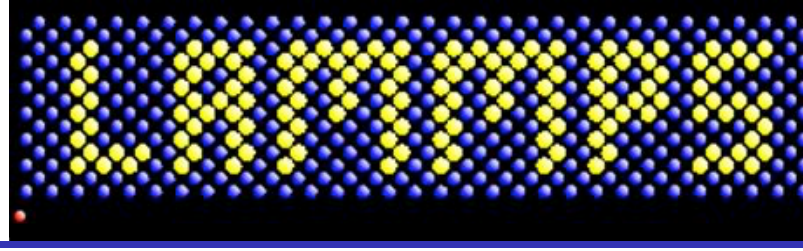


Atomic scale simulations with Lammps in material science: from polymers to metallurgy

R. Veiga, O. Waseda, A. Makke, W. Goncalves, J. Morthomas, P. Chantrenne, J. Amodeo and Michel Perez

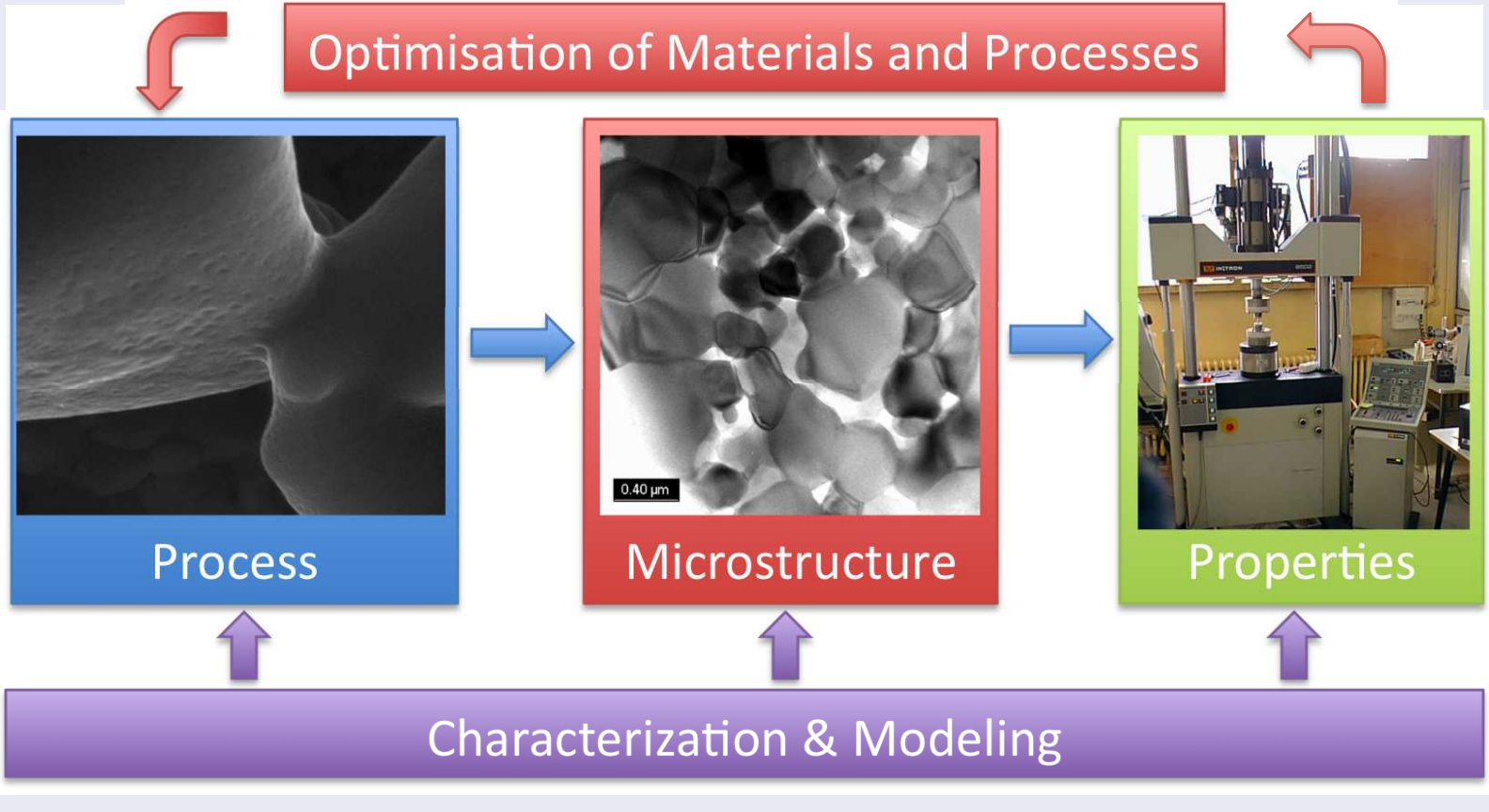
Université de Lyon - INSA Lyon - MATEIS - UMR CNRS 5512

26 juin 2018

Outline...

MATEIS: MATerials Engineering and Sciences

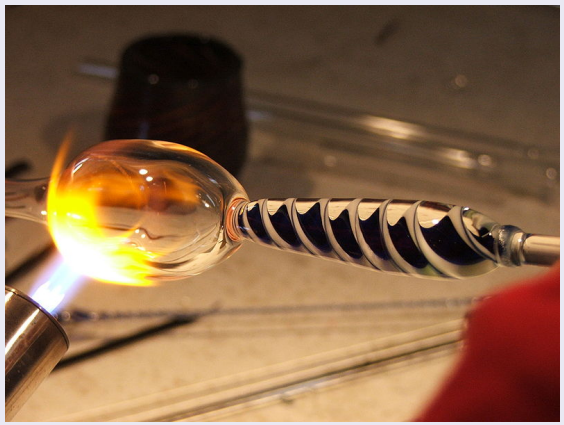
Strategy of the group



Recyclable polymers ?

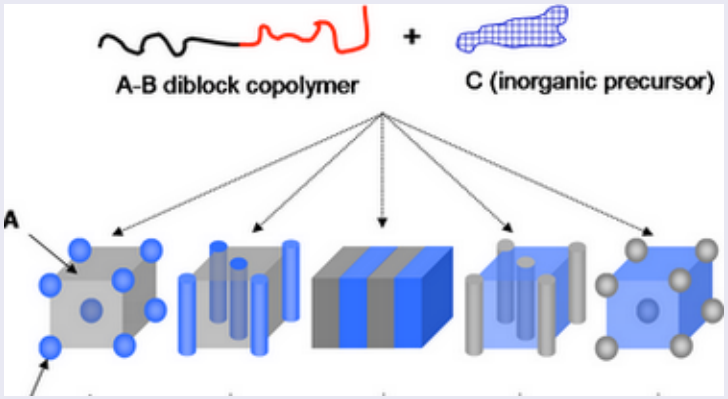
Elastomers *vs* thermoplastics

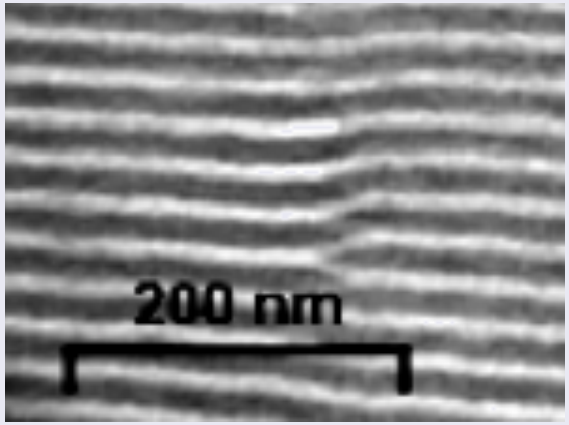
- Elastomers
  - Liquid solids!
  - amazing elastic properties (thanks to entropy)
- Thermoplastics
  - soften when heated
  - reversible ($\rightarrow$ recyclable !)



Copolymers

Many structures...

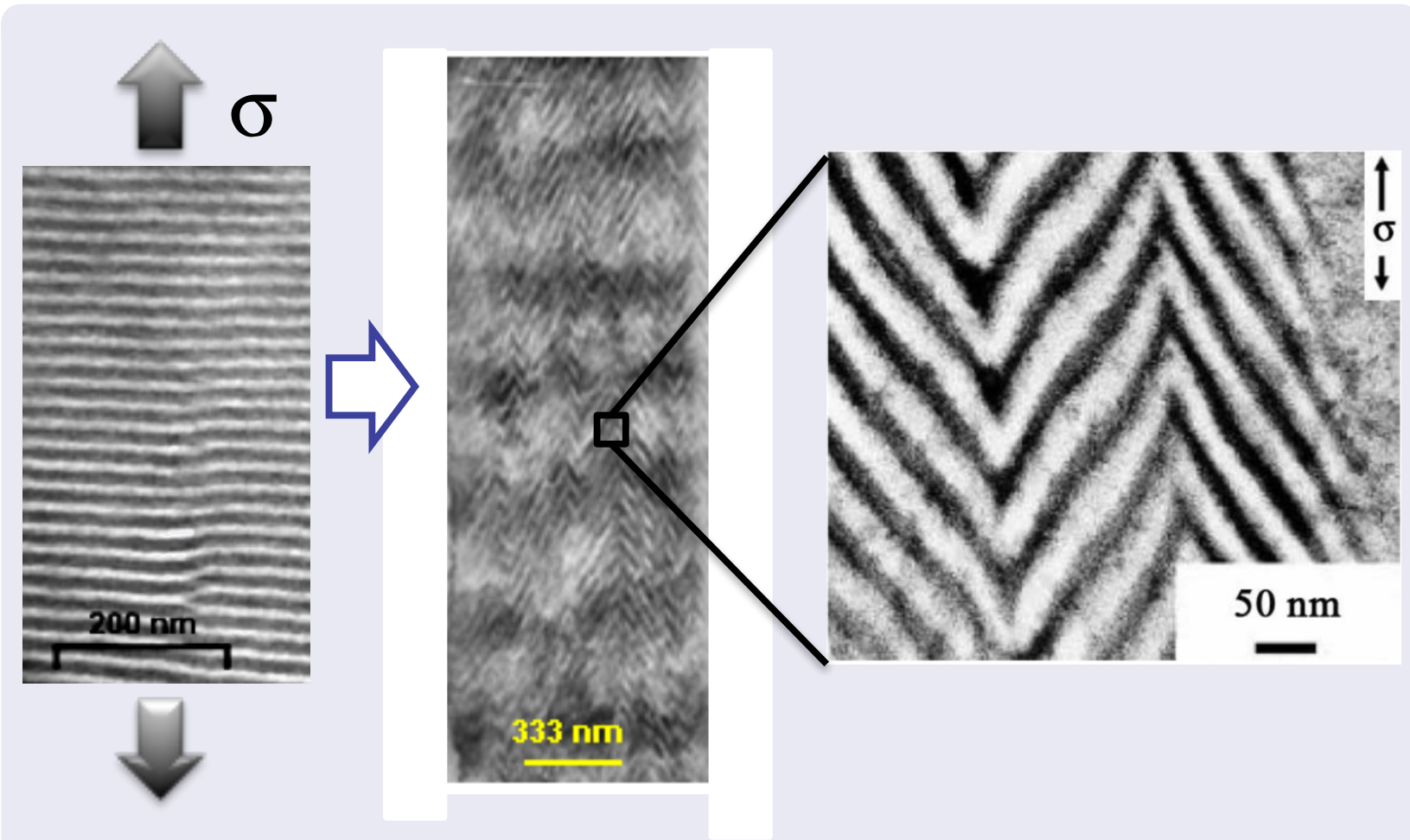




... but, always

- a hard phase ($T < T_g$)
- a soft phase ($T > T_g$)

Strange coupling between phases

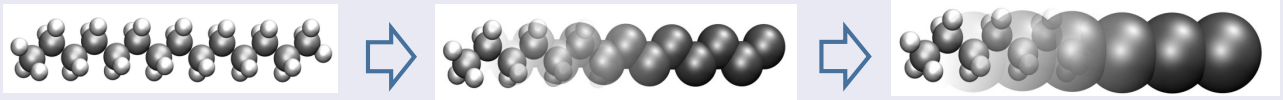


Method: Molecular Dynamics

Principle

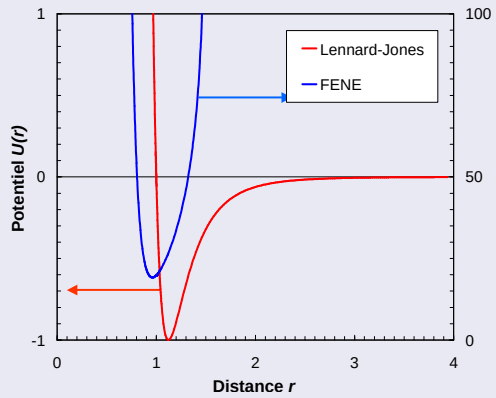
- Newtons 2nd law $m_i \frac{d\mathbf{v}}{dt} = \mathbf{f_i}$
- Interactions de paires: $\mathbf{f_i} = \sum_j \mathbf{f_{ij}} = \sum_j \mathbf{grad}\, V_{ij}$

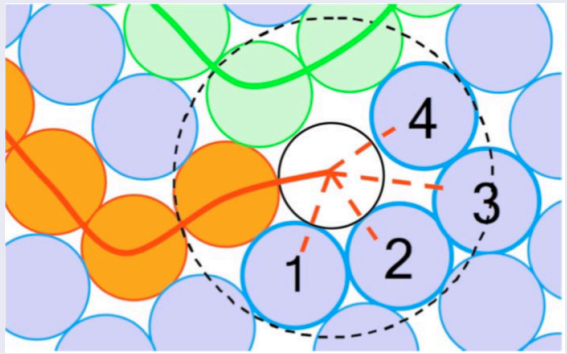
"Coarse grained" MD



Tri-block generation: Radical-like Polymerization (lammps fix)


[Mahaud, *Comp. Soft.* **24** (2018)]





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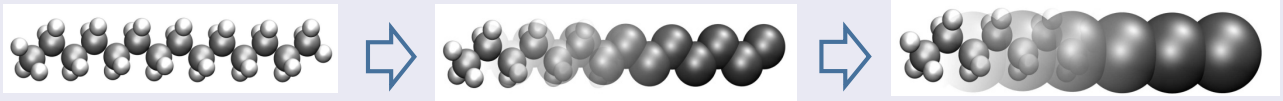

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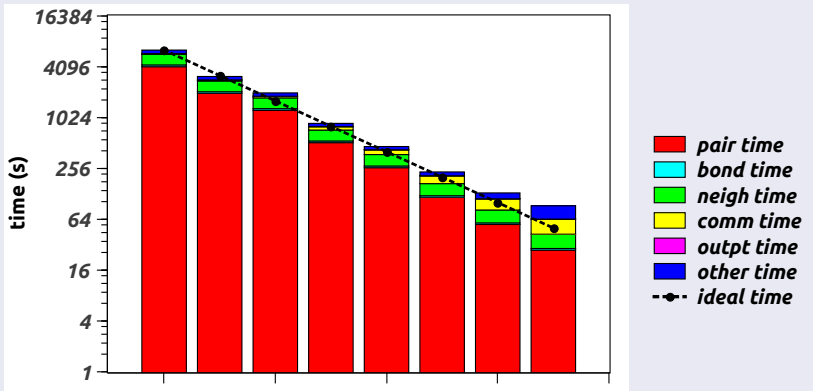
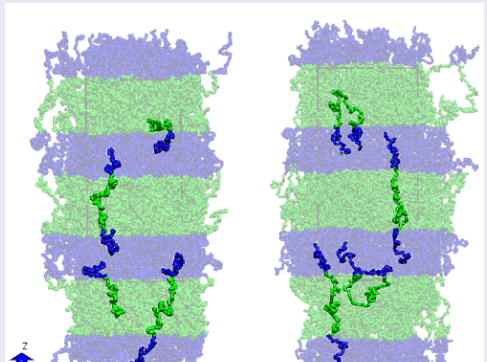
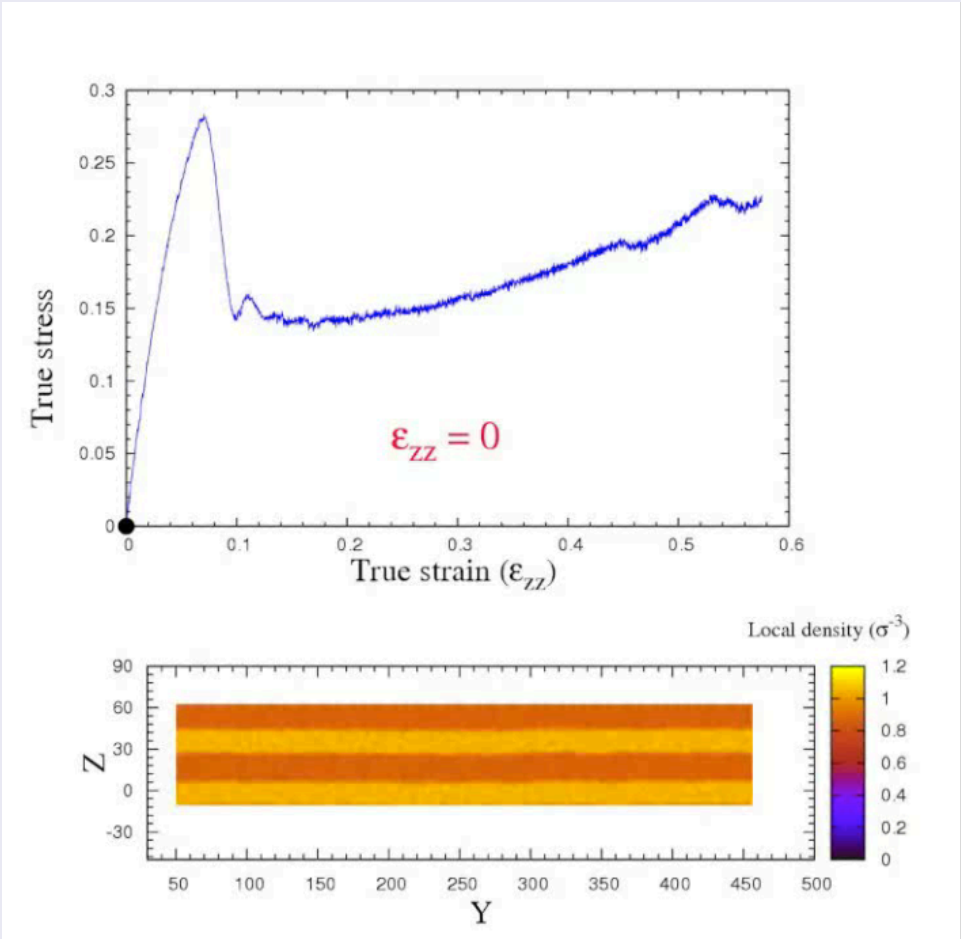
[Mahaud, *Comp. Soft.* **24** (2018)]





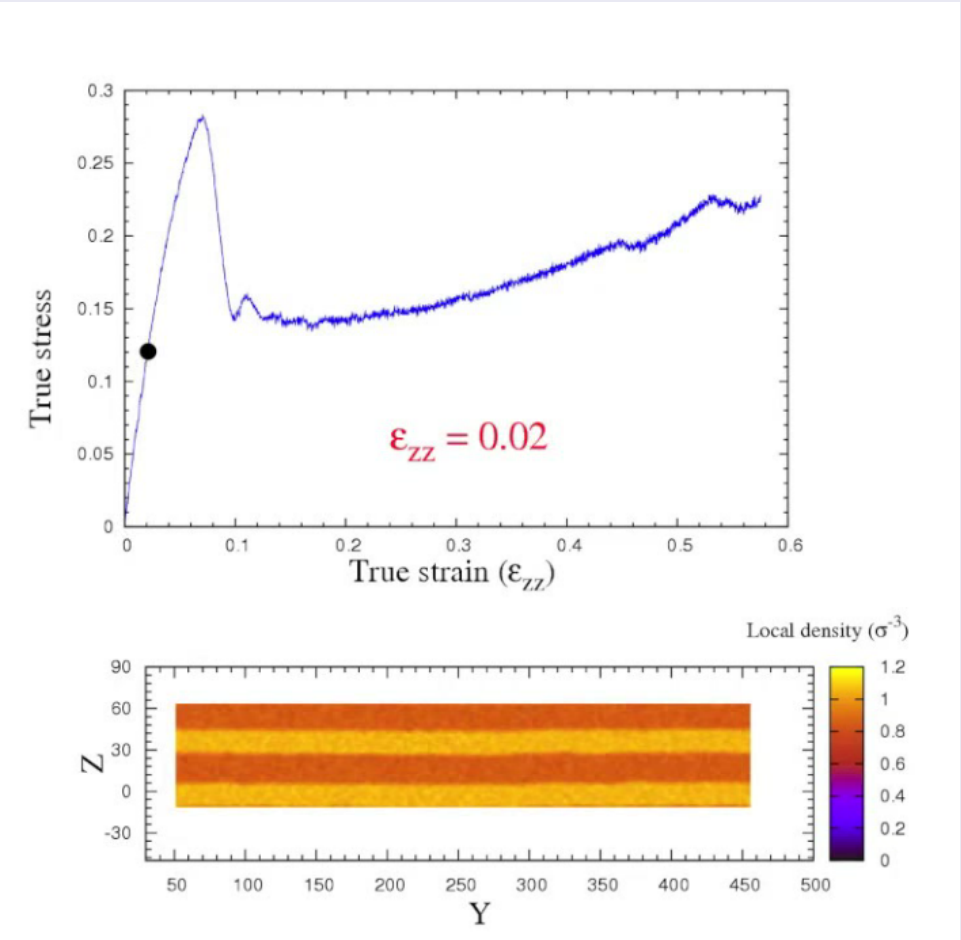
Tensile test

Perpendicular to lamellae



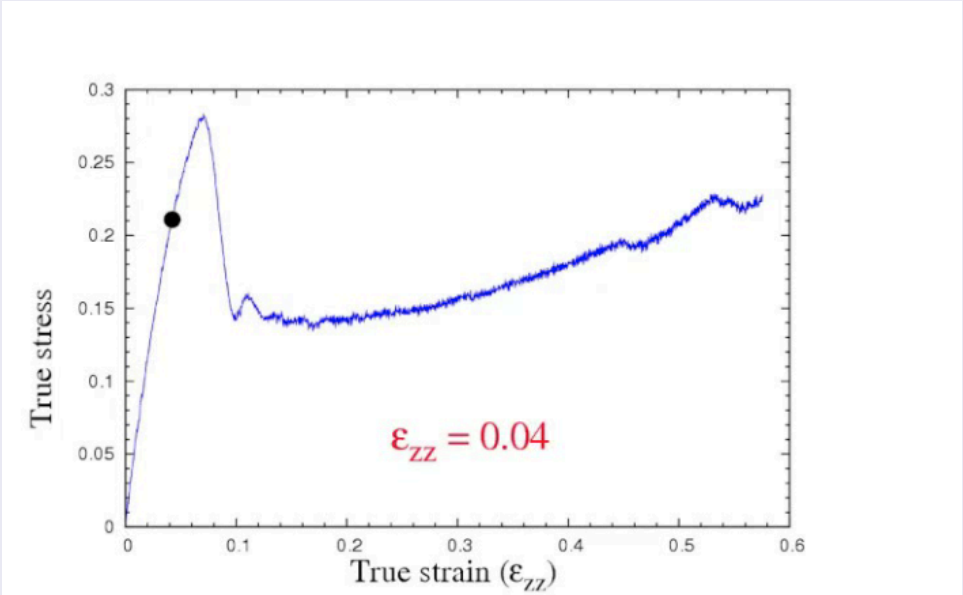
Tensile test

Perpendicular to lamellae



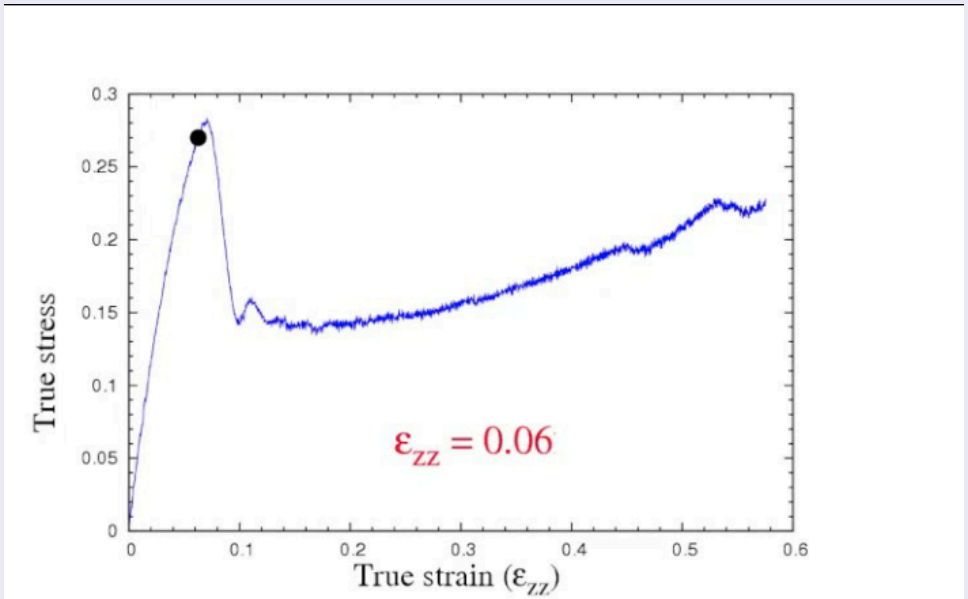
Tensile test

Perpendicular to lamellae



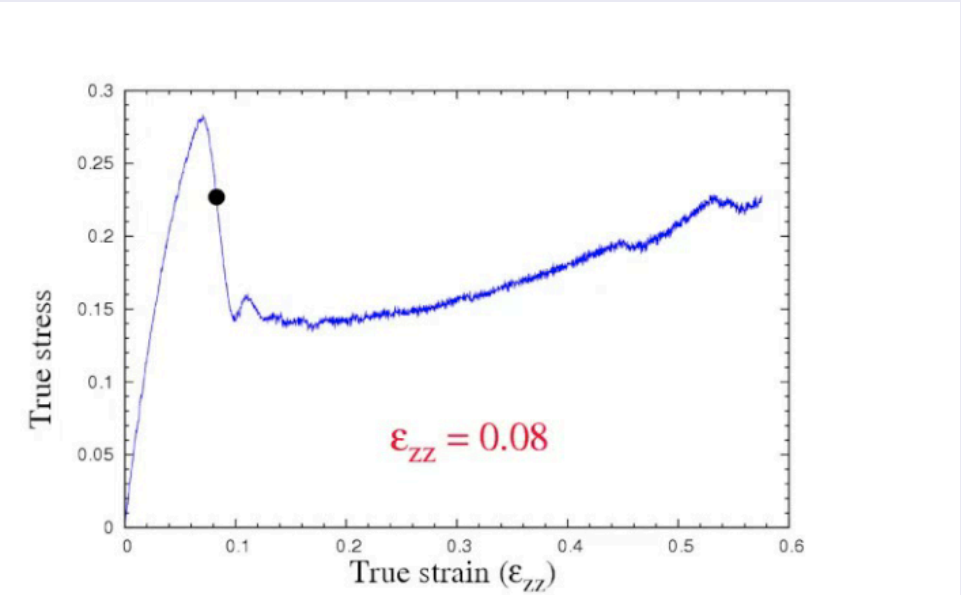
Tensile test

Perpendicular to lamellae



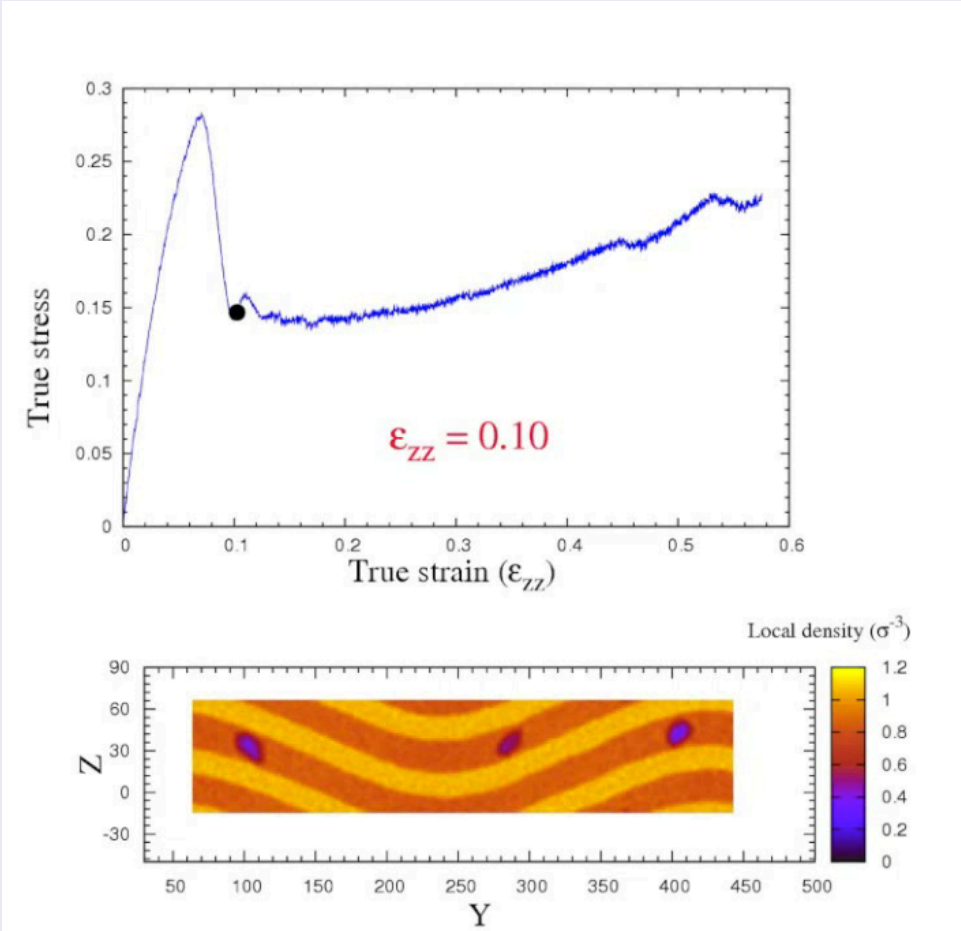
Tensile test

Perpendicular to lamellae



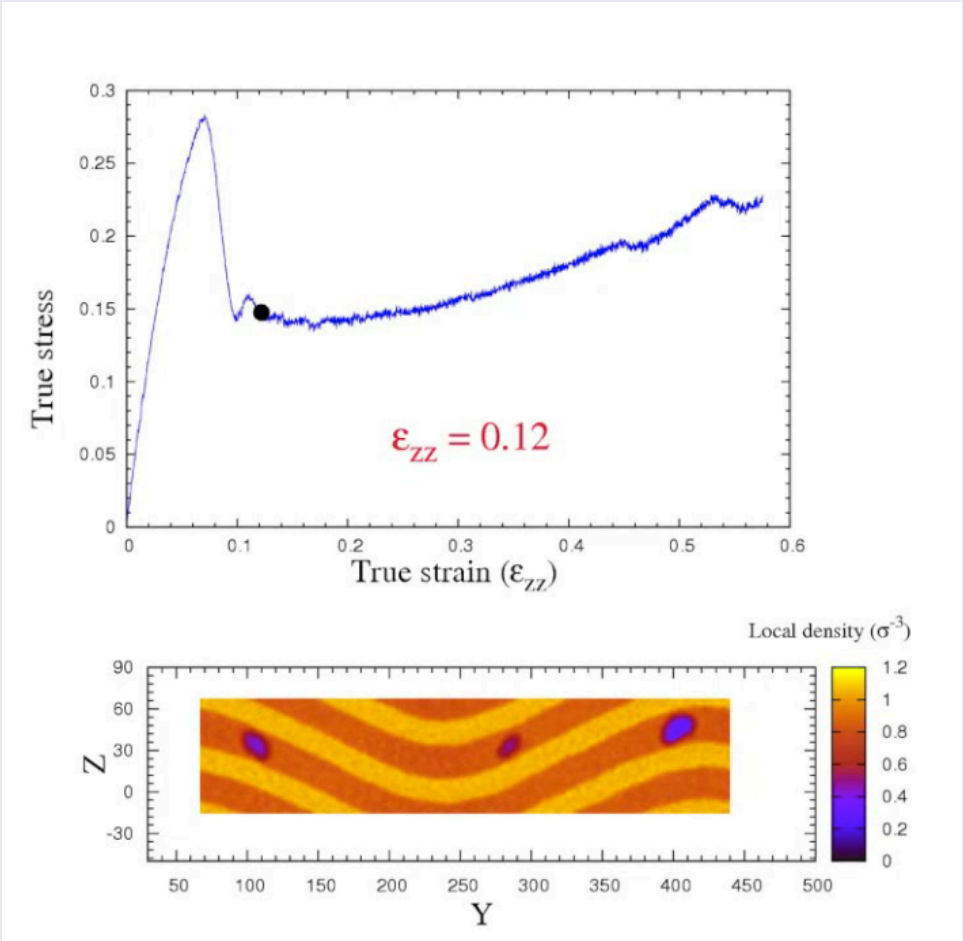
Tensile test

Perpendicular to lamellae



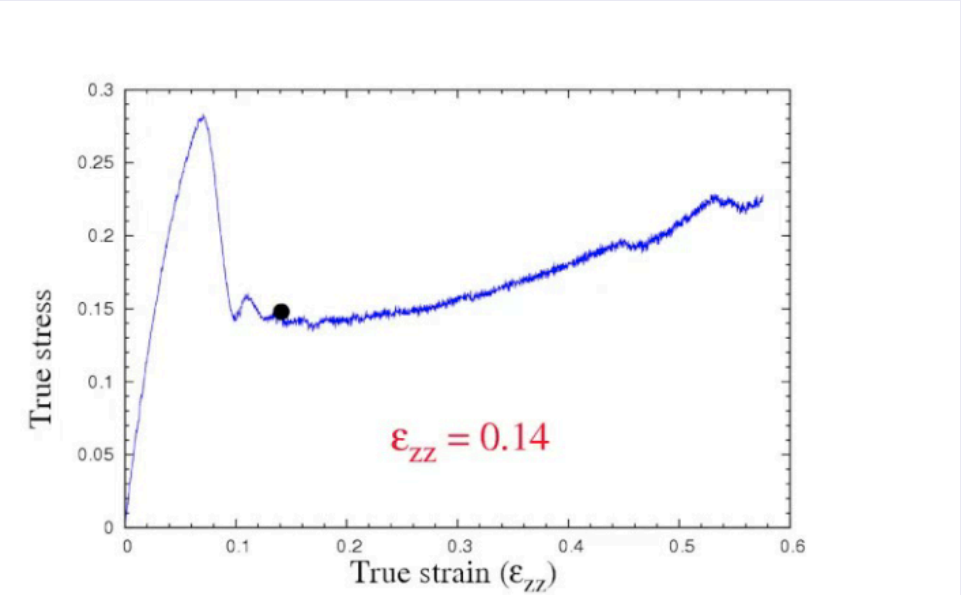
Tensile test

Perpendicular to lamellae



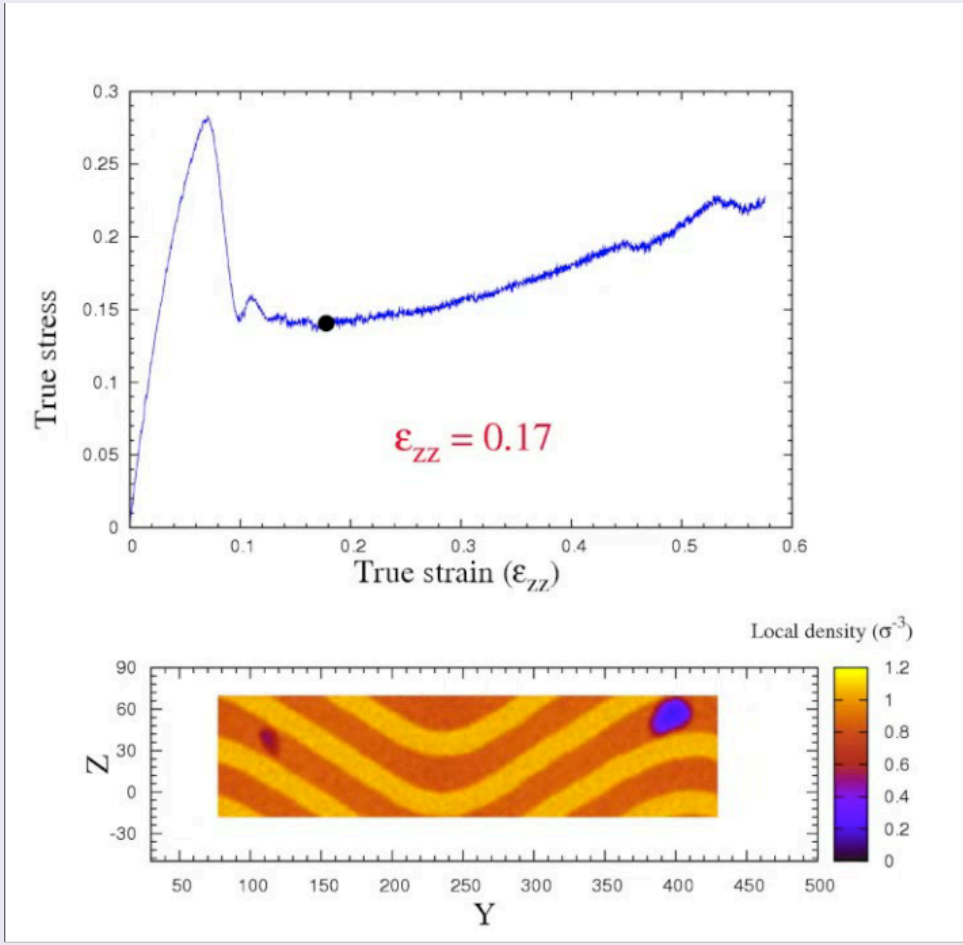
Tensile test

Perpendicular to lamellae



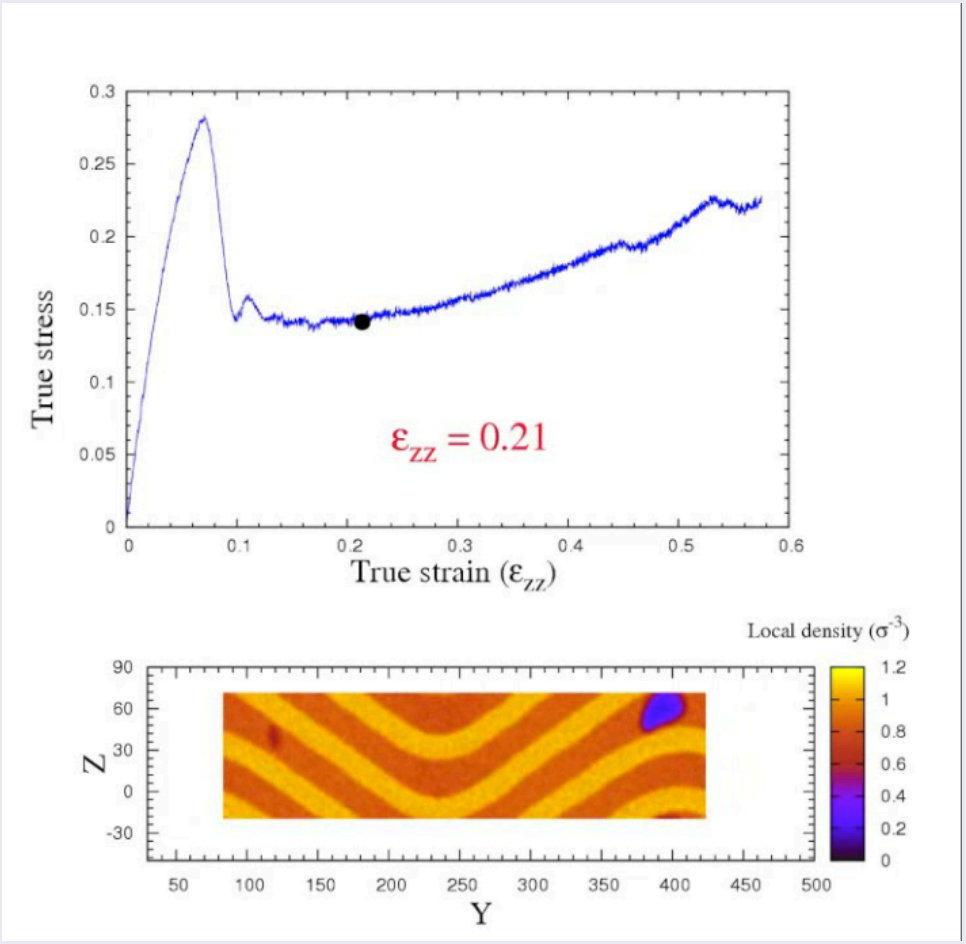
Tensile test

Perpendicular to lamellae



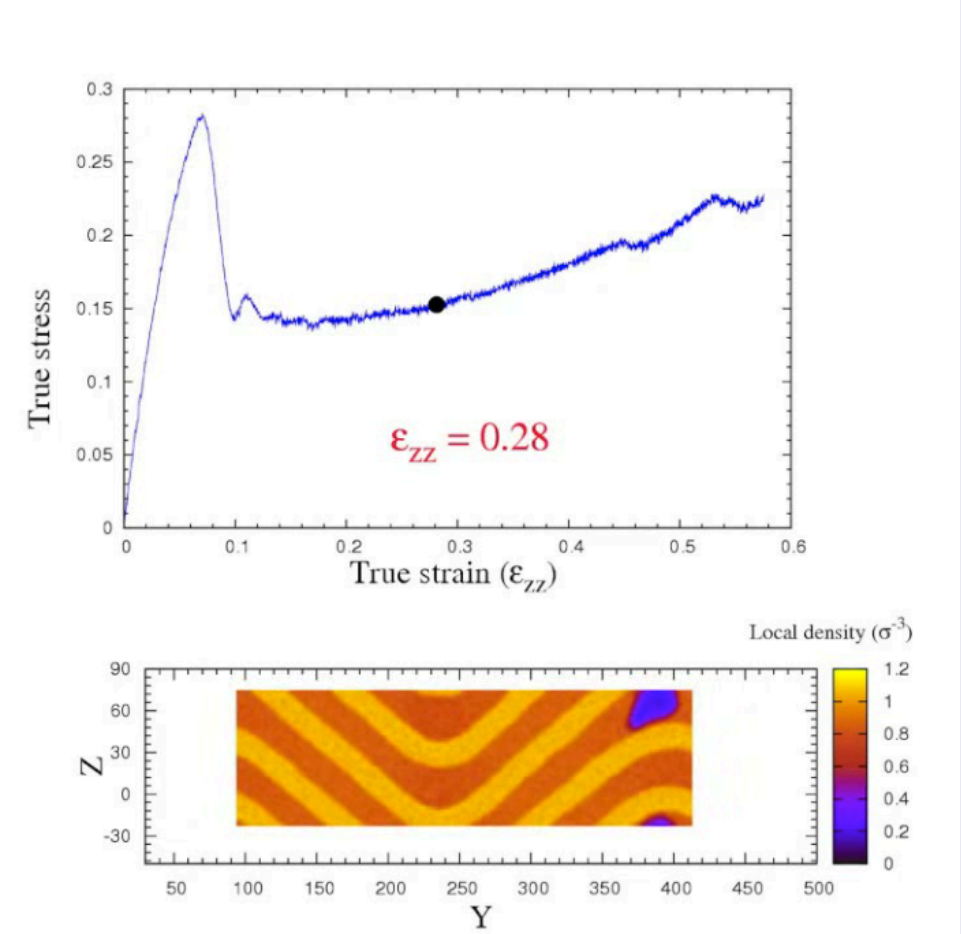
Tensile test

Perpendicular to lamellae



Tensile test

Perpendicular to lamellae



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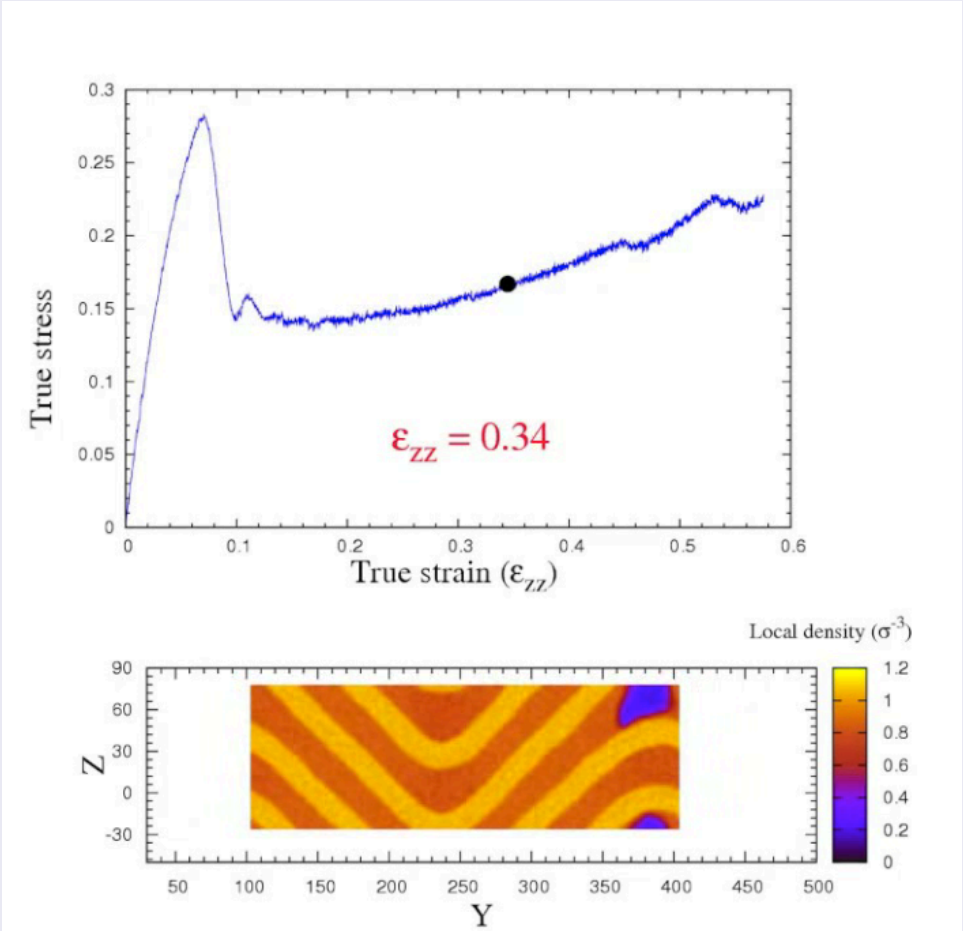
Perpendicular to lamellae



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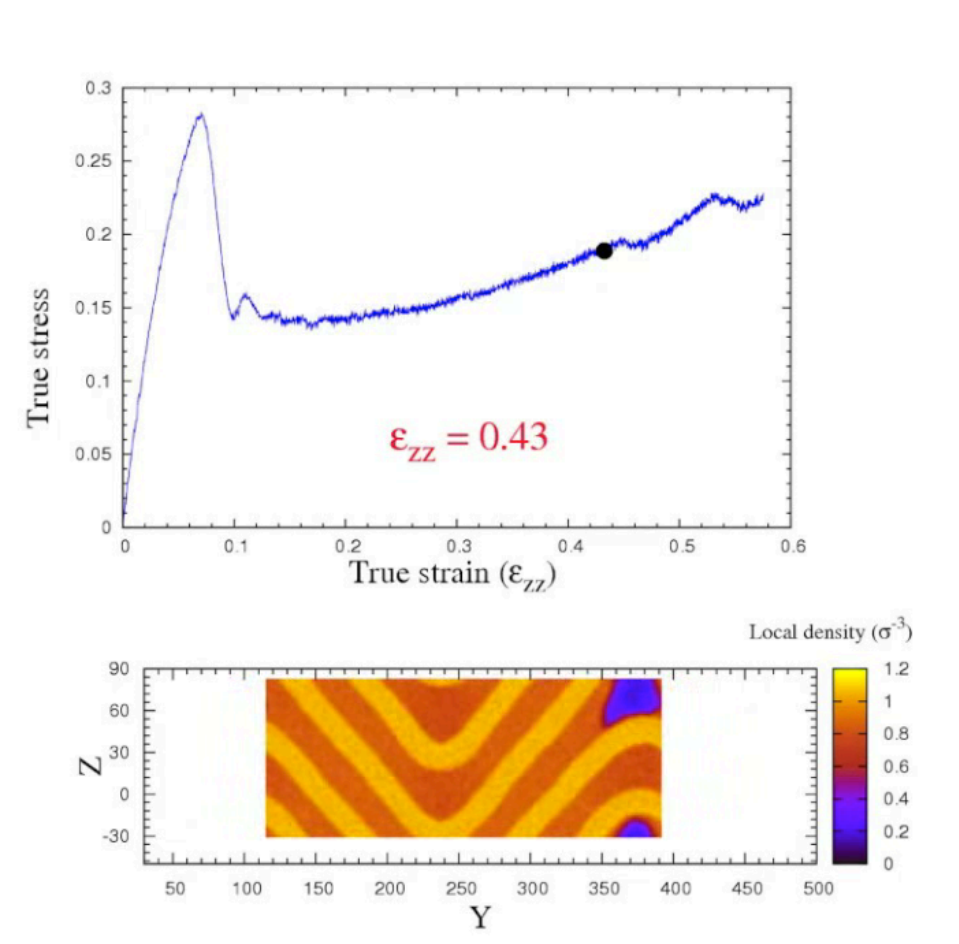
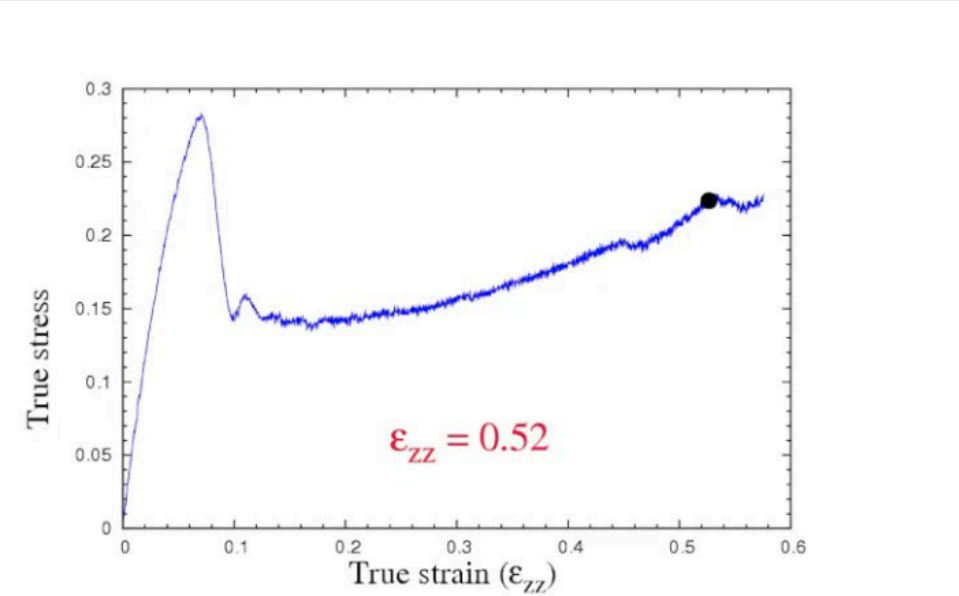


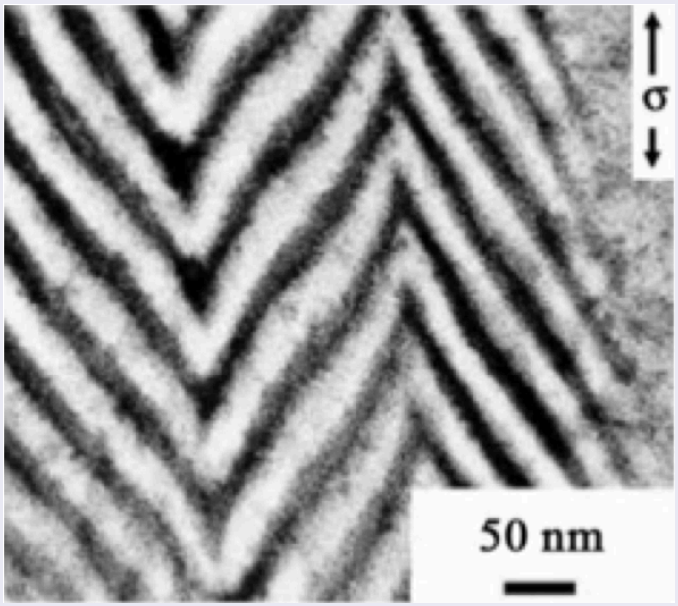
Tensile test

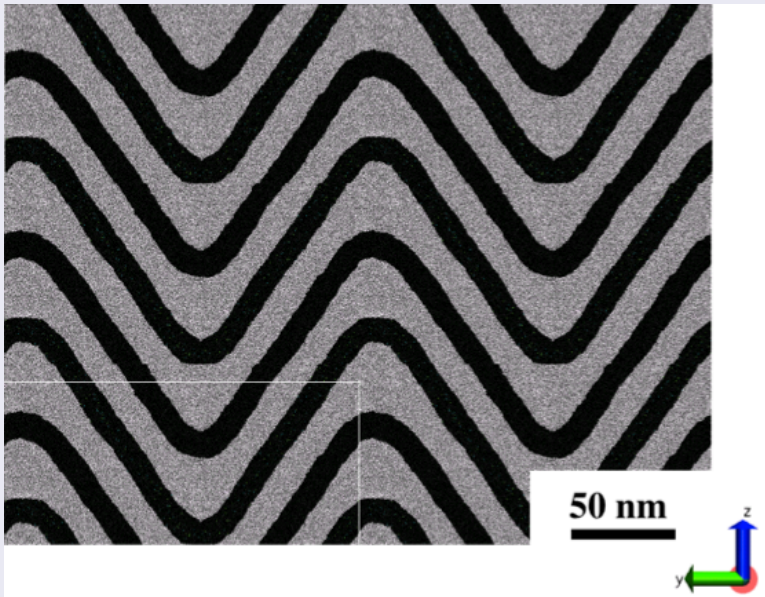
Perpendicular to lamellae



Problem solved !

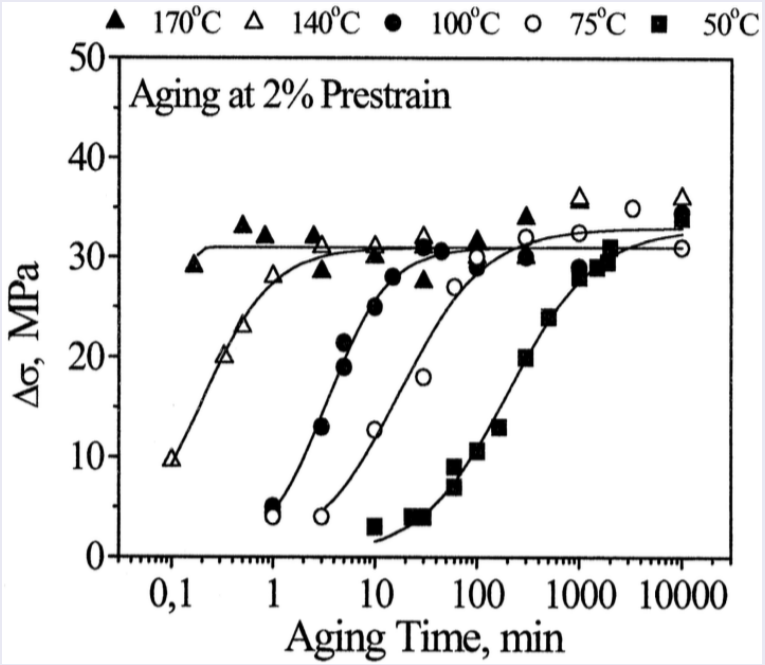
Experiment *vs* simulations

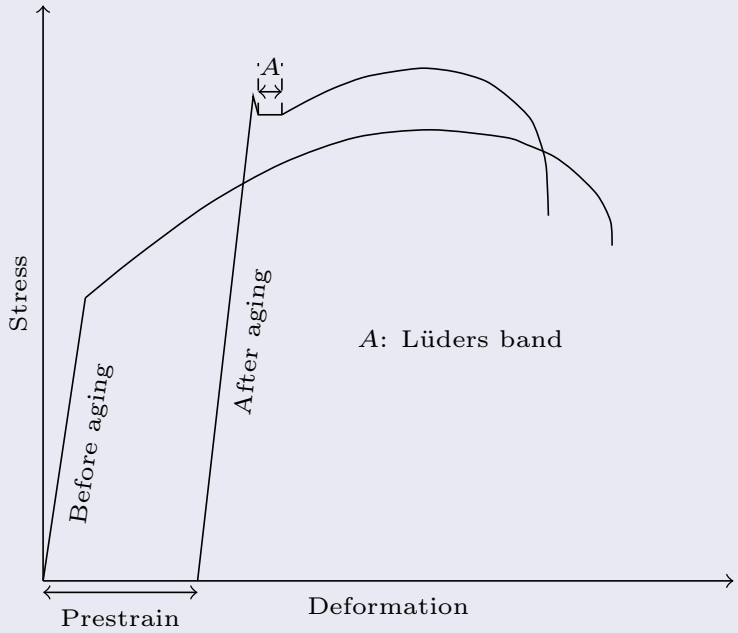




- Buckling phenomena reproduced
- Due to mechanical coupling between hard and soft phases

Ageing in steels





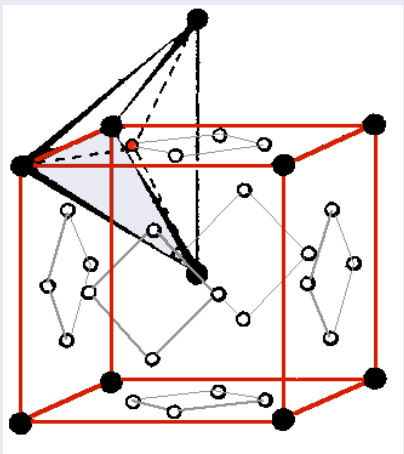
[De *et al*, *Scripta Mater.* **41** (1999)]

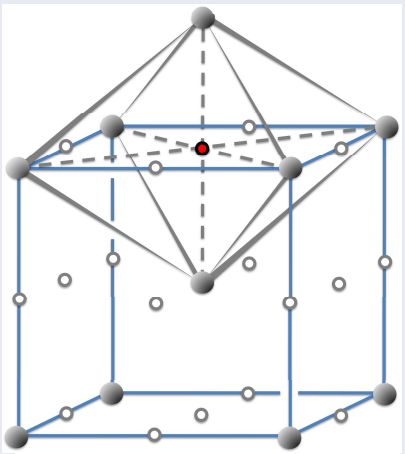
- Higher yield stress
- Higher brittle/ductile transition temperature
- Lüddering

A Fe-C interatomic potential

From *ab-Initio* modelling

- Goal: Fe-C interaction potential for Molecular Dynamics
- Two reference configurations:
  - C in octahedral and tetrahedral sites





- Correct energy barrier for diffusion: 0.815 eV

A Fe-C interatomic potential

From *ab-Initio* modelling

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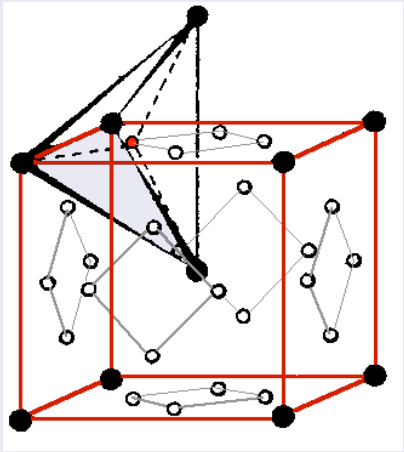
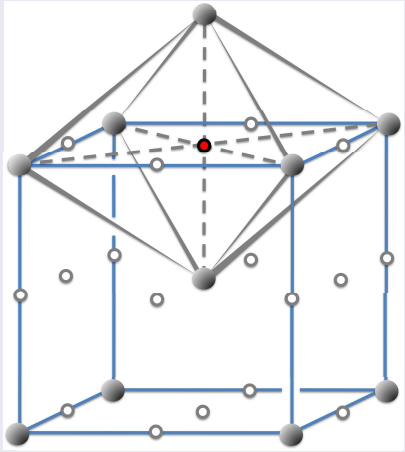
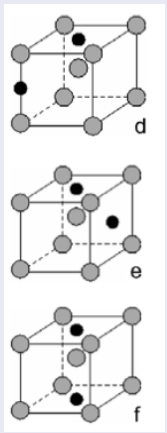
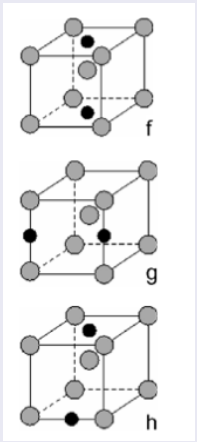








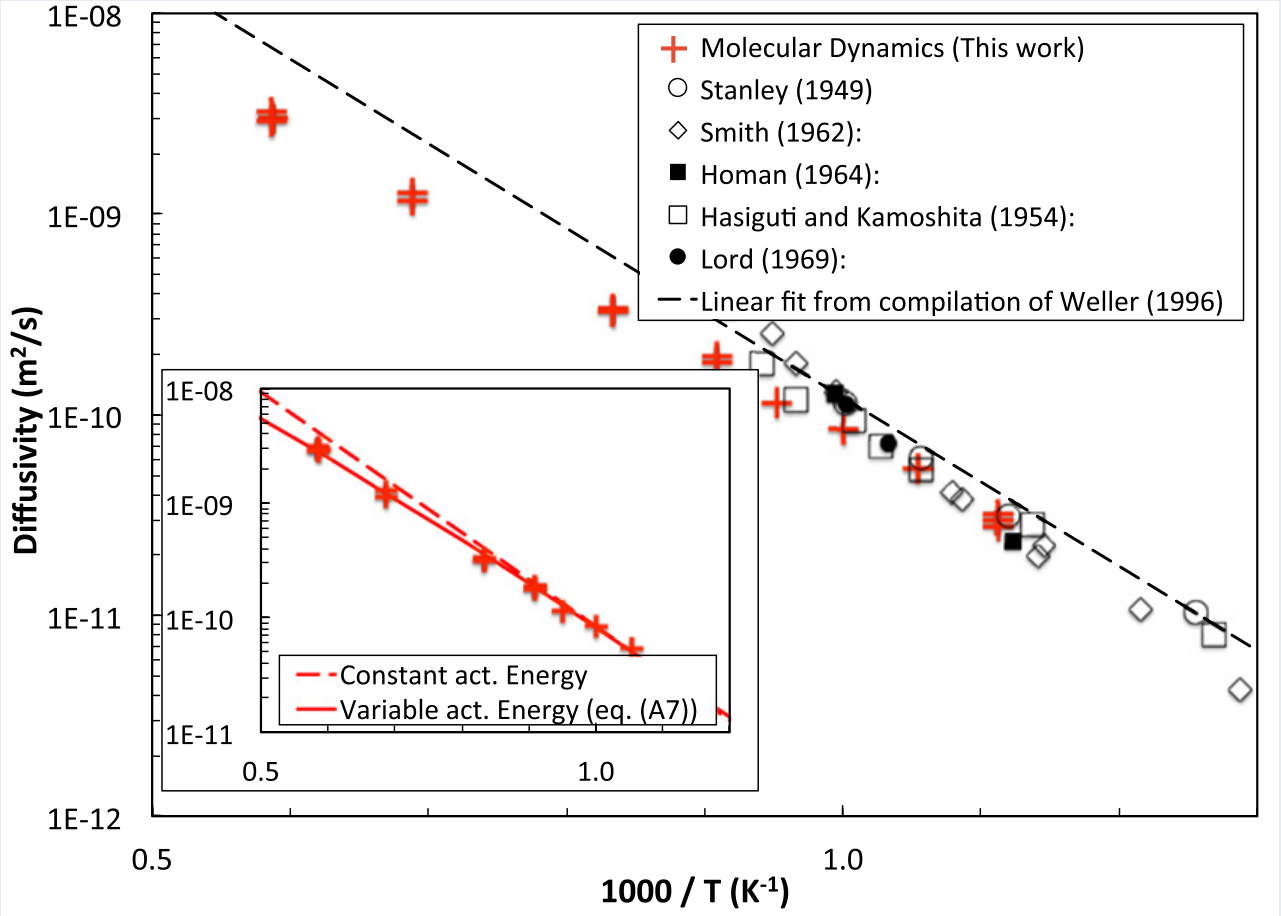
- Correct energy barrier for diffusion: 0.815 eV
- Test on many configurations (C, Fe, Va)

Tabulated potential for Mol. Dyn. and Monte-Carlo

[Becquart *el al*, *Comp. Mat. Sc.* **40** (2007)]

C diffusion in pure Fe

MD results

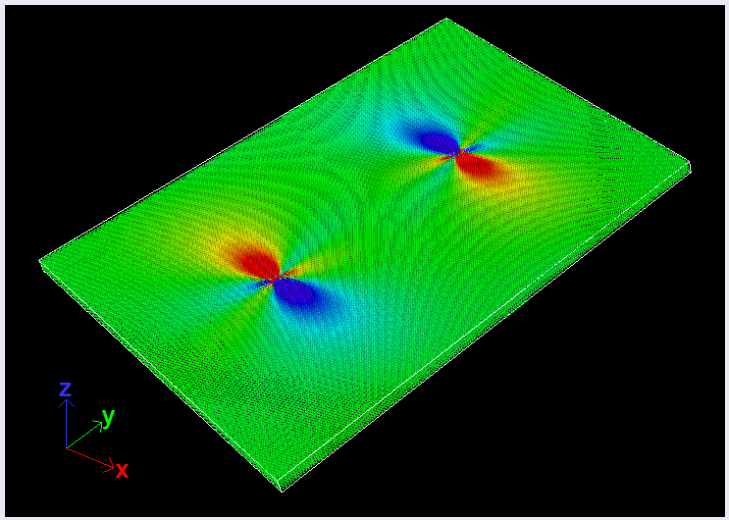


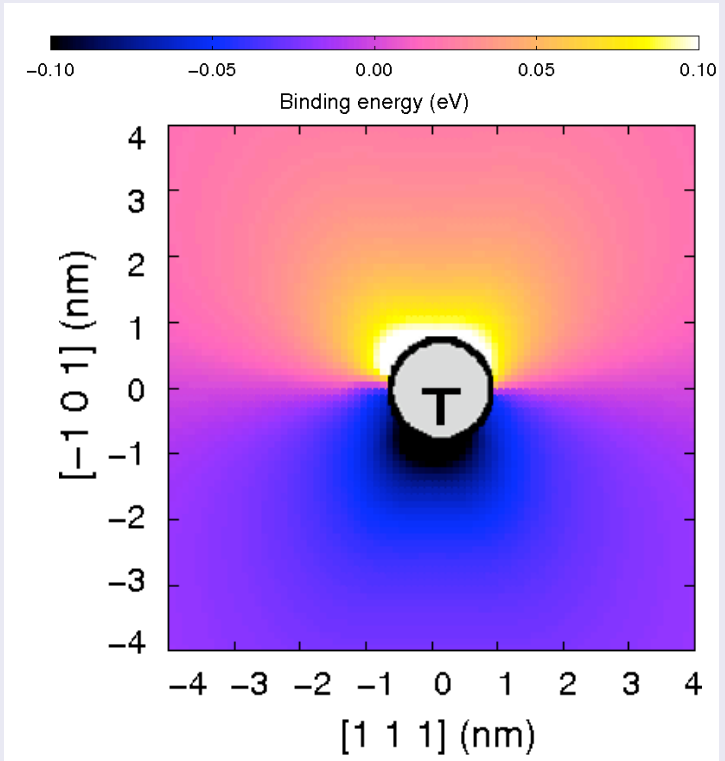
- Not following experiments...
- ... but we understand MD non linearity!

Fe, C and dislocations

Binding energy of C around dislocation core

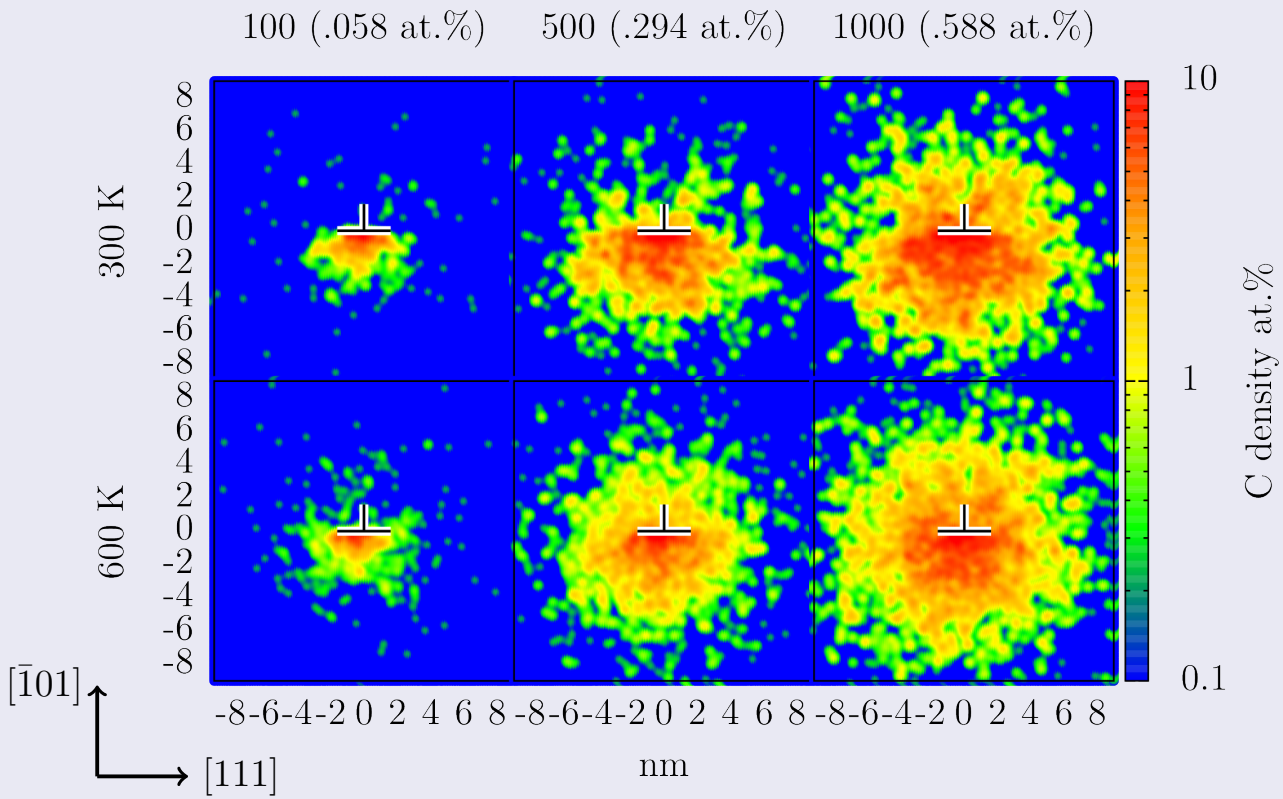
[Veiga, *PhD* **INSA-Lyon** (2011)]





Metropolis Monte-Carlo

Equilibrium Cottrell atmospheres (from different C levels)

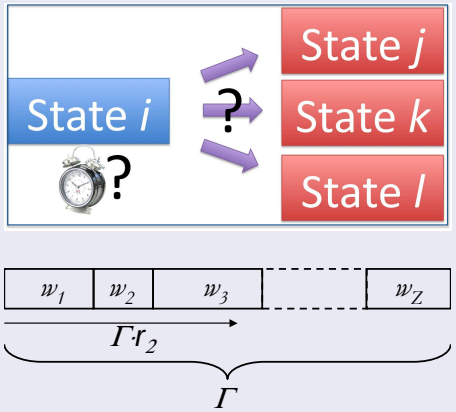


[Waseda *et al*, *Scripta Mater.* **129** (2016)]

- ≈150 C atoms per nm (same as measured with TAP)
- Max. C concentration: 8.8% (TAP: 8%)

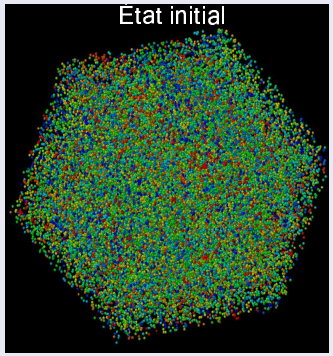
Kinetic Monte-Carlo

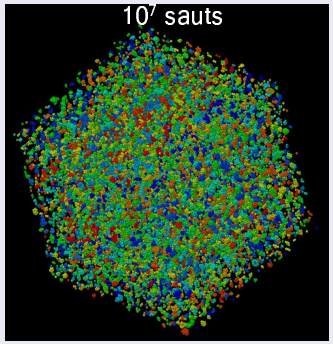
Principle

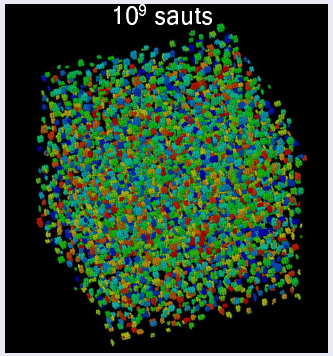


- Transition frequency from $i \rightarrow j$:
  $w_j^i = w_0 \exp\left(\frac{-\Delta E_{ij}}{kT}\right)$ $w_0 \approx 10^{14}$ Hz
- Residence time i
  
  $r_1 \rightarrow \tau_R = -\frac{\ln r_1}{\sum_j w_j}$
- Choice of a particular transition  r_2

Example: precipitation from a supersaturated solid solution



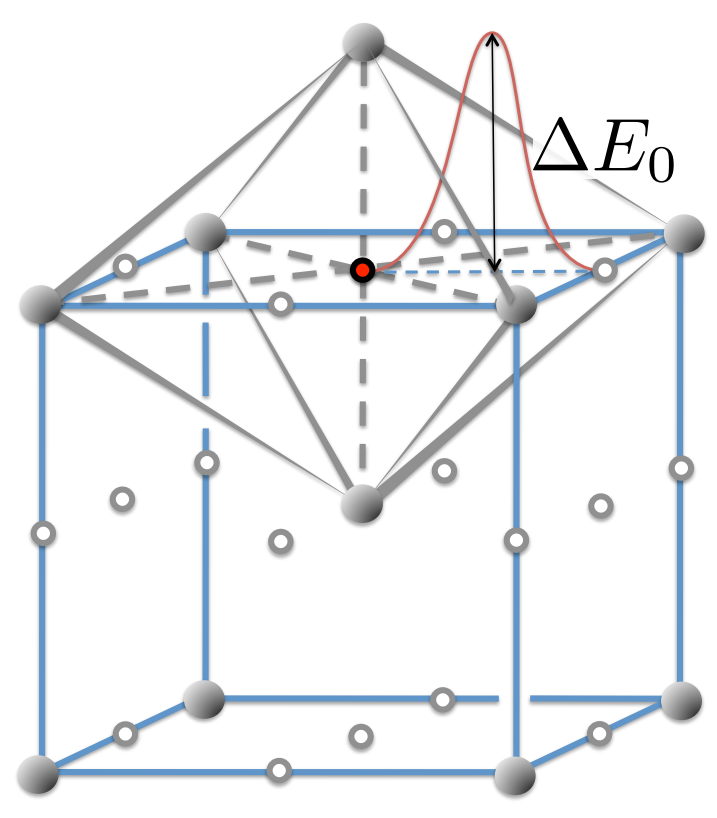


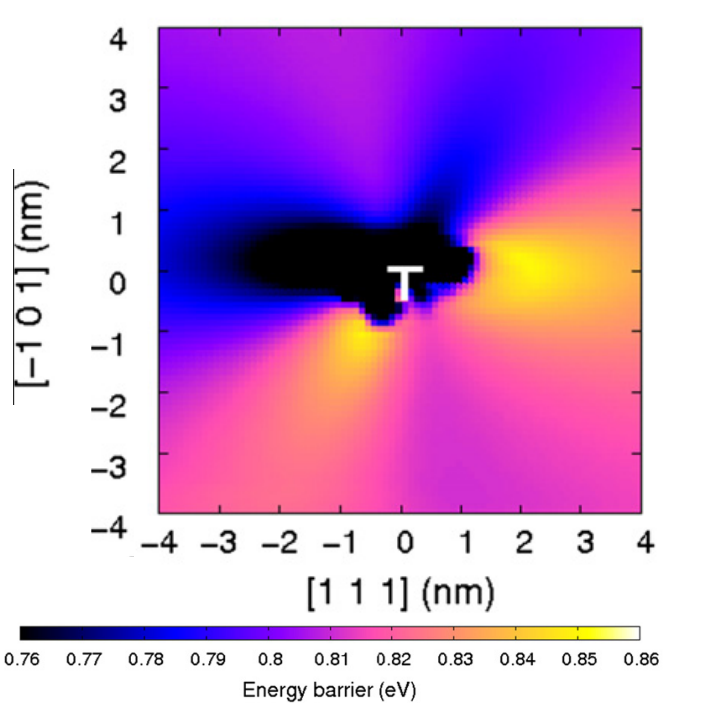


Brute force

Migration energy of C around dislocation core

[Veiga *et al*, *Acta Mater.* **59** (2011)]

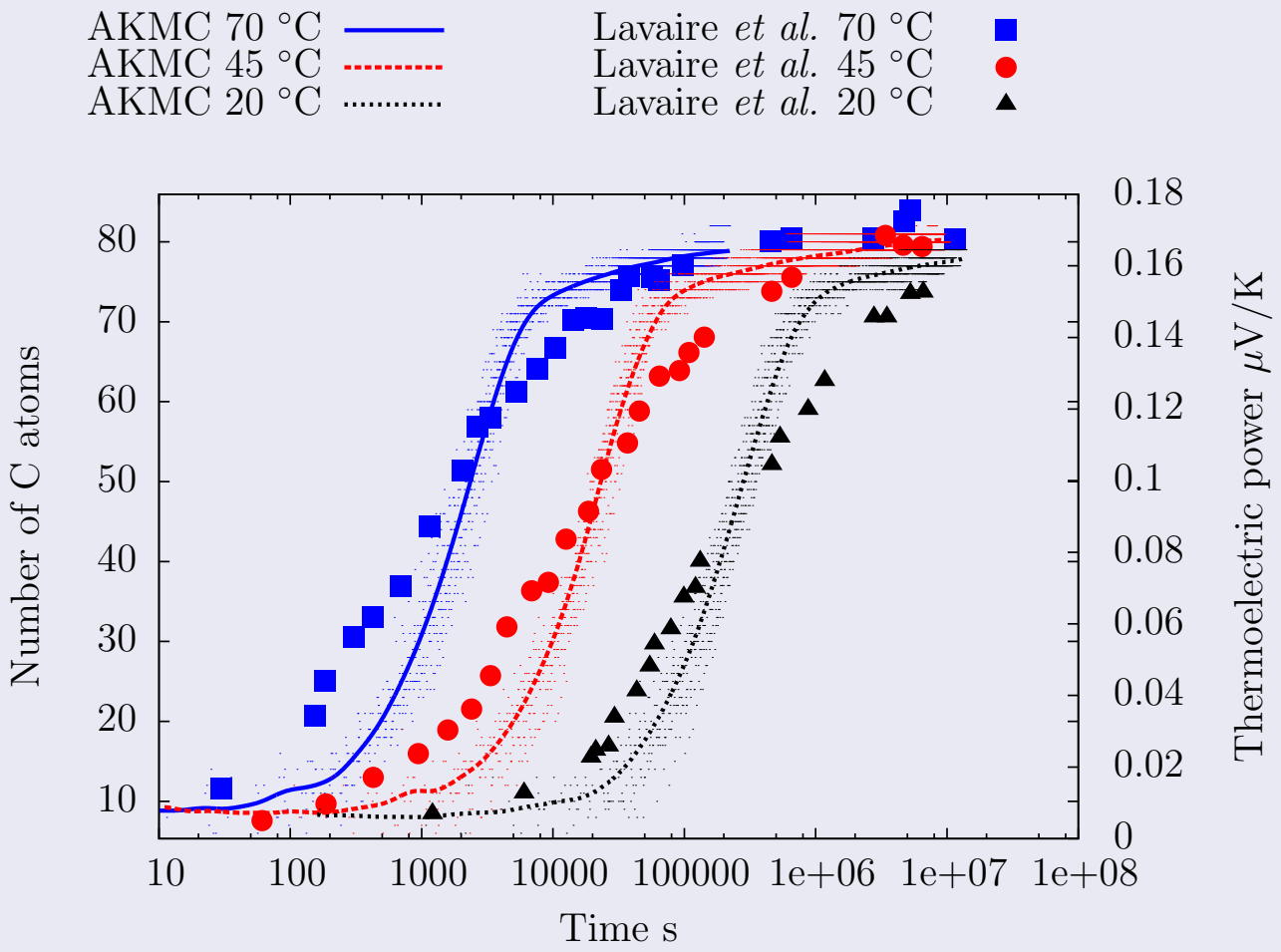




- All saddle point energy for all possible transition around a dislocation !

Kinetic Monte-Carlo

Formation kinetics: AKMC *vs* ThermoElectric Power



- Same kinetics **without any adjustable parameter**

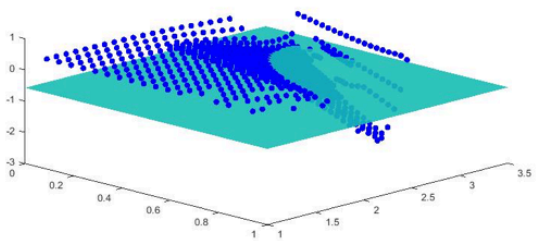
And now... carbides !

Needs for stronger C-C interactions

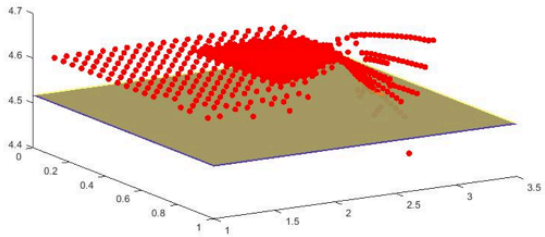
Initial Screening of $\varepsilon = 0 - 1$ & $\sigma = 1 - 3.5$

$$V_{LJ} = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right.$$

ΔEc



a



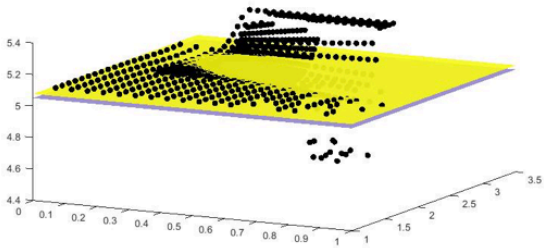
THÈSE DE DOCTORAT
Spécialité: Physique
École Doctorale de Physique d'Ile-de-France (n° 564)

présentée par
Thomas Schuler

pour l'obtention du grade de
DOCTEUR DE L'UNIVERSITÉ PARIS SUD XI

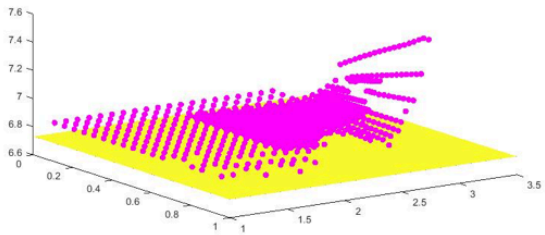
Influence des amas lacunes - solutés sur le vieillissement des solutions solides de Fer-α

b



$$\Delta E_C(\alpha - \mathrm{Fe/Fe_3C}) = 0.57 + 1.47 k_B T$$

c



- to be continued...

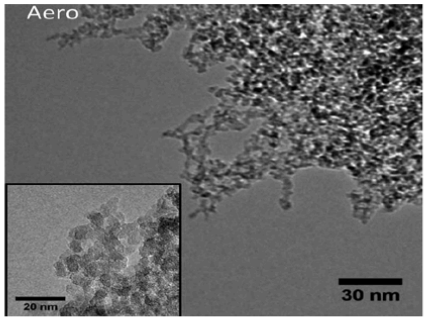
Silica Aerogel

Amazing thermal properties

- But poor (and not understood) **mechanical properties**

Molecular dynamics on large volume

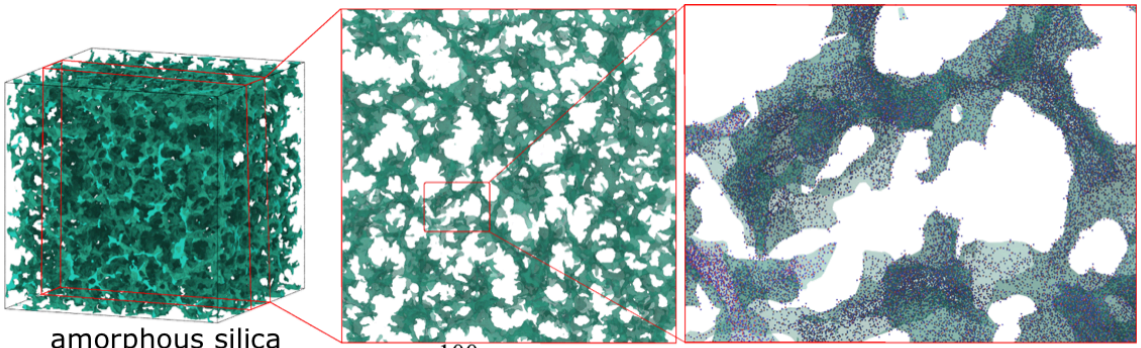
Need for a new potential



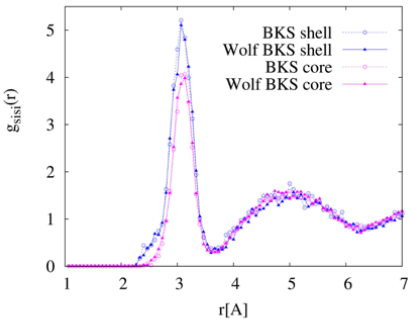
nano-particles ~ 3 nm

Typical pore size: 10 nm

Simulation box size for mechanics > ?



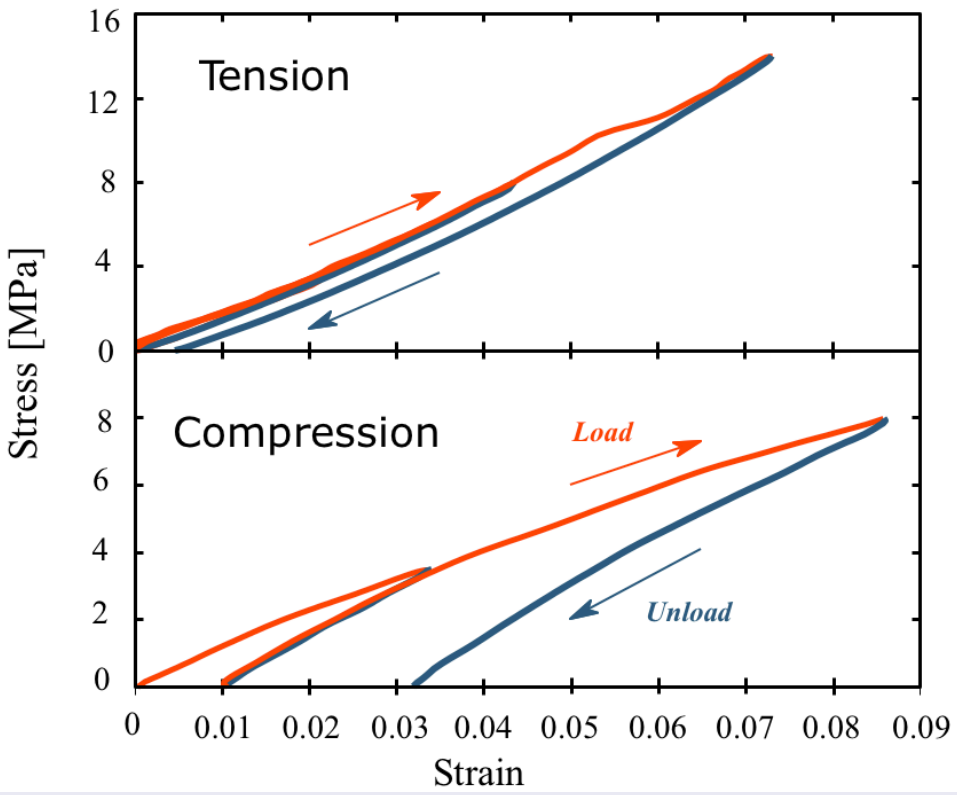
amorphous silica areogel



- 7 million atoms !
- [Goncalves *et al*, *J. Non. Cryst. Sol.* (2016)]

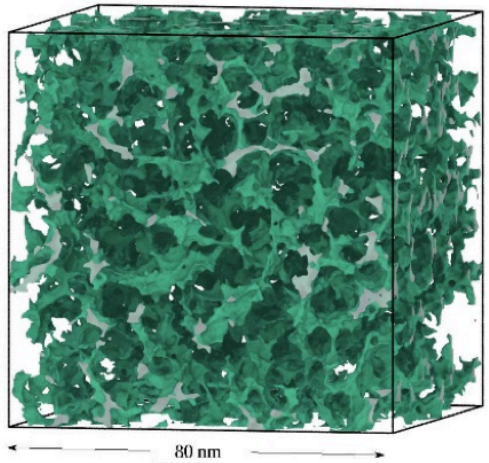
Molecular dynamics on large volume

Tensile test



ligament buckling ?

capillary effects ?



- Capillarity effects
- [Goncalves *et al*, *Acta Mater.* (2018)]

Conclusions

Take home messages

- LAMMPS is great !
- Strong need to develop new potentials
- LAMMPS as a library is convenient (but not fast !)
- Need for a place to publish/share new fixes

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