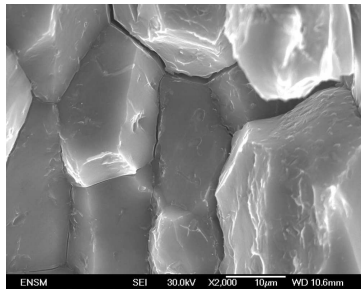
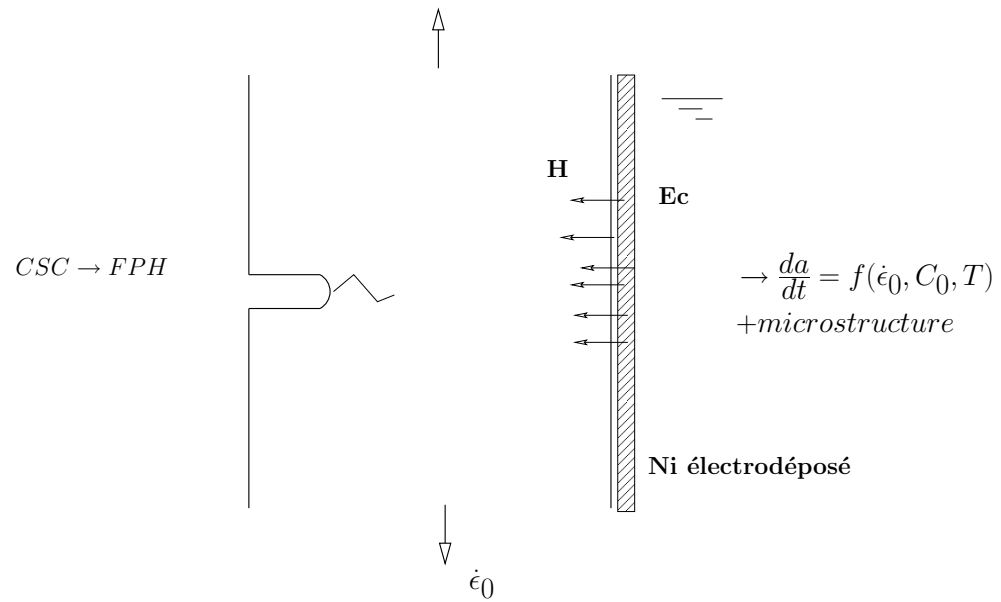
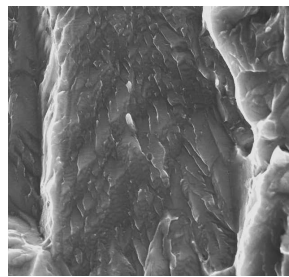


Rupture et plasticité en pointe de fissure.

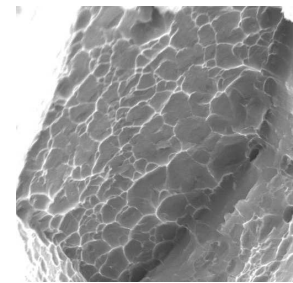
Dôme TANGUY
CNRS, UMR 5146
SMS/Ecole des Mines de Saint-Etienne
tanguy@emse.fr



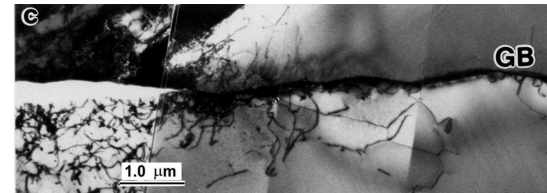
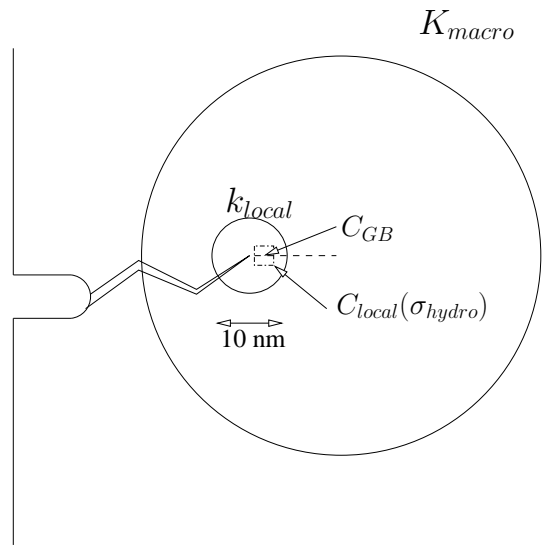
$$\dot{\epsilon}_0 = 2 \cdot 10^{-7} s^{-1}$$



$$\dot{\epsilon}_0 = 10^{-5} s^{-1}$$



$$\dot{\epsilon}_0 = 2 \cdot 10^{-4} s^{-1}$$

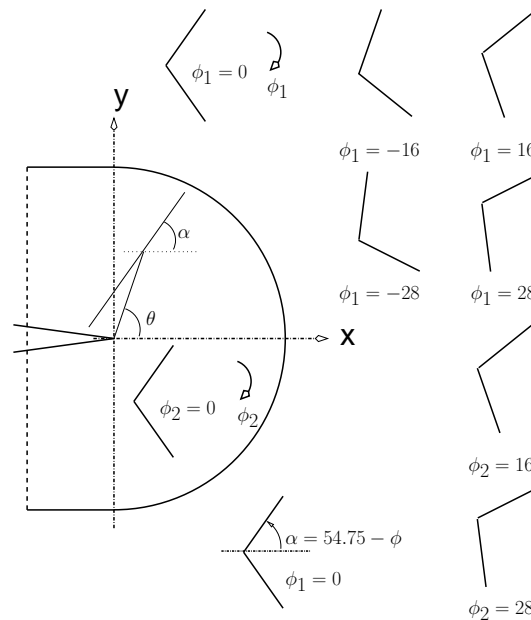


Ni + S + H

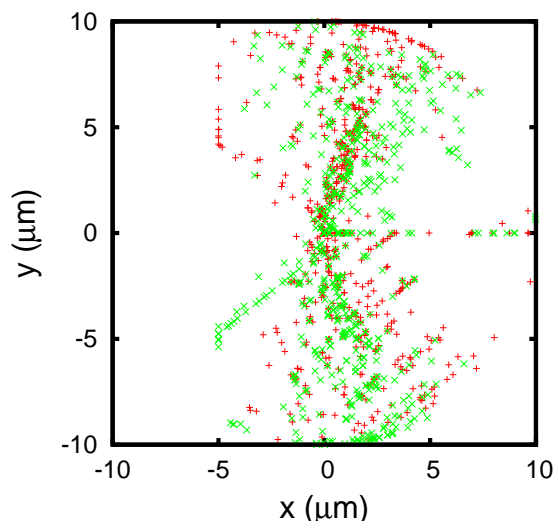
Ian Robertson, Univ. Illinois Urbana Champaign

- vitesses de propagation expérimentales lentes **1nm/100ms** (1mm/20h)
- plasticité (rupture semi fragile). Role $\dot{\epsilon}_0$ sur la transition intergranulaire / transgranulaire.
- piégeage sur les défauts (joints de grains, dislocations, précipités, lacunes)

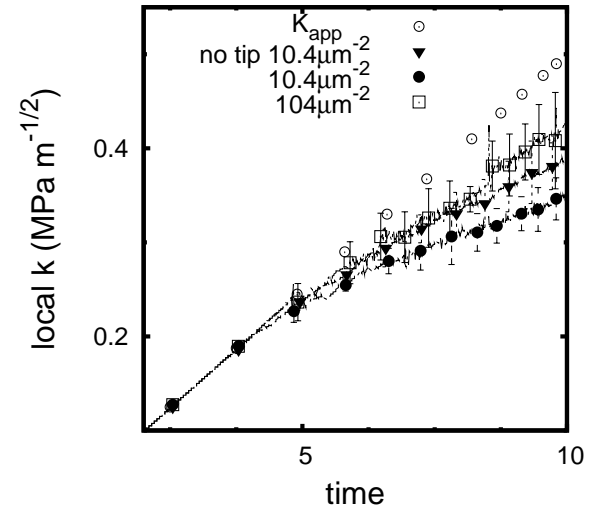
Modélisation de la zone plastique en dynamique des dislocations: Phil. Mag. 2010



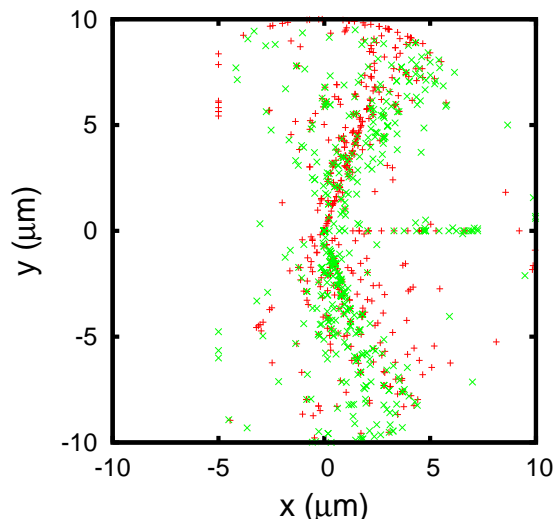
- dislocations coin parallèles au front de fissure: 2D
- interactions dislocation-fissure et dislocation-dislocation: élastique: potentiels complexes (analytique). Chargement extérieur: K_{app} .
- dynamique: $\vec{v}_i = \alpha \vec{f}$; $\vec{f} = \sigma \vec{b} \wedge \vec{\xi}$
- règles locales: émission (fissure ou source), annihilation, jonction, obstacles



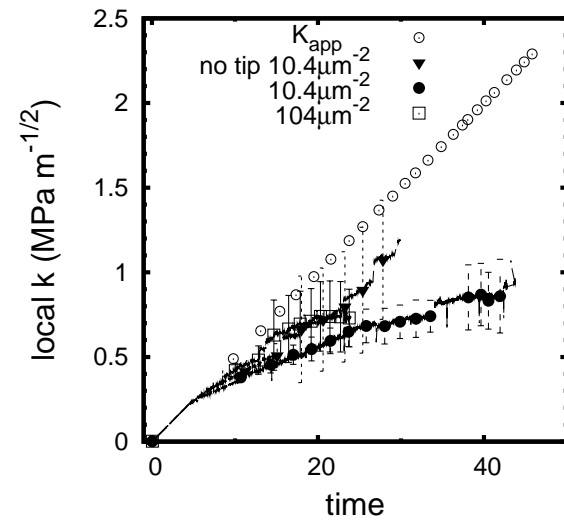
(a)



(a)



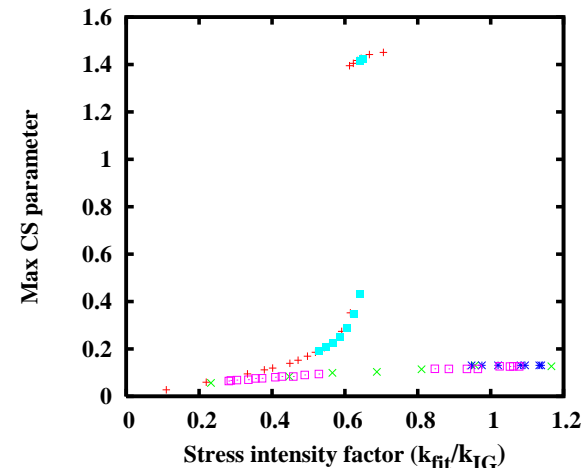
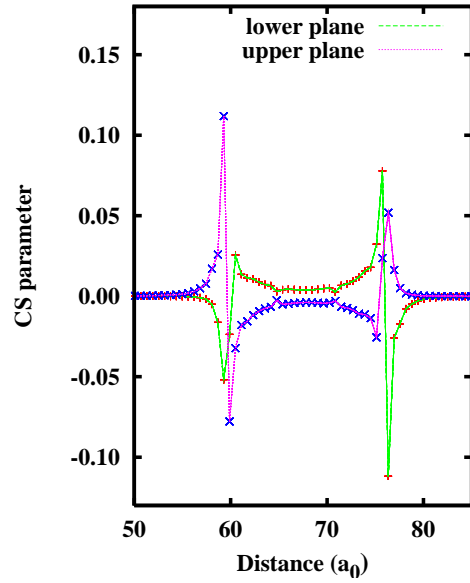
(b)



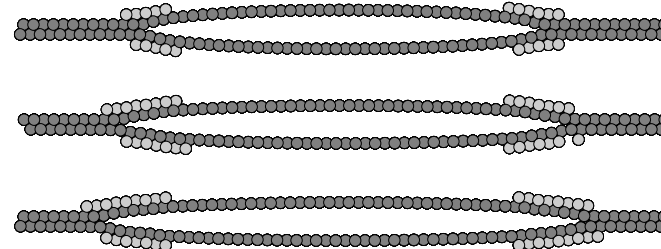
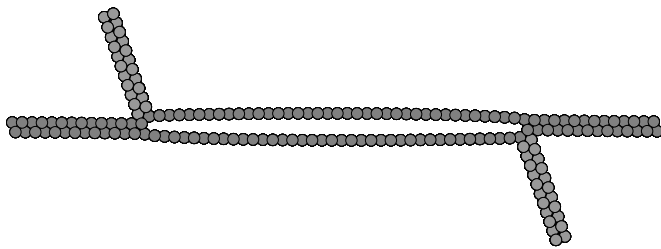
(b)

Problème: faible valeur de K_{app} qd $k = k_c$, même avec émission depuis la pointe

Calculer k_c et k_e à l'échelle atomique. Phys. Rev. B 2007

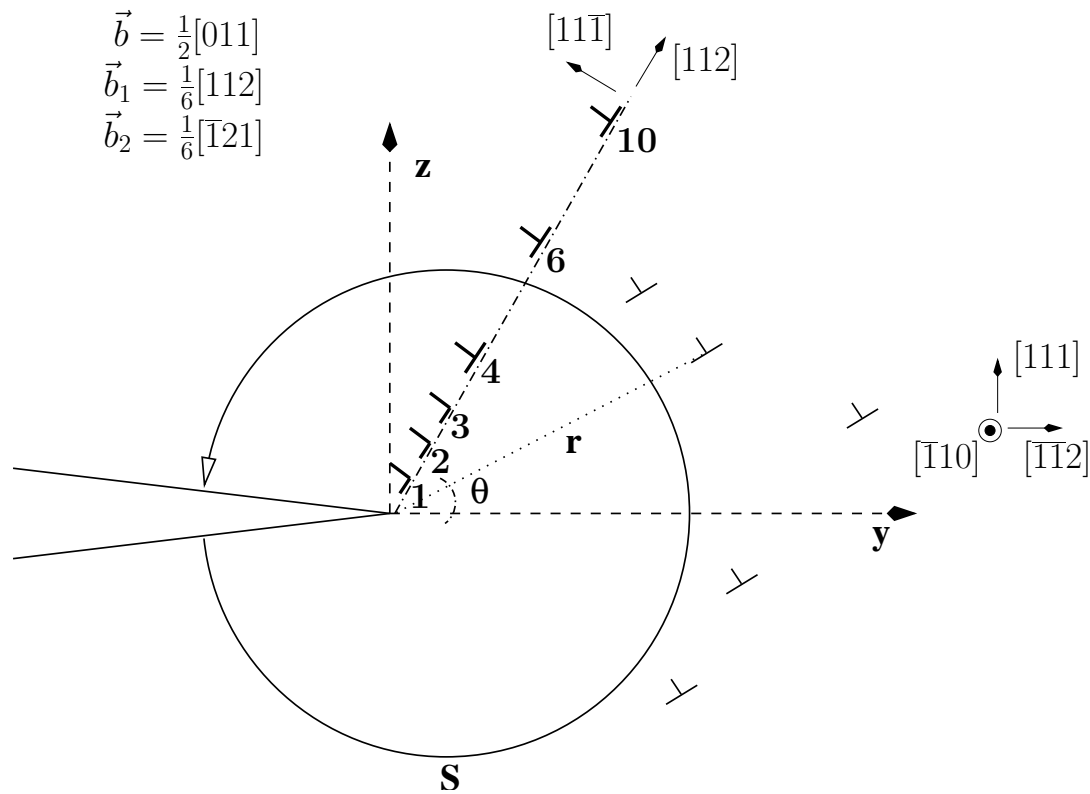


$$CS_i = \sum_j (\vec{q}_j - \vec{q}_i + q_{j+6} - \vec{q}_i) \cdot \vec{b}$$

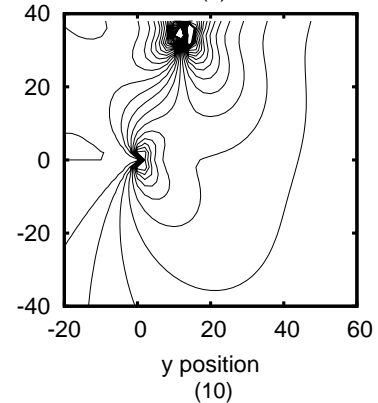
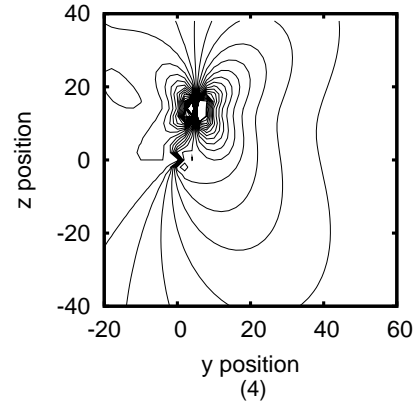
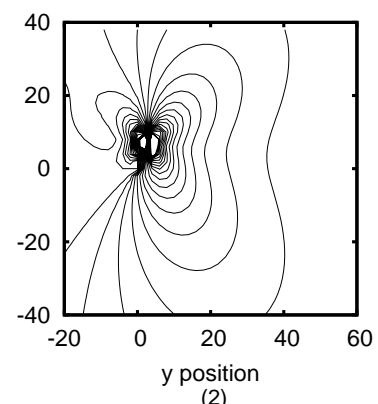
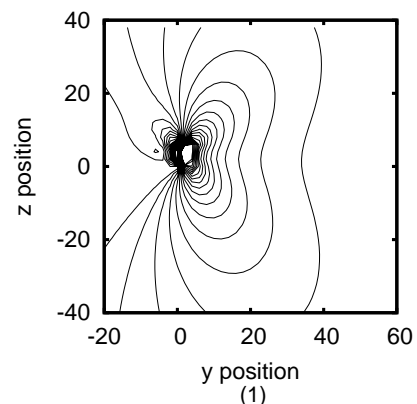
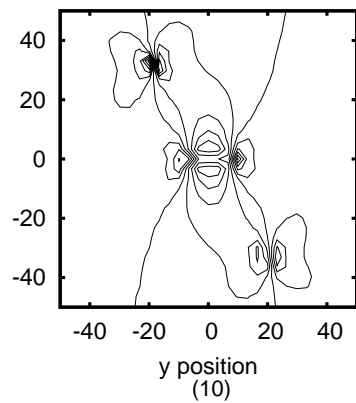
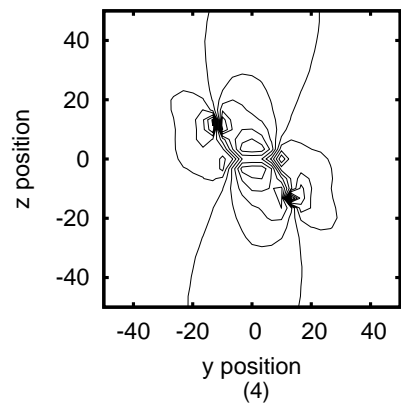
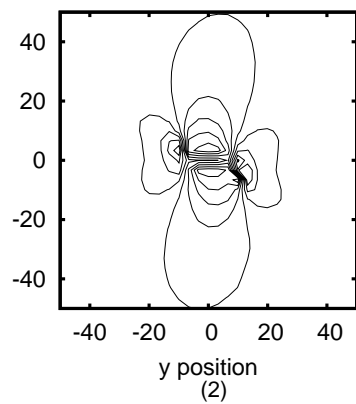
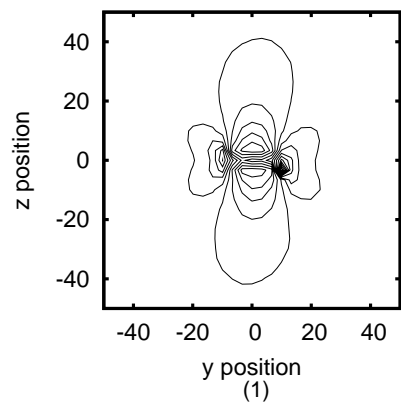


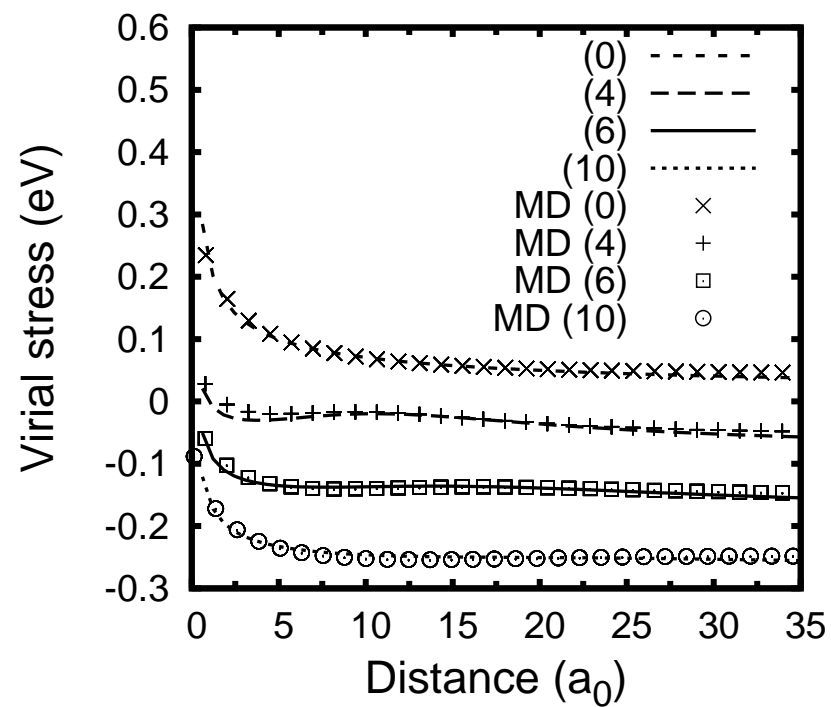
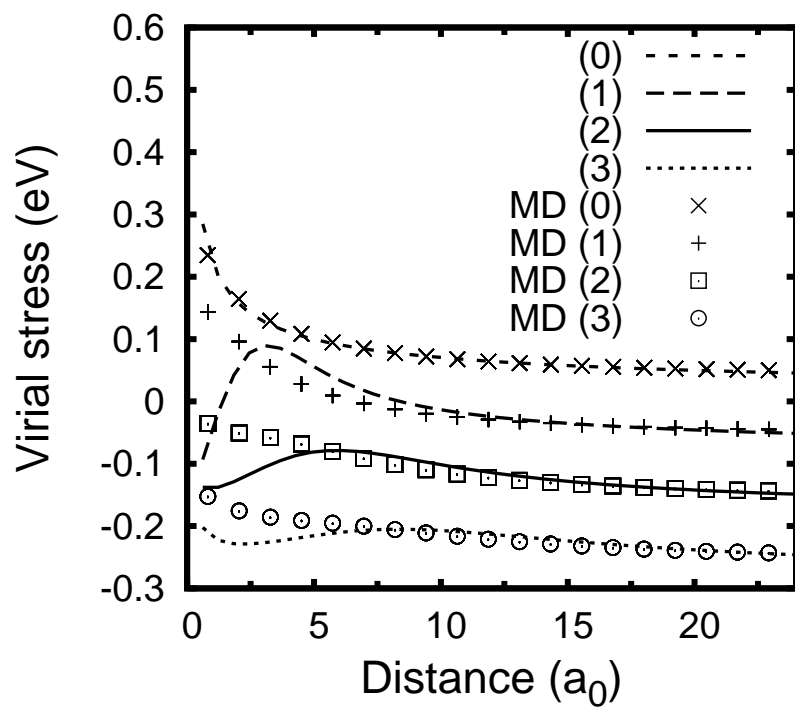
Epingler les dislocations:

$$\begin{aligned}\vec{b} &= \frac{1}{2}[011] \\ \vec{b}_1 &= \frac{1}{6}[112] \\ \vec{b}_2 &= \frac{1}{6}[\bar{1}21]\end{aligned}$$



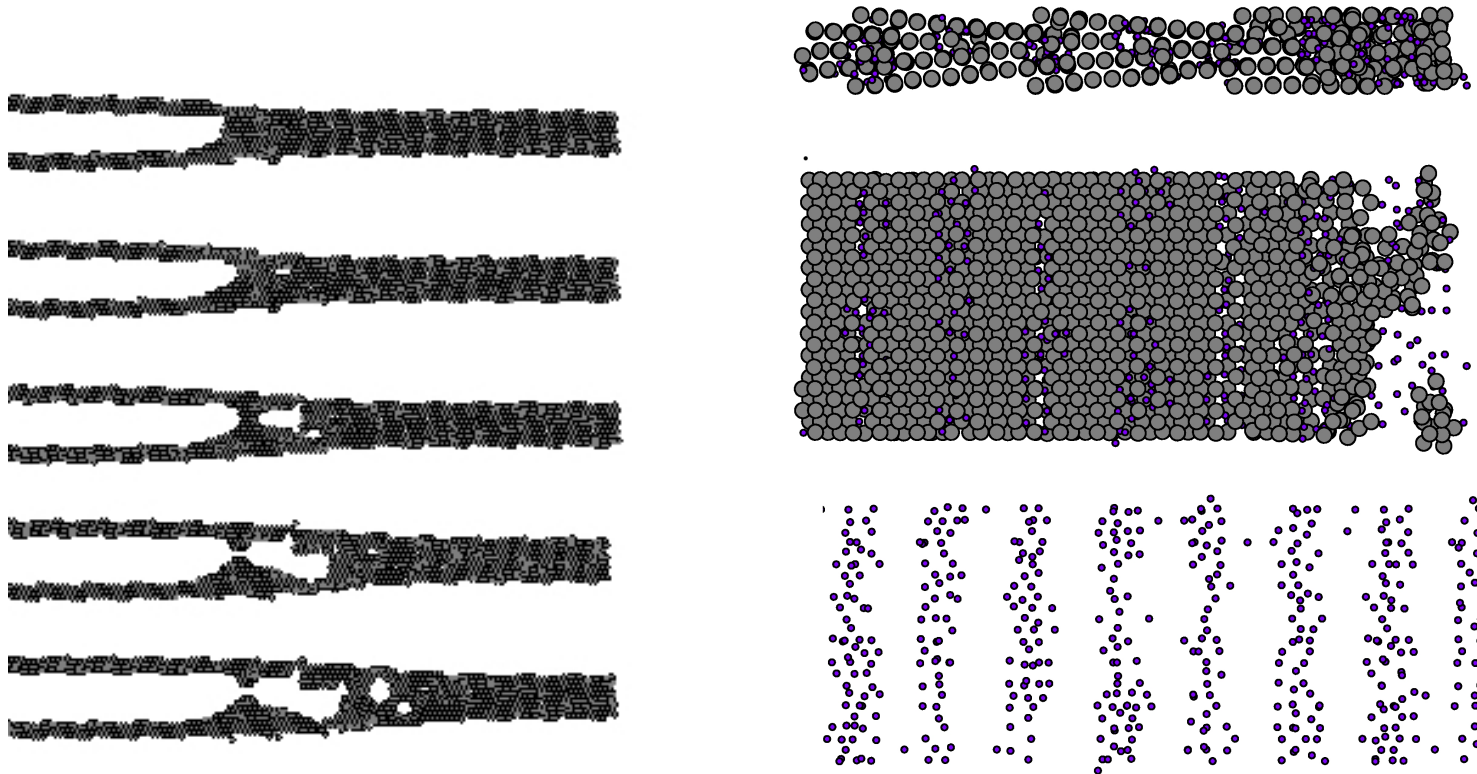
un problème élastique - un problème atomique





Objectif: inclure cette distance critique dans DD pour mieux modéliser l'écrantage.

Calculer k_{Ic} pour un joint avec T (et t): échelle de temps en MD



Objectif: accélérer la dynamique (avec Art. Voter).

Autre chose: Monte Carlo avec lacunes (Grand Canonique ou pas) Phys. Rev. B 2005 et 2009

$$\mathcal{Q}_c(M, \mu, V, T) = \sum_{N=0}^M \sum_{\{p_n\}} \frac{1}{\Lambda^{3N}} \int_{W.S} d\vec{u}^N \times \exp(-\beta(\mathcal{H}(\{p_n\}, (\vec{u})^N) - N\mu))$$

