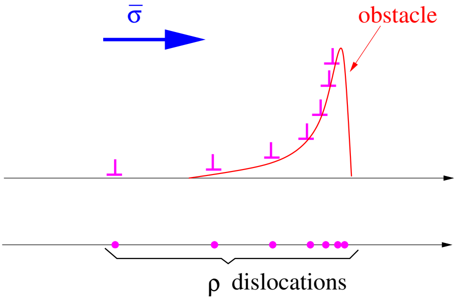
Effective Hamiltonian $\bar{H}(\rho, \bar{\sigma})$



Pinning effect if $\int_{[0,1)} \sigma = 0$




$\overline{\sigma}$
$\overline{H}>0$
pinning effect
$\overline{H}=0$
ρ
$\overline{H}<0$
barriers as $1/\rho$

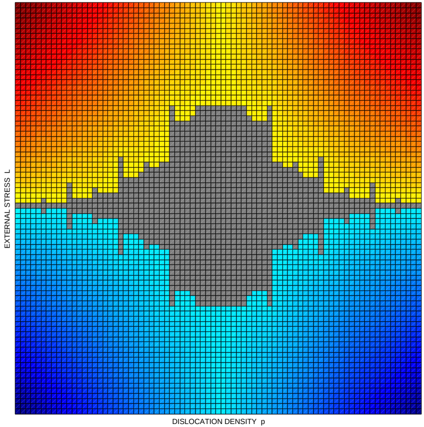


$$\overline{\sigma} = \frac{\sigma^{\mathsf{obst}}}{\rho}$$

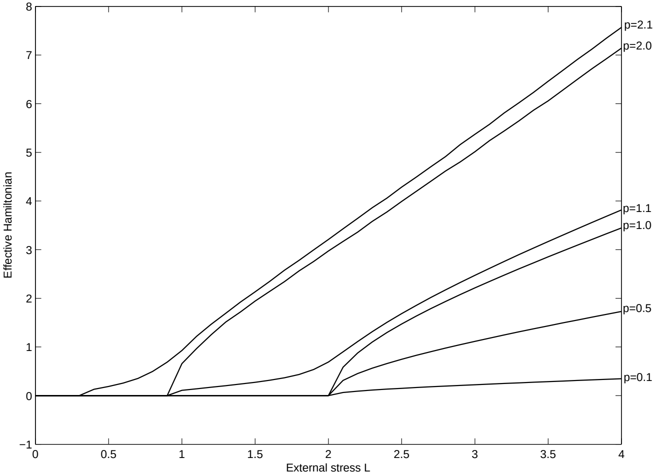
[Hirth, Lothe (1992), p. 766]

Effective Hamiltonian $\bar{H}(\rho, \bar{\sigma})$ (Numerics)

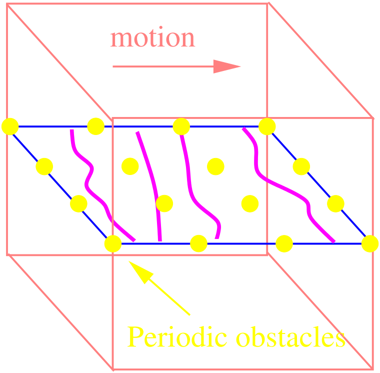
[Cacace, Chambolle, M. (2012)]



Effective Hamiltonian $\bar{\sigma} \mapsto \overline{H}(\rho, \bar{\sigma})$

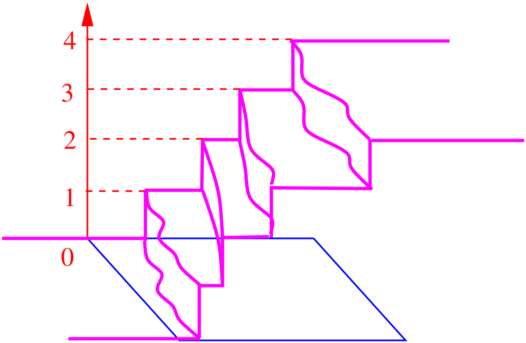


Homogenization of dislocation curves

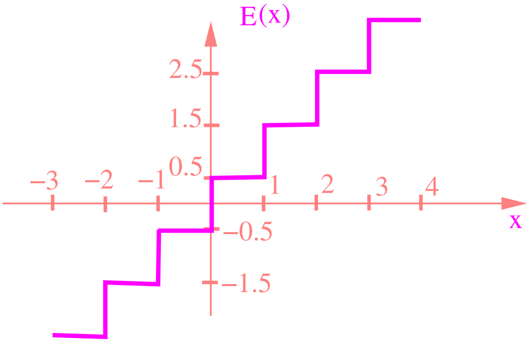


Limit for density of curves ?

Plastic displacement



$$E(w) = l + \frac{1}{2} \quad \text{for} \quad l \leq w < l+1, \quad l \in \mathbb{Z}$$



Level sets formulation

$$w_t = |\nabla w| \; c[w] \quad \text{on} \quad \mathbb{R}^N \times (0, +\infty)$$

with

$$(c[w])(x) = c(x) + (J \star E \{w(\cdot, t) - w(x, t)\})(x)$$

Level sets formulation

$$w_t = |\nabla w| \; c[w] \quad \text{on} \quad \mathbb{R}^N \times (0, +\infty)$$

with

$$(c[w])(x) = c(x) + (J \star E\{w(\cdot,t) - w(x,t)\})(x)$$

where $c(x)$ represents the (periodic) obstacles :

$$c(x+k) = c(x) \quad \text{for all} \quad k \in \mathbb{Z}^N$$

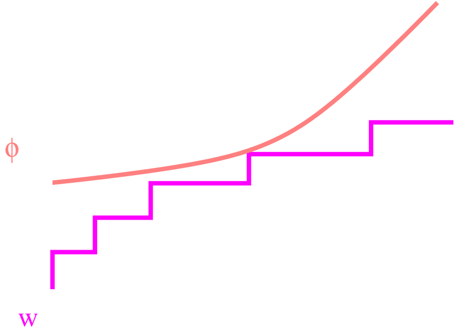
and

$$J(z) = \frac{1}{|z|^{N+1}} \cdot 1_{\{|z| \geq \delta\}} \quad \text{for some fixed} \quad \delta > 0$$

$$c[w] = c + J \star E\left\{w(\cdot,t) - w(x,t)\right\}$$

We set

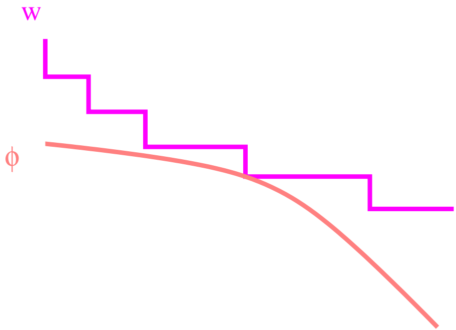
$$\left\{\begin{array}{l} c^*[w] := c + J \star E^*\left\{...\right\} \\ \\ c_*[w] := c + J \star E_*\left\{...\right\} \end{array}\right.$$



subsolution :

$$\phi_t \leq |\nabla \phi| \cdot c^*[w] \quad \text{at the contact point}$$

“$Slepčev$ viscosity solution”



supersolution :

$$\phi_t \geq |\nabla \phi| \cdot c_*[w] \quad \text{at the contact point}$$

Let

$$w^{\varepsilon}(x,t) = \varepsilon w\left(\frac{x}{\varepsilon}, \frac{t}{\varepsilon}\right)$$

Thm 3' (Convergence DD → CP) [Forcadel, Imbert, M. (2009)]

As $\varepsilon \to 0$, we have

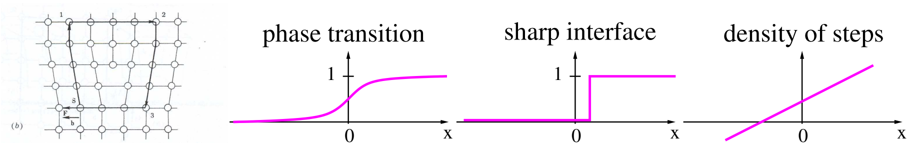
$$w^{\varepsilon} \to w^0 \quad \text{in} \quad L^{\infty}_{loc}(\mathbb{R}^N \times [0,+\infty))$$

where w^0 is the solution of the limit equation for some suitable function $\bar{H}$:

$$w^0_t = \bar{H}(\nabla w^0, \Delta^{\frac{1}{2}} w^0) \quad \text{on} \quad \mathbb{R}^N \times (0,+\infty)$$

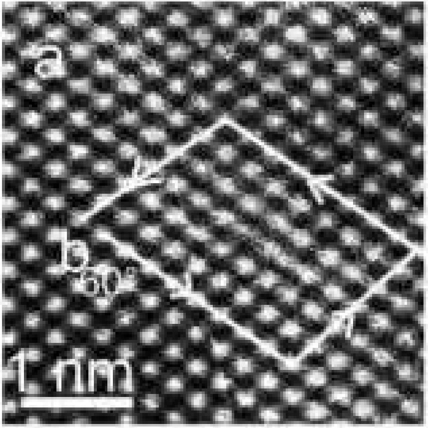
Conclusion

Hierarchy of scales and models



“FK” $\Longrightarrow$ PN $\Longrightarrow$ DD $\Longrightarrow$ Crystal plasticity

A dislocation in cubic Boron Nitride



High Resolution Transmission Electronic Microscopy