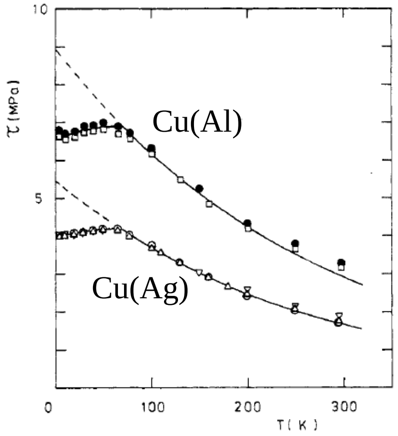
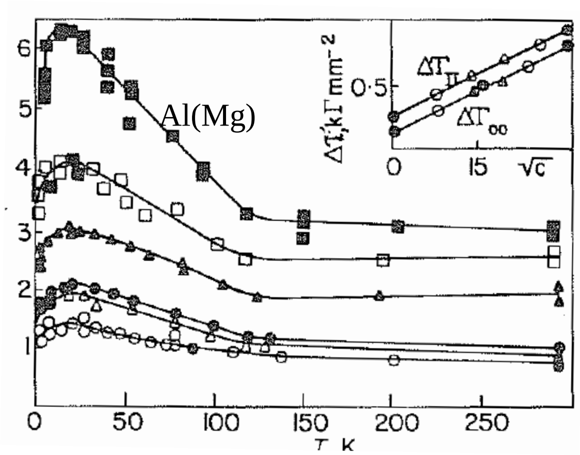
Statistique des dislocations en solution solide

Collaboration: S. Patinet PhD thesis, D. Rodney

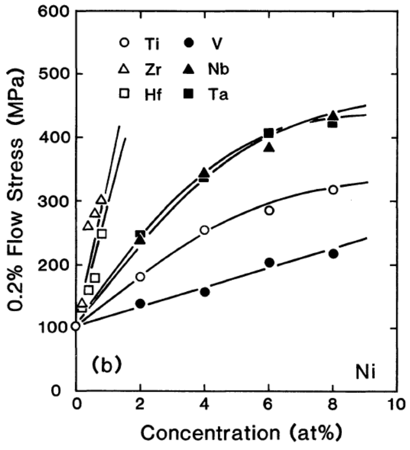
Motivations:



Basinski, Scr. Metall. (1972)



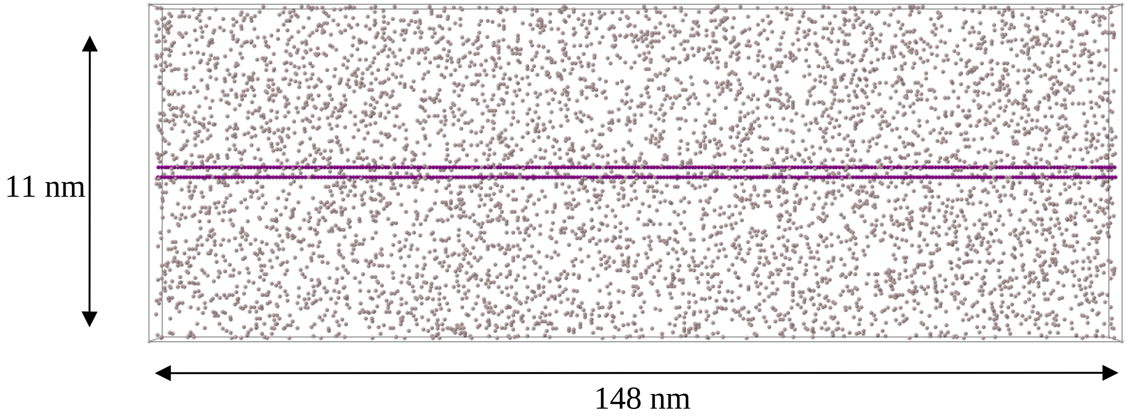
V. P. Podkuyko, Criogenics (1978)



Mishima, Trans. Jap. Inst. Of Met. (1986)

CEA-SRMP

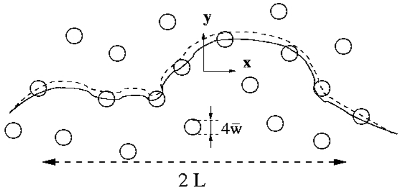
Screw dislocation in Al(Mg) c_s= 2 at. %



Jmol

$$\tau_c = \left(\frac{c^2 v f_m^4}{b^3 s^2 \Gamma_s}\right)^{1/3}$$

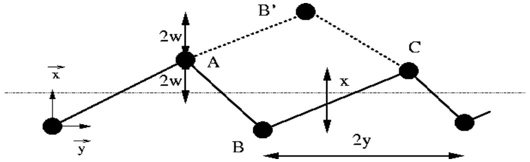
Mott-Nabarro-Labush



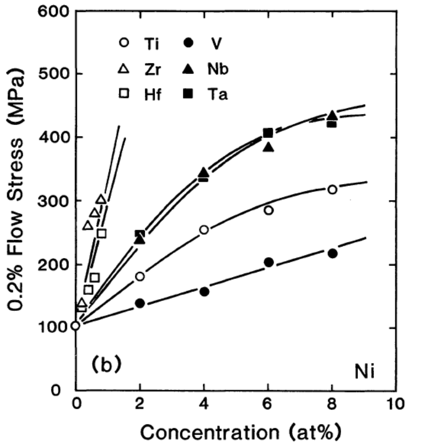
$\tau_c \sim c^{2/3}$

Friedel-Mott-Suzuki

$$\tau_c = \frac{f_m \bar{w} c}{s b}$$



$\tau_c \sim c$



Mishima, Trans. Jap. Inst. Of Met. (1986)

Quantitative prediction of solute strengthening in aluminium alloys

Gerard Paul M. Leyson[1], William A. Curtin[1]*, Louis G. Hector Jr[2] and Christopher F. Woodward[3]

$$\tau_{y0} = \frac{\pi}{2}\frac{\Delta E_b}{b\zeta_c(w_c)w_c} = 1.01\left(\frac{c^2 \Delta \tilde{E}_p{}^4(w_c)}{\Gamma b^5 w_c{}^5}\right)^{\frac{1}{3}}$$

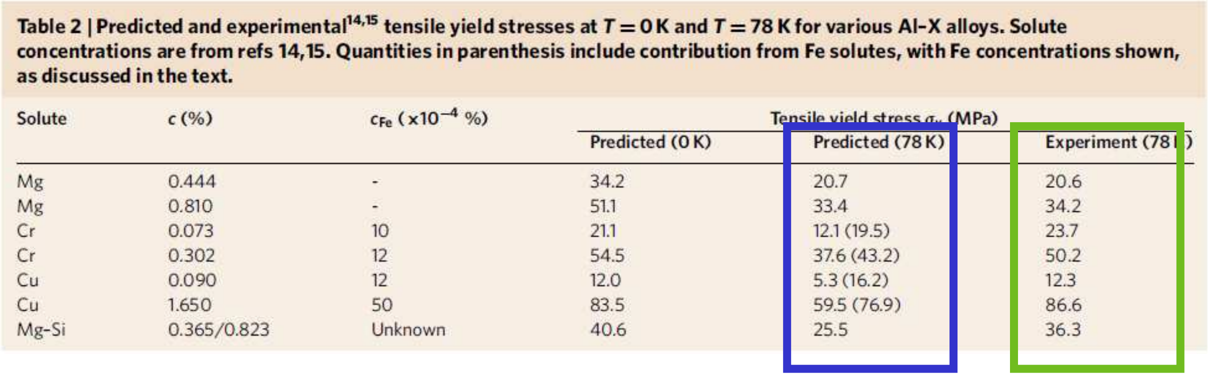
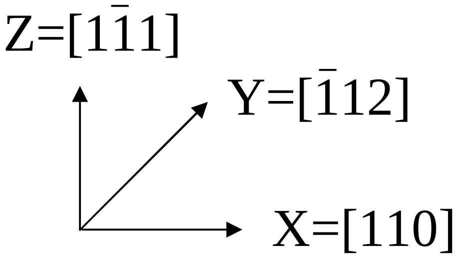


Table 2 | Predicted and experimental[14,15] tensile yield stresses at $T = 0$ K and $T = 78$ K for various Al-X alloys. Solute concentrations are from refs 14,15. Quantities in parenthesis include contribution from Fe solutes, with Fe concentrations shown, as discussed in the text.

Solute	c (%)	c_{Fe} ($\times 10^{-4}$ %)	Tensile yield stress σ_y (MPa) Predicted (0 K)	Predicted (78 K)	Experiment (78 K)
Mg	0.444	-	34.2	20.7	20.6
Mg	0.810	-	51.1	33.4	34.2
Cr	0.073	10	21.1	12.1 (19.5)	23.7
Cr	0.302	12	54.5	37.6 (43.2)	50.2
Cu	0.090	12	12.0	5.3 (16.2)	12.3
Cu	1.650	50	83.5	59.5 (76.9)	86.6
Mg-Si	0.365/0.823	Unknown	40.6	25.5	36.3

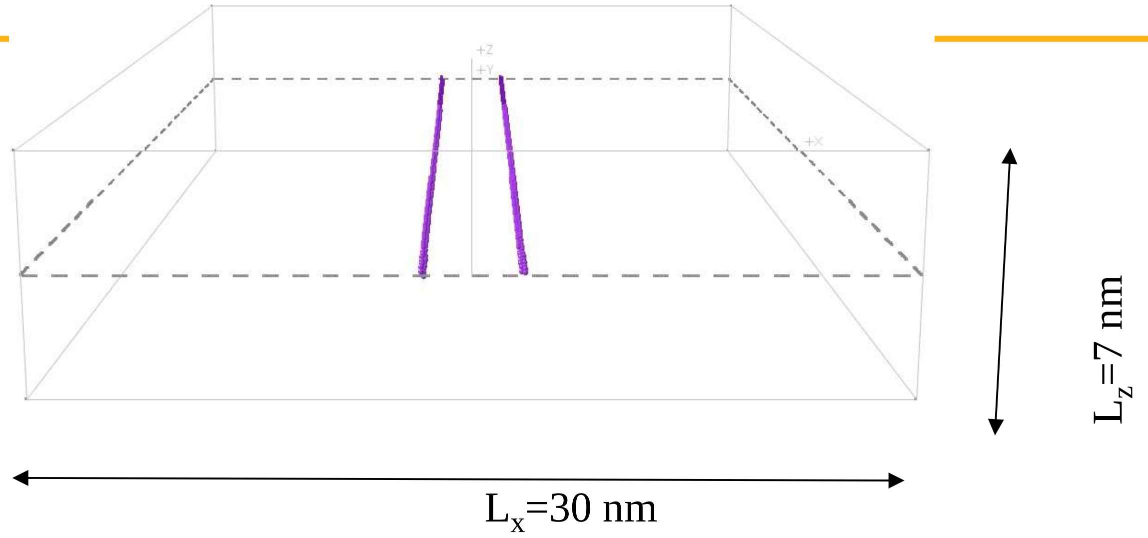
Pure Metal

fcc crystal

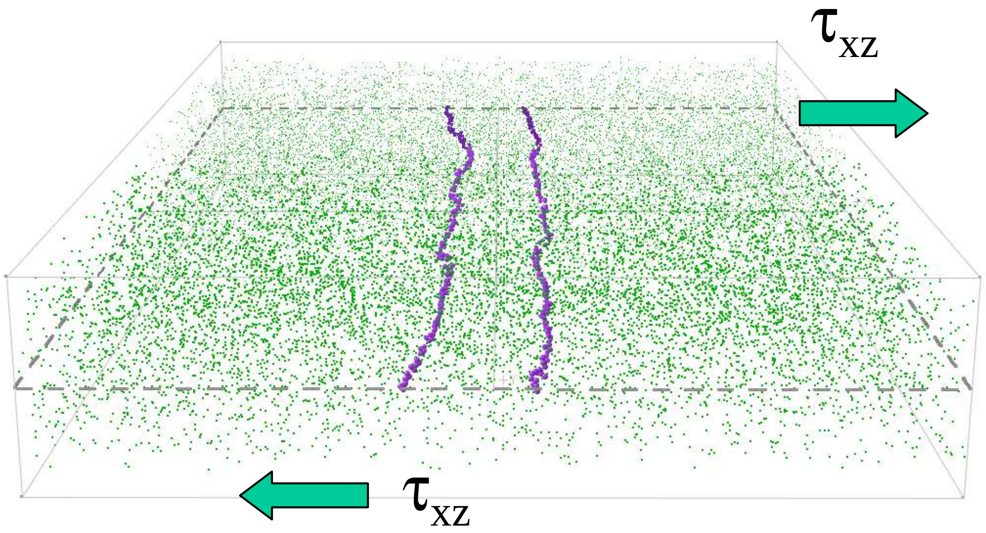

Z=$[1\bar{1}1]$

Y=$[\bar{1}12]$

X=$[110]$



Edge dislocation $a/2[110](1\bar{1}1)$



Solid solution
(3% at. Al in Ni)

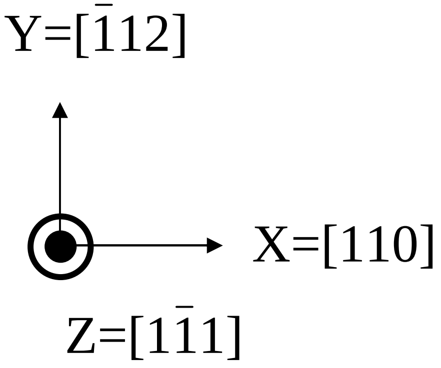
Solid solution hardening in Ni(Al) and Al(Mg)

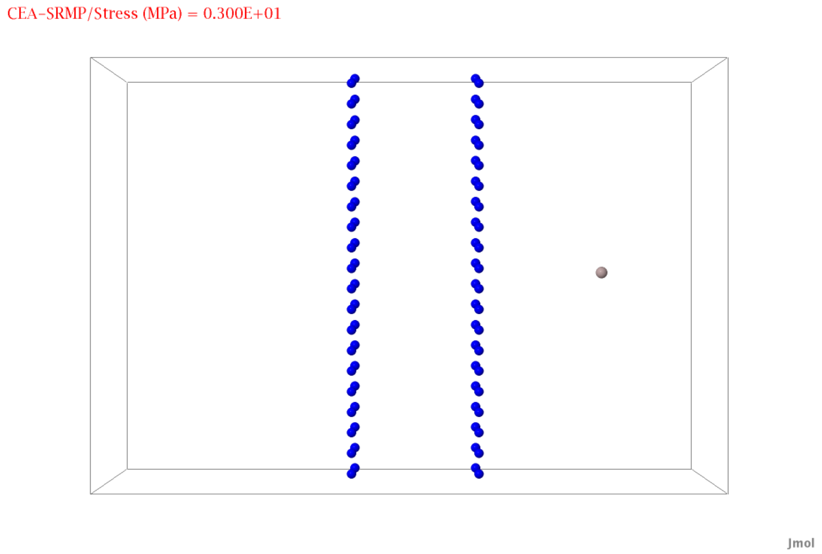
Atomistic model: Embeded atom method (Murray S. Daw and M. I. Baskes PRB 1984)

Ni-Ni Angelo *et al.*: *Modell. Simul. Mater. Sci. Eng. 3, 289 (1995).*
Al-Al Voter and Chen: *Mater. Res. Soc. Symp. Proc. 82, 175 (1987).*
Ni-Al Rodary *et al.*: *Phys. Rev. B 70, 054111 (2004).*

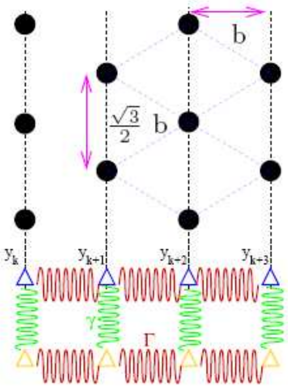
Mg-Mg X.-Y. Liu, P. P. Ohotnicky, J. B. Adams, C. L. Rohrer, and J. R. W. Hyland, Surf. Sci. 373, 357 (1996).
Al-Mg X.-Y. Liu, J. B. Adams, F. Ercolessi, and J. Moriarty, Modelling Simul. Mater. Sci. Eng. 4, 293 (1996)

Simulation avec un seul obstacle





1D elastic line model:



$$\lambda \dot{y_k} = \frac{\Gamma}{\sqrt{3}}\Delta_k y_k - \gamma[y_k - y'_k - 2d/b] + \tau s$$
$$- \sum_i V'_A(y_k - a_{k,i}) + V'_B(y_k - b_{k,i})$$

Forces images

$$F_s = \gamma_I - \alpha\frac{\mu b^2}{2\pi}[\frac{1}{r} + \sum - \frac{1}{(jL_y) - r} + \frac{1}{(jL_y) + r}]$$

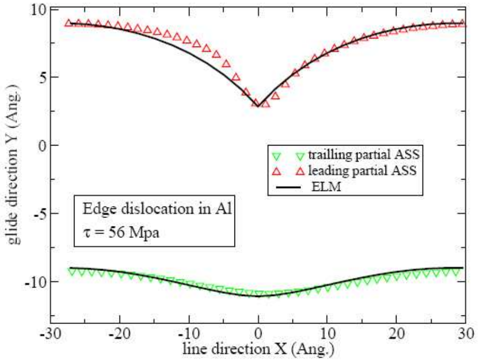
$$F_s(r) = \gamma_I - \alpha\frac{\mu b^2}{2L_y}[\cot(\frac{\pi r}{L_y})]$$

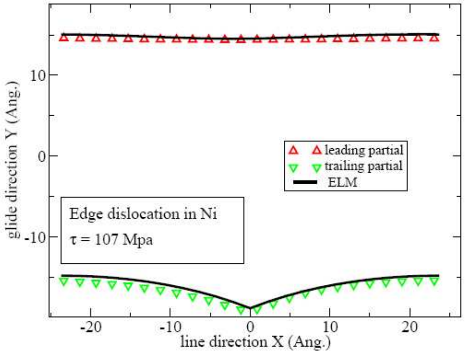
$$d_{\mathrm{SPD}} = \frac{L_y}{\pi}\arctan(\frac{\alpha\mu b^2}{2L_y\gamma_I})$$

$$F_s(r) = -\frac{\alpha\pi\mu b^2}{2L_y^2 \sin(\frac{\pi d_{\mathrm{SPD}}}{L_y})^2}(r - d_{\mathrm{SPD}})$$

Hirth & Lothe p. 315

Hypothèse: γ_I et d varient peu avec c_s



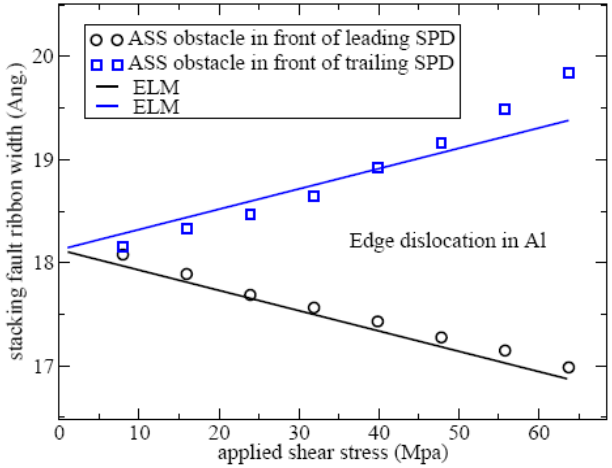


$$\Gamma_{Al} = 0.158 \text{ nN}$$
$$\Gamma_{Ni} = 0.324 \text{ nN}$$

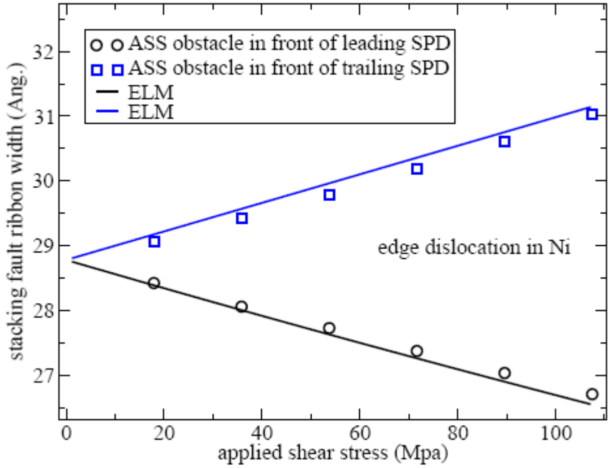
$$\Gamma = \mu b^2 \frac{1-2\nu}{4\pi(1-\nu)}\ln(L_z/2b),$$

H. & L. p. 180

$$\Gamma_{Al} = 0.18 \text{ nN}$$
$$\Gamma_{Ni} = 0.47 \text{ nN}$$

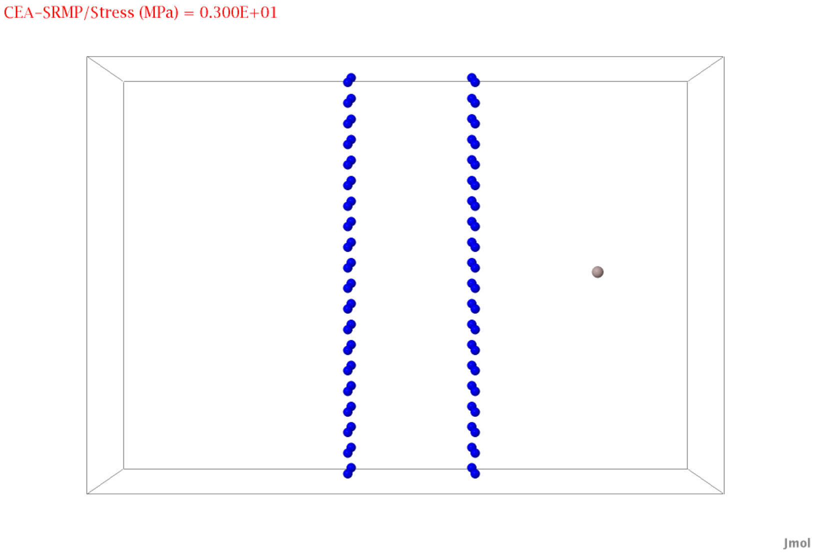

ASS obstacle in front of leading SPD
ASS obstacle in front of trailing SPD
ELM
ELM
Edge dislocation in Al
stacking fault ribbon width (Ang.)
17
18
19
20
0
10
20
30
40
50
60
applied shear stress (Mpa)

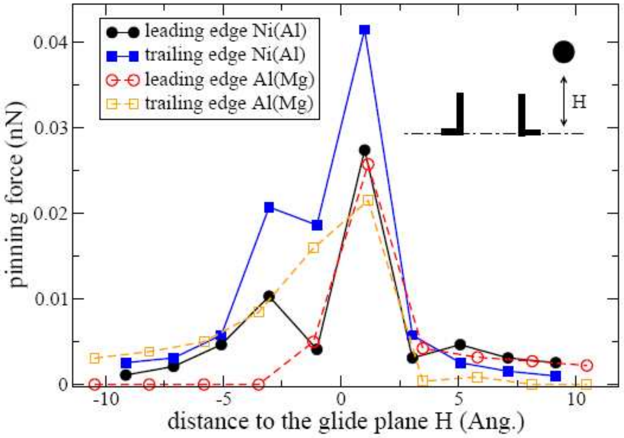
(a)


ASS obstacle in front of leading SPD
ASS obstacle in front of trailing SPD
ELM
ELM
edge dislocation in Ni
stacking fault ribbon width (Ang.)
27
28
29
30
31
32
0
20
40
60
80
100
applied shear stress (Mpa)

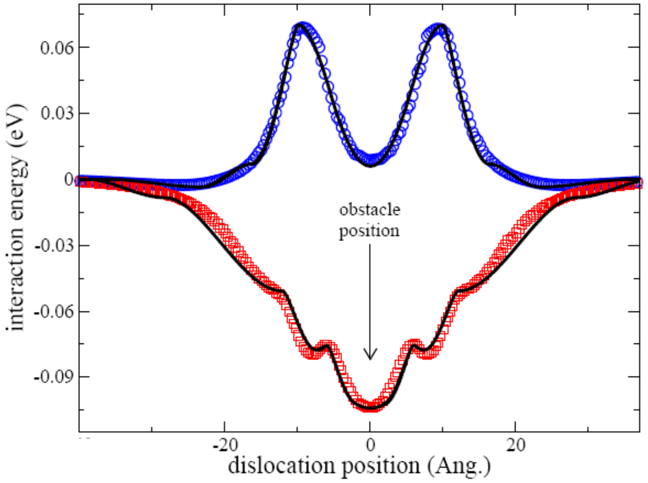
(b)

dislocation-obstacle interaction potential

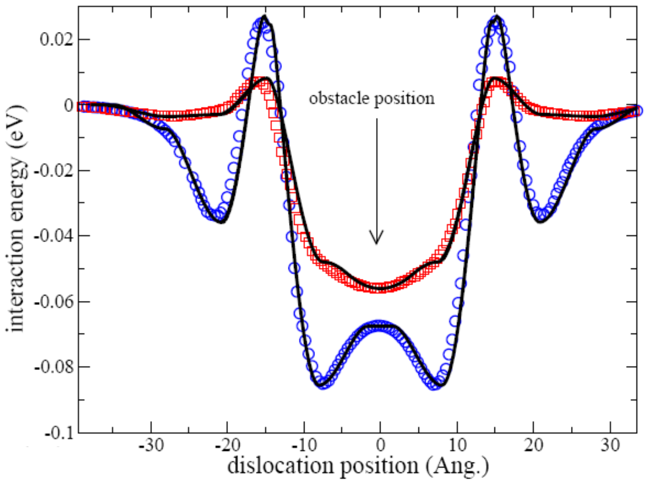


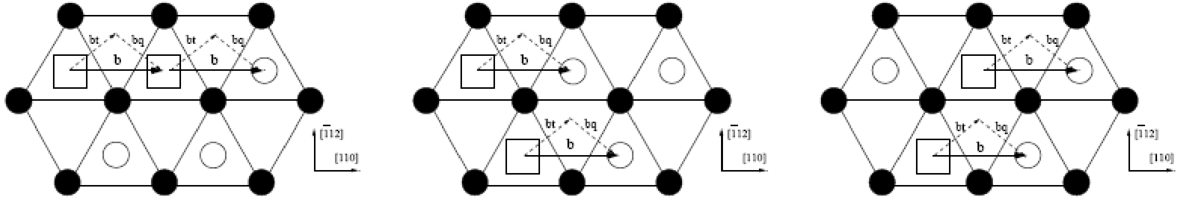


Al(Mg)



Ni(Al)




bt
bq
b
[$\bar{1}$12]
[110]

(a) (b) (c)

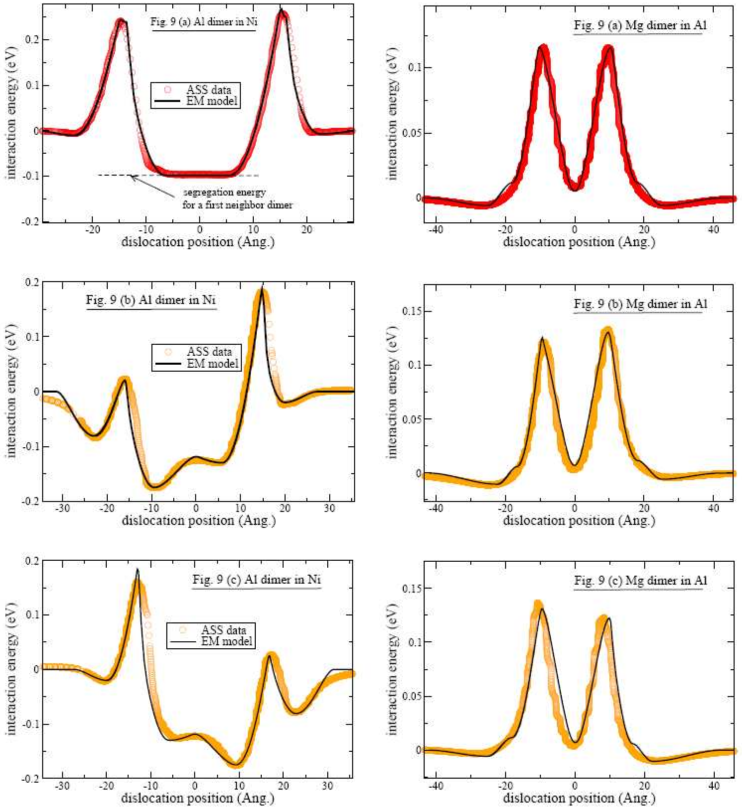
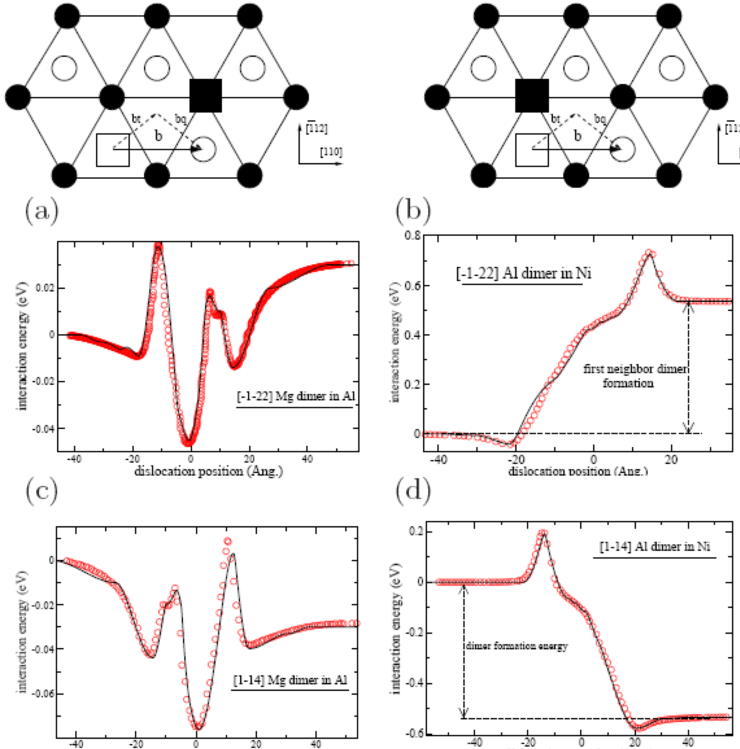
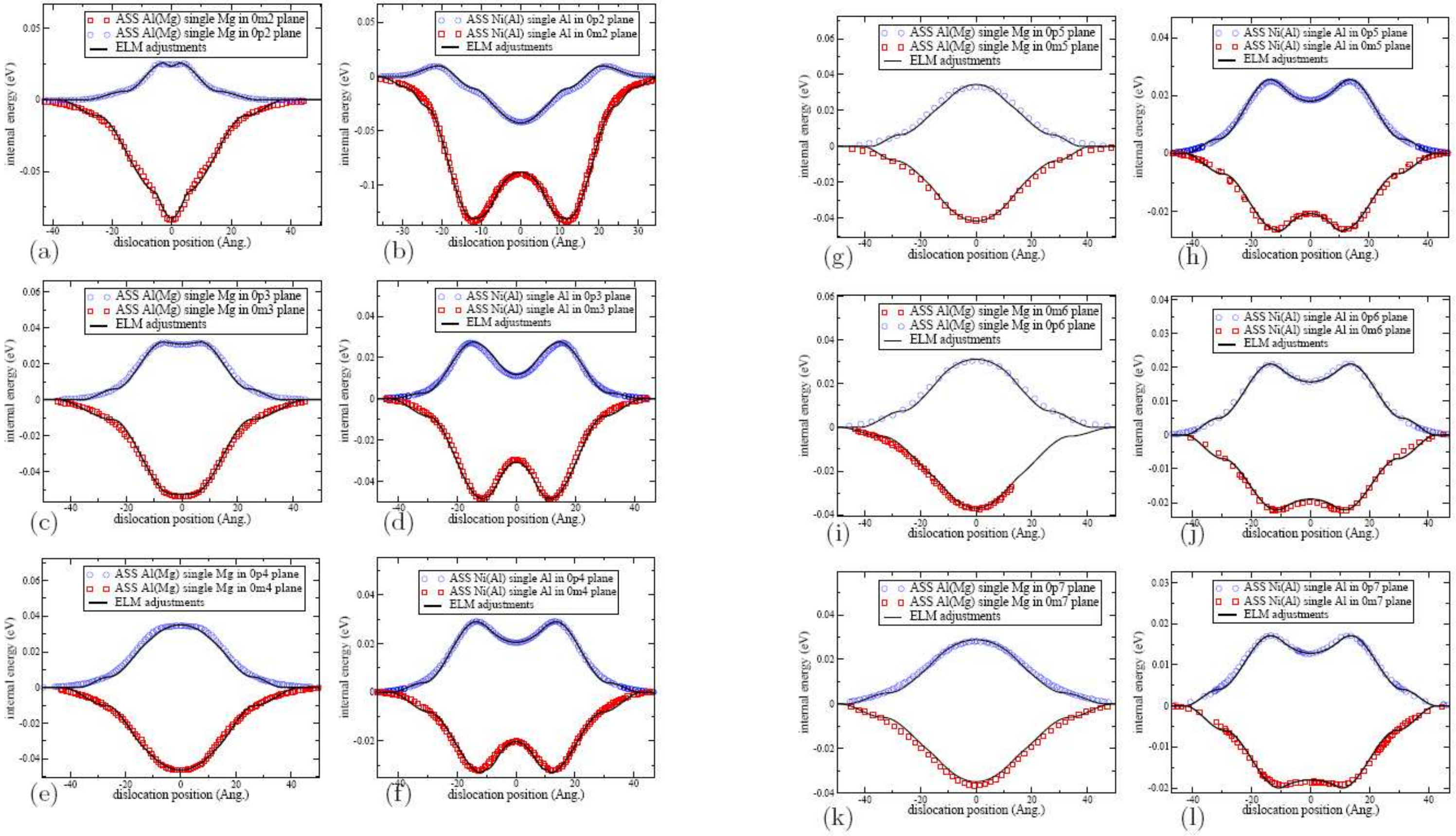


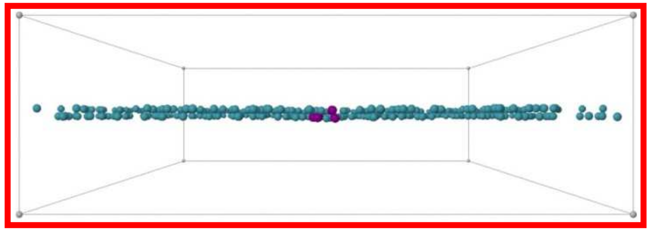
Fig. 9 (a) Al dimer in Ni
ASS data
EM model
segregation energy for a first neighbor dimer
interaction energy (eV)
dislocation position (Ang.)
Fig. 9 (a) Mg dimer in Al
Fig. 9 (b) Al dimer in Ni
Fig. 9 (b) Mg dimer in Al
Fig. 9 (c) Al dimer in Ni
Fig. 9 (c) Mg dimer in Al

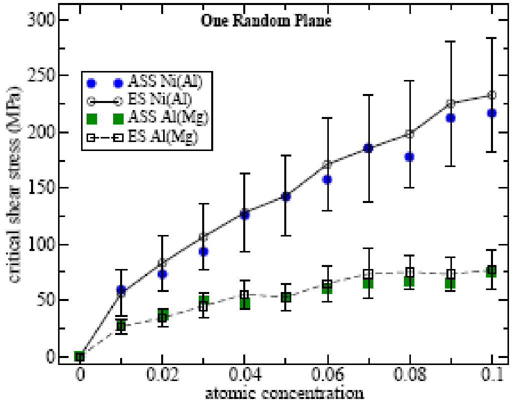

bt
bq
b
[$\bar{1}$12]
[110]
[-1-22] Mg dimer in Al
[-1-22] Al dimer in Ni
first neighbor dimer formation
[1-14] Mg dimer in Al
[1-14] Al dimer in Ni
dimer formation energy
interaction energy (eV)
dislocation position (Ang.)

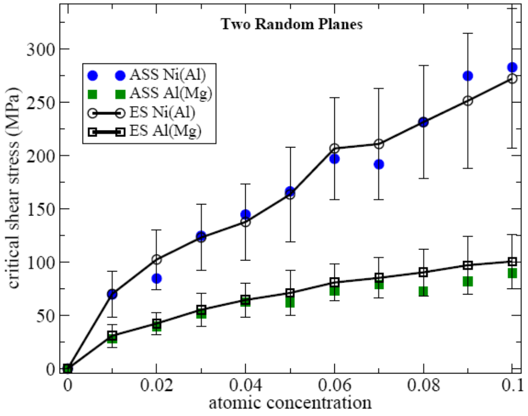
(a) (b) (c) (d) (e) (f)

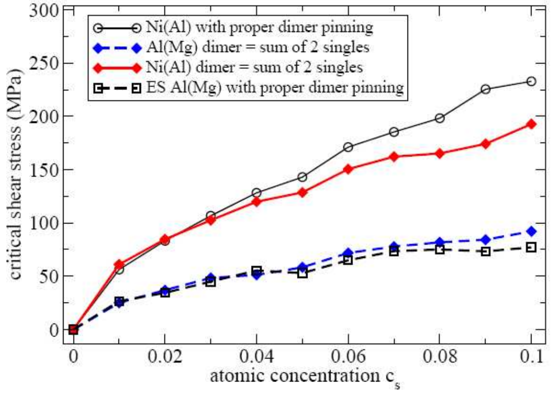

(a)
ASS Al(Mg) single Mg in 0m2 plane
ASS Al(Mg) single Mg in 0p2 plane
ELM adjustments
(b)
ASS Ni(Al) single Al in 0p2 plane
ASS Ni(Al) single Al in 0m2 plane
ELM adjustments
(c)
ASS Al(Mg) single Mg in 0p3 plane
ASS Al(Mg) single Mg in 0m3 plane
ELM adjustments
(d)
ASS Ni(Al) single Al in 0p3 plane
ASS Ni(Al) single Al in 0m3 plane
ELM adjustments
(e)
ASS Al(Mg) single Mg in 0p4 plane
ASS Al(Mg) single Mg in 0m4 plane
ELM adjustments
(f)
ASS Ni(Al) single Al in 0p4 plane
ASS Ni(Al) single Al in 0m4 plane
ELM adjustments
(g)
ASS Al(Mg) single Mg in 0p5 plane
ASS Al(Mg) single Mg in 0m5 plane
ELM adjustments
(h)
ASS Ni(Al) single Al in 0p5 plane
ASS Ni(Al) single Al in 0m5 plane
ELM adjustments
(i)
ASS Al(Mg) single Mg in 0m6 plane
ASS Al(Mg) single Mg in 0p6 plane
ELM adjustments
(j)
ASS Ni(Al) single Al in 0p6 plane
ASS Ni(Al) single Al in 0m6 plane
ELM adjustments
(k)
ASS Al(Mg) single Mg in 0p7 plane
ASS Al(Mg) single Mg in 0m7 plane
ELM adjustments
(l)
ASS Ni(Al) single Al in 0p7 plane
ASS Ni(Al) single Al in 0m7 plane
ELM adjustments
internal energy (eV)
dislocation position (Ang.)

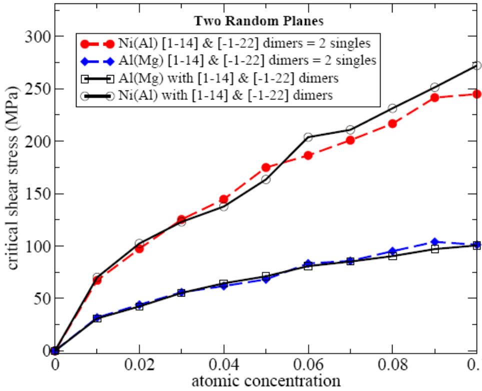
- obstacles in plane contiguous to the glide plane

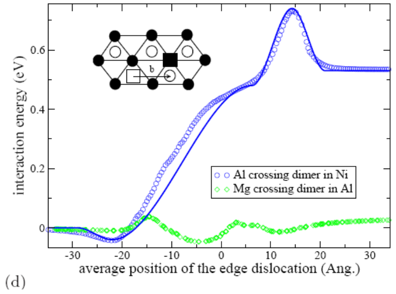


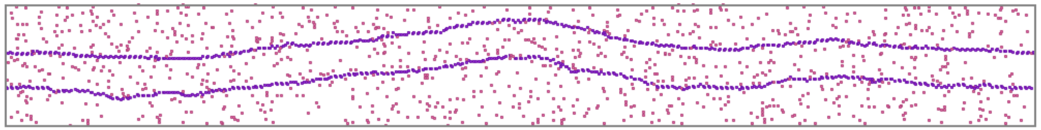




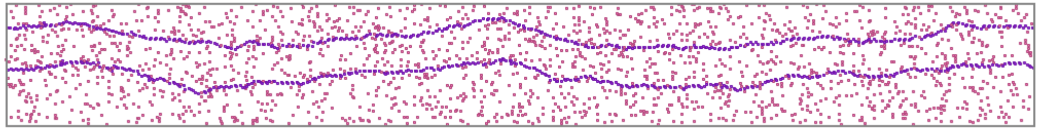




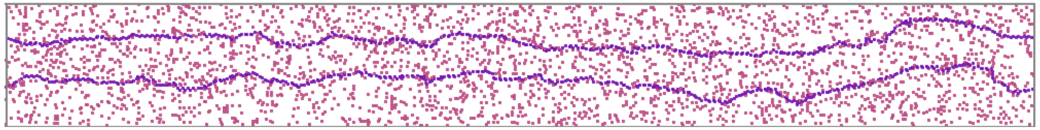




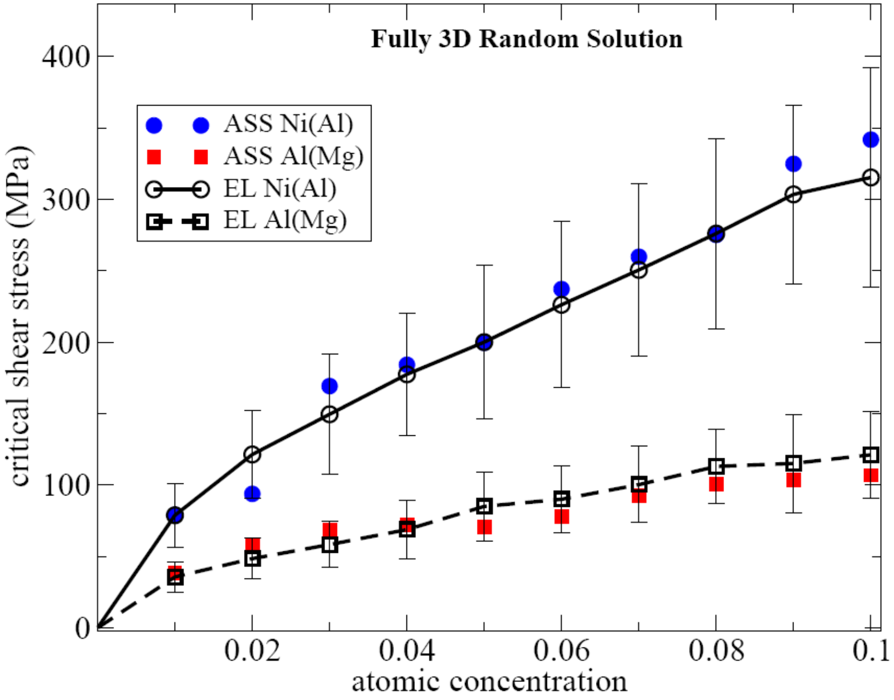
C_{Al}=3%

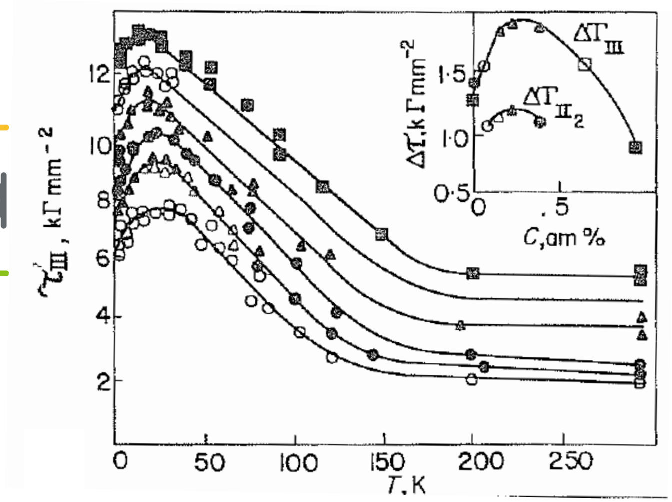


C_{Al}=6%

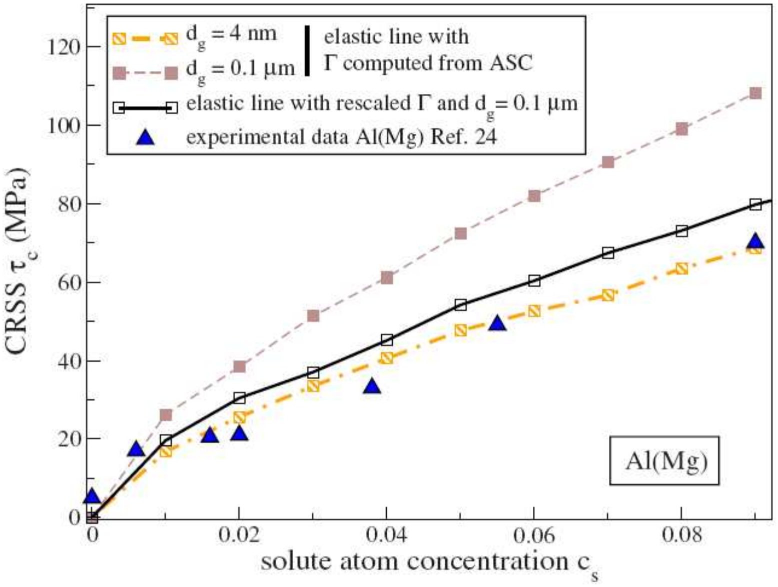


C_{Al}=9%





V. P. Podkuyko, Criogenics (1978)



$$\tau_c = A(c_s)\ln(d_g)^\alpha$$

[L. Proville, J. Stat. Phys. **137**, 717 (2009)]

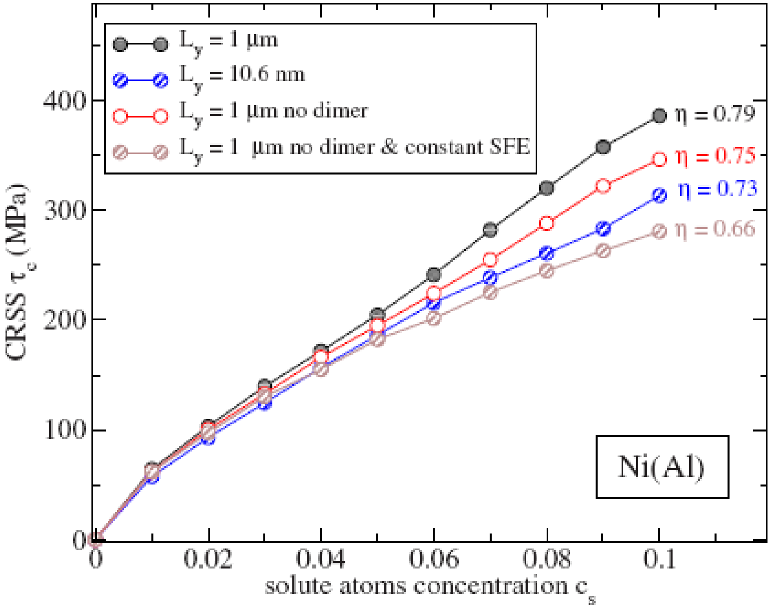
$\alpha = a_0 - a_1 \ln(c_s)$

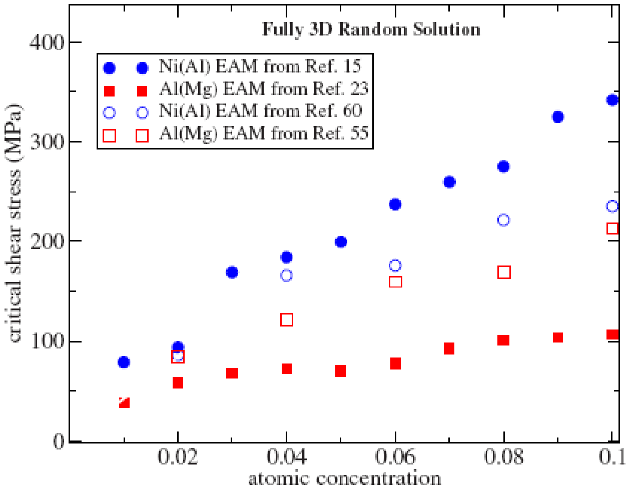
Orowan relation : $\epsilon = \rho_d b d_g$ $d_g = 100\ \mathrm{nm}$ $\epsilon = 2.5 10^{-5}\ \%$

$\rho_d \approx 10^{12}\ \mathrm{m}^{-2}$

$\varepsilon = 0.1\ \%$ ➔ $d_g = 1$ mm

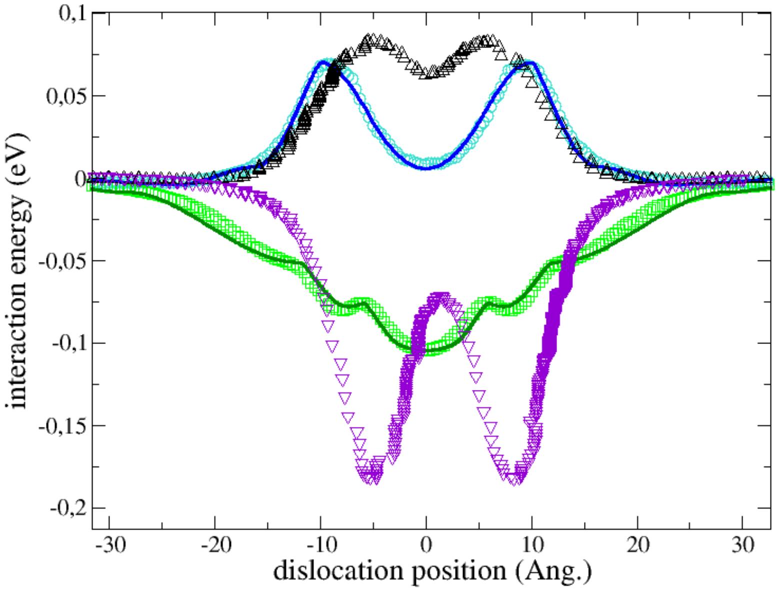
$\tau_c = A c_s^\eta$ $\eta = 0.67$ for d_g = 100 nm


L_y = 1 µm
L_y = 10.6 nm
L_y = 1 µm no dimer
L_y = 1 µm no dimer & constant SFE
η = 0.79
η = 0.75
η = 0.73
η = 0.66
Ni(Al)
CRSS τ_c (MPa)
0
100
200
300
400
0
0.02
0.04
0.06
0.08
0.1
solute atoms concentration c_s

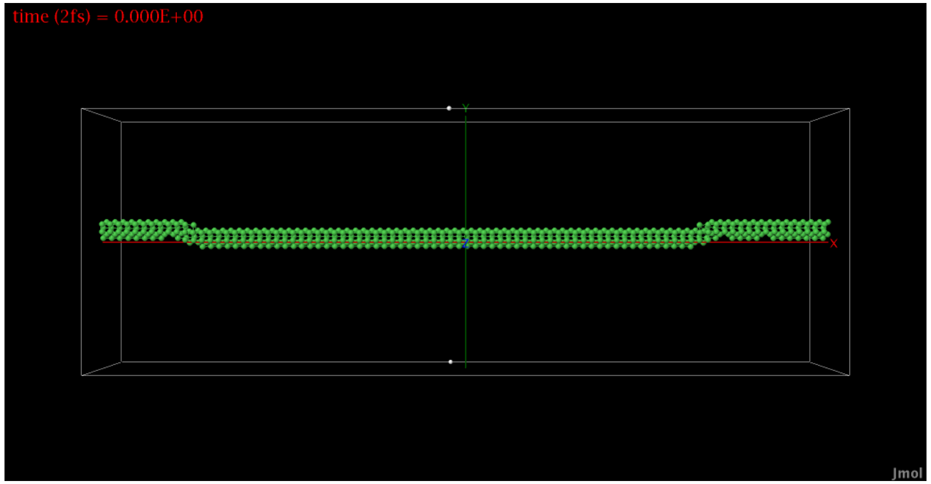


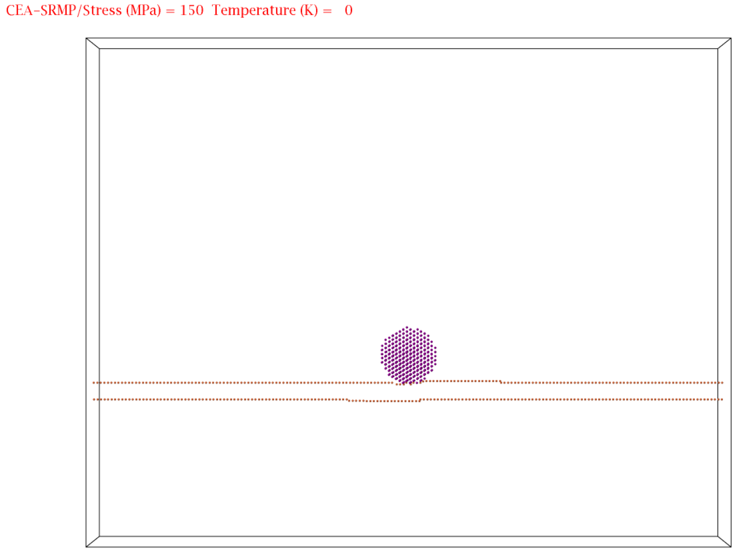
Ni(Al) G. P. Purja Pun and Y. Mishin, Philos. Mag. **89**, 3245 2009.

Al(Mg) M.I. Mendelev *et al.*, Philos. Mag. **89**, 3269 (2009).



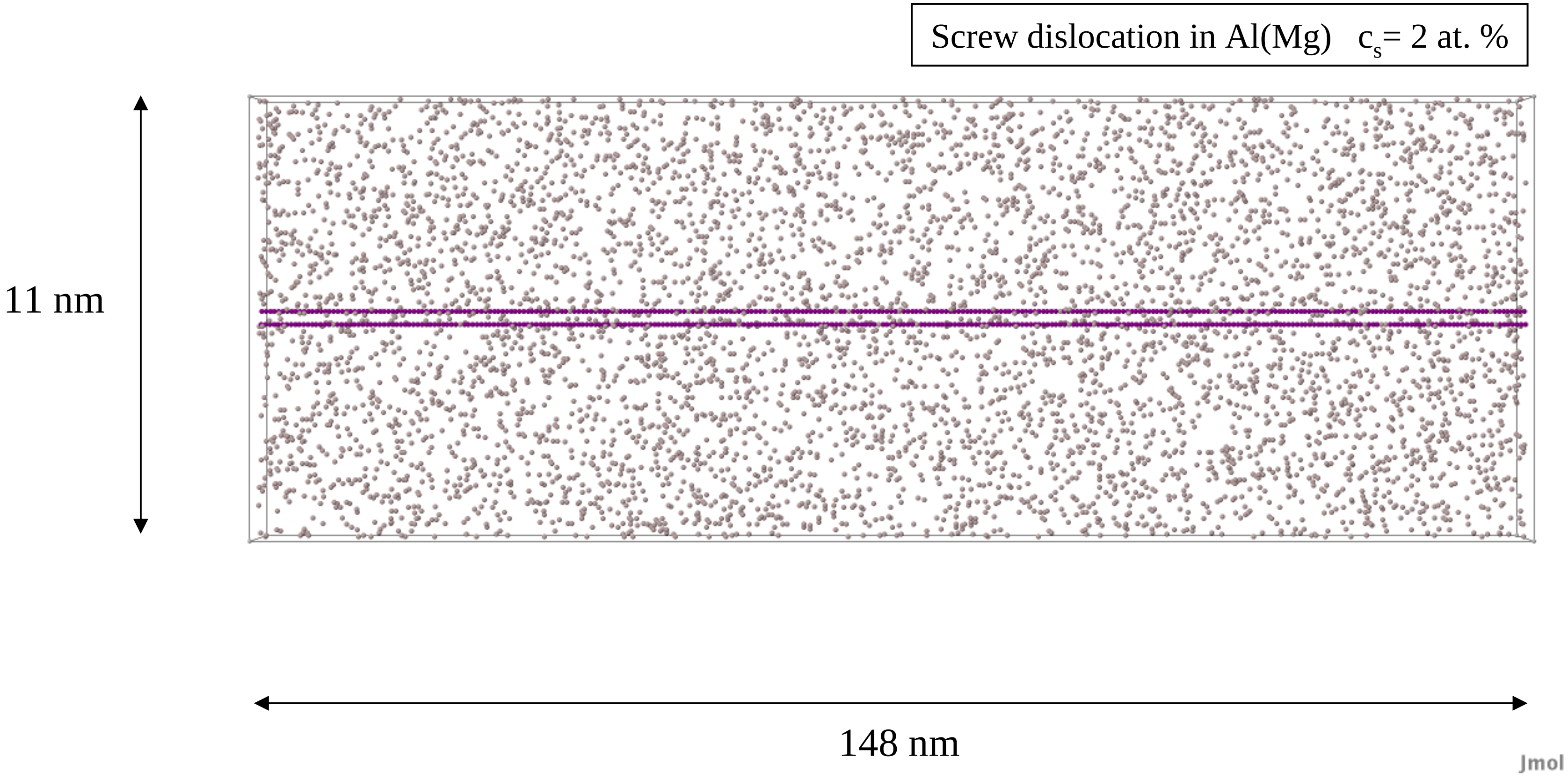
- ASS allows to capture the dislocation core details
- The 1D elastic line model allows scale transitions + good understanding
- Projects:
  - study solid solution hardening in bcc (ELM model development)
  - effect of temperature in the elastic line model (solute atom diffusion)



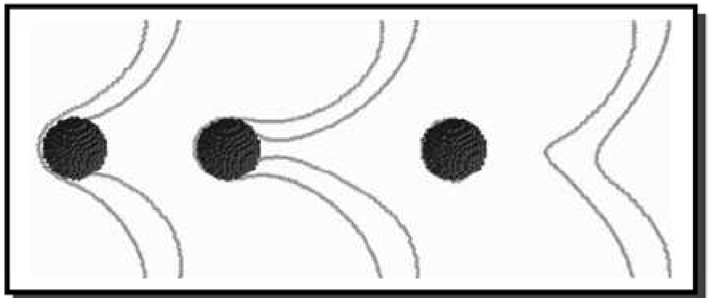


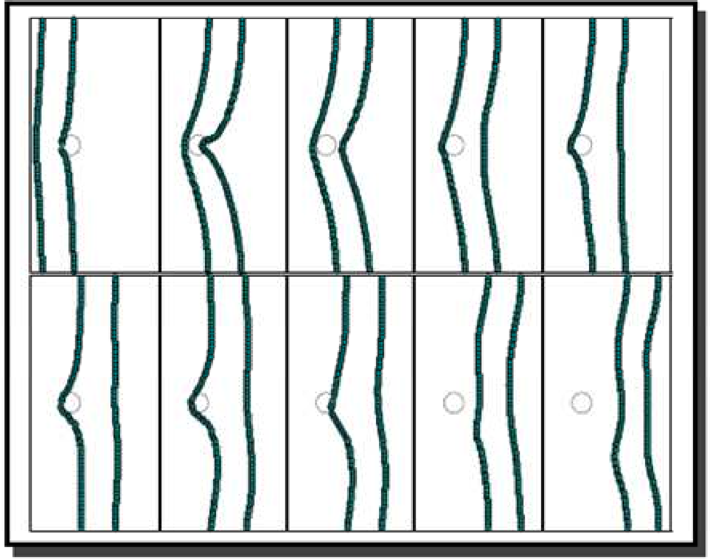
CEA-SRMP

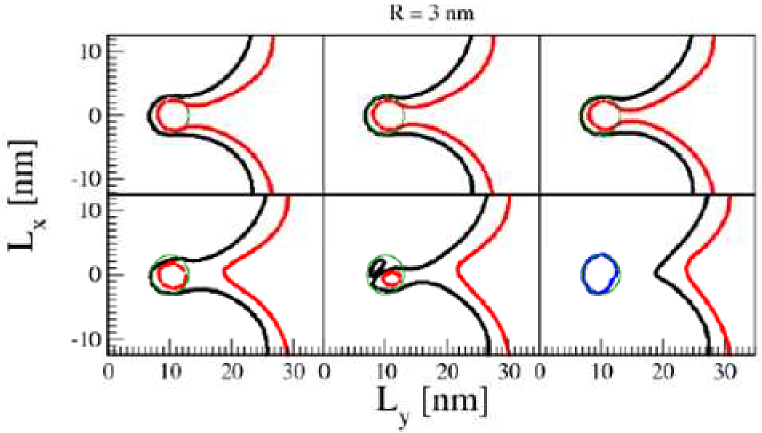
Screw dislocation in Al(Mg) c_s= 2 at. %



Depinning of edge dislocations







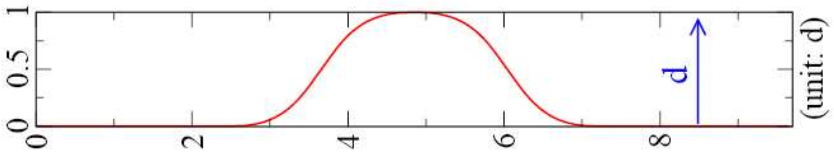
- up to a critical value $r_{\mathrm{crit}} \approx 1.5$nm the dislocation cuts through the Ni_3Al precipitate;
- the depinning stress is proportional to the square of the radius, r^2.
- above the critical value r_{crit} the partials relax into a loop circumventing the nanophase.

Modèle de tension de ligne pour une approche multi-echelle de la formation des paires de décrochement

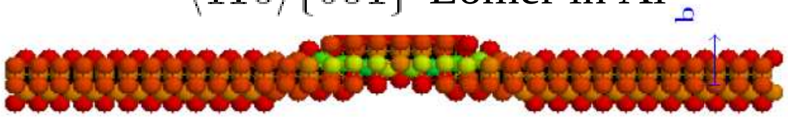
Auteurs : D. Rodney[a] et L. Proville[b]
a) b) CEA, DMN Service de Recherches de Métallurgie Physique

Tension de ligne :

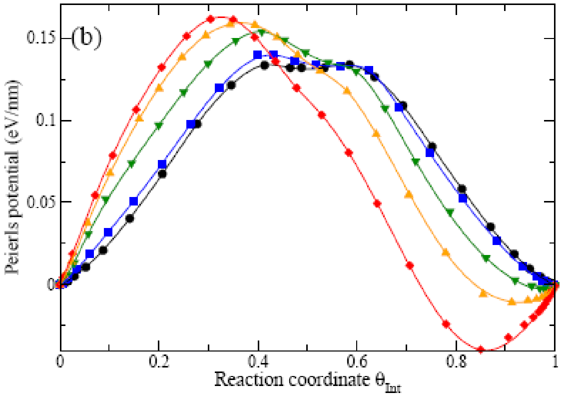
$$-V_P'(y(x)) + \sigma_A b + T\frac{\partial^2 y}{\partial x^2} = 0$$

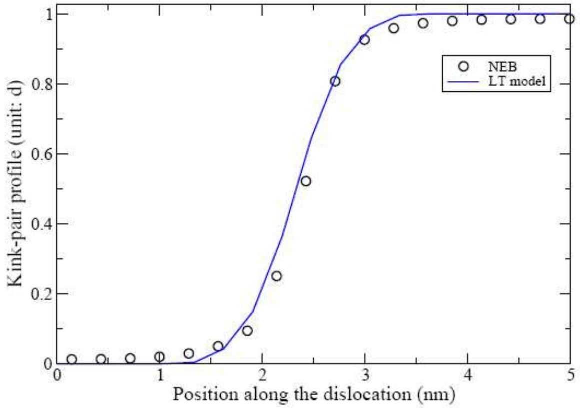


$\langle 110\rangle\{001\}$ Lomer in Al



Potentiel de Peierls variable avec la contrainte appliquée



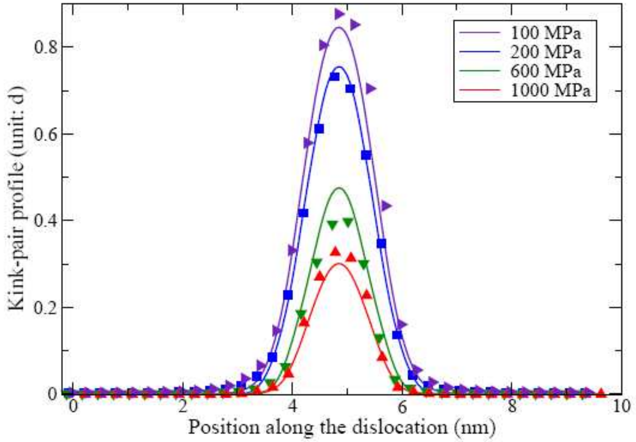


Profile d'un décrochement
Calcul atomistique +
Tension de ligne

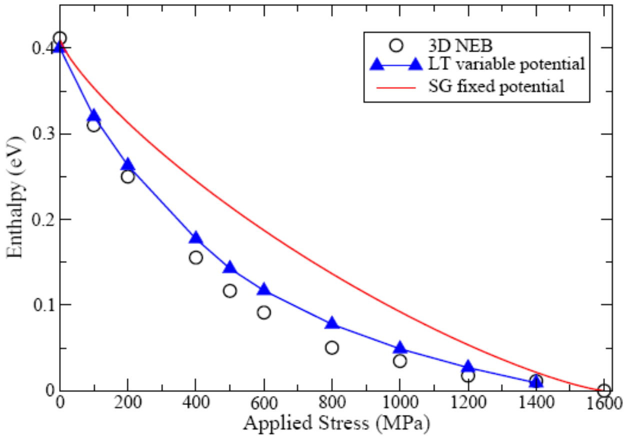
$$T = 0.36\ \text{eV}.\mathring{A}^{-1}$$

Prédictions du modèle de tension de ligne comparées au résultats de simulation atomistique

Profiles des paires de décrochement à différentes contraintes

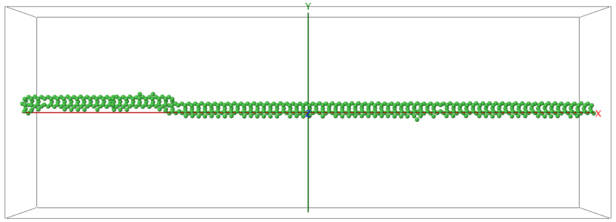


Enthalpie de formation en fonction de la contraintes



time (2fs) = 0.100E+03

Dislocation de Lomer Al
σ =500 MPa T = 20 K



D. Rodney and L. Proville, Physical Review B, Vol. 79, 094108 (2009)

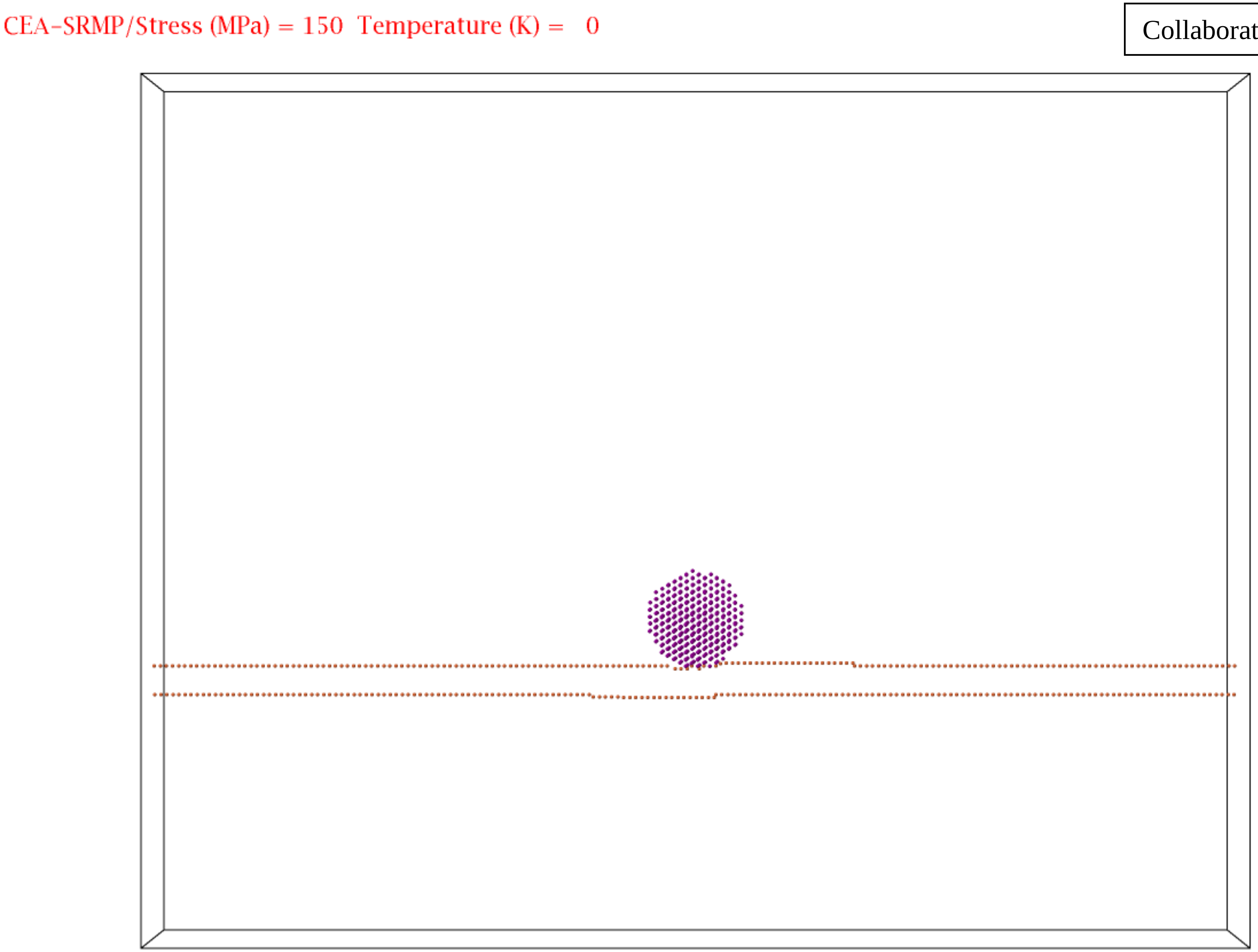
Jmol

Conclusions

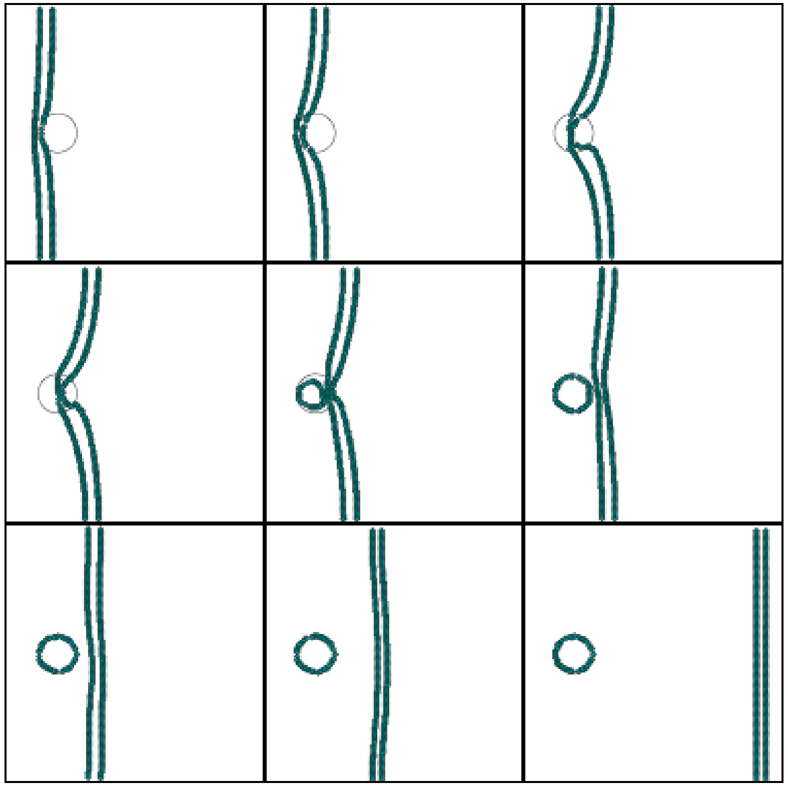
- Dislocations cut nanophases under a radius r_c,
  above Orowan loops are formed at low temperature
- The loop formation is different for screw and edge
- For cutting mechanism, the critical stress varies as r^2
- For Orowan mechanism, the log prefactor is $\mu b(2-\nu)/8(1-\nu)$
  for edge dislocations
- Projects:
  - effect of solid solution
  - effect of temperature (climb)

II. Ni_3Al nanophase strengthening for Ni based alloys

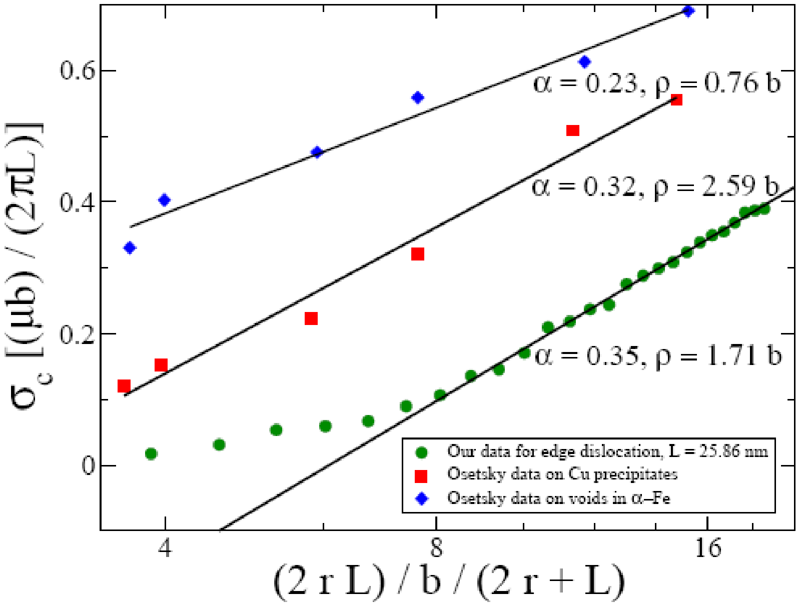
Collaboration: B. Bako



Depinning of a screw dislocation



Orowan looping – Theory



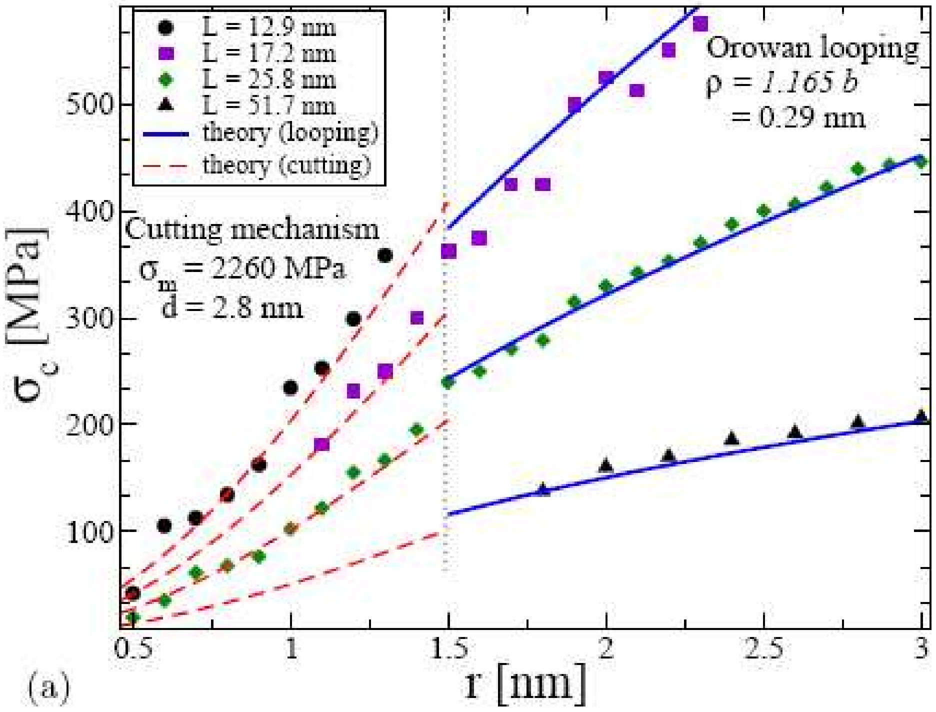
- Analytical phenomenological model based on DD (Bacon, Kocks, and Scattergood – 1973)

$$\sigma_c = \frac{\mu b}{2\pi L} \ln\left[\frac{2rL}{\rho(2r+L)}\right]$$

(for the edge dislocation)

- Works with voids, ODS, precipitates in FCC and BCC, but
- Requires an unknown rescaling parameter α
- There is no theory for the depinning stress in the cutting regime.

$$\sigma_{\text{cut}} = \sigma_m \frac{\cos^2(\frac{\theta}{4})[\theta - \sin(\theta)]}{2L/r + 1}, \quad \sigma_{\text{Orowan}} = \frac{2-\nu}{4(1-\nu)} \frac{\mu b}{2L - \pi r} \left[\ln\left(\frac{4r}{\rho}\right) - 2 \right]$$

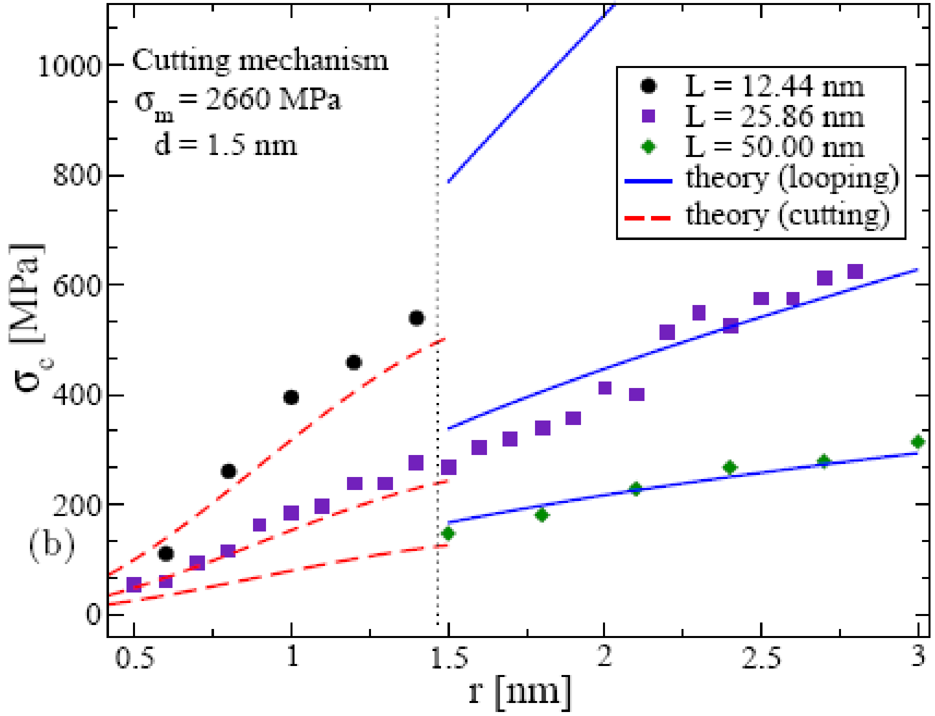


$\cos^2(\theta/4) = \frac{r}{2d}$, where

d: separation distance of the dislocation

σ_m the CRSS required for a straight dislocation to penetrate a semi-infinite Ni_3Al phase with $L1_2$ order.

All parameters of the theory can be calculated by MD, no fitting is required.


Cutting mechanism
σm = 2660 MPa
d = 1.5 nm
L = 12.44 nm
L = 25.86 nm
L = 50.00 nm
theory (looping)
theory (cutting)
(b)
σc [MPa]
0
200
400
600
800
1000
0.5
1
1.5
2
2.5
3
r [nm]

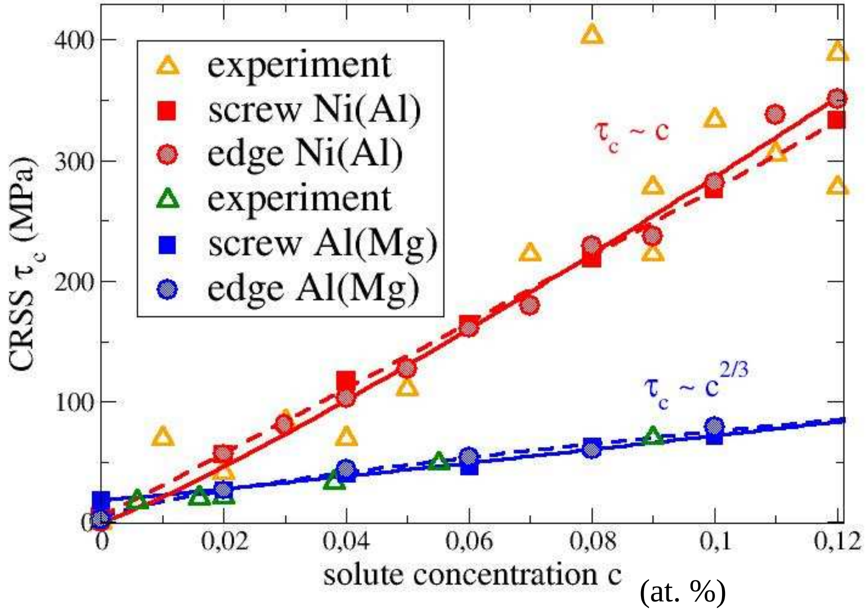
Ancrage d'une dislocation vis dans une solution solide modèle CFC

Thèse de S. Patinet

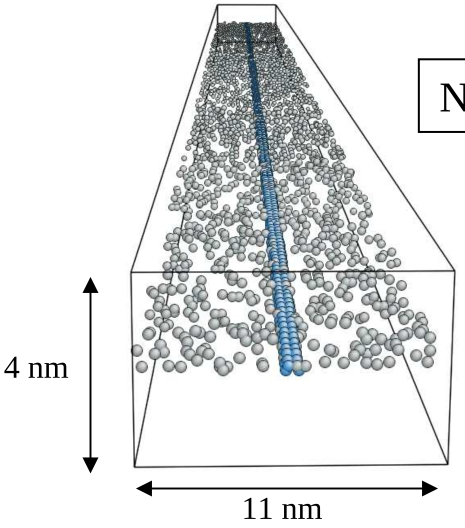
Etude à l'échelle atomique avec potentiels inter-atomique EAM

Calcul du seuil de décrochage statique

Contrainte critique résolue pour différents alliages
En fonction de la densité d'obstacles



(at. %)



Ni(Al) 6% at.

- ➔ Bon accord expérience simulation
- ➔ différentes lois de durcissement pour 2 alliages FCC

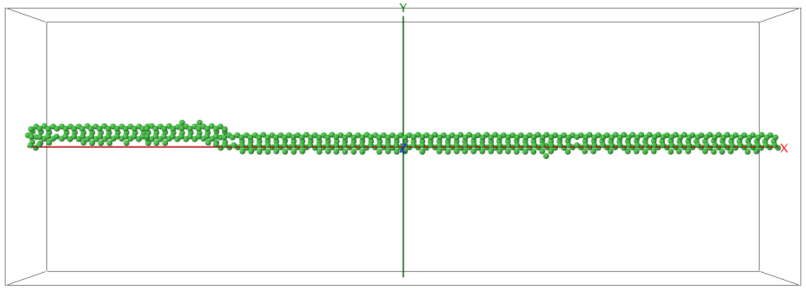
Attention taille de simulation << exp !!

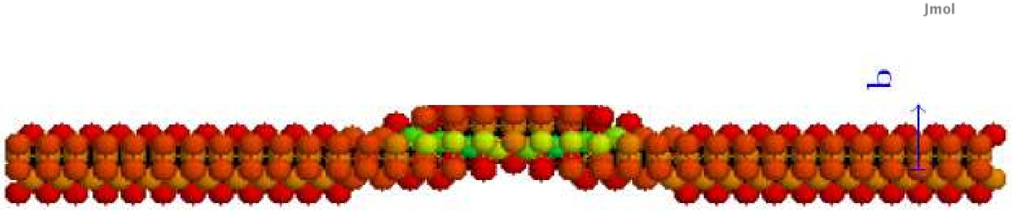
PHYSICAL REVIEW B **78**, 104109 (2008)

I. Peierls mechanism

Collaboration: D. Rodney
INP Grenoble, Science et Ingénierie Matériaux Procédés

- ➔In bcc thermal activation of dislocation glide proceeds through kink pair nucleation on screw
- ➔ Interatomic forces model = Embedded Atom method
- ➔ Not yet efficient at modeling screw dislocation in bcc metals
- ➔ Lomer dislocation in Al-Al F. Ercolessi and J. Adams, Europhys. Lett.

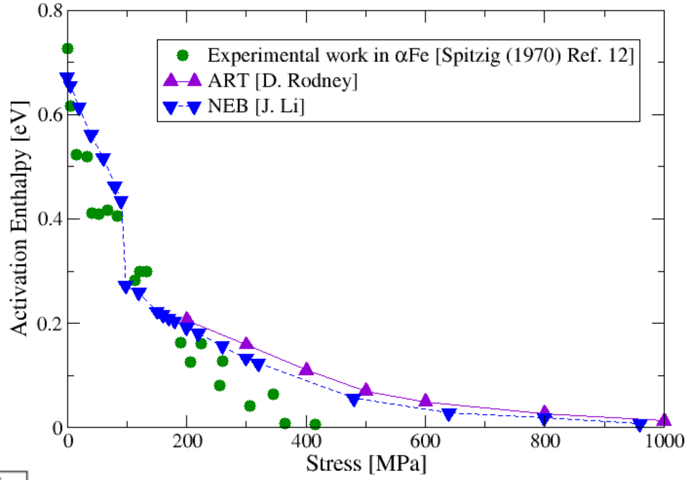




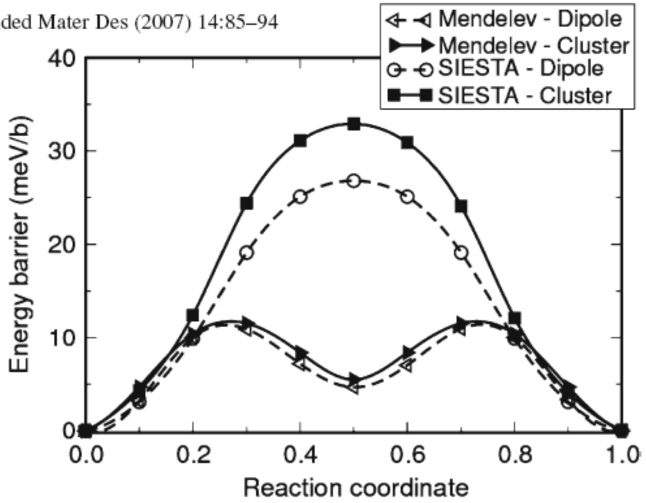
D. Rodney and L. Proville, Phys. Rev. B **79**, 094108 (2009).

Mécanisme de Peierls

Enthalpie d'activation d'une paire de décrochement sur
La dislocation vis modèle de Mendelev (Phil. Mag. 2003) pour Fe cc



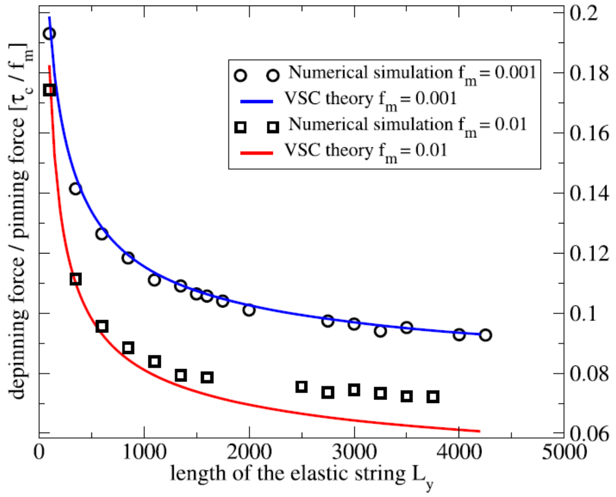
L. Ventelon & F. Willaime
J Computer-Aided Mater Des (2007) 14:85–94



	Fe	Ta	Mo	K	W
τ_p (MPa) (exp.)	390 [1, 3, 12]	340	710 [13]	2.7 [14, 15]	900 [6]
τ_p (MPa) (theory)	933 [10]/1200[16]	1730 [9]	2730[9, 17]	6.9 [8, 18]	2400 [19]

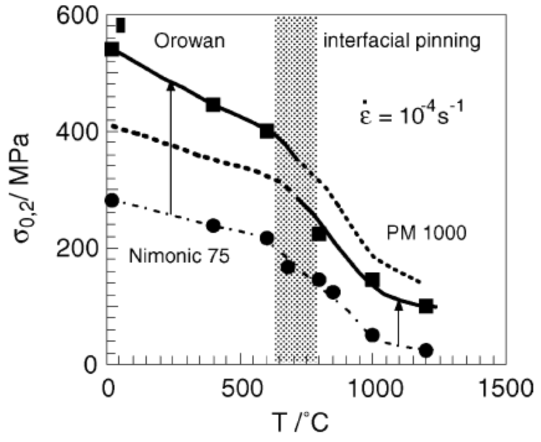
L. Proville, Annals of Physics,
accepted for publication
http://lanl.arxiv.org/abs/0904.3357.

L. Proville, J. Stat. Phys. **137**, 717 (2009)



Conclusion:

- le modèle de ligne élastique peut être développé afin d'intégrer la complexité du niveau atomique.
- possibilité de paramétrer % calcul AB-initio ➔ éviter artefact des potentiels EAM
- transition d'échelle vers DDD envisageable


600
400
200
0
$\sigma_{0,2}$/ MPa
Orowan
interfacial pinning
$\dot{\varepsilon} = 10^{-4} s^{-1}$
PM 1000
Nimonic 75
0
500
1000
1500
T /°C