Plasticité des minéraux du manteau terrestre

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Université de Lille 1
Villeneuve d'Ascq

Le laboratoire

UMET
Unité Matériaux Et Transformations

se décline en quatre équipes :

Matériaux Moléculaires et Thérapeutiques

Métallurgie Physique et Génie des Matériaux

Physique des Minéraux

Ingénierie des Systèmes Polymères.

Equipe : Métallurgie Physique

Modélisation multi-échelle de matériaux métalliques au voisinage ou loin de l'équilibre thermodynamique, en présence ou non de sollicitations extérieures (chocs, irradiation, contraintes mécaniques)

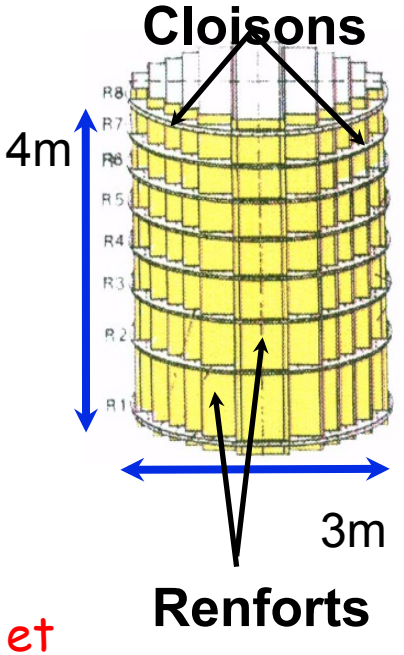
Permanents :
A. Legris
R. Besson
L. Thuinet
C. Becquart
Post doctorants :
A. De Backer
J. Boisse
J.B. Piochaud
Doctorants :
H. Rouchette
J. Kwon

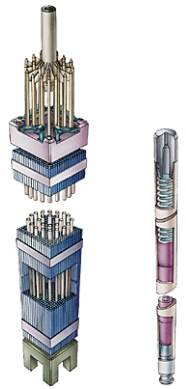
-Alliages de Zr

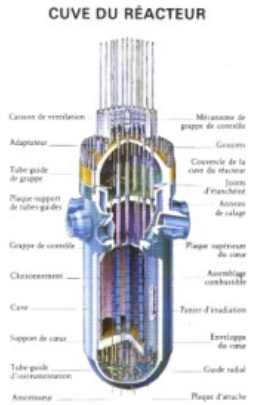
-Aciers ferritiques et austénitiques

-W

-NiAl



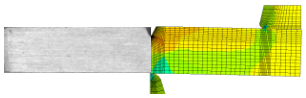




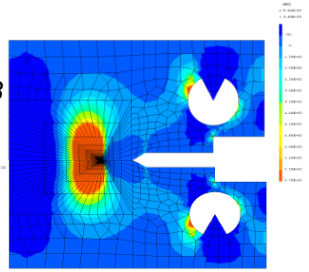
Equipe : Métallurgie Physique

m^3

10 years

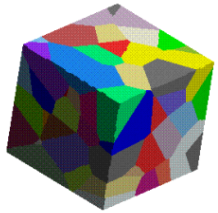


Finite elements

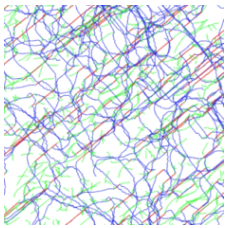


cm^3

Micro-macro



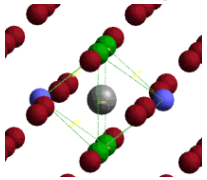
μm^3



Dislocation dynamics

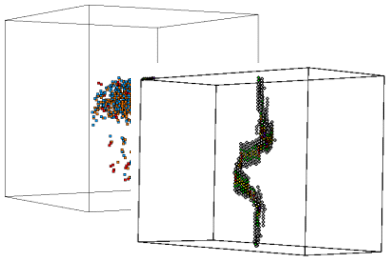
ab initio, dft

$1nm^3$, 0- ps

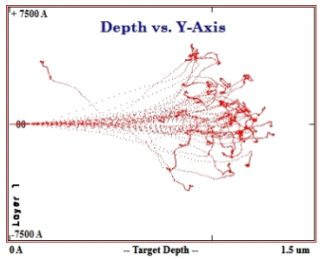


Molecular dynamics

($10\ nm^3$), ns



Binary collision approximation



-Alliages de Zr

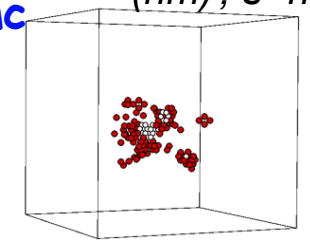
-Aciers ferritiques et austénitiques

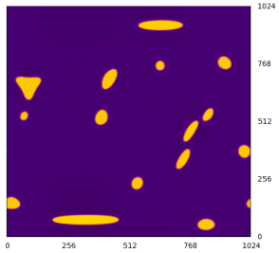
-W

-NiAl

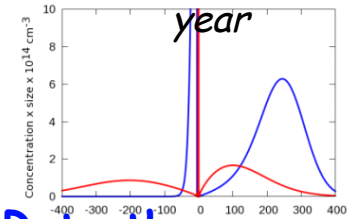
Akmc

(nm) , s- h

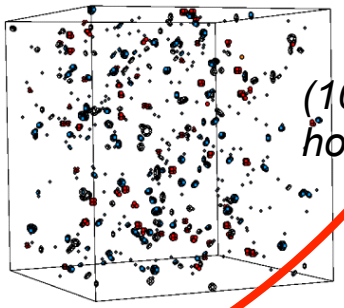




Phase Field



Rate theory



($100\ nm^3$)

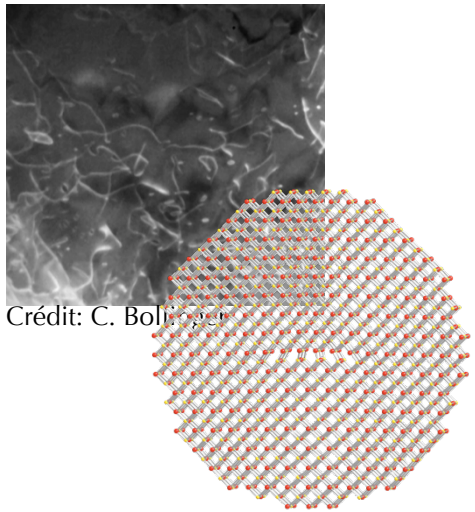
hour- year

Okmc

Equipe : Physique des Minéraux

=> astrominéralogie

=> **plasticité** des minéraux sous haute pression


Crédit: C. Bolliger

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Doctorants :
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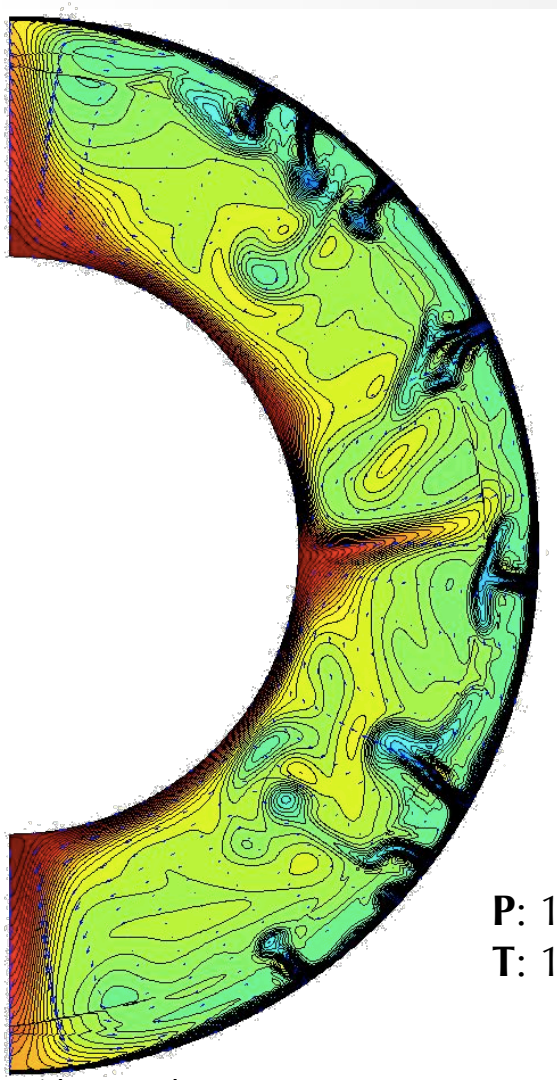
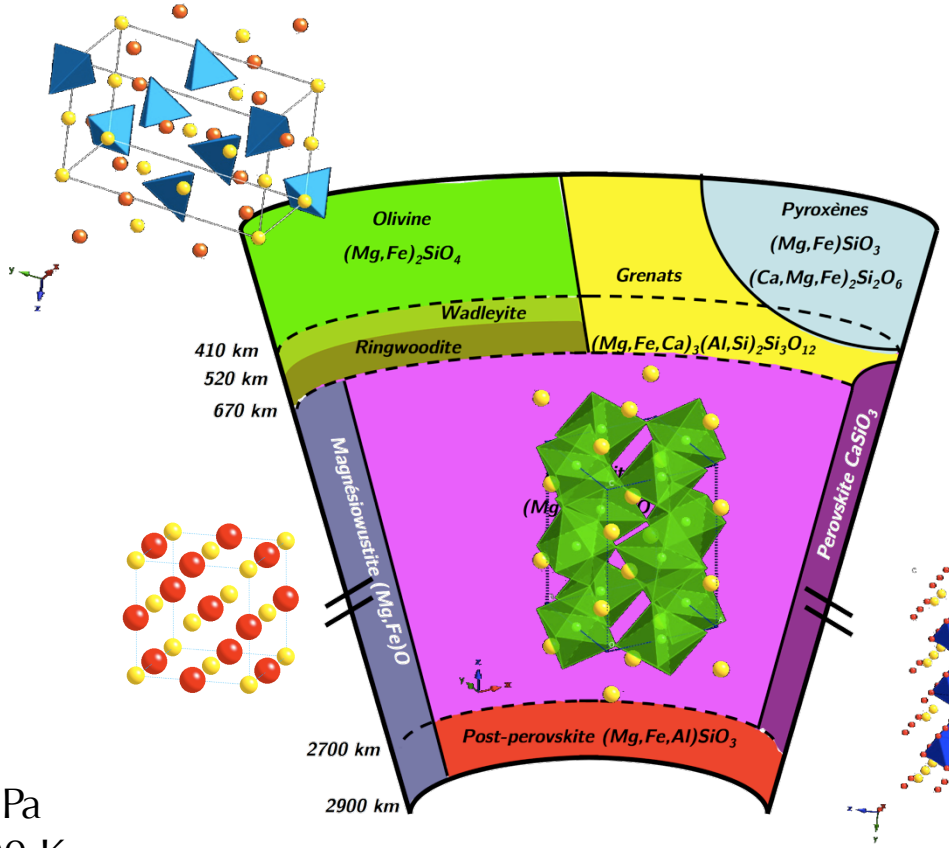
Projet ERC Adv. Grant RheoMan

Plasticité des minéraux du manteau terrestre

Convection et deformation



Crédit: S. Bulter



Mg

Si

Ca, Al

Fe

Ni

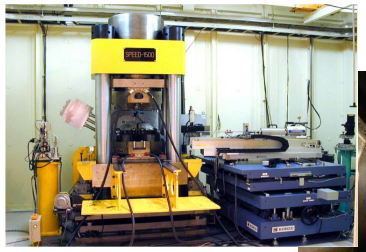
O

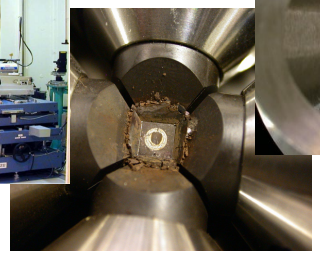
P: 10 – 130 GPa
T: 1000 – 3000 K

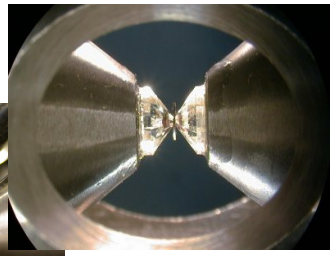
Mécanismes de déformation ?

La plasticité des minéraux: du point de vue expérimental

Conditions (P,T,$\dot{\varepsilon}$) sont particulièrement difficiles à reproduire dans les conditions du laboratoire



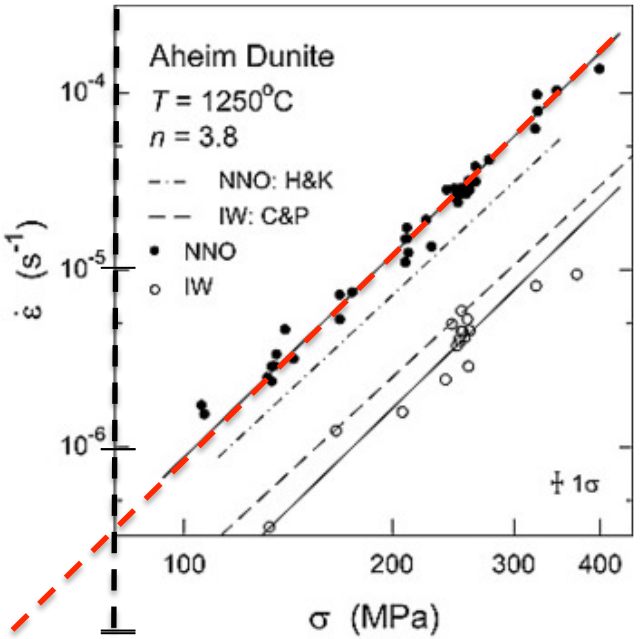




Presse Gros Volume
P_{max} = 20-80 GPa

D-Dia
P_{max}=20 GPa

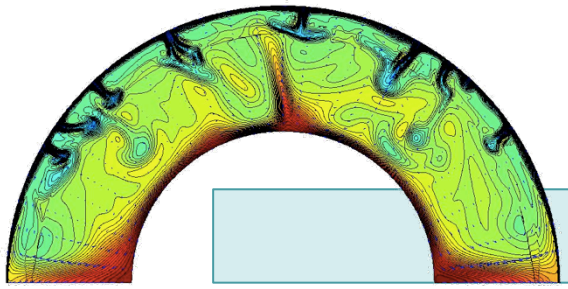
Diamant anvil cell (DAC)
P_{max}=400 GPa



Mackwell et al. 2008

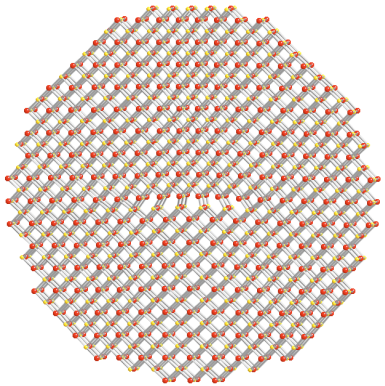
$$\dot{\varepsilon} = \dot{\varepsilon}_0.\sigma^n.exp[-Q/RT]$$

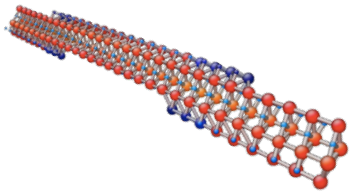
$$Q = E+PV$$

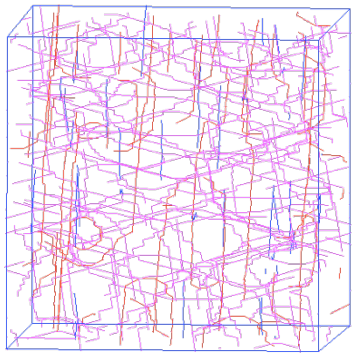


?

L'approche numérique: Objectifs







. Structures de cœur de dislocations dans les minéraux du manteau

. Friction de réseau et Contrainte de Peierls

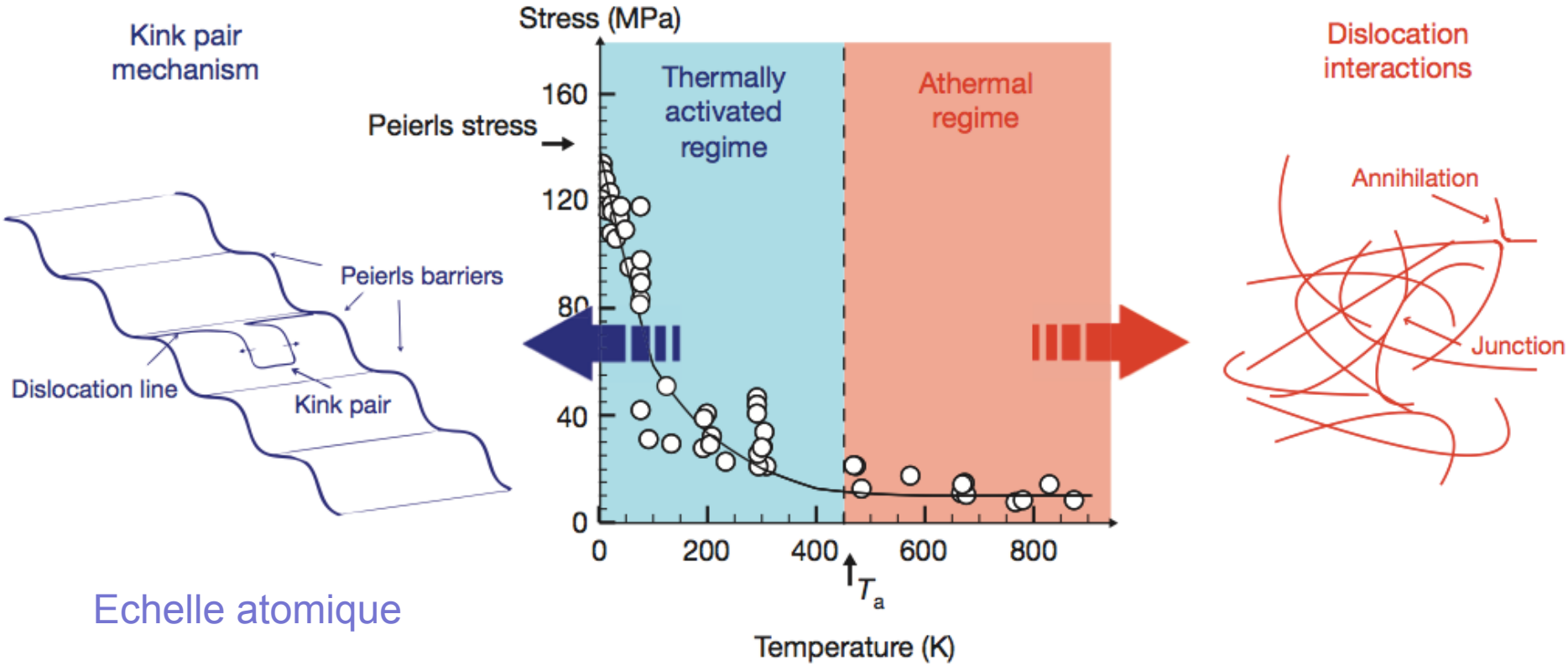
. Effet de pression

. Effet de température et mobilité

. Fluage

Modélisation des CRSS

Echelle mésoscopique / code DD



Echelle atomique

DFT/calculs par potentiels

DFT

b-initio VASP ackage ienna imulation

Taille des volumes simulés / nombre d'atomes dans les mailles élémentaires (> 20)

Calcul de γ-surface (énergie de faute d'empilement généralisé)

Approche semi-continu de type Peierls-Nabarro

Potentiels

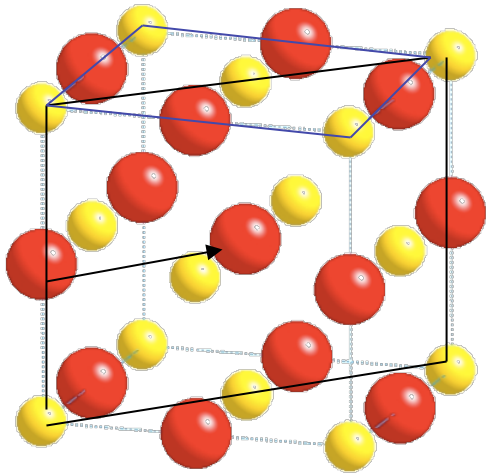
$$V_{ij}(r_{ij}) = \frac{q_i q_j}{r_{ij}} + A_{ij}\exp(-r_{ij}/\rho_{ij}) - \frac{C_{ij}}{r_{ij}^6}$$

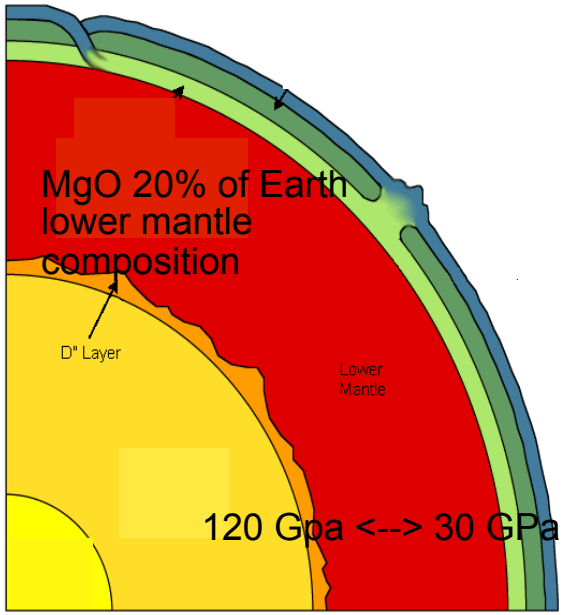
LAMMPS

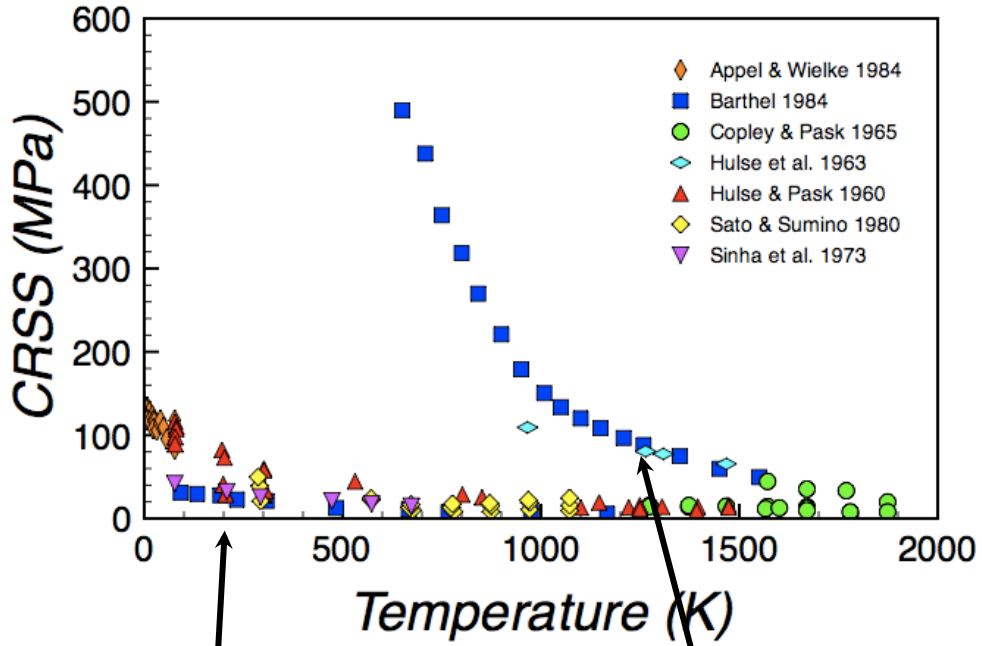
GULP

Illustration

dislocation vis de vecteur de Burgers ½<110> dans MgO

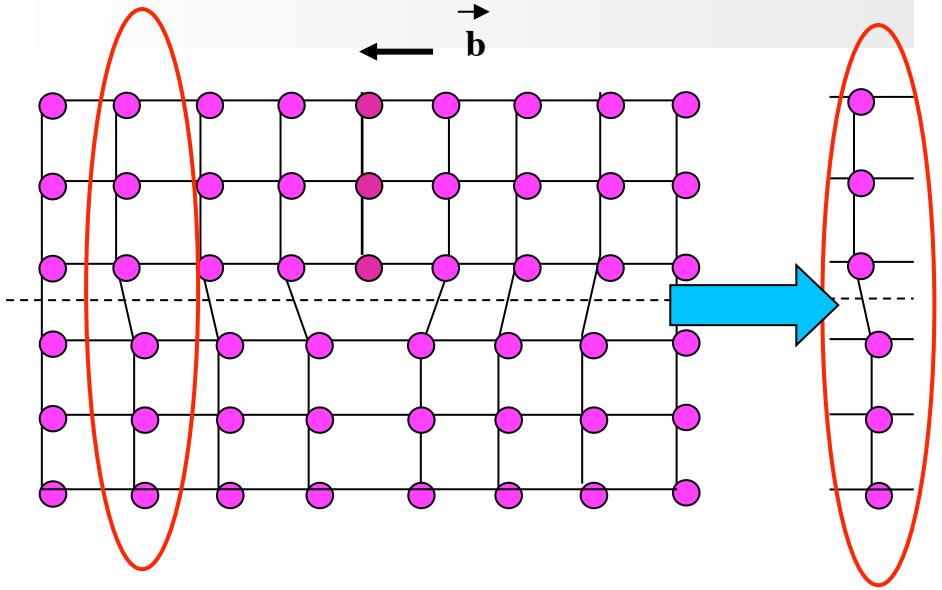


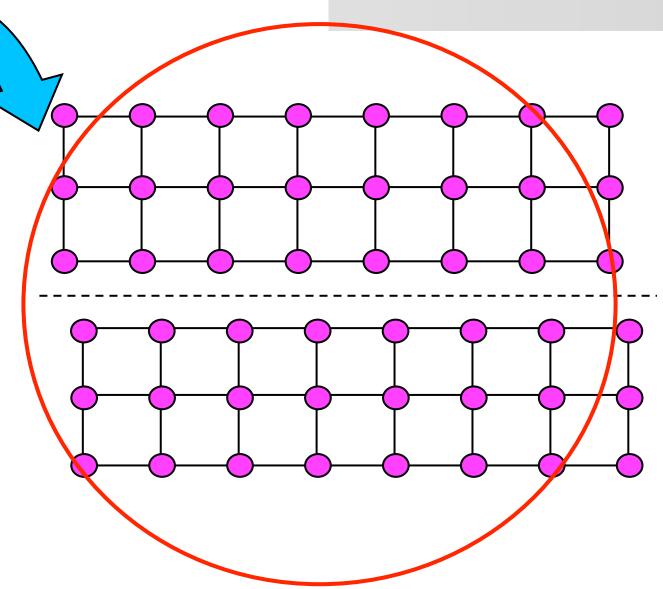


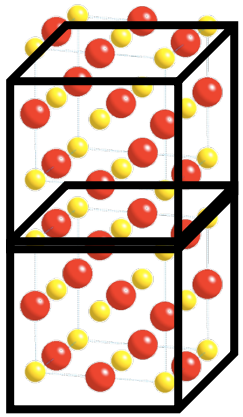


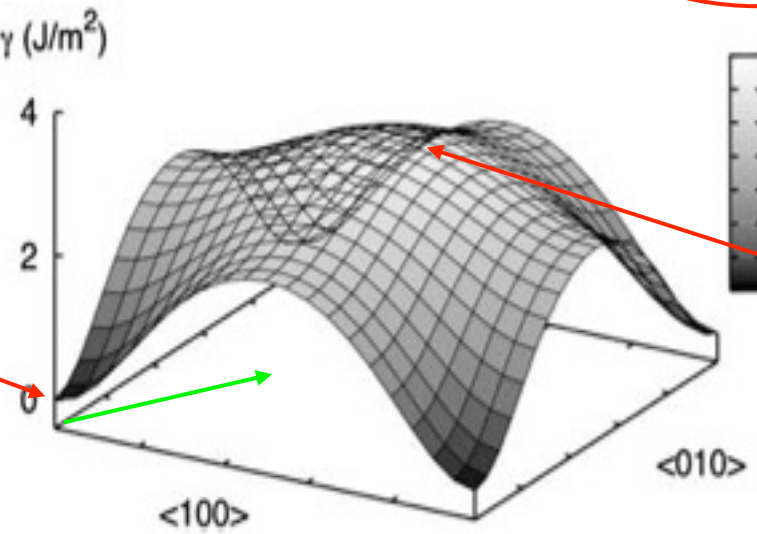
1/2<110>{110} and 1/2<110>{100}

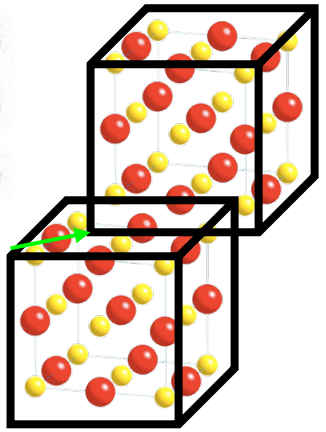
Faute d'empilement généralisée et γ-surface







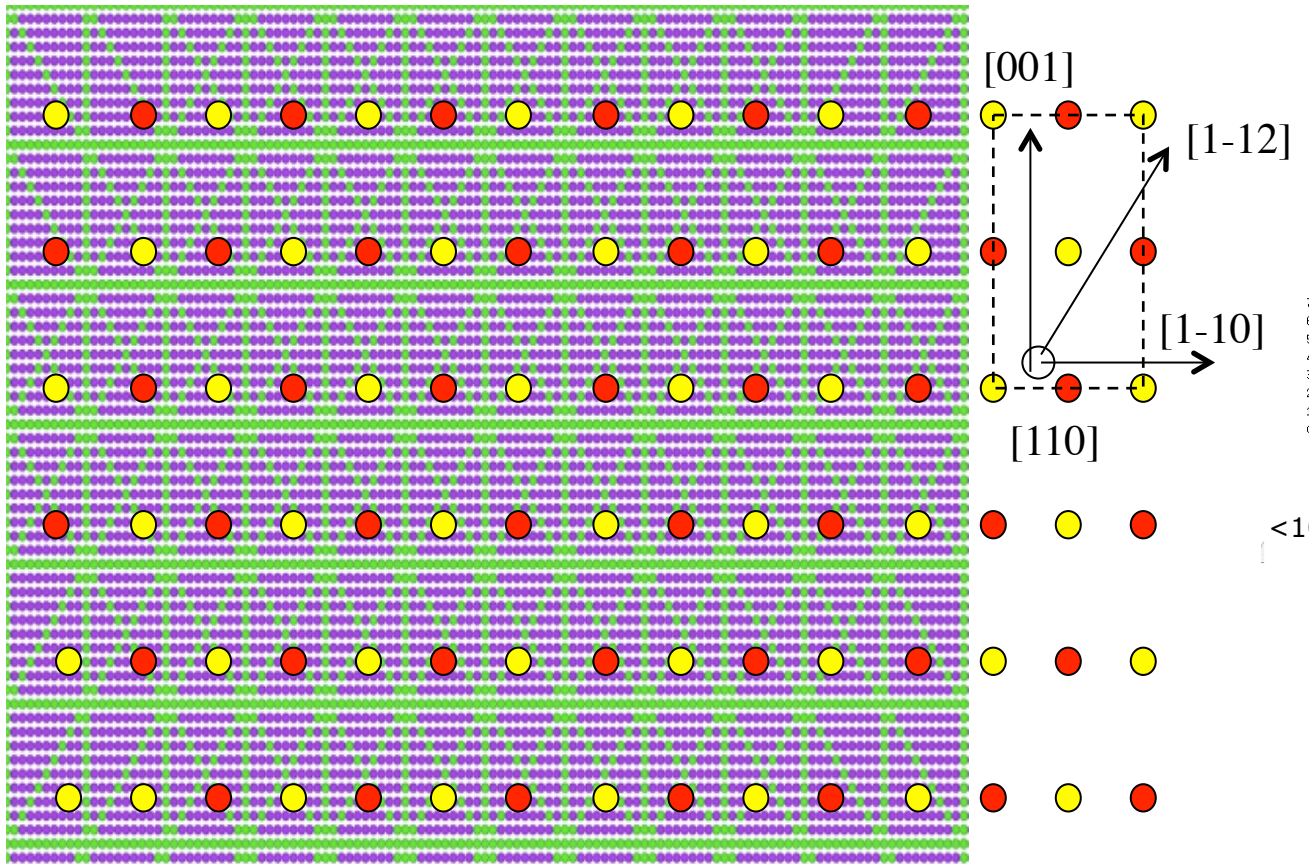




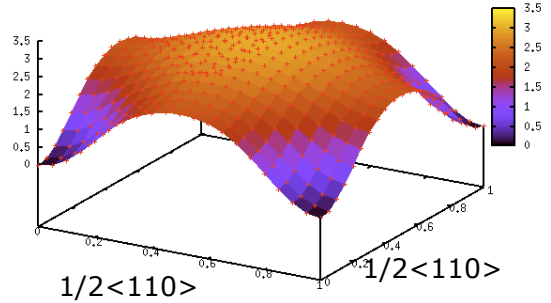
Le modèle de Peierls-Nabarro-Galerkin

dislocation vis de vecteur de Burgers ½<110>

$$\int_V \left\{ E^e[u,S] + \frac{1}{2}\Omega \dot{u}^2 \right\} dV + \int_\Sigma E^{isf}[S]\, d\Sigma$$



{100}



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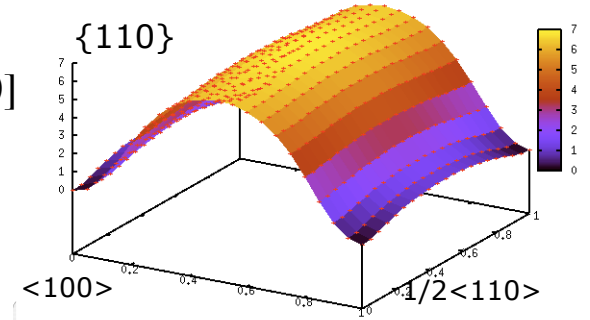
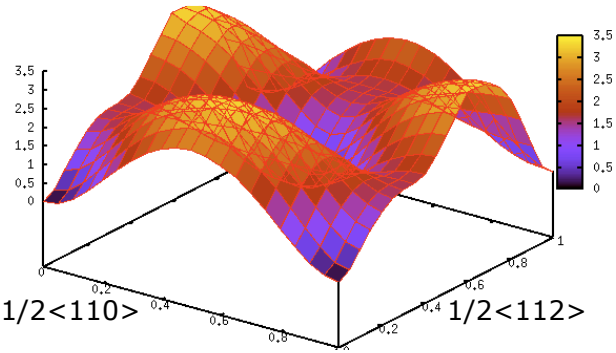


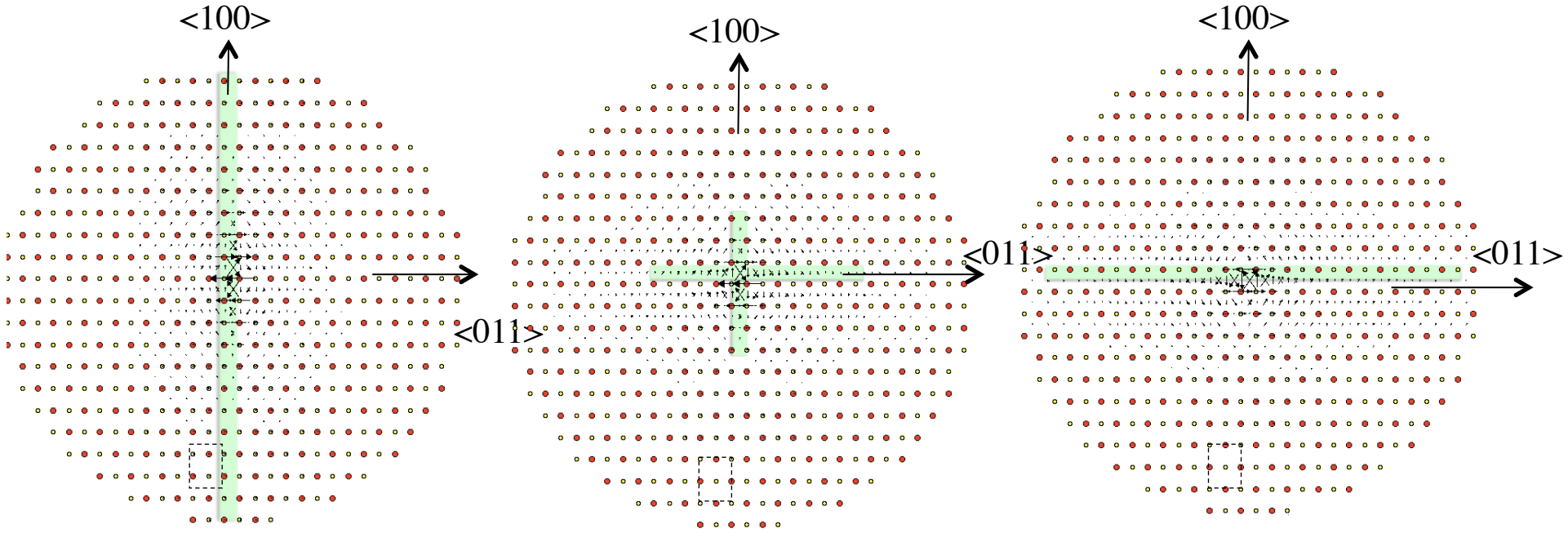
{111}



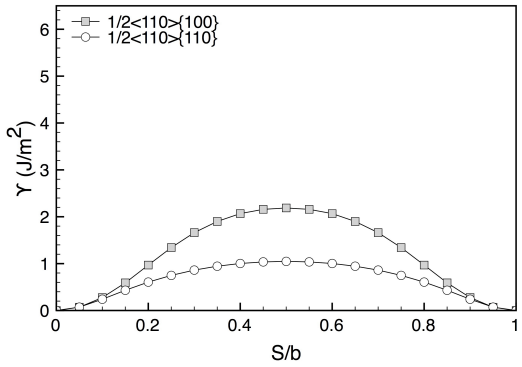
Code de calcul Cod²*ex* développé au CEA/DAM

L'effet de la pression sur la structure de cœur de la dislocation vis ½<110> dans MgO

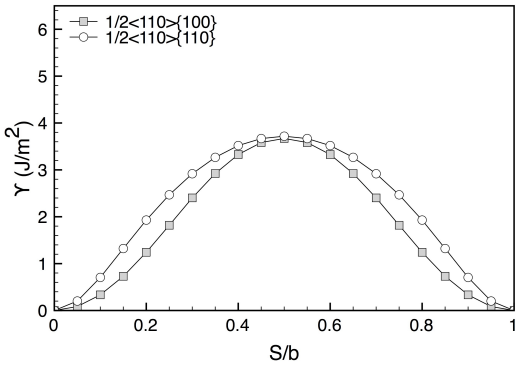
Evolution de la structure de cœur d'une dislocation vis de vecteur de Burgers ½<110> dans MgO



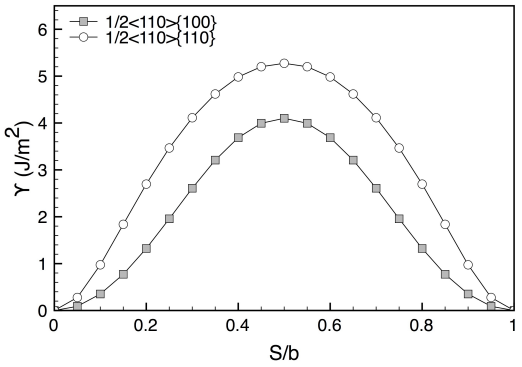
P=0 GPa



P=60 GPa



P=100 GPa

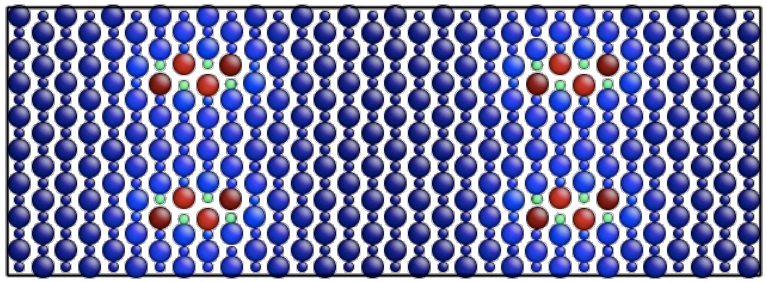


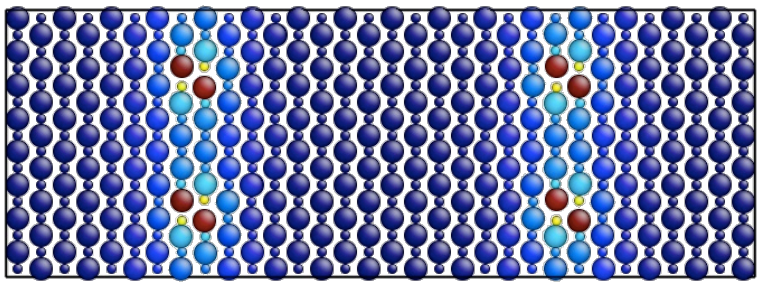
L'effet de la pression sur la structure de coeur de la dislocation vis ½<110> dans MgO

(001)

0 GPa

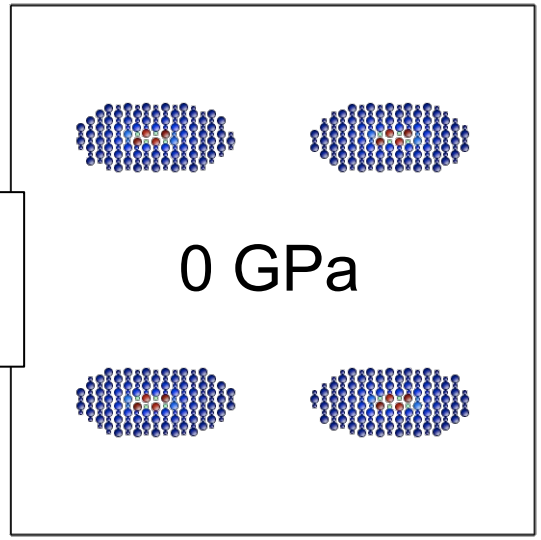
60 GPa





DFT

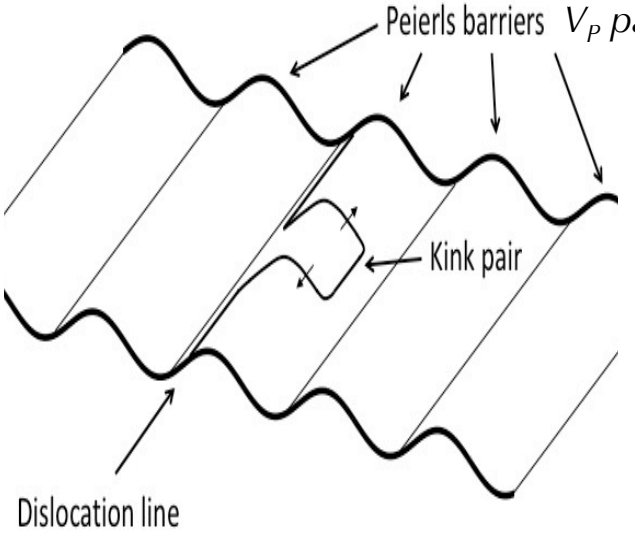
Potentiels Buck.



(110)

Local von Mises shear strain invariant coloring

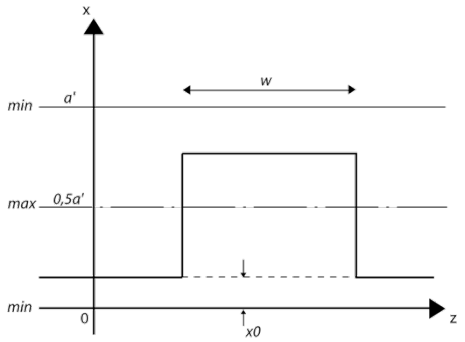
Enthalpie critique de nucléation d'un double décrochement



V_P paramétrées sur le calcul de σ_p

$$\begin{cases} \Delta H(h,w) = \Delta E(h,w) + \Delta P(h,w) - W(h,w) \\ \dfrac{\partial \Delta H}{\partial h} = \dfrac{\partial \Delta H}{\partial w} = 0 \end{cases}$$

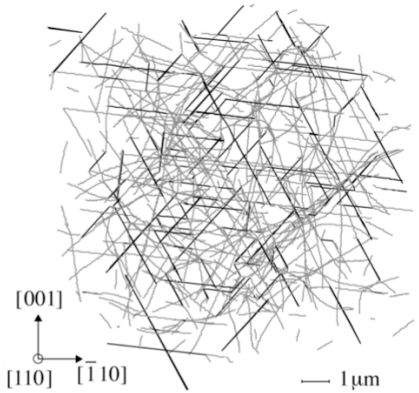
- Elastic Interactions Theory (*Koizumi et al., 1993*)

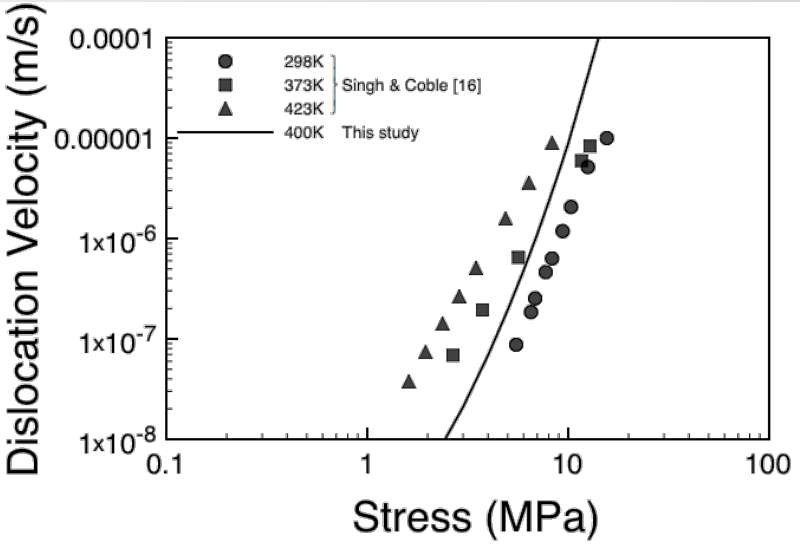


$h^*, w^*, \Delta H^*$

Confrontation aux données expérimentales

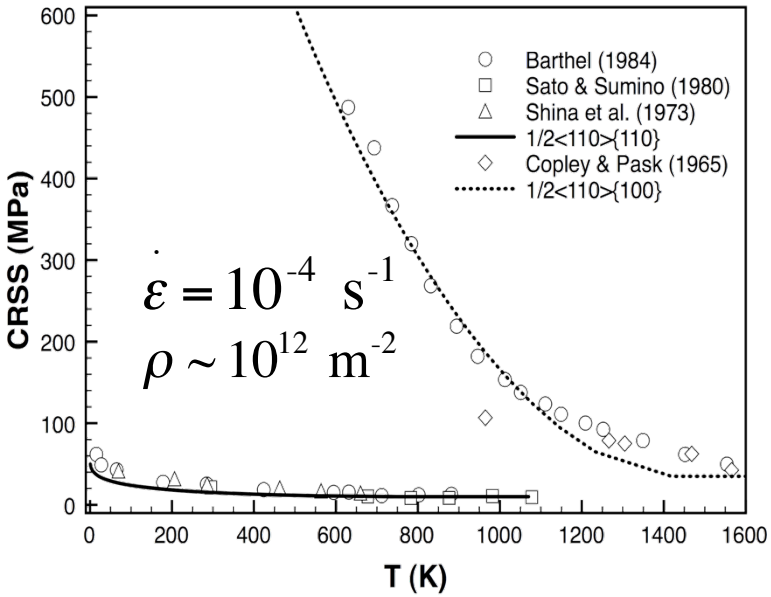
$$v = a' . \frac{L}{w^*(\tau)} . \frac{\nu_D b}{w^*(\tau)} . \exp\left(-\frac{\Delta H^*(\tau)}{kT}\right)$$





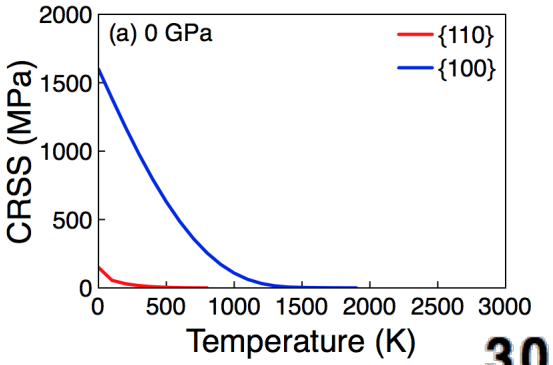
Loi d'Orowan $\dot{\varepsilon} = \rho\, b\, v$

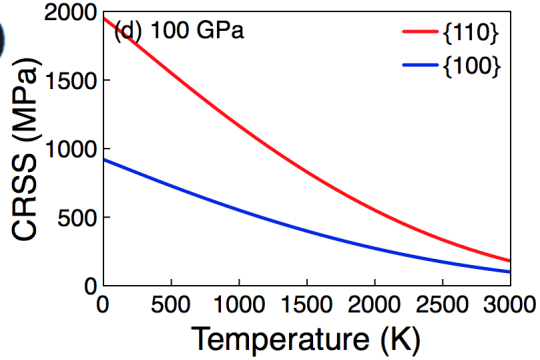
$$\dot{\varepsilon} = \sqrt{\rho}\frac{\upsilon_D a' b^2}{2w_c^2}\exp(-\Delta H^*(\tau)/kT)$$

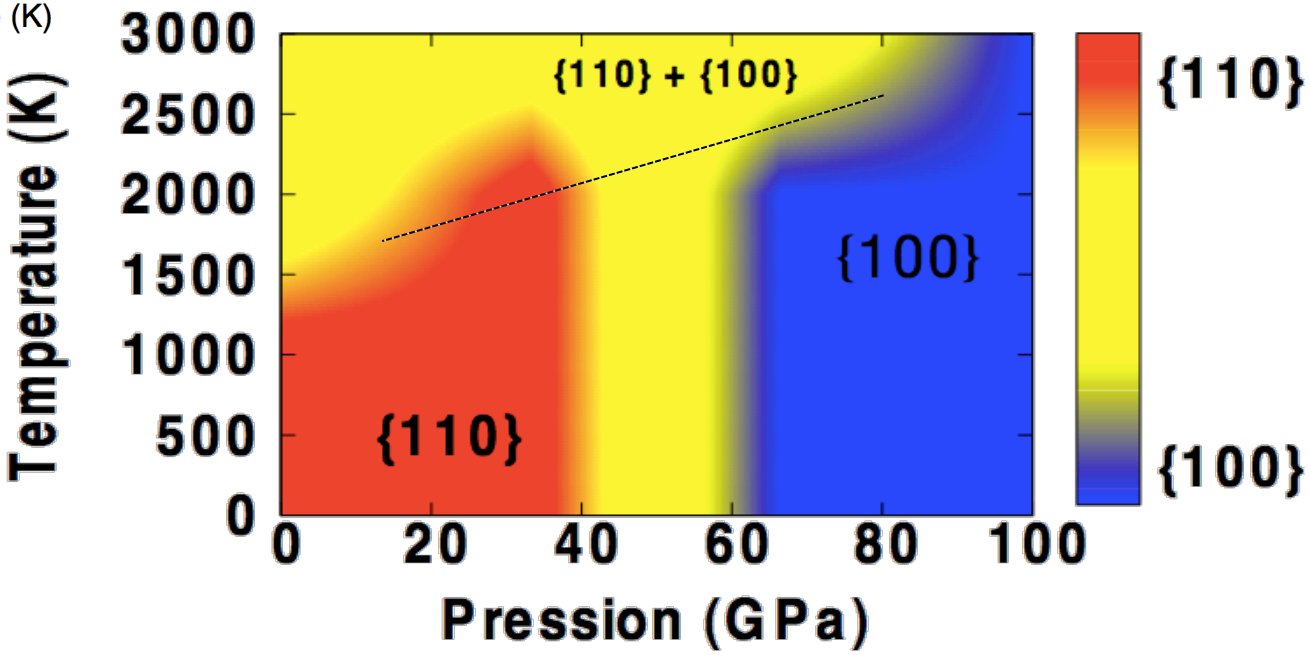


Evolution des CRSS de MgO en fonction de la pression

$$\dot{\varepsilon} = \sqrt{\rho}\frac{\upsilon_D a' b^2}{2w_e^2}\exp(-\Delta H^*(\tau)/kT)$$



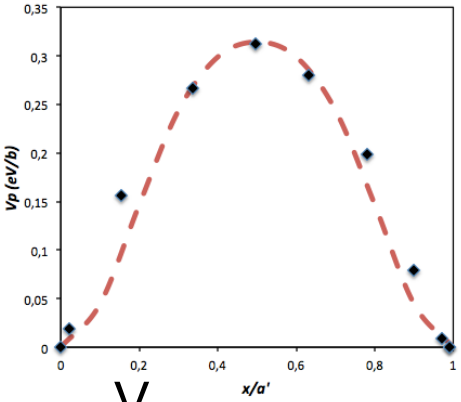




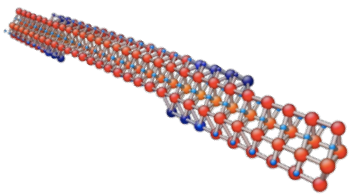
Confirmation expérimentale -> Girard et al. (2012)

Conclusion

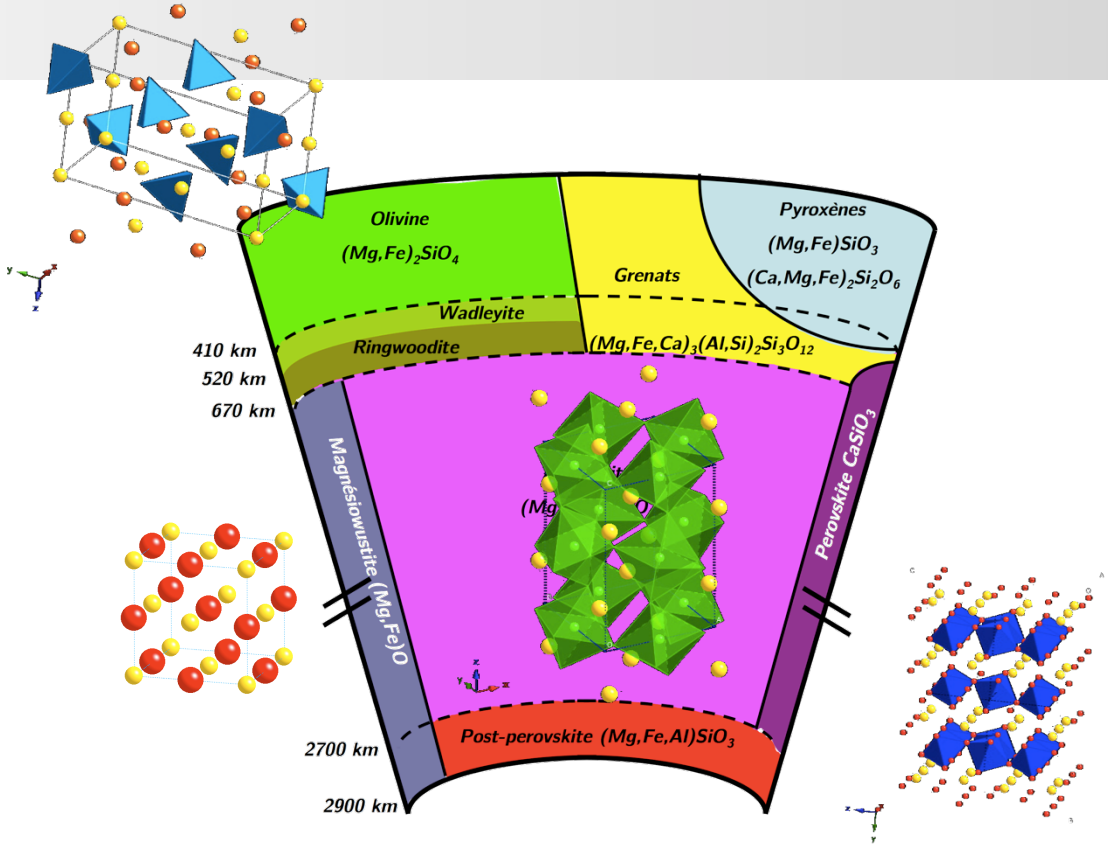
NEB



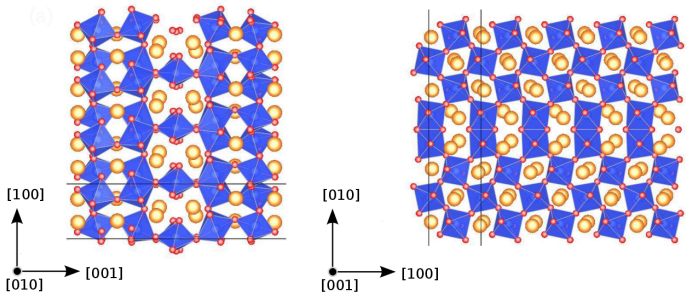
V_p

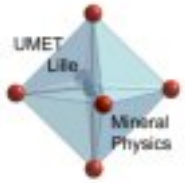


$\Delta H(\tau)$



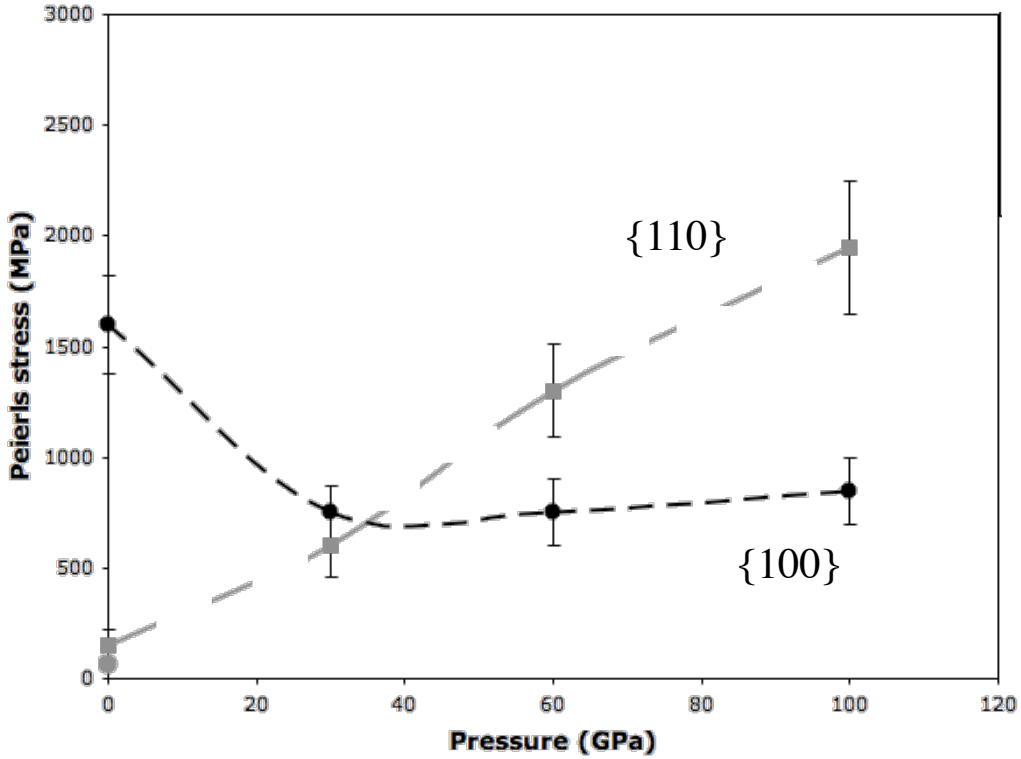
Perovskite: vis [100]




UMET
Lille
Mineral
Physics

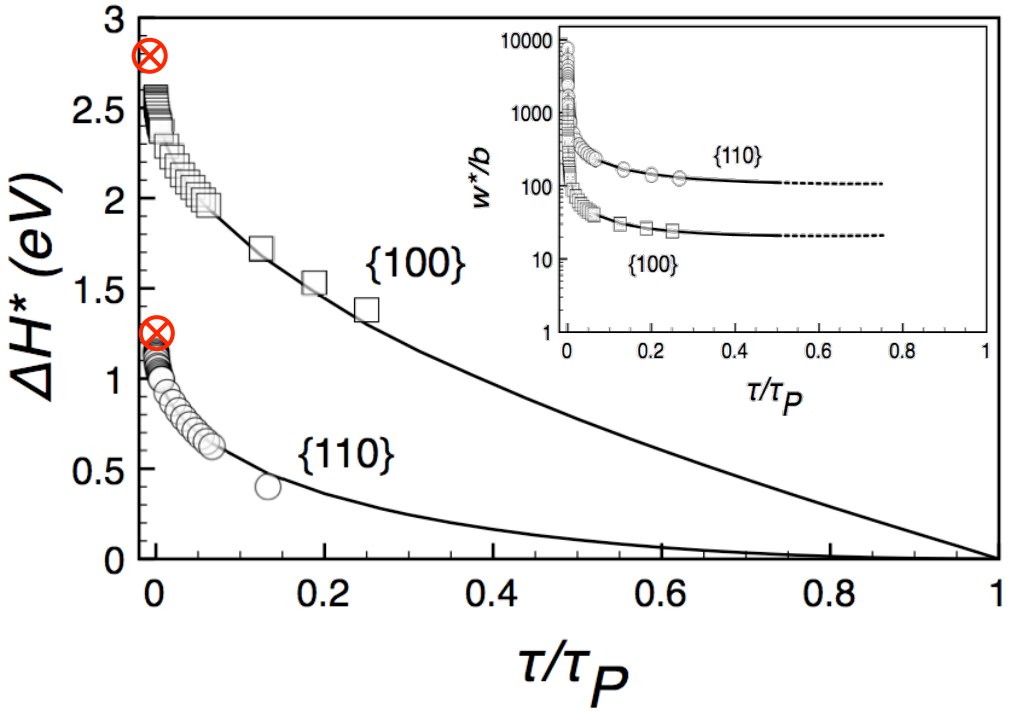
L'effet de la pression sur la structure de coeur de la dislocation vis ½<110> dans MgO

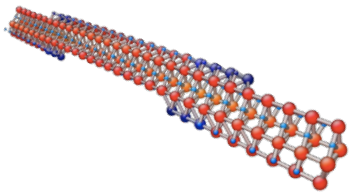
A P=0 GPa, étalement du cœur de la dislocation dans {110} => $\sigma_p^{\{110\}} << \sigma_p^{\{100\}}$

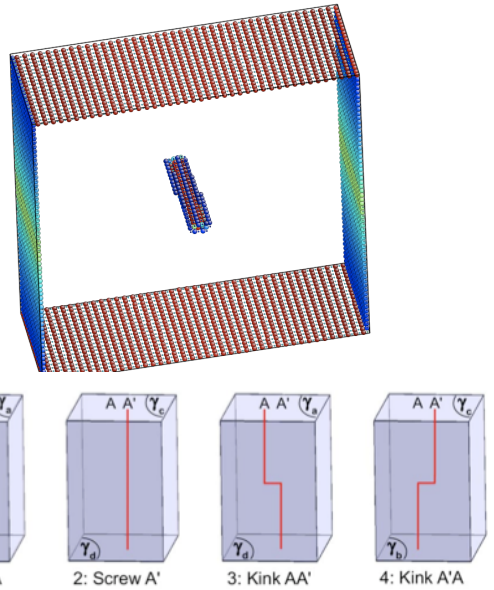


A P=100 GPa, étalement du cœur de la dislocation dans {100}
=> $\sigma_p^{\{100\}} < \sigma_p^{\{110\}}$

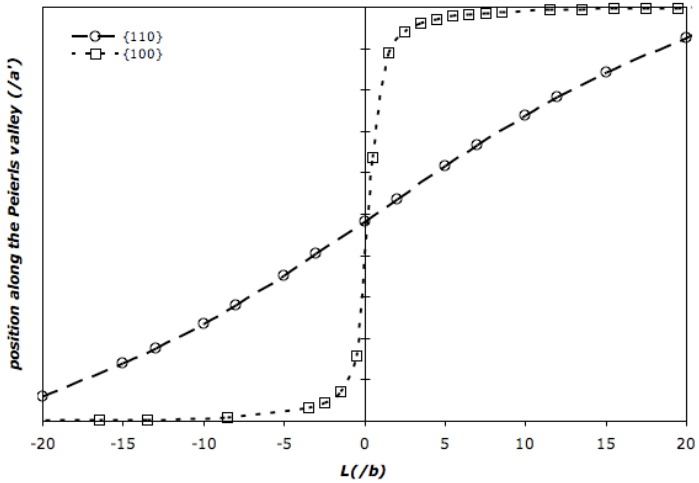
Enthalpie critique de nucléation d'un double décrochement





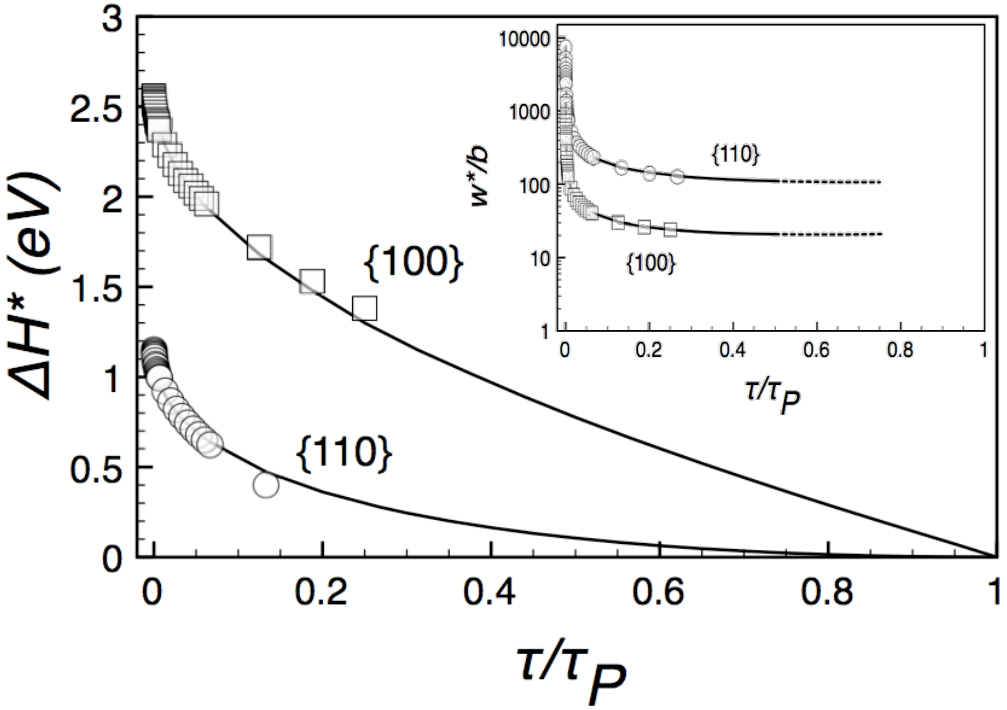


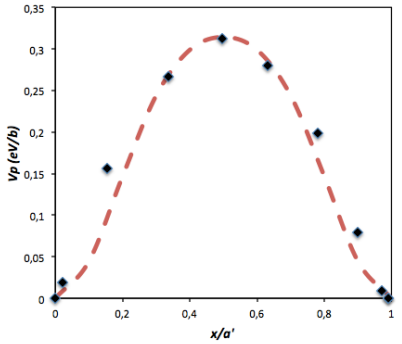
Pizzagalli et al. (2008)



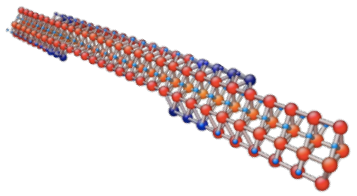
Enthalpie critique de nucléation d'un double décrochement

NEB+climbing image





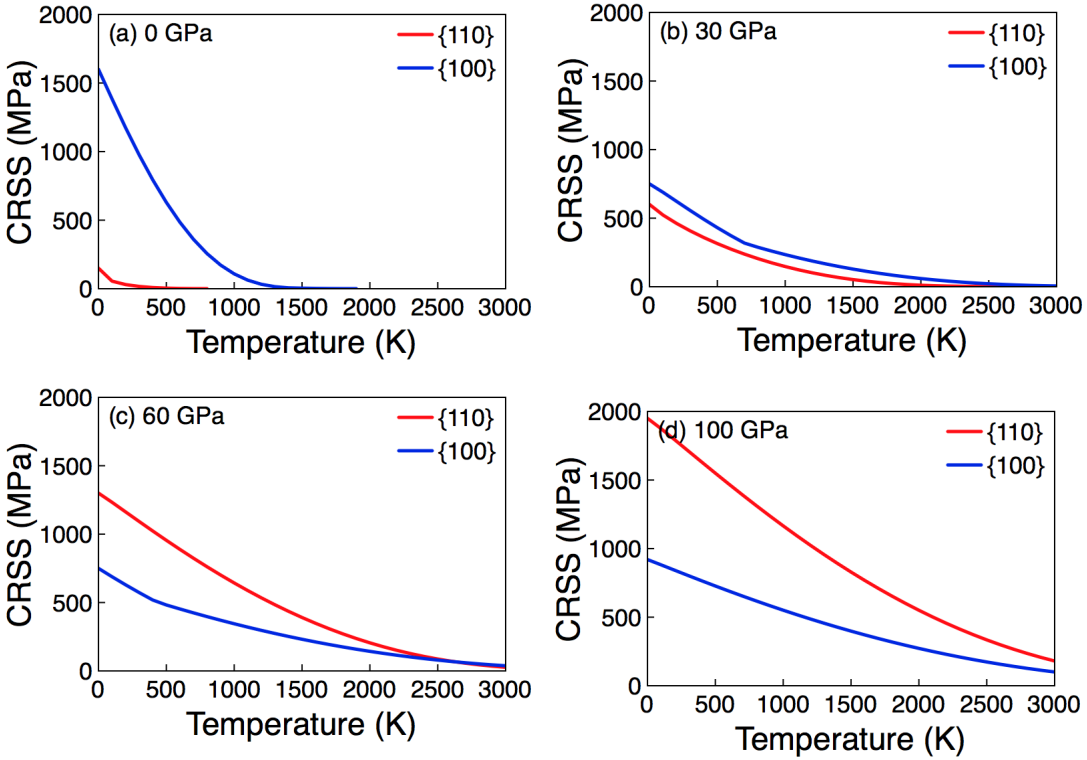
Vp



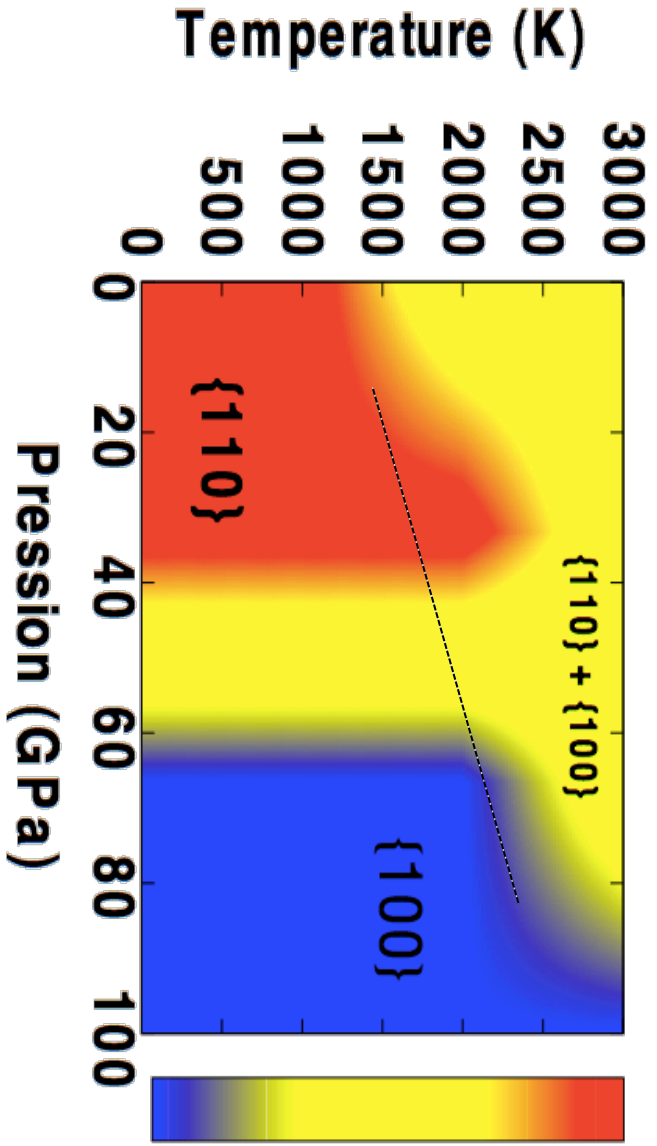
ΔH(τ)

Evolution des CRSS de MgO en fonction de la pression

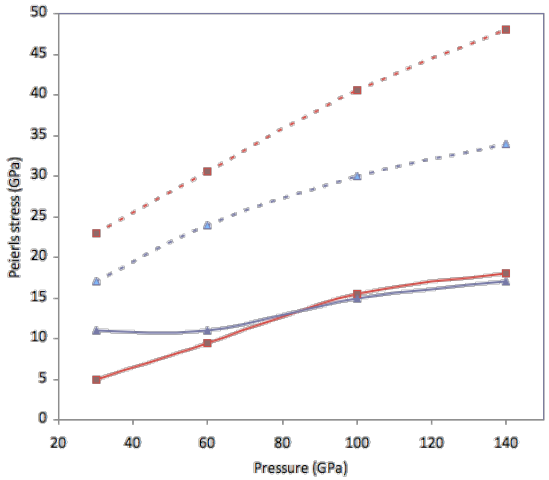
$$\dot{\varepsilon} = \sqrt{\rho}\frac{\upsilon_D a' b^2}{2w_e^2}\exp(-\Delta H^*(\tau)/kT)$$

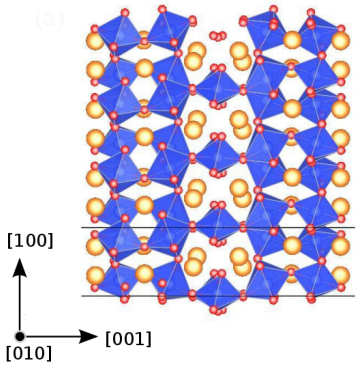


Amodeo et al. (2012)

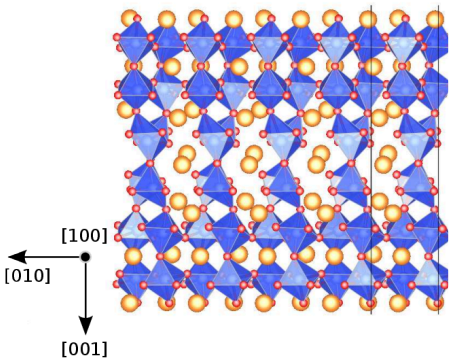


Partie III: Calculs par potentiels



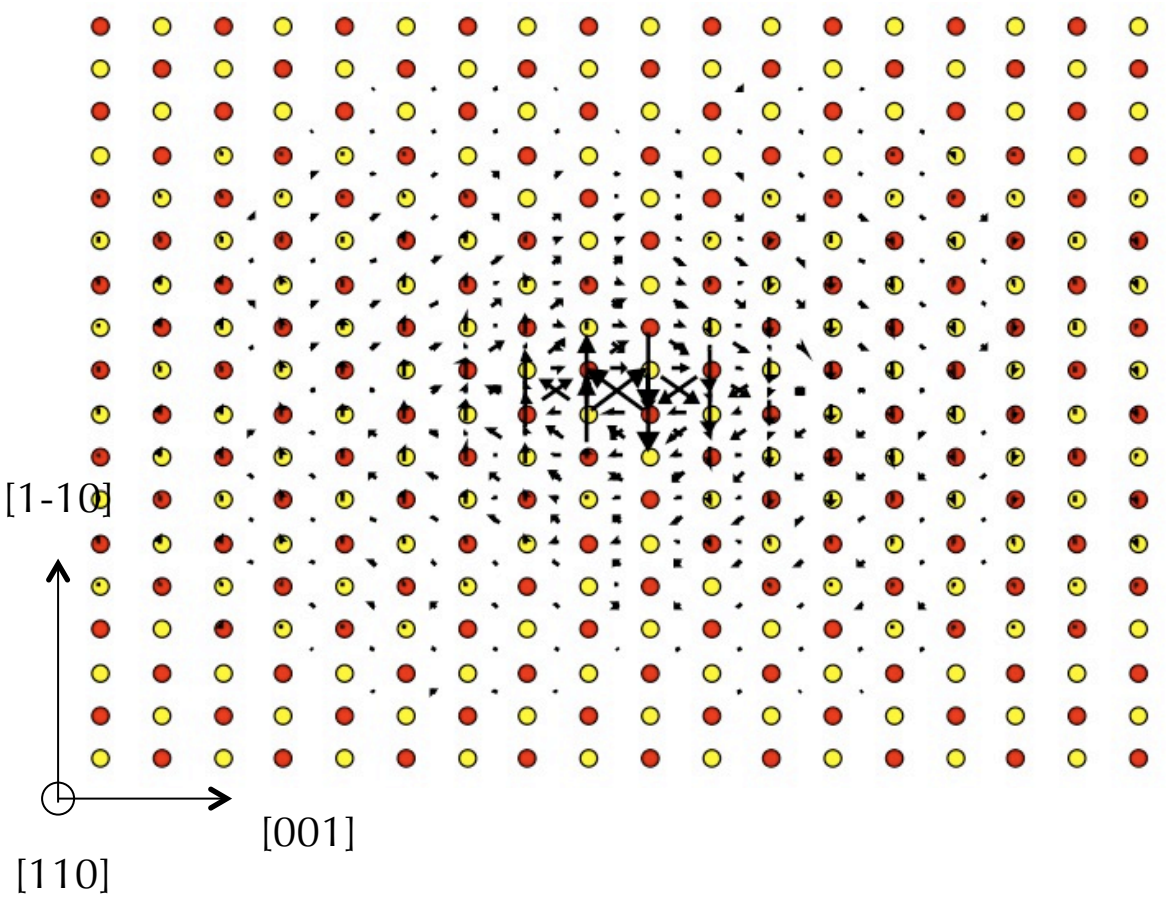


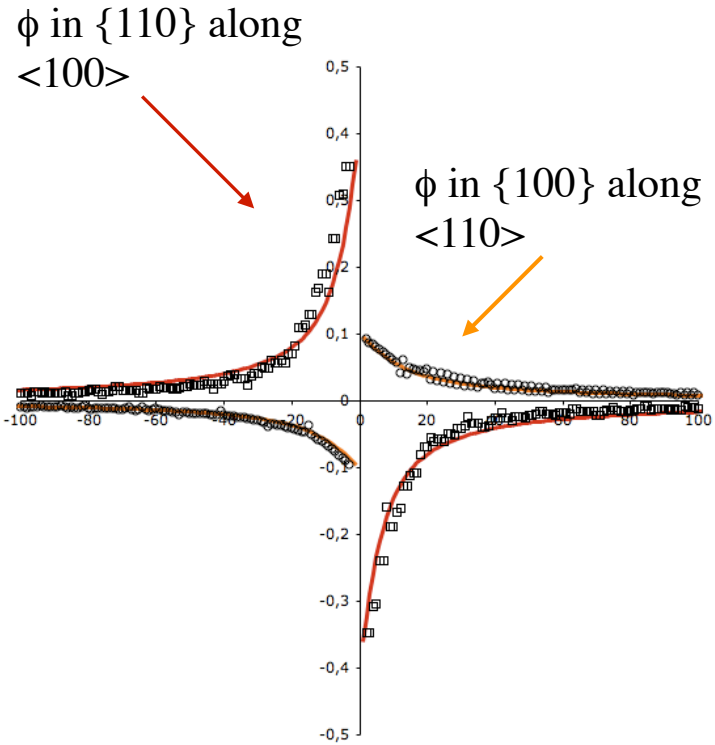
Perovskite $MgSiO_3$



Thèse A. Kraych

1/2<110> screw core structure





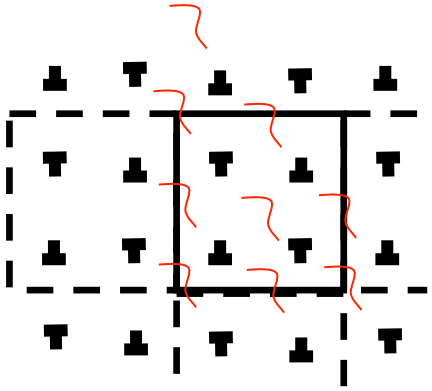
Quadrupole energy

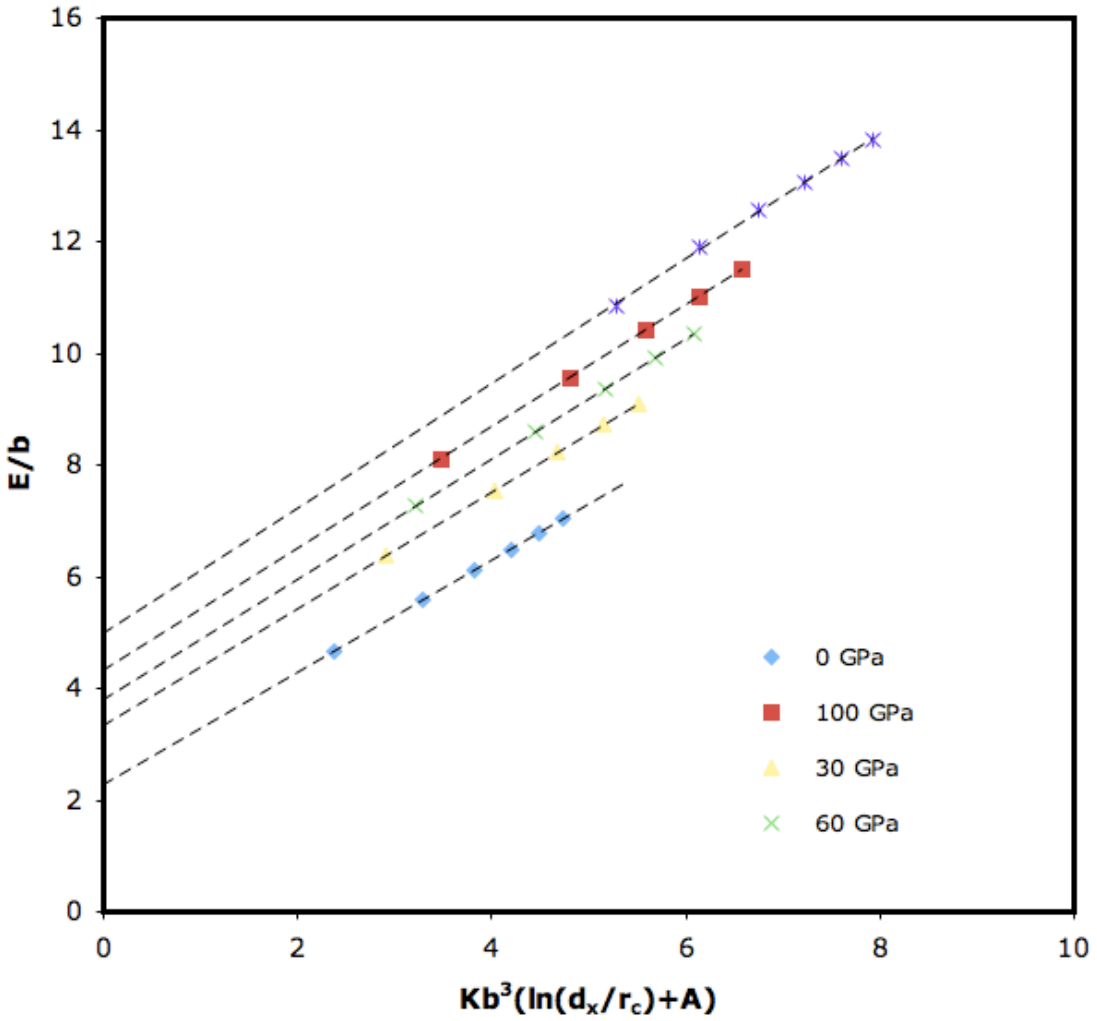
$$W_{1-2}/L = -\frac{\mu b_1 b_2}{2\pi}\ln(R/R_a) = \pm 2Kb^2\ln(d/r_c)$$

In a quadrupole, energy per dislocation per b is then given by

$$E = E_c(r_c) + Kb^3\left(\ln(d/r_c) + A\right)$$

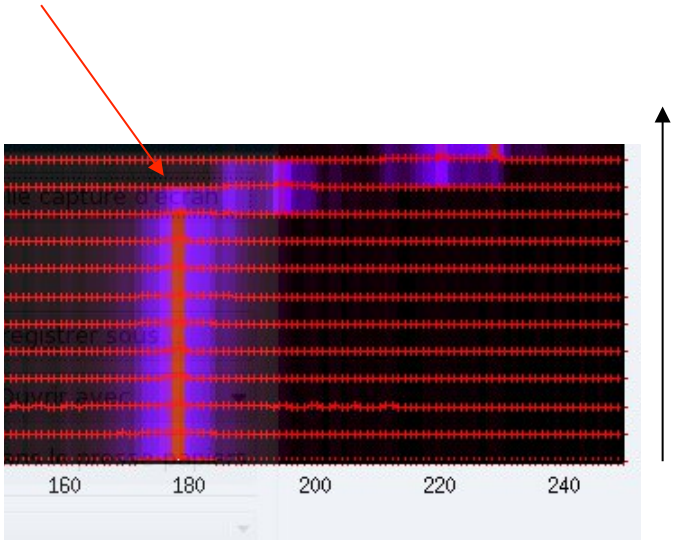
A contains all the effect of the infinite sums of dislocation interactions (A=0.545)

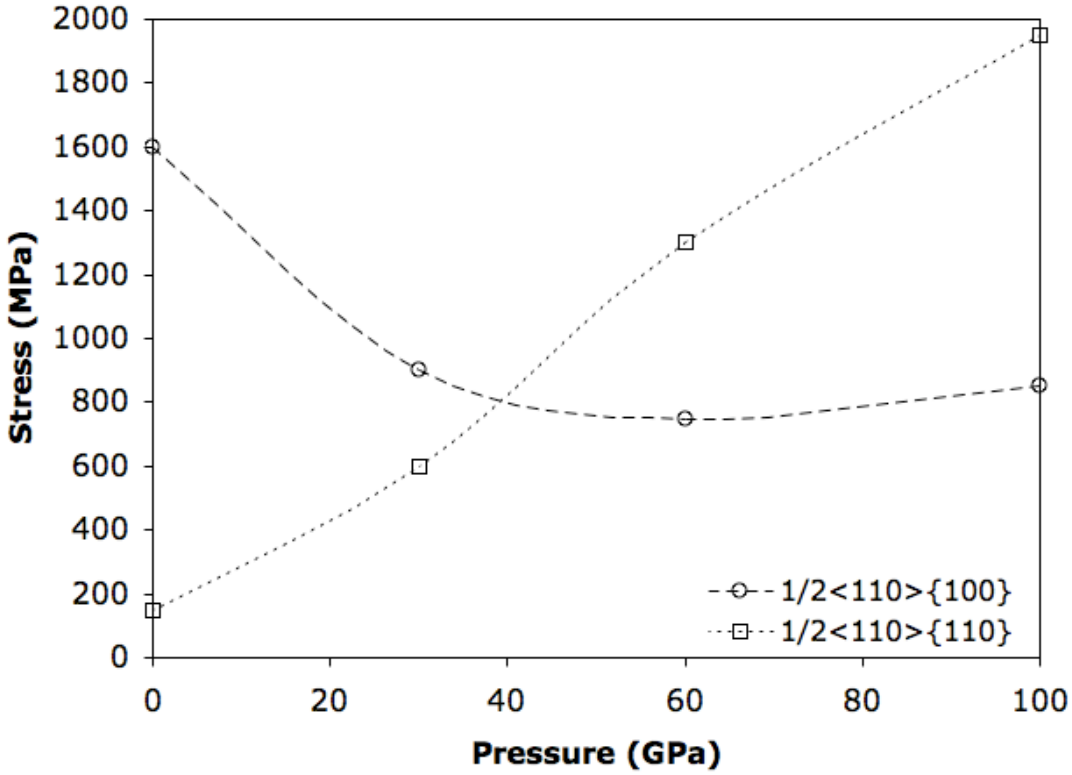




Effect of Pressure on Peierls stresses of screw dislocation

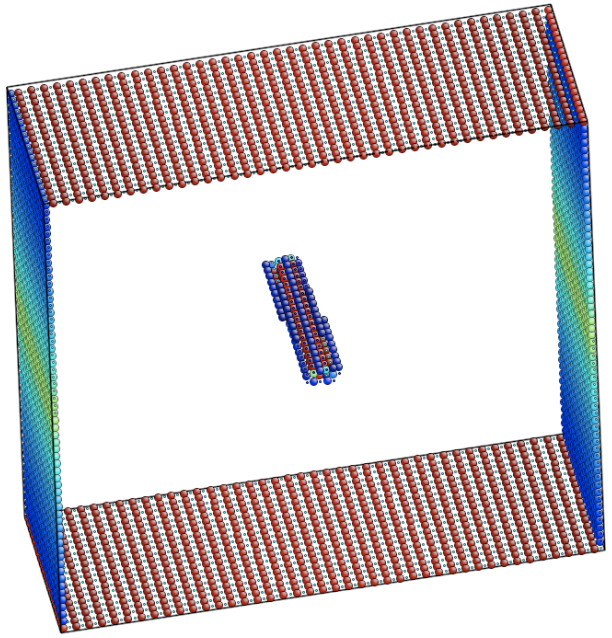
As core spreads from {110} to {100}, Peierls stresses evolve and ones may expect a change in favourable slip system from 1/2<110>{110} to 1/2<110>{100}

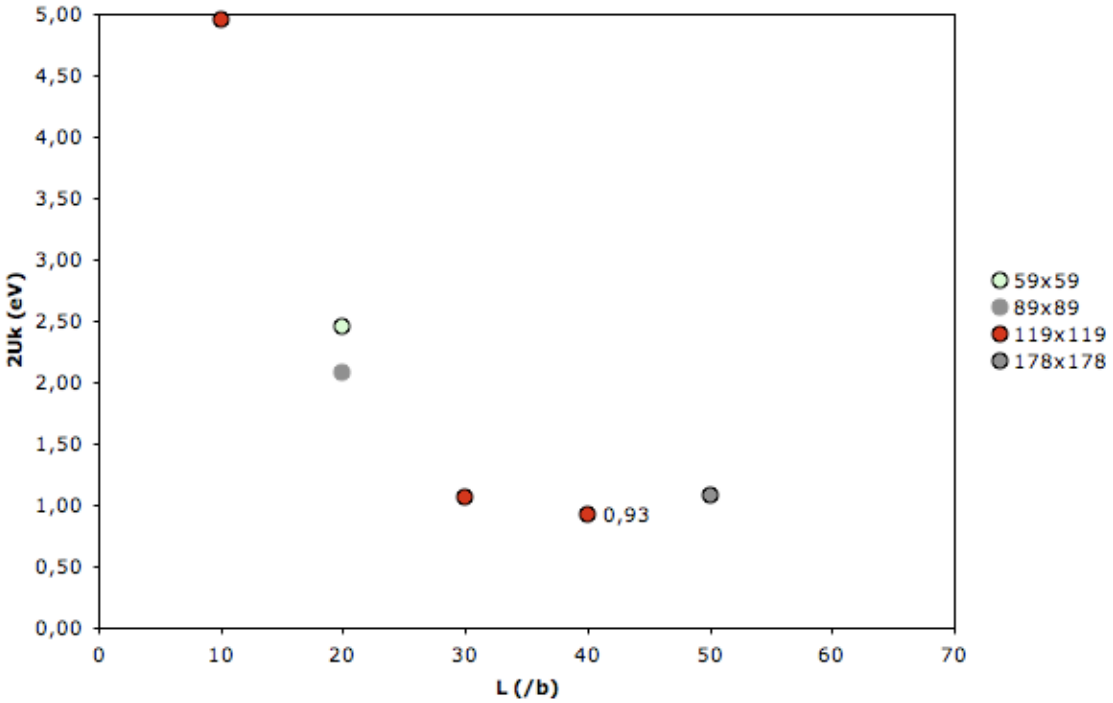




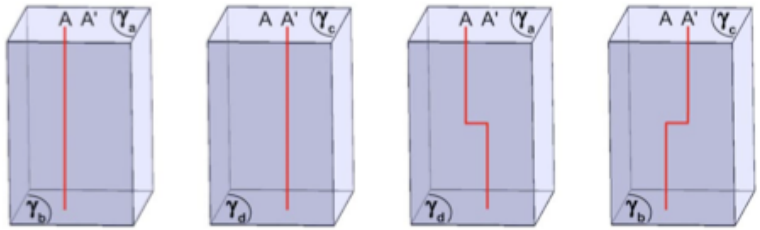
Stretton et al. (2001), Merkel et al. (2002), Heidelbach et al. 2003

Isolated kink and U_k



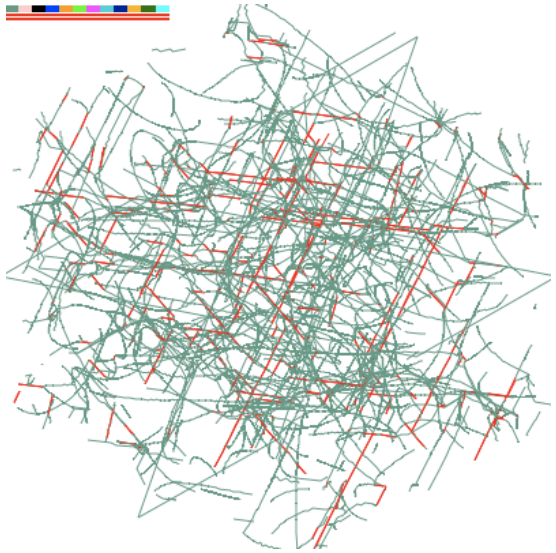


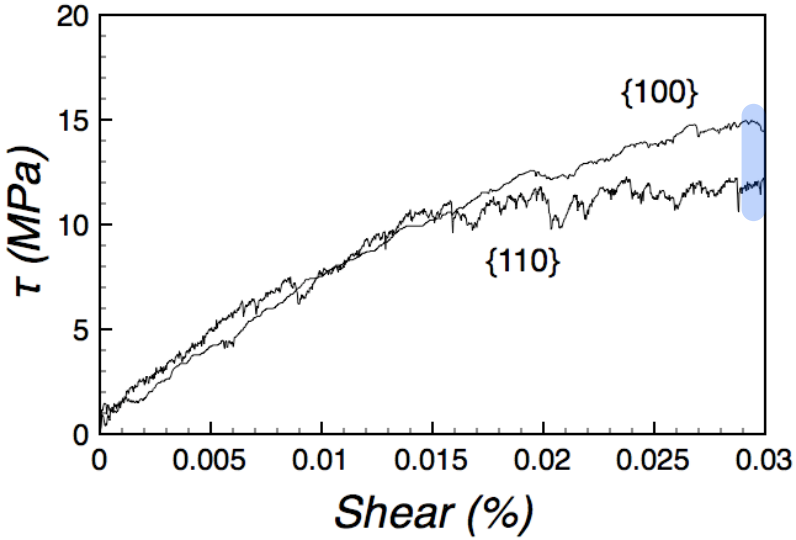
Following Pizzagalli et al. (2008)



$2U_k = (E_3+E_4)-(E_1+E_2)$

DD results in Forest regime

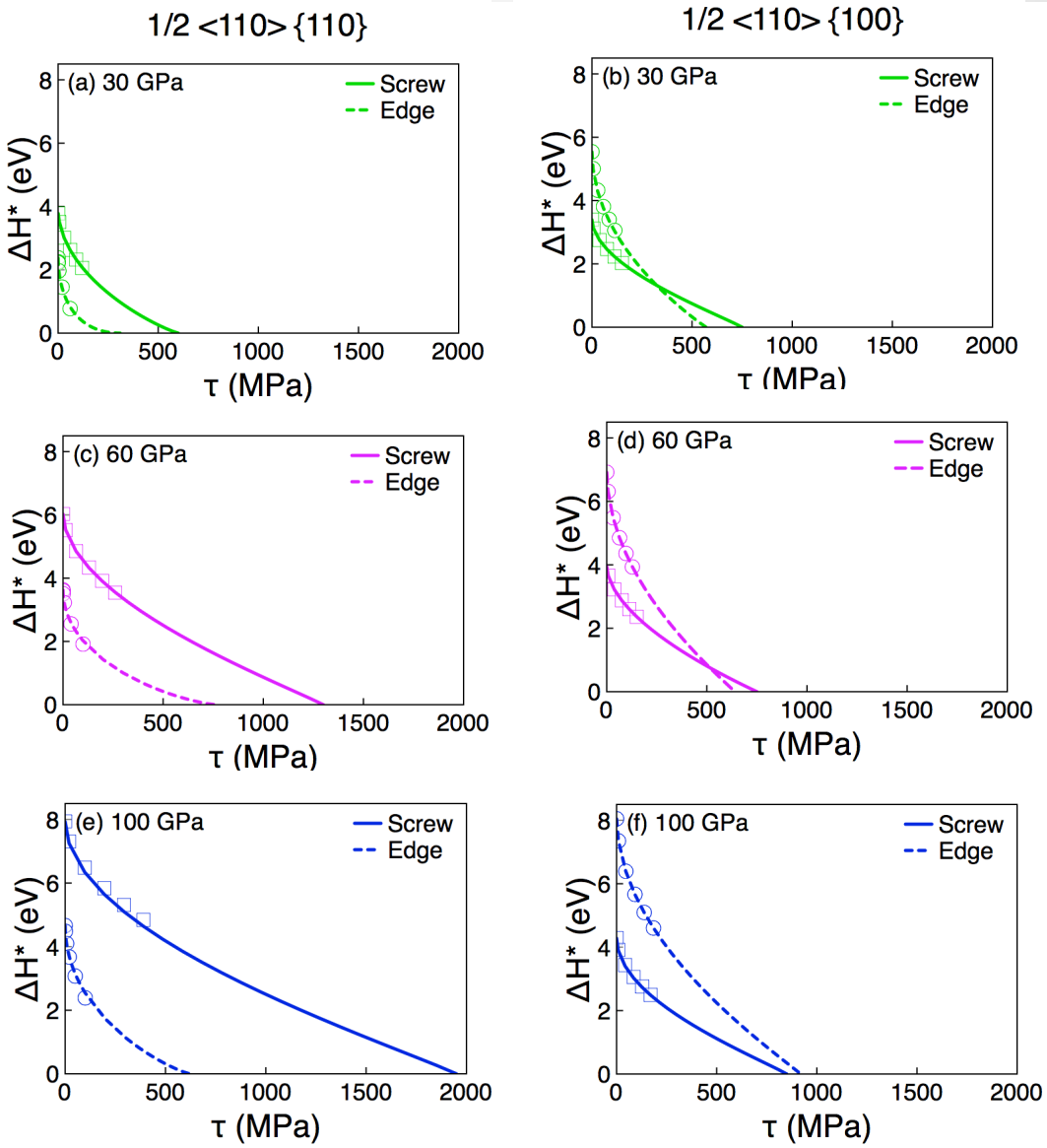




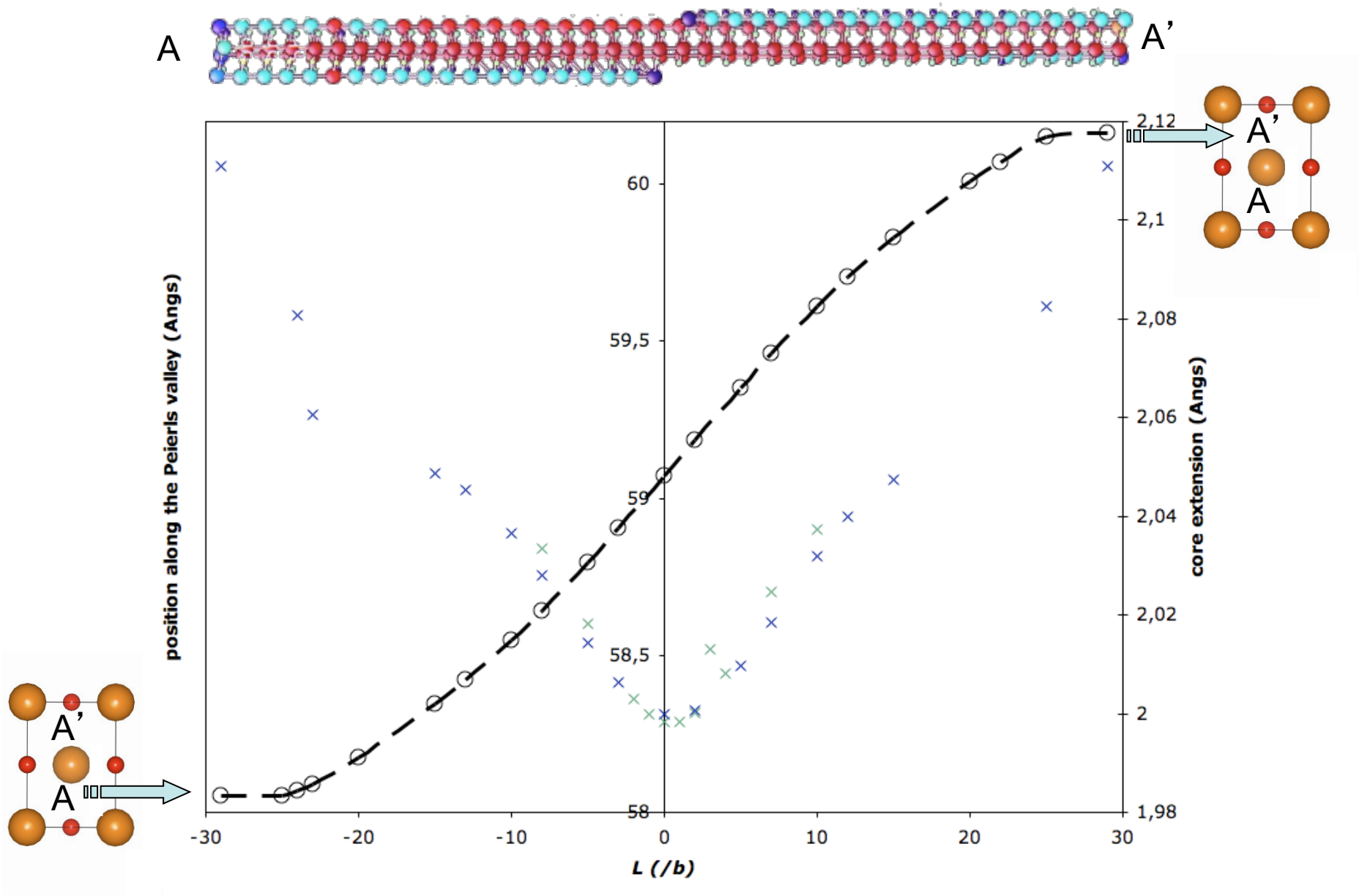
- ~10^{12} m^{-2} Dislocation density, equaly allocated to the 6 slip systems, for both glide family Dislocation density has to be consistent with the experimental value of τ_μ (~15 MPa)

- Strain rate chosen in the range of the dislocation dynamic behavior : strain has to be governed by forest interactions (dynamic behavior) not by dislocation velocity (quasi static behavior)

Kink pair nucleation enthalpy



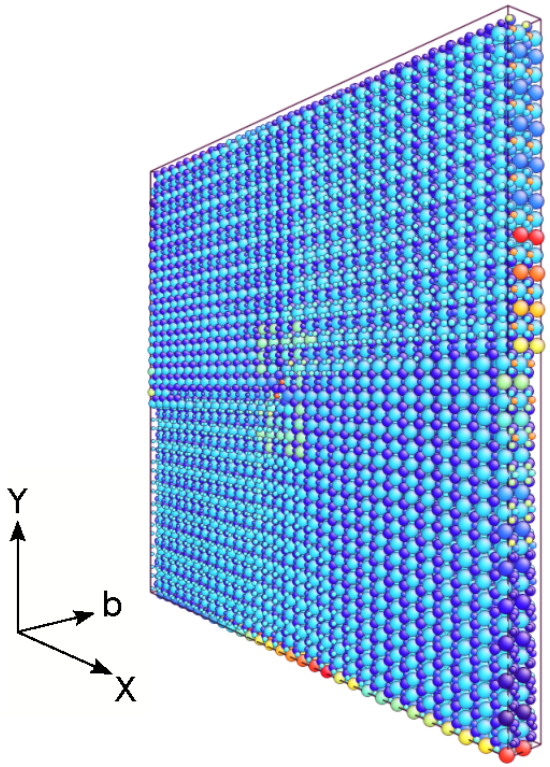
(*Amodeo et al. 2012*)


A
A'
A'
A
A'
A
position along the Peierls valley (Angs)
core extension (Angs)
L (/b)
60
59,5
59
58,5
58
2,12
2,1
2,08
2,06
2,04
2,02
2
1,98
-30
-20
-10
0
10
20
30

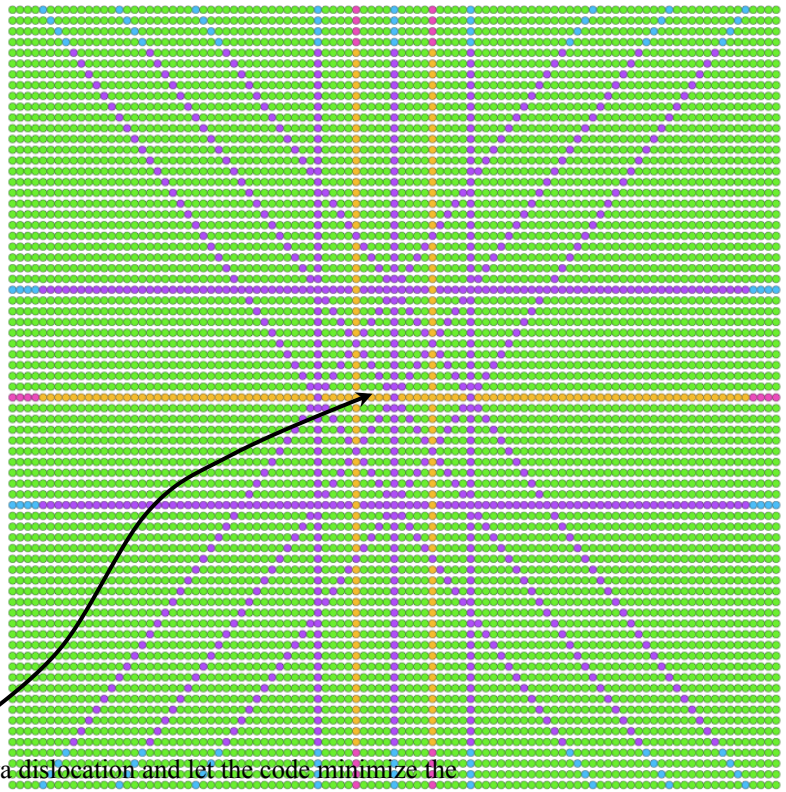
Dislocation core structures using either "cluster" approach or Peierls-Nabarro method

Atomistic "Cluster" approach

Single screw dislocation in a 300 Å x 300 Å x b cell with fixed region to elastic displacement field



Peierls-Nabarro-Galerkin method (Denoual 2004,2007)



Introduce a Volterra dislocation and let the code minimize the structure

Numerical examination of PN equations is performed using a nodal mesh, taking into account for a dislocation density in given plane Pi, interaction between dislocation density distributed in Pj, balanced with inelastic staking fault (from gamma-surface) attributed to Pi plane

[100] screw dislocations: (010), (001), (011) γ-surfaces

[010] screw dislocations: (100), (001), (101) γ-surfaces