Deformation of mantle minerals

Patrick Cordier

Mineral Physics Gourp
Unité Matériaux et Transformations
UMR 8207 - Université Lille 1 - CNRS

Structure and Dynamics of the Earth's Deep Mantle
November 13th and 14th, 2012

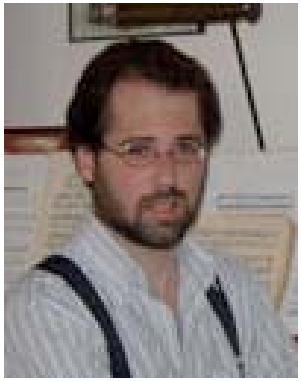
Funding: *ERC advanced grant n°290424*
Multiscale Modeling of the Rheology of the Mantle (RheoMan)

Deformation of mantle minerals


Ph. Carrez


K. Gouriet


A. Kraych


S. Ritterbex


P. Hirel

RheoMan

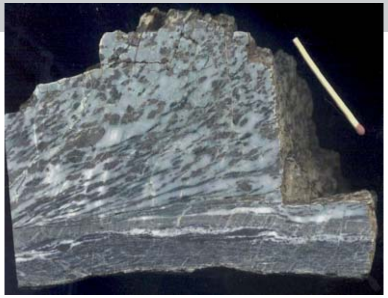
European Research Council

Funding: *ERC advanced grant n°290424*
Multiscale Modeling of the Rheology of the Mantle (RheoMan)

Convection in a solid mantle

$$\dot{\varepsilon} = 10^{-15} s^{-1}$$

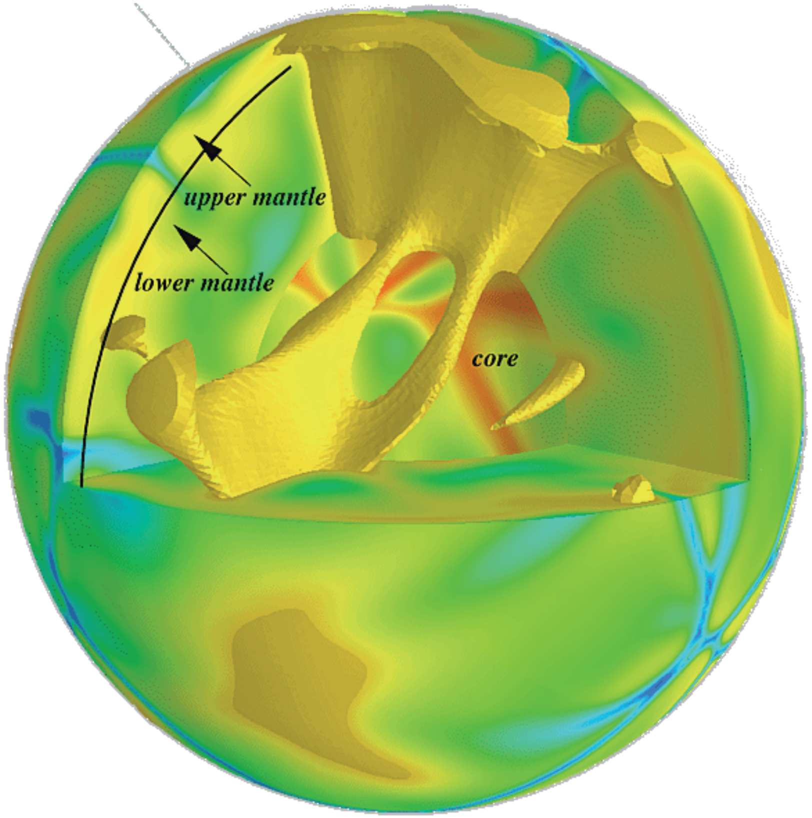
$$\text{Mantle: rocks}$$



$$5 \ km < \text{Depth} < 2900 \ km$$

$$\eta = 10^{22} Pa.s$$

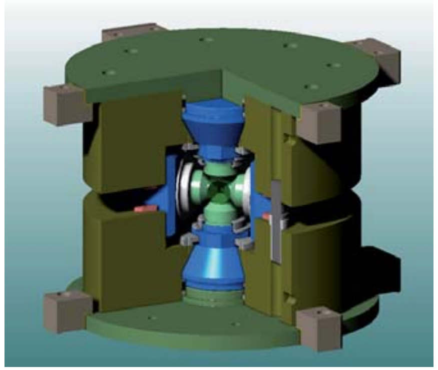
$$\sigma = 10 \ MPa$$



$$10 \ GPa < P < 130 \ GPa$$

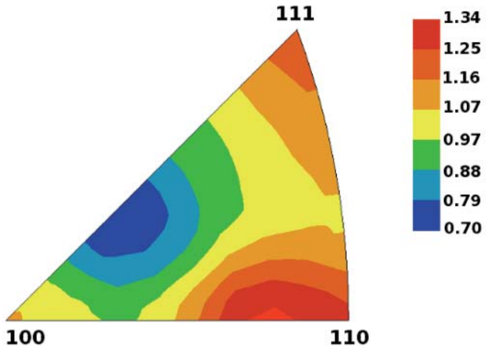
$$1000 \ K < T < 3000 \ K$$

Deformation of mantle minerals



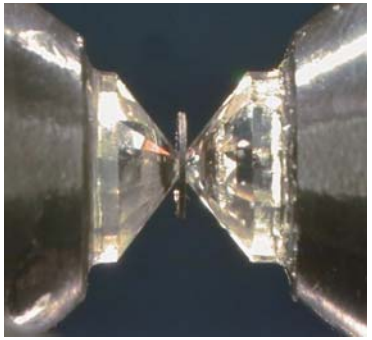
Y. Wang, W. Durham, Y. Getting and D. Weidner (2003)

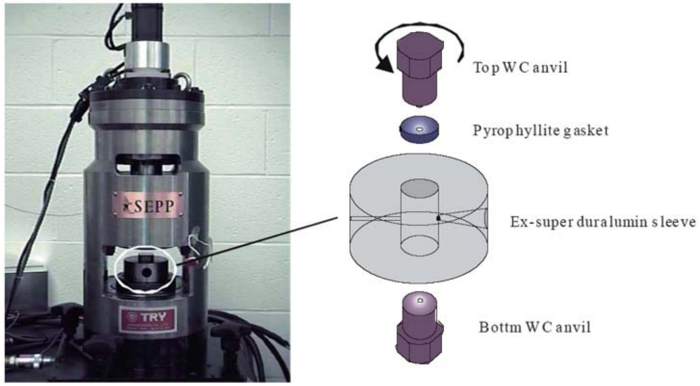
The experimental Approach:



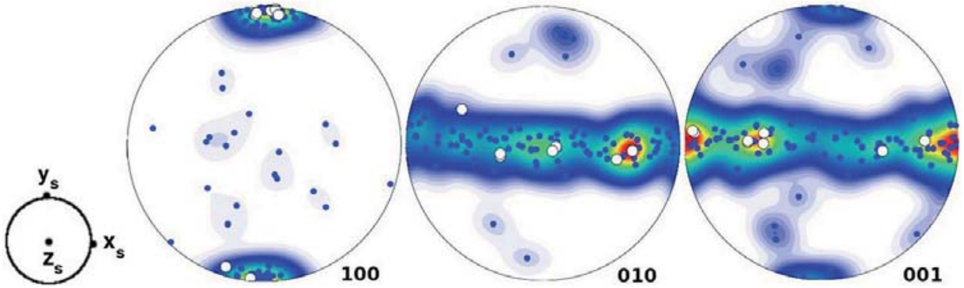
FCC iron 16.5 Gpa – 976 K
Courtesy S. Merkel

Ringwoodite 22 GPa



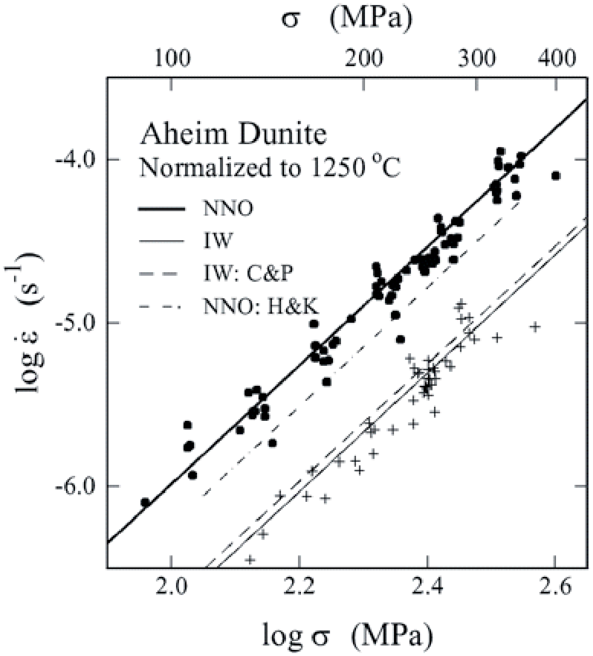


Yamasaki & Karato (2001)

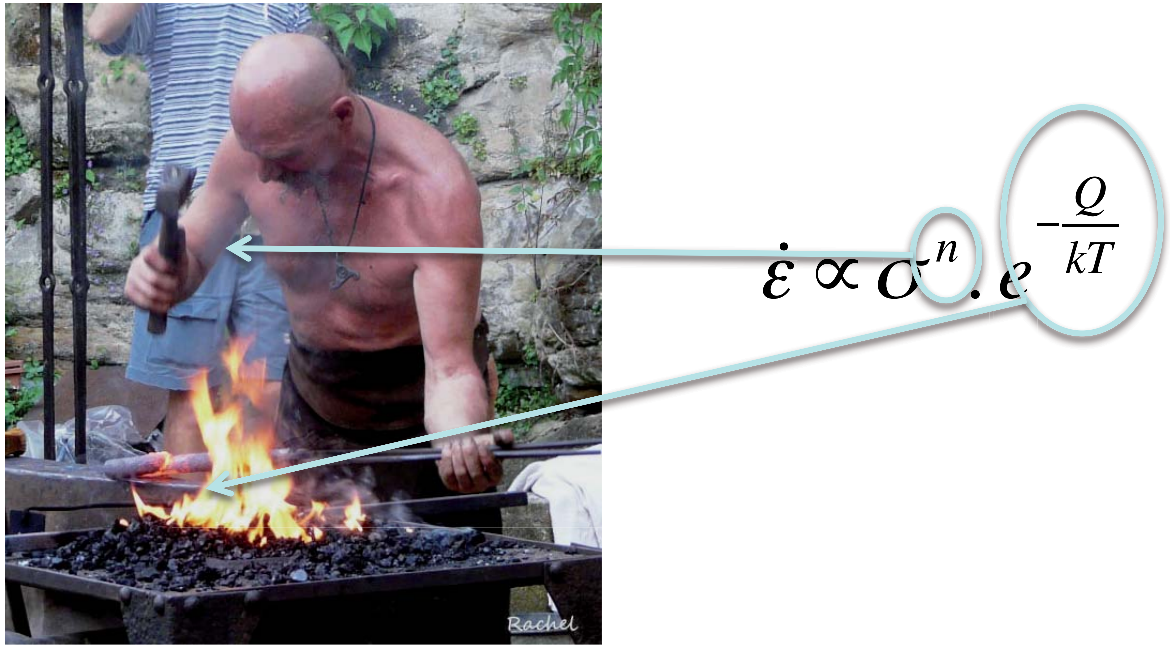


$MgGeO_3$ post-perovskite at 90 GPa – Nisr et al (2012)

The empirical approach



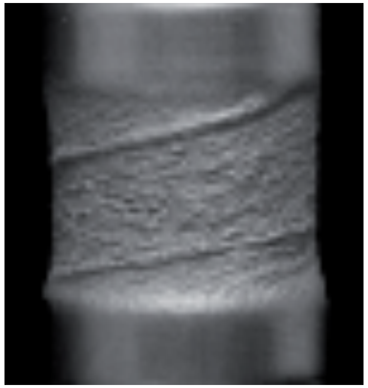
Mackwell, 2008



$$\dot{\varepsilon} \propto \sigma^{n} . e^{-\frac{Q}{kT}}$$

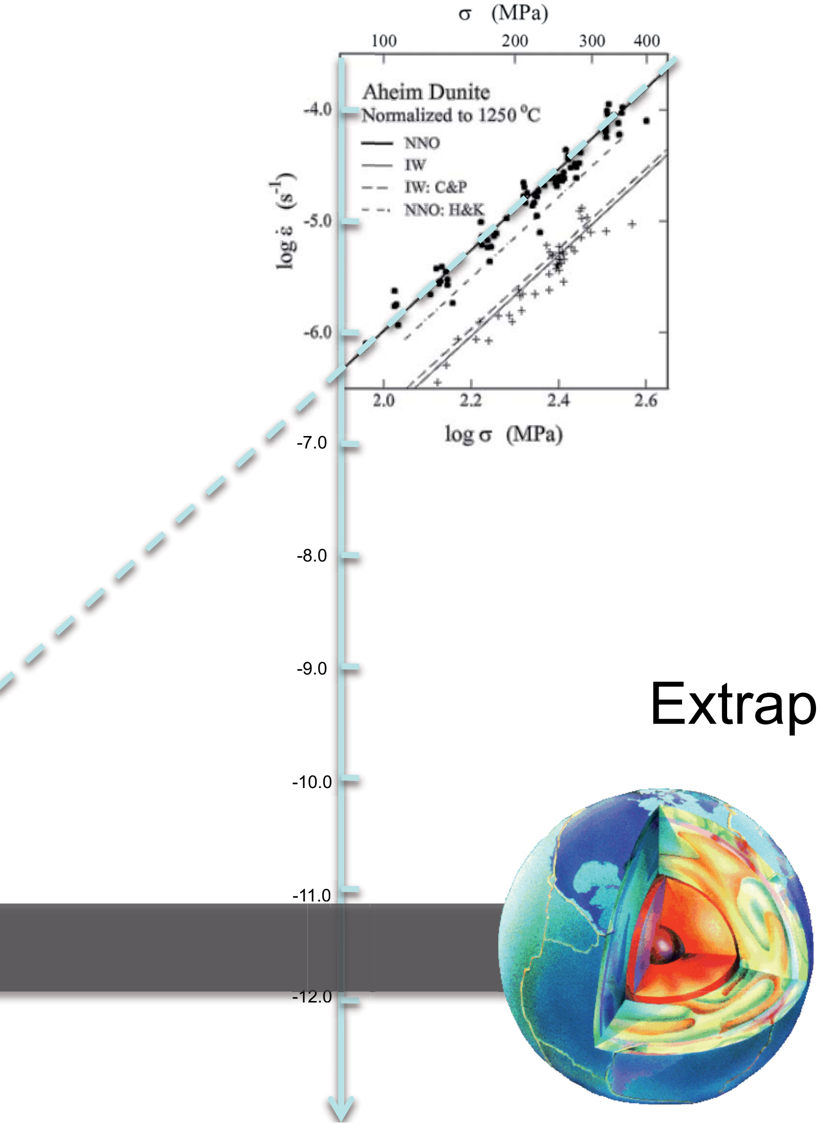
The empirical approach

Experiments



Phenomenological laws

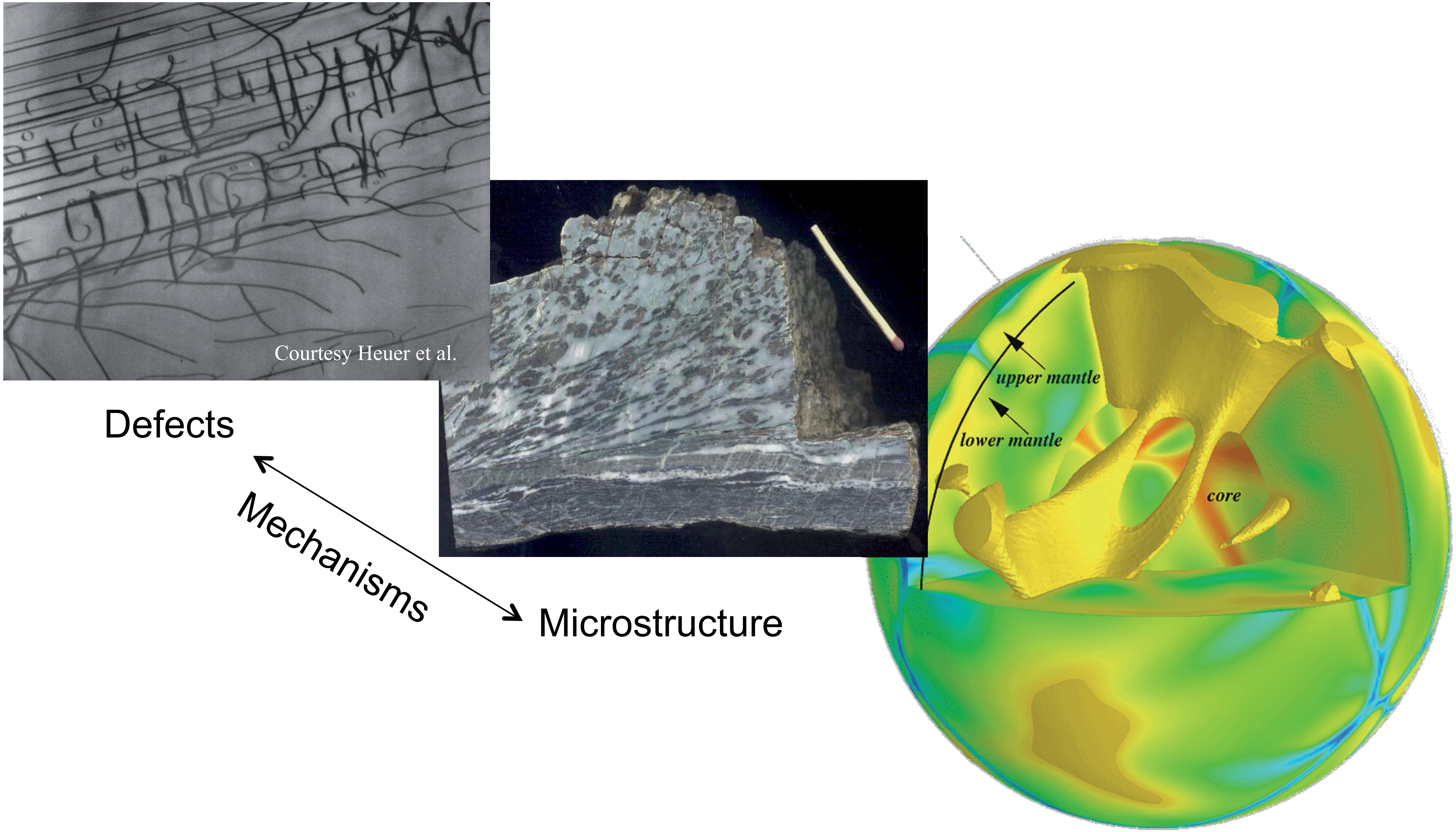
$$\dot{\varepsilon} = \dot{\varepsilon}_0 \sigma^n f_{O_2}^m \exp\left(-\frac{Q}{RT}\right)$$



Extrapolation to natural conditions

Also need to take high-pressure into account...

Behind mantle convection:
the physics of solid-state flow



Courtesy Heuer et al.

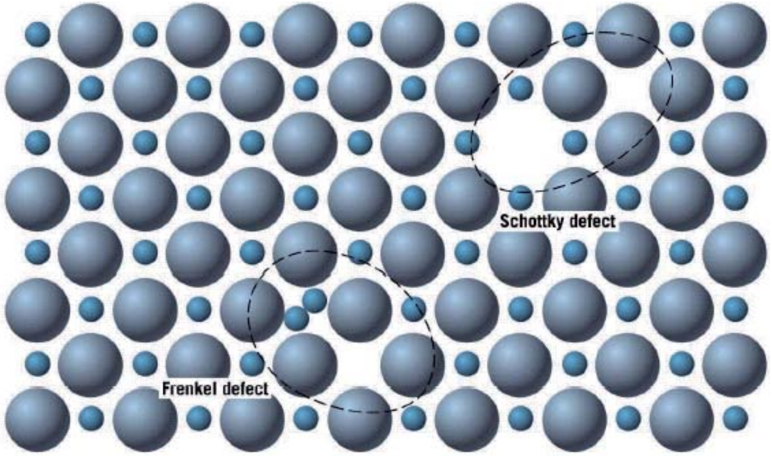
Defects

Mechanisms

Microstructure

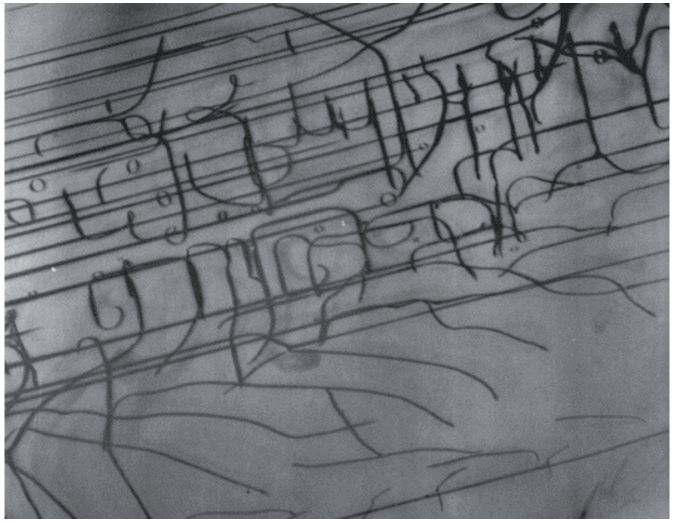
Behind mantle convection:
the physics of solid-state flow

- Transport of matter



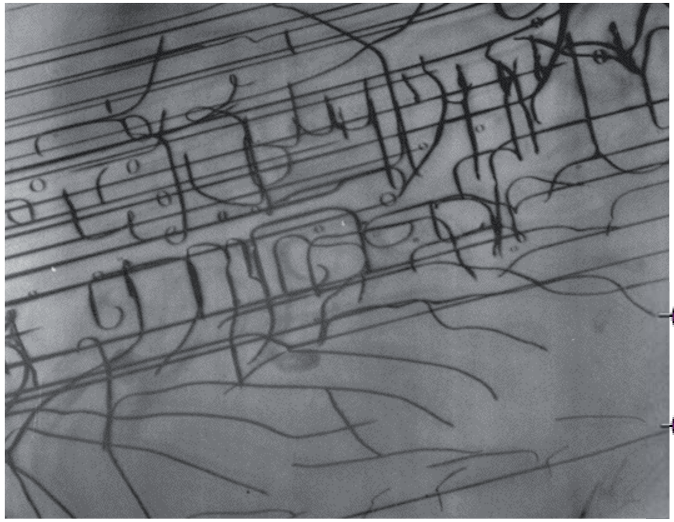
  - Atomic diffusion
  - Point defects

- Transport of shear

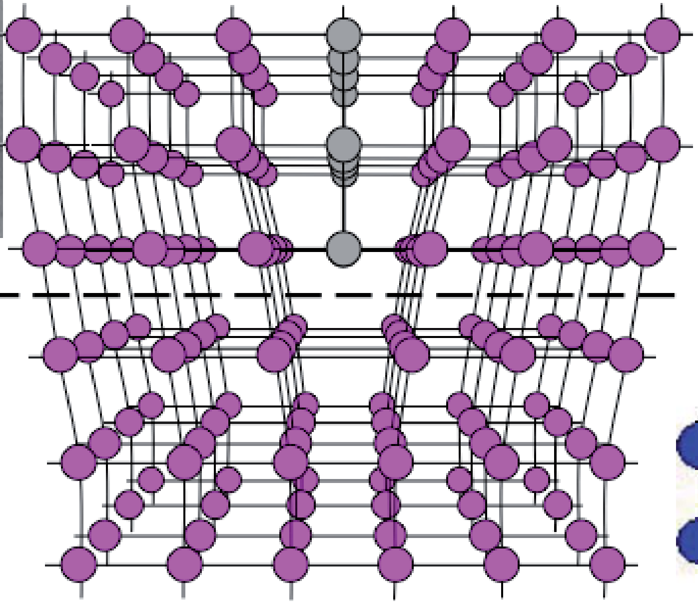


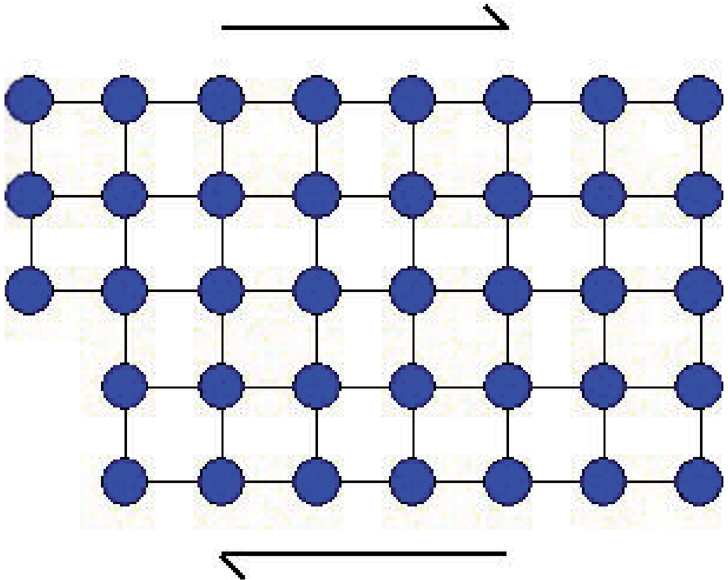
  - Dislocations

Behind mantle convection:
crystal defects: dislocations



Courtesy Heuer et al.





Goals

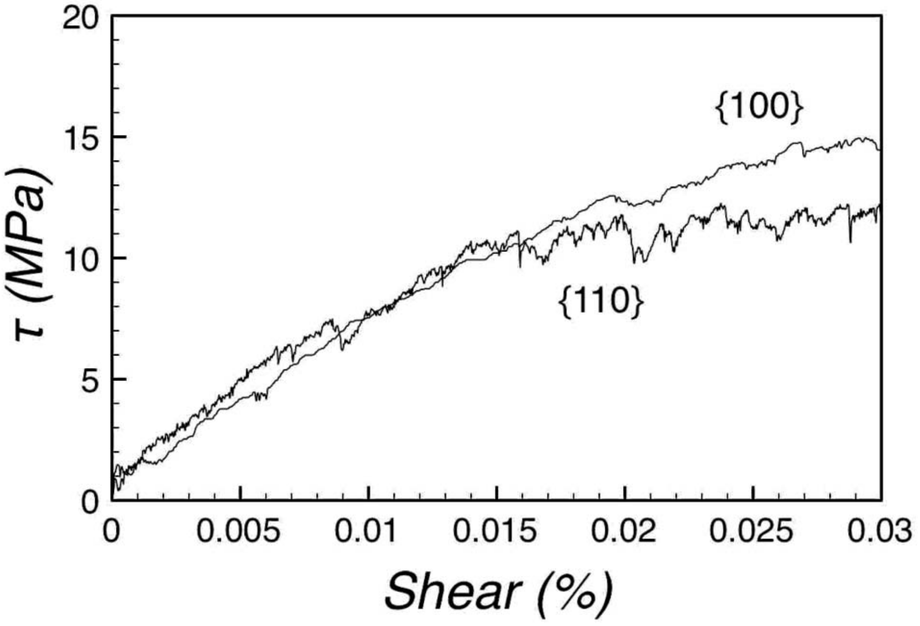
- Addressing the rheology of mantle minerals by numerical modeling and based on the physics of plastic deformation

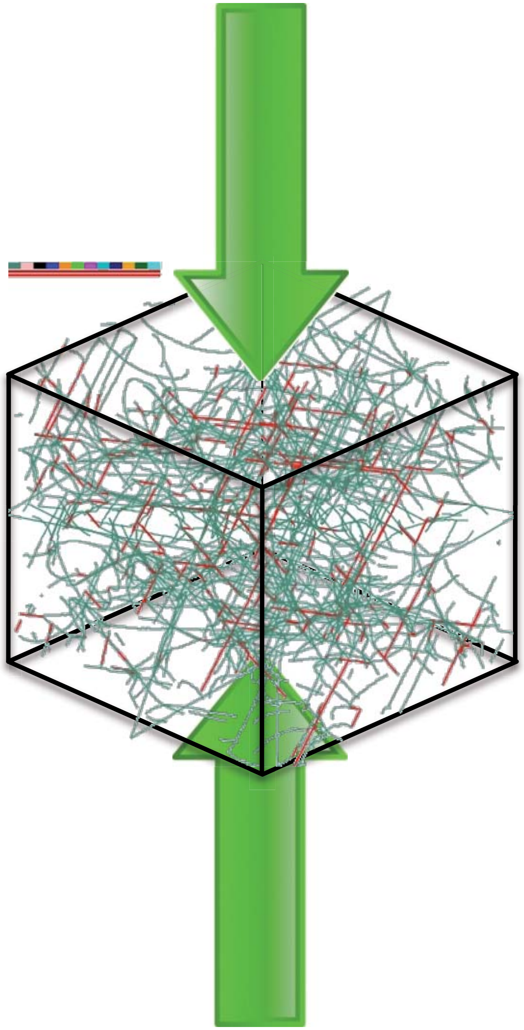
- Intrinsic flow properties

(influence of impurities (water), grain boundaries, secondary phase, melt, … will come later)

- Taking into account the influence of:
  - Pressure
  - Temperature
  - Strain-rate

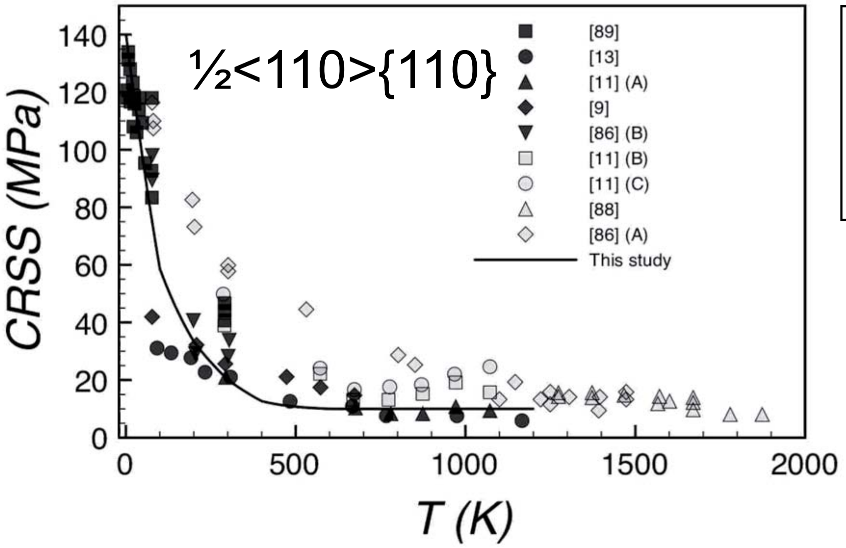
Numerical deformation experiments



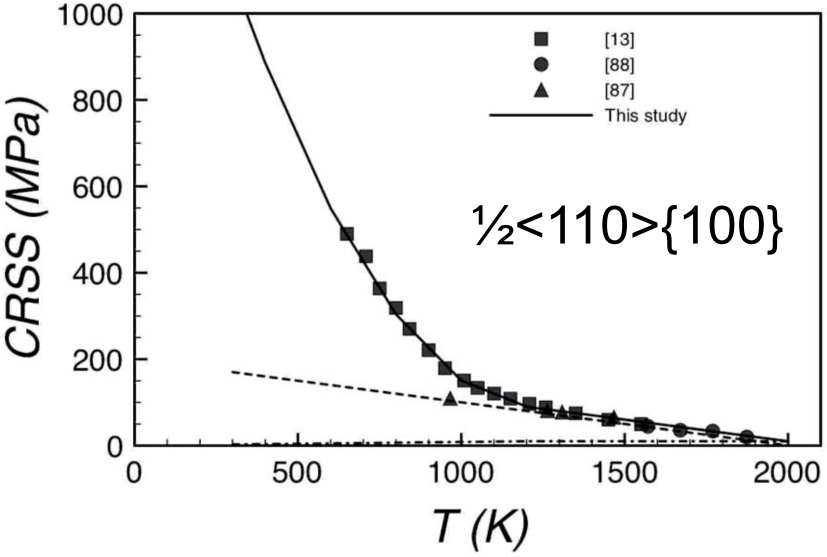


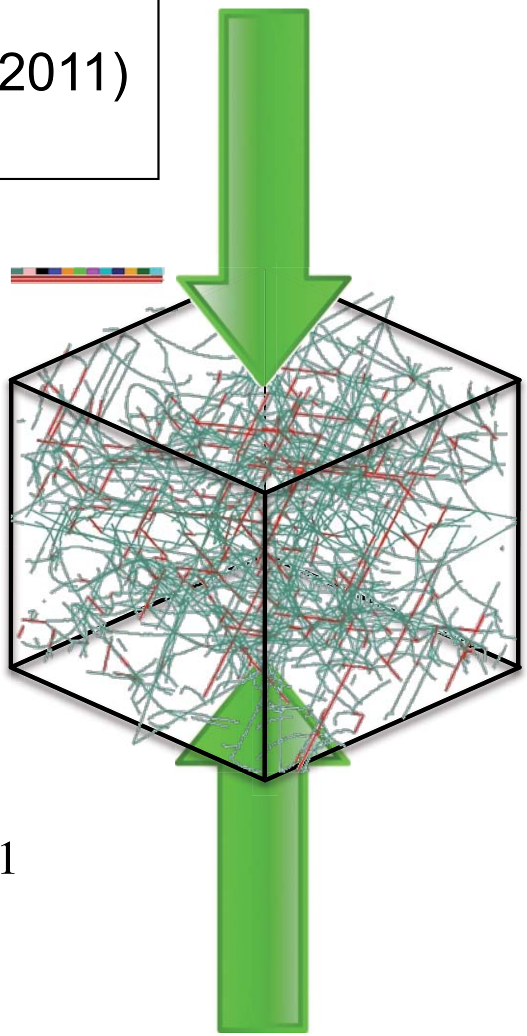
Modelling the intrinsic flow properties of a given phase under extreme pressure, temperature and strain-rate conditions

Proof of concept: Modelling MgO plasticity at ambiant P and laboratory strain-rates



Amodeo *et al.*
Acta Materialia (2011)
59, 2291–2301

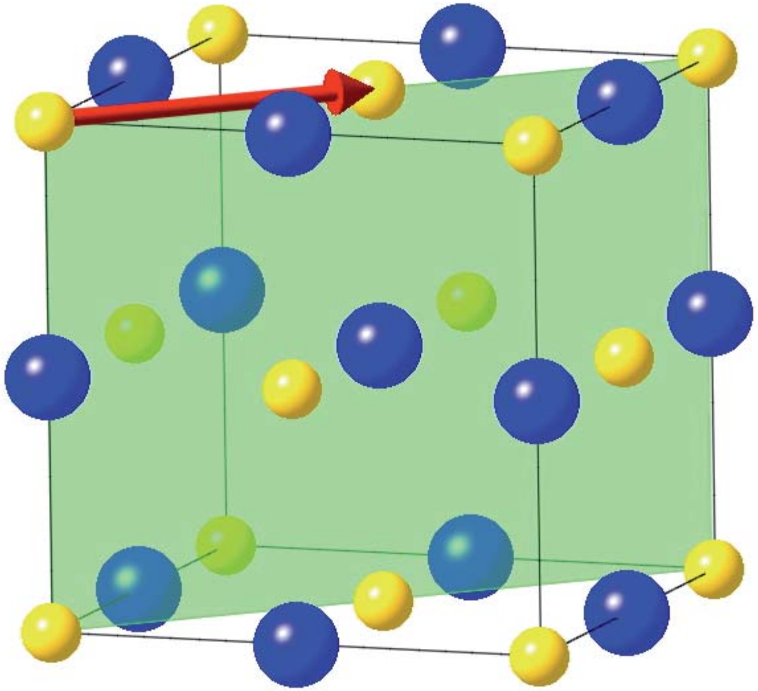




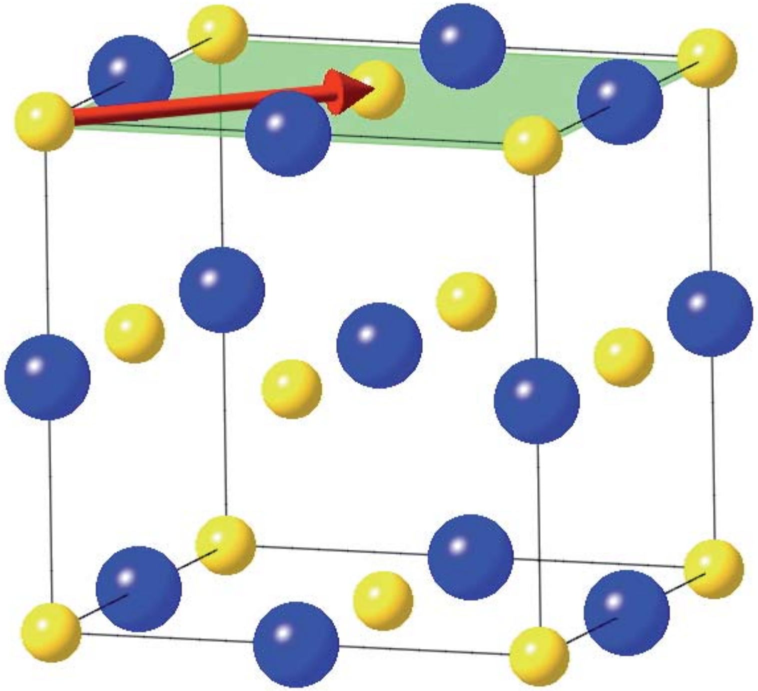
$$\dot{\varepsilon} = 10^{-4}\, s^{-1}$$

Slip systems in MgO

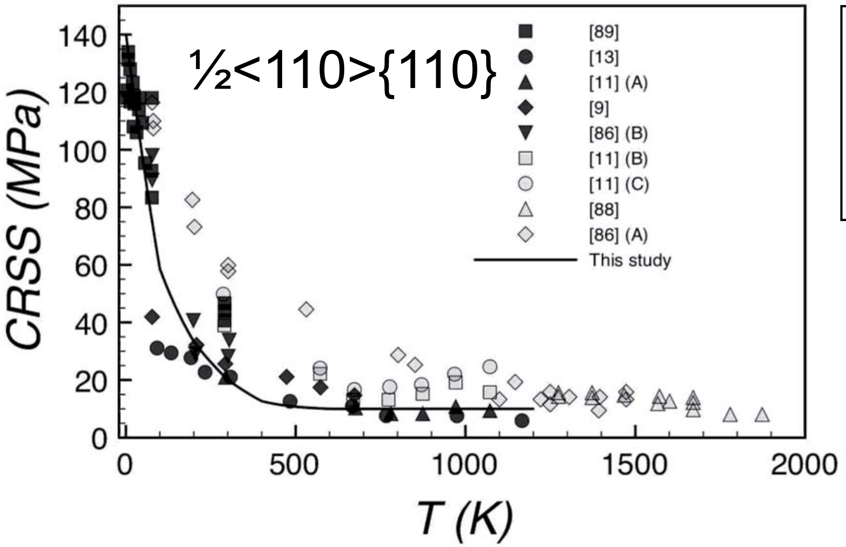
½<110>{110}



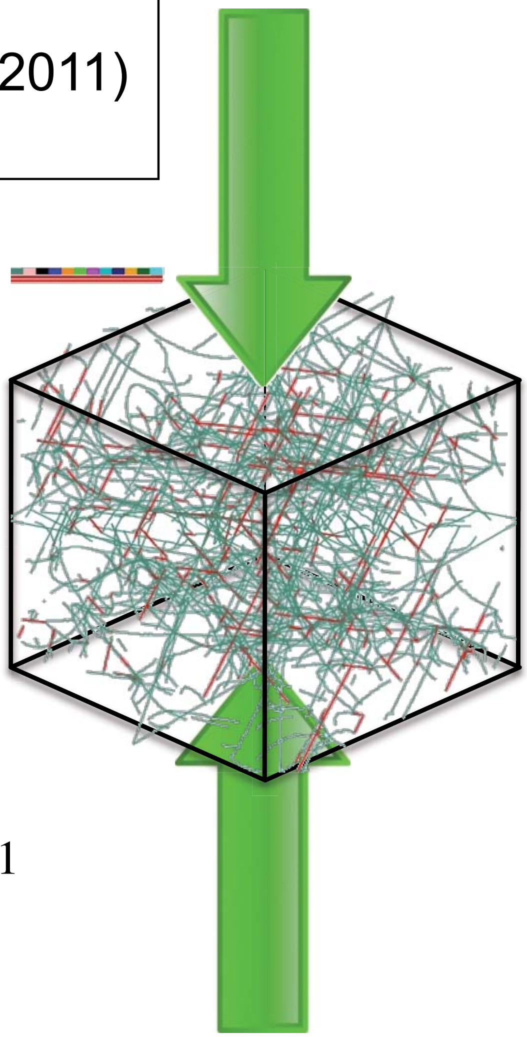
½<110>{100}

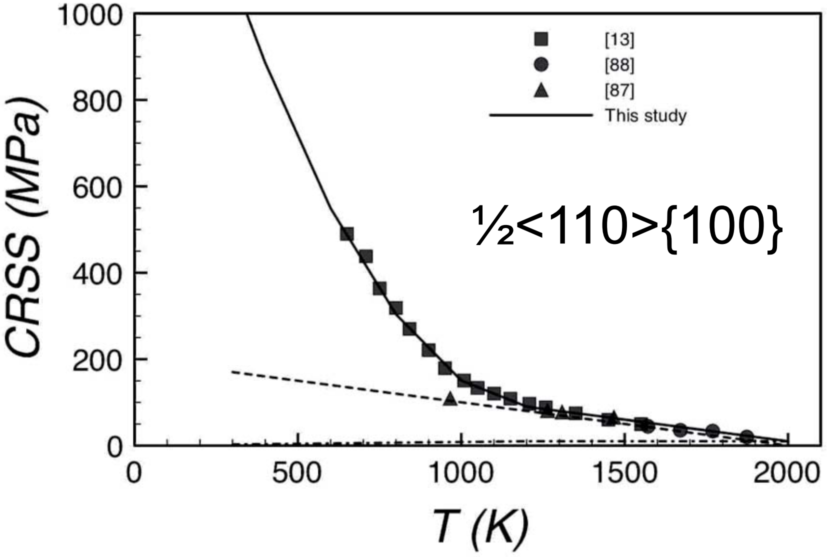


Proof of concept: Modelling MgO plasticity at ambiant P and laboratory strain-rates



Amodeo *et al.*
Acta Materialia (2011)
59, 2291–2301

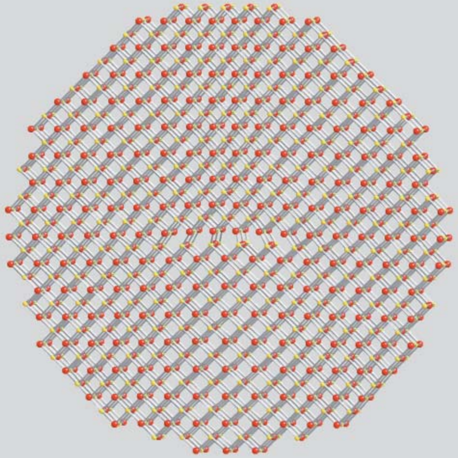




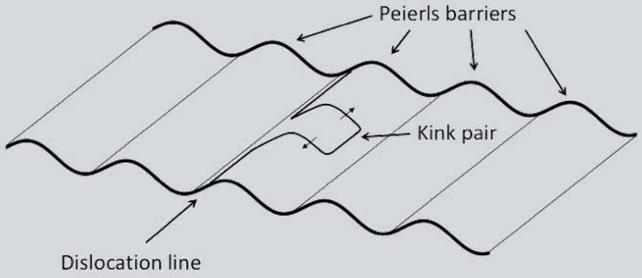
$$\dot{\varepsilon} = 10^{-4}\, s^{-1}$$

How do we do that ?

1. Modeling the defects

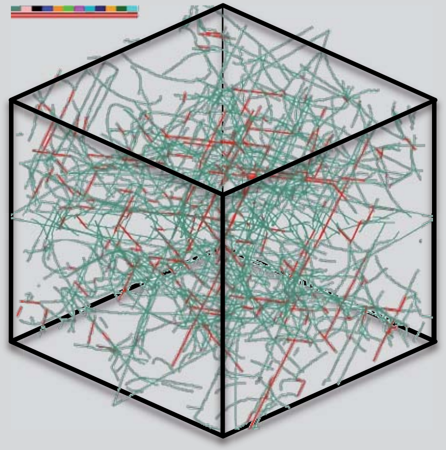


2. Modeling their mobility (σ, T)

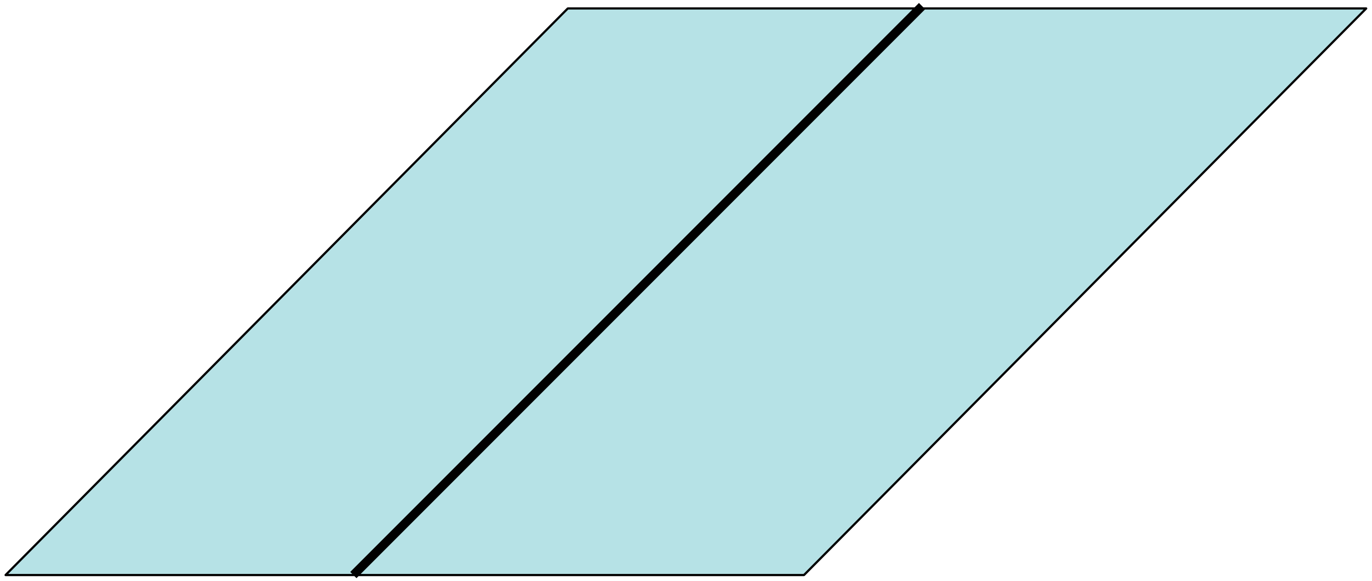


3. Modeling flow laws

$$\dot{\varepsilon} = \rho b v$$



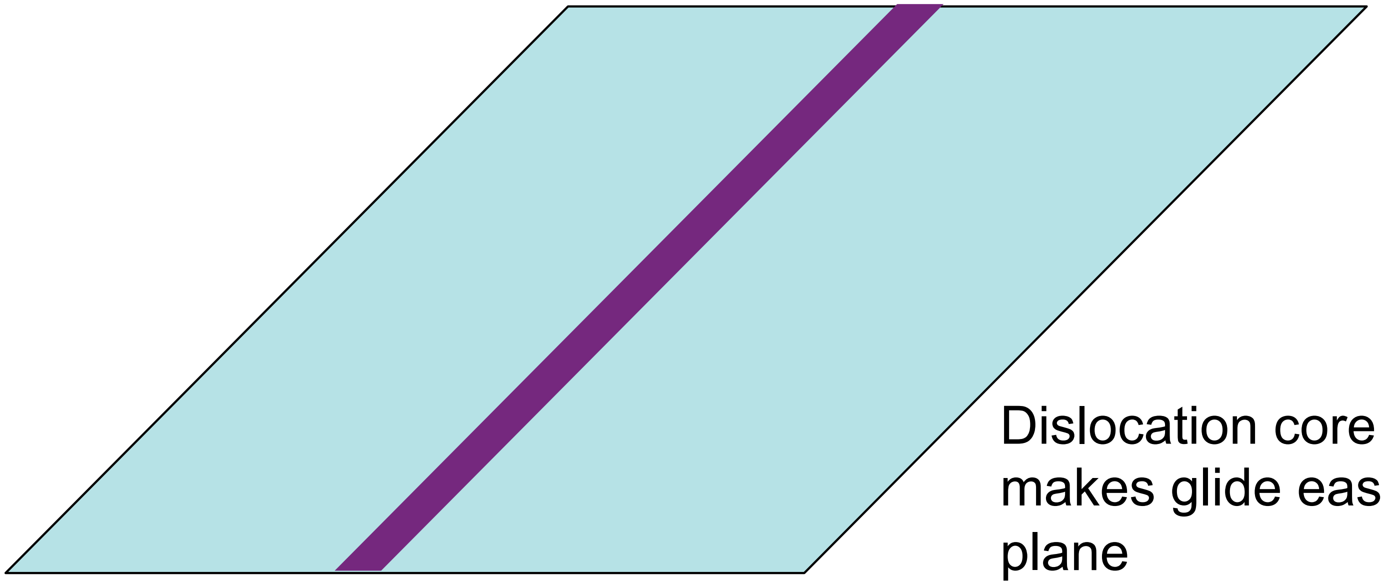
Dislocation core structure: influence on dynamics



Glide plane

Dislocation line

Dislocation core structure: influence on dynamics

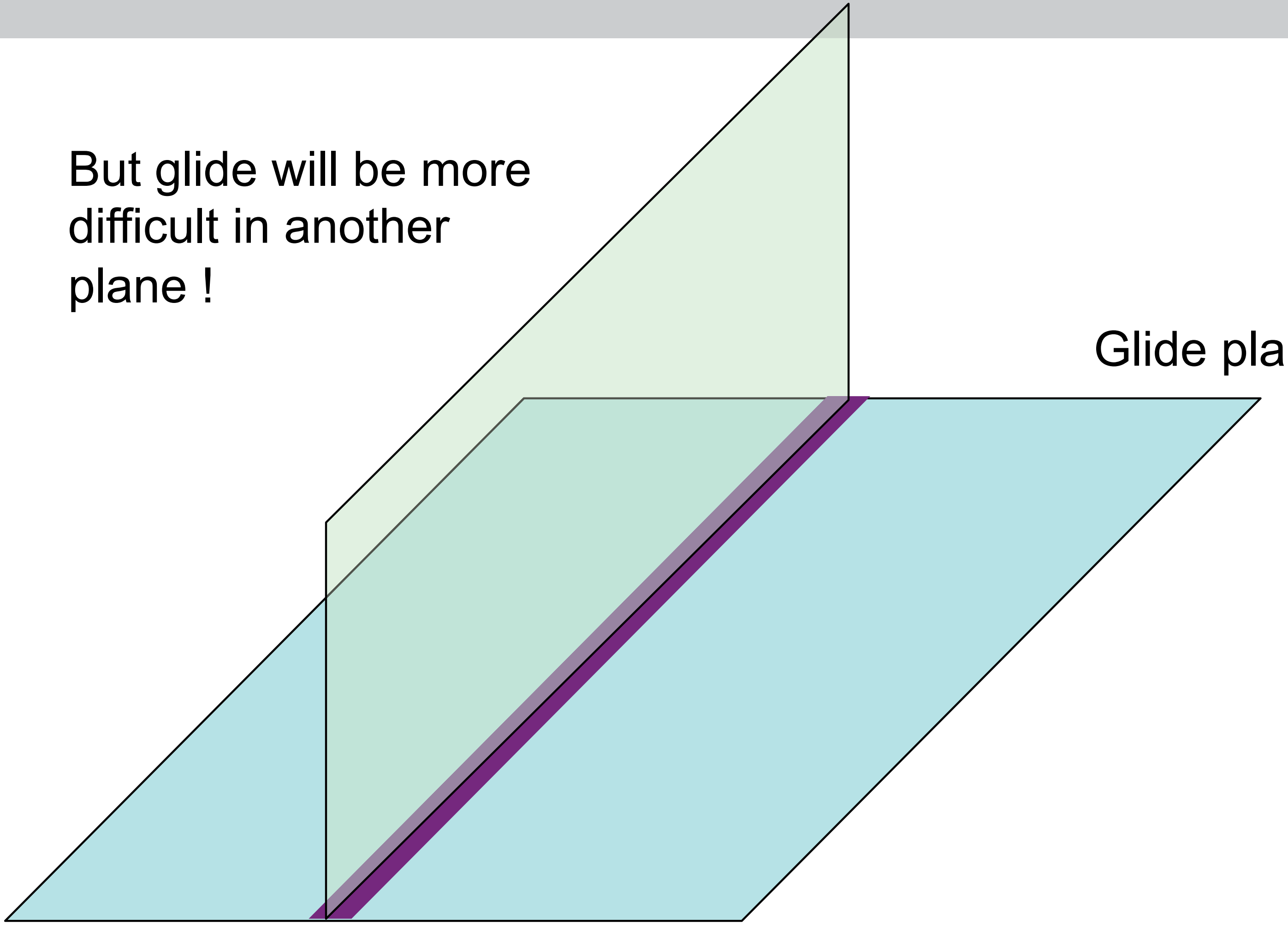


Glide plane

Dislocation core spreading makes glide easier in this plane

Dislocation line

Dislocation core structure: influence on dynamics

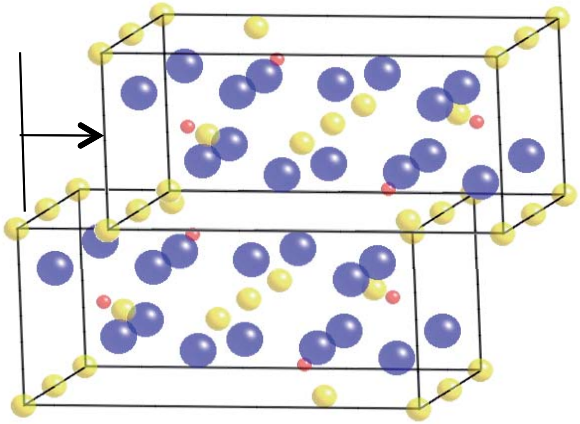


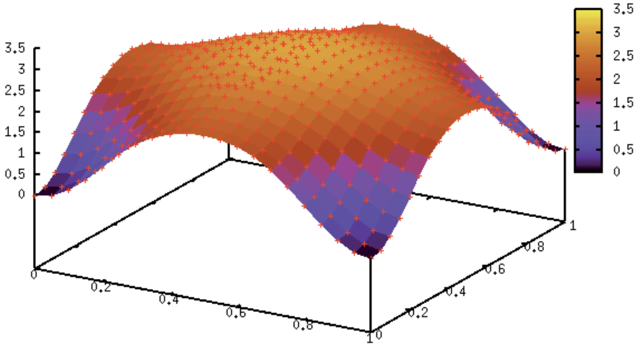
But glide will be more difficult in another plane !

Glide plane

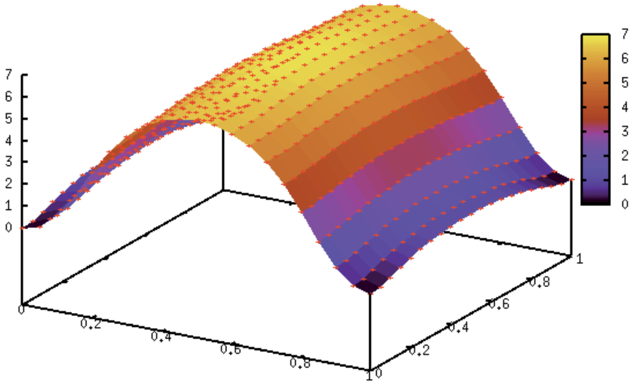
Dislocation line

Shearing crystals: Generalized Stacking Fault (GSF)





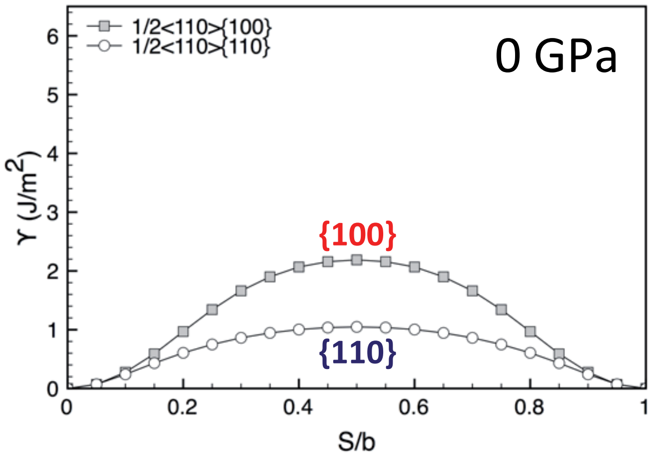
{100}

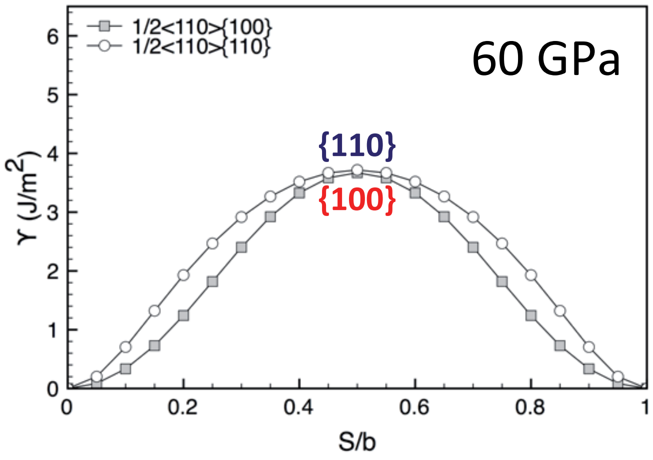


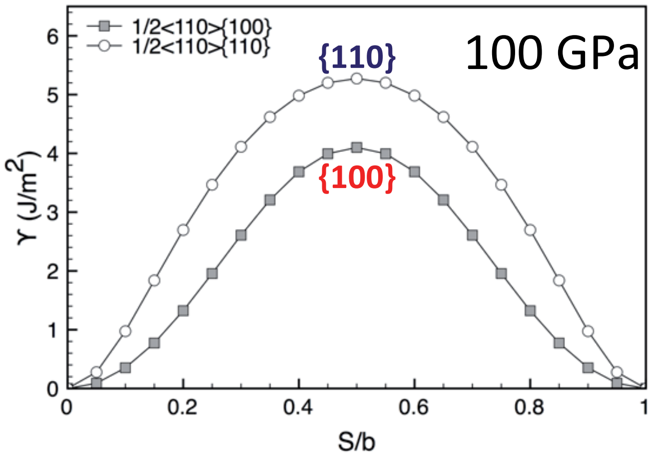
{110}

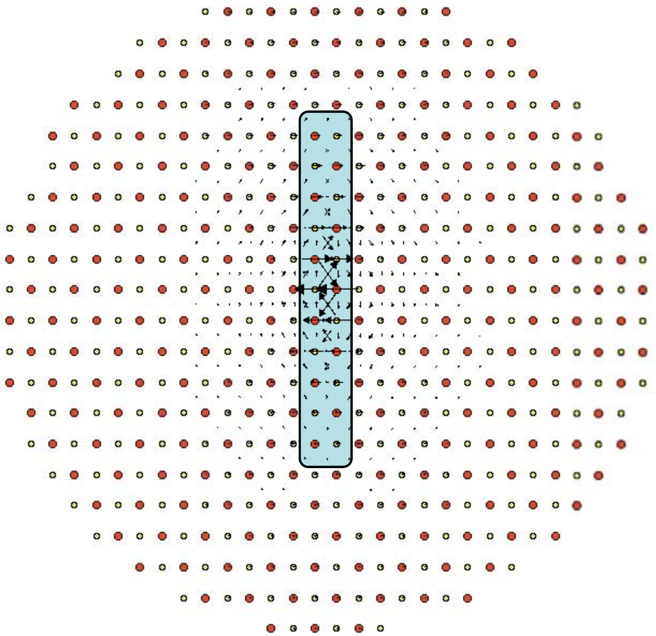
Dislocation core modeling in MgO

Screw dislocations

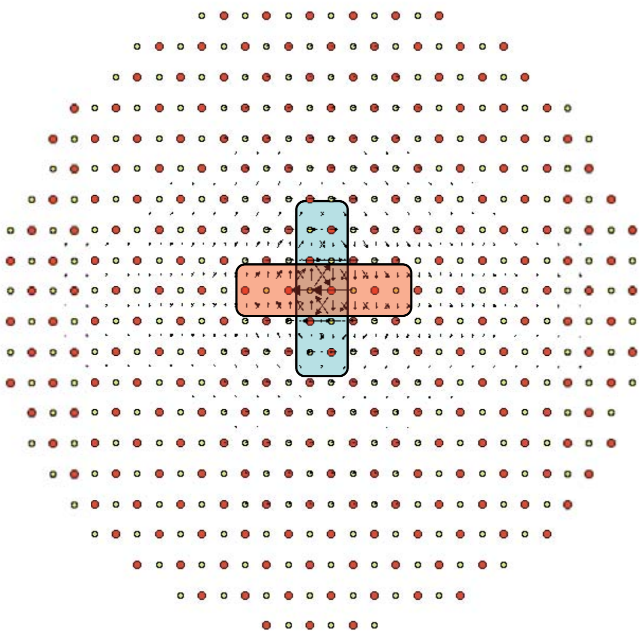


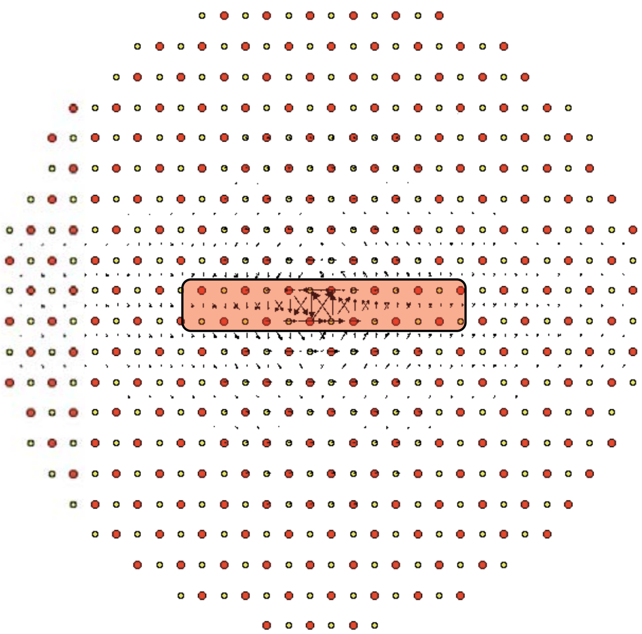






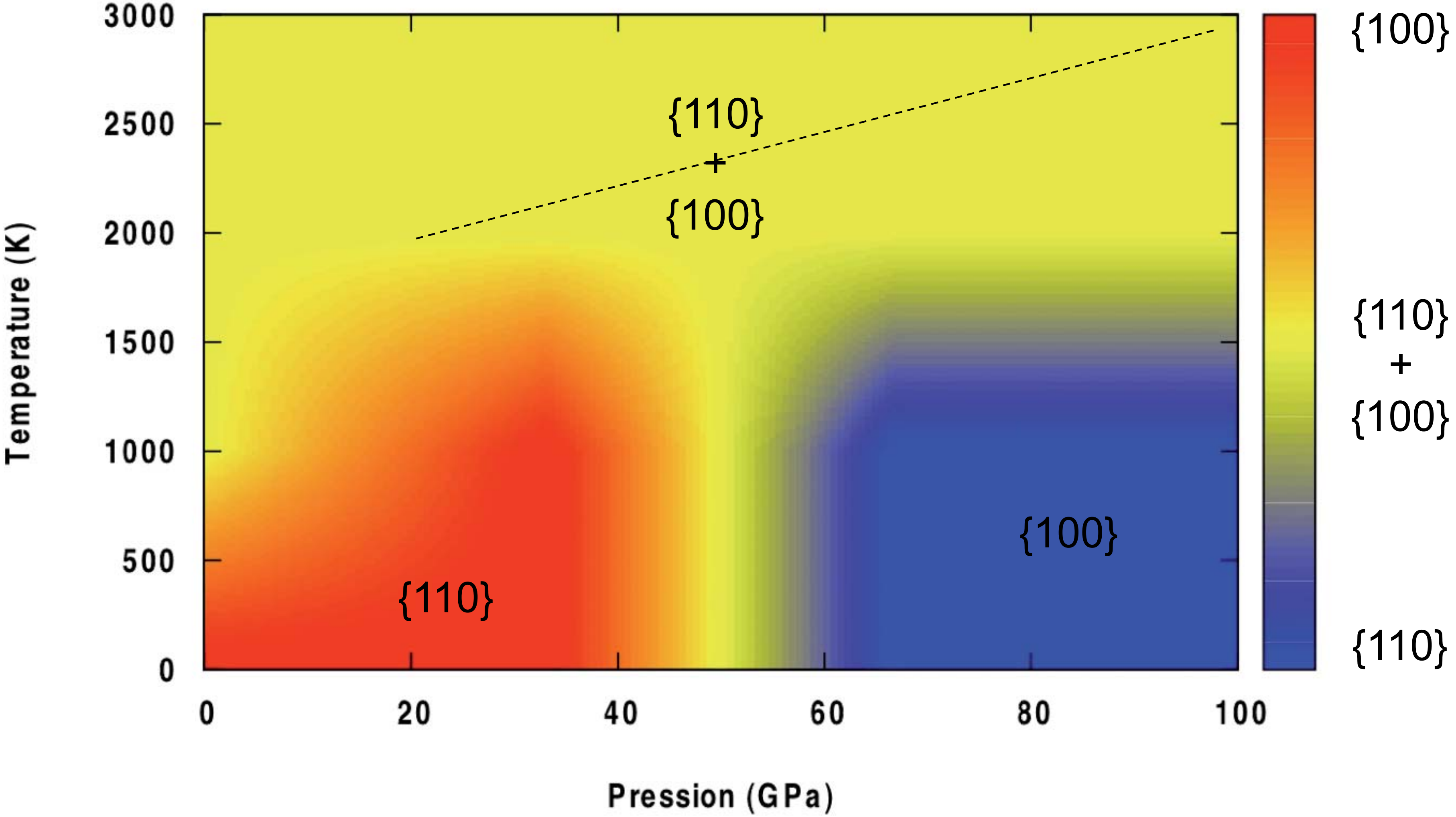
Glide in {110}



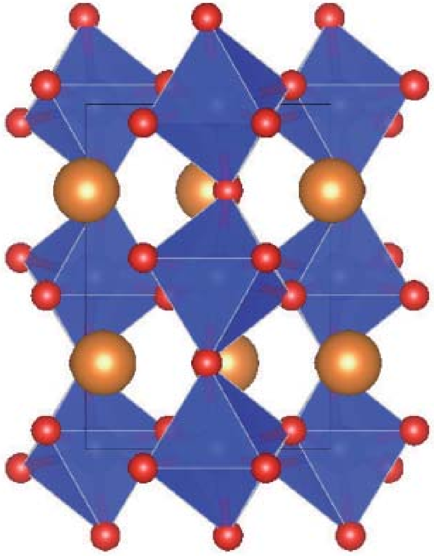


Glide in {100}

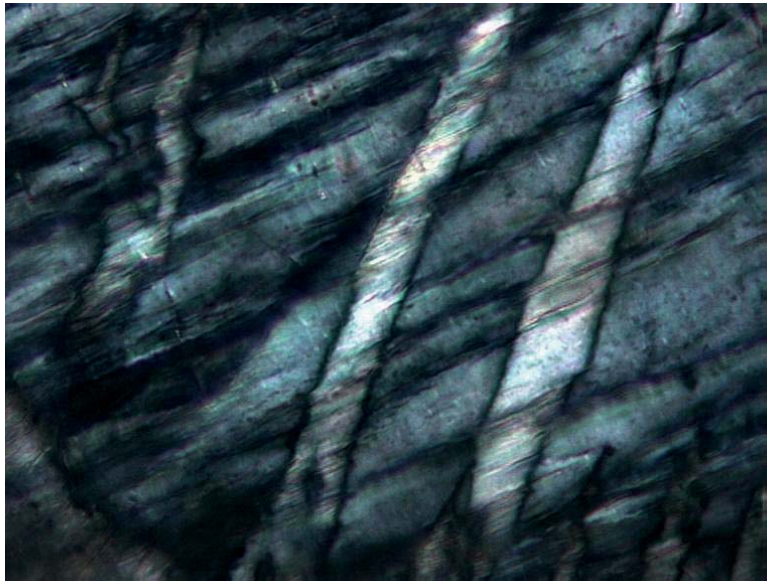
$$\dot{\varepsilon} = 10^{-16}\ s^{-1};\ \rho = 10^{12}\ m^{-2}$$



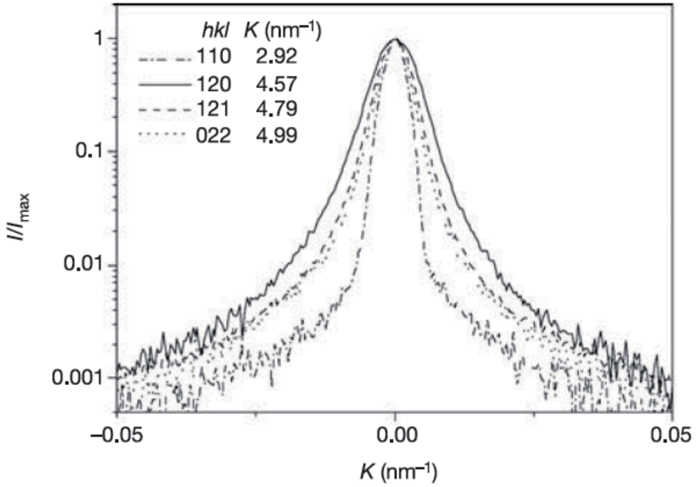
$MgSiO_3$ Perovskite



Experimental deformation in the multianvil apparatus
25 GPa, 1400°C
Cordier *et al.* (2004) Nature, **428**, 837.



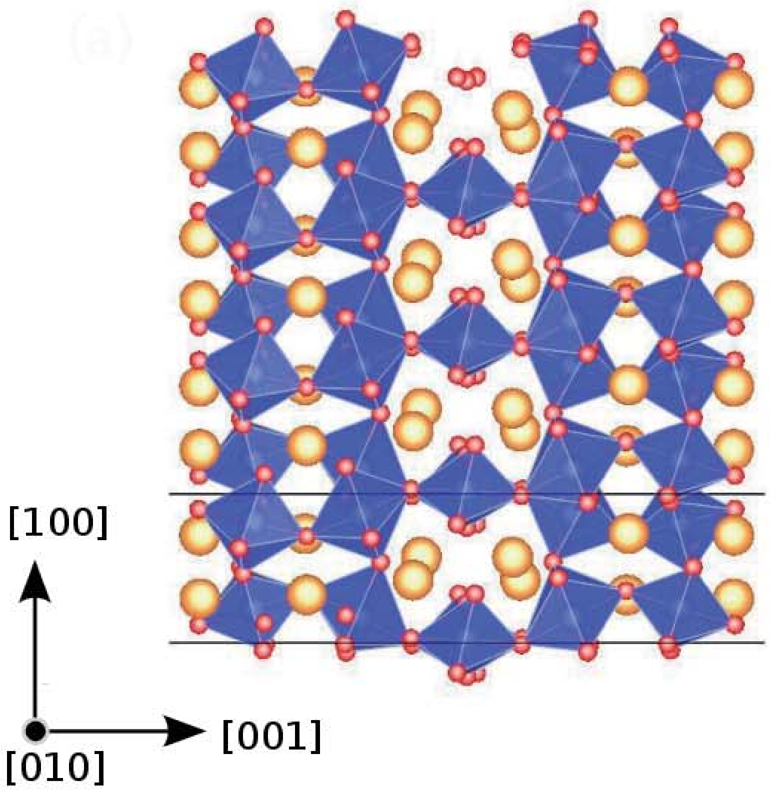
Peak line broadening analysis

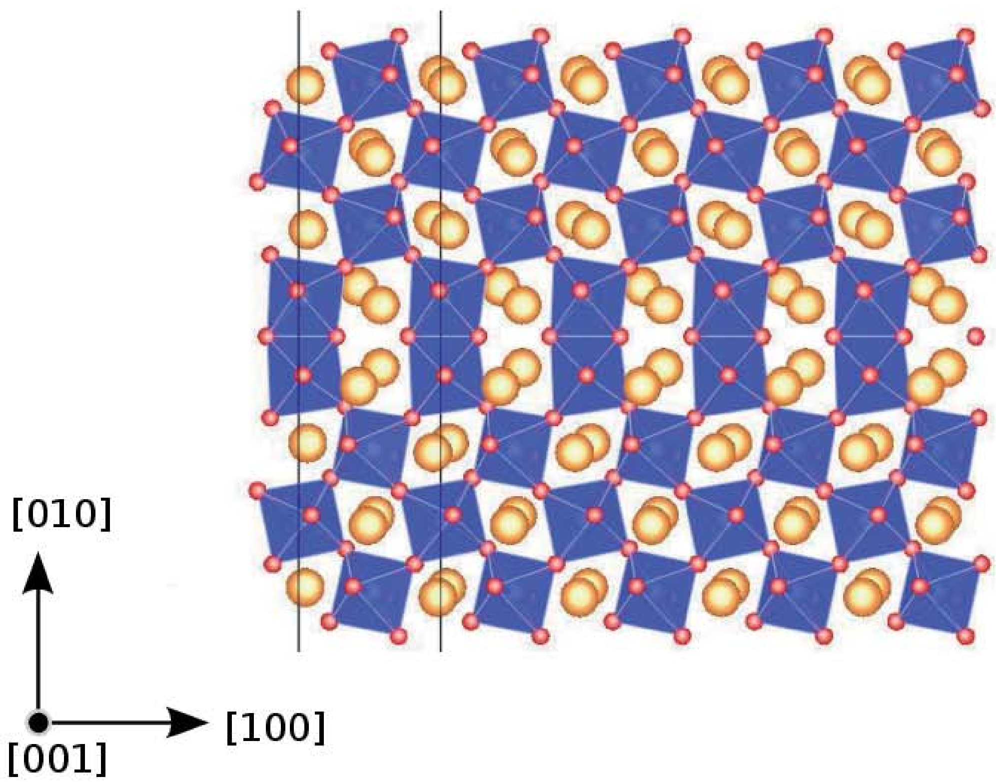


Dominant slip systems:
[100](010)
[010](100)

Dislocation core modeling in $MgSiO_3$ Perovskite

Screw dislocation; Burgers vector [100]

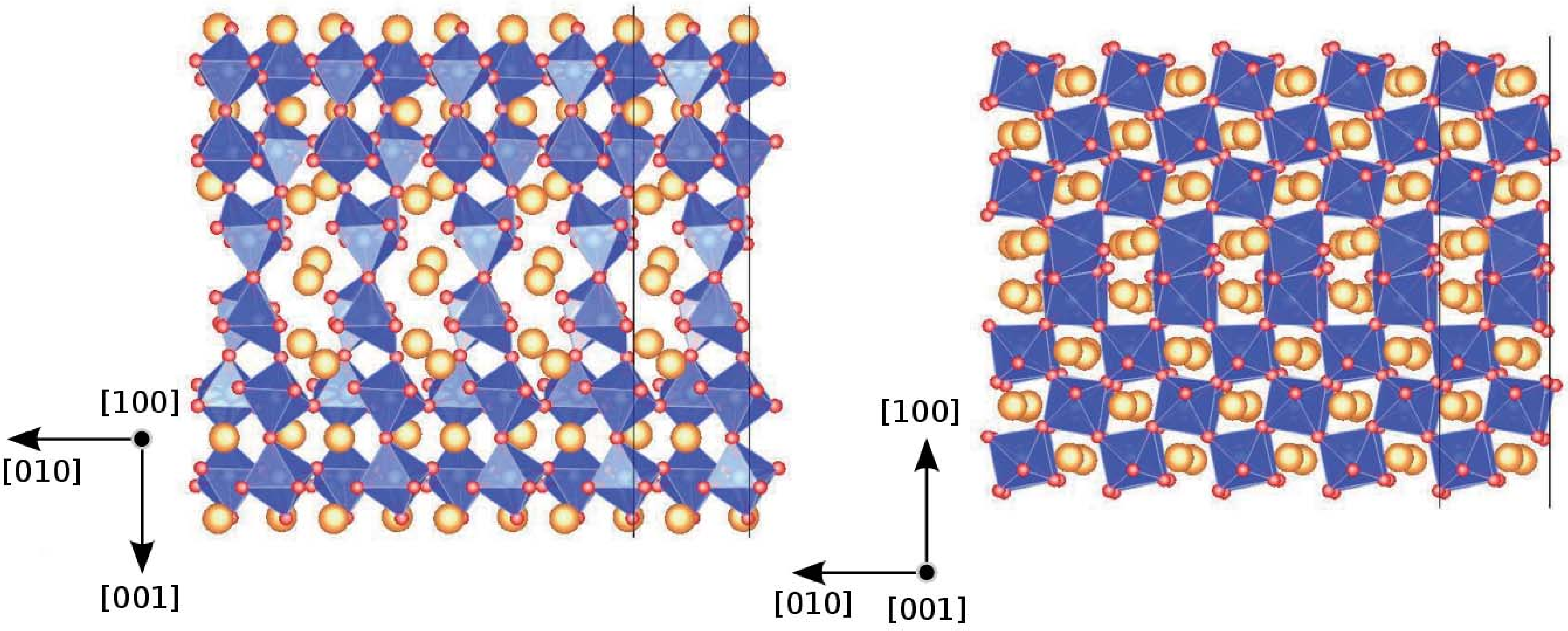




See Antoine Kraych's poster !

Dislocation core modeling in $MgSiO_3$ Perovskite

Screw dislocations; Burgers vector [010]



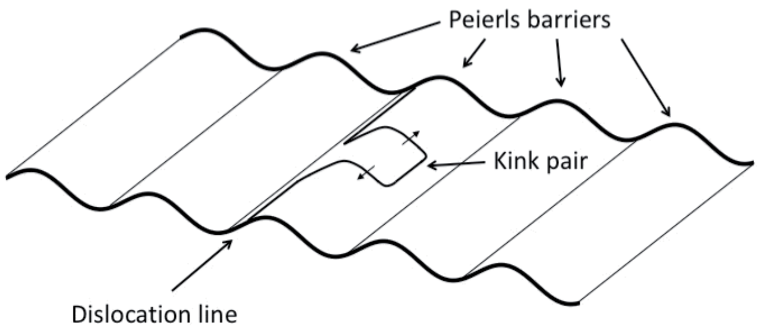
See Antoine Kraych's poster !

Dislocation mobility at finite temperature

Frequency of the vibrational mode responsible for the jump: $\dfrac{\nu_D b}{w^*(\tau)}$

Number of sites: $\dfrac{L}{w^*(\tau)}$

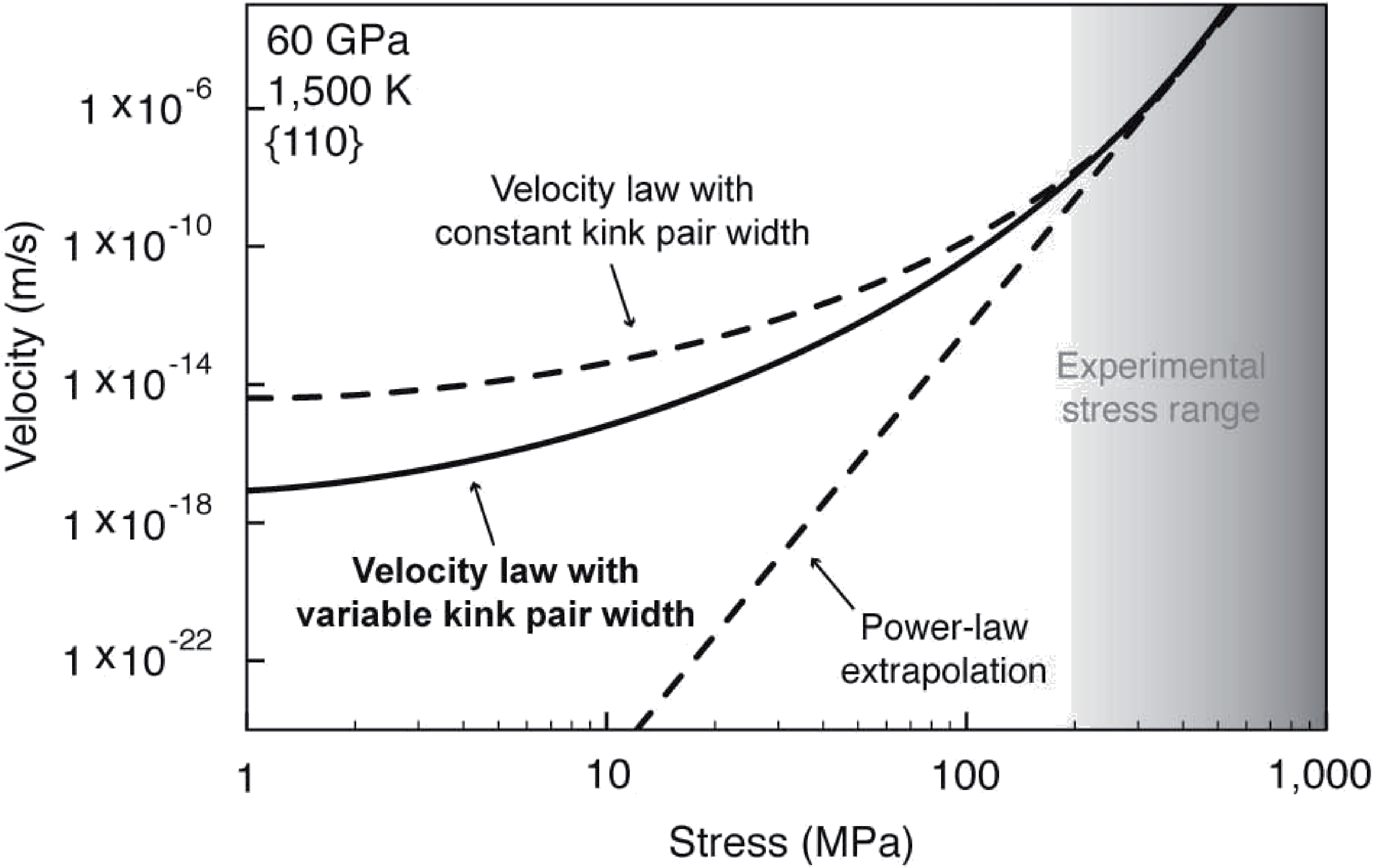
Probability of a successful jump: $e^{-\frac{\Delta H^*(\tau)}{kT}}$



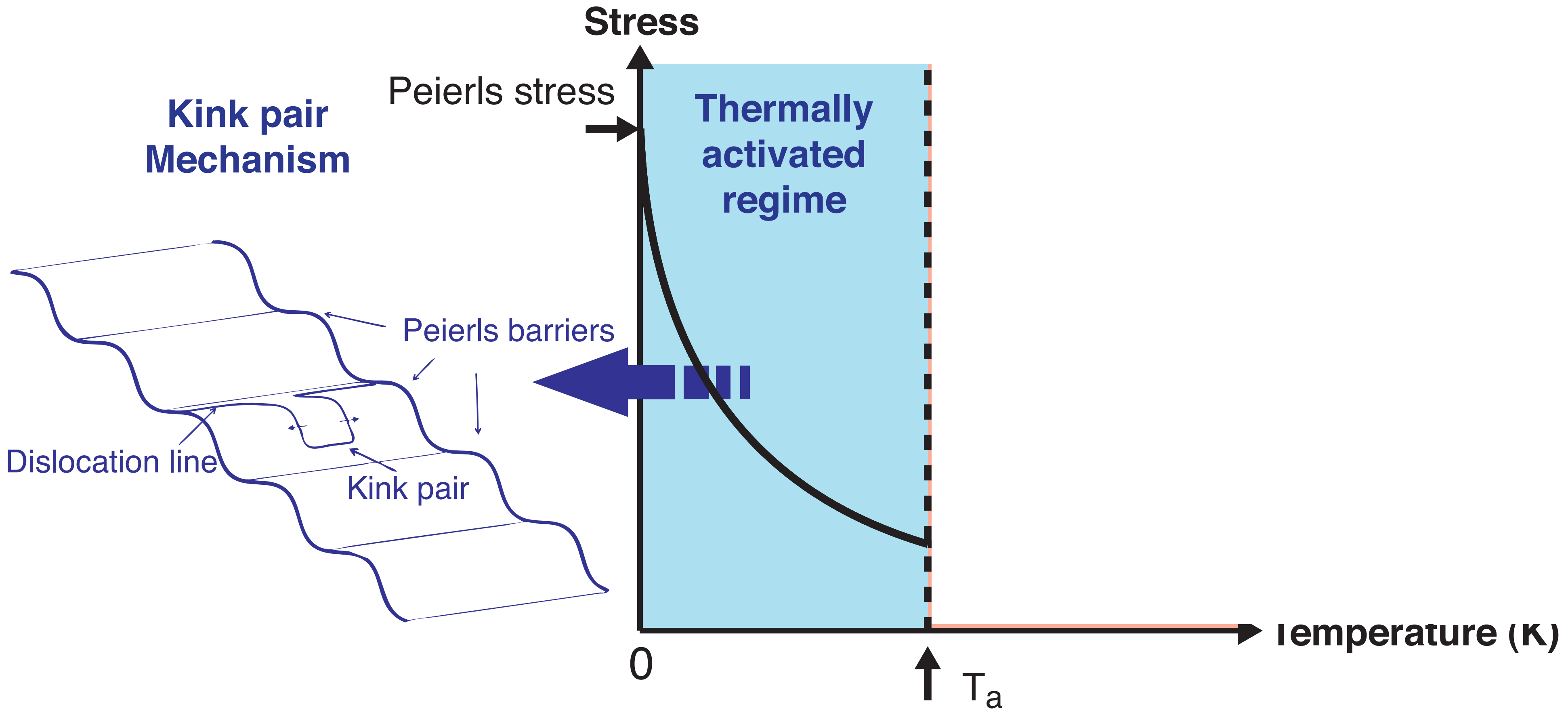
$$\Rightarrow v = a' . \frac{L}{w^*(\tau)} . \frac{\nu_D b}{w^*(\tau)} . \exp\left(-\frac{\Delta H^*(\tau)}{kT}\right)$$

Dislocation mobility

$$v = a' \nu_D b . \frac{L}{w^*(\tau)^2} . \exp\left(- \frac{\Delta H_0}{kT} \right)$$



Thermally activated regime

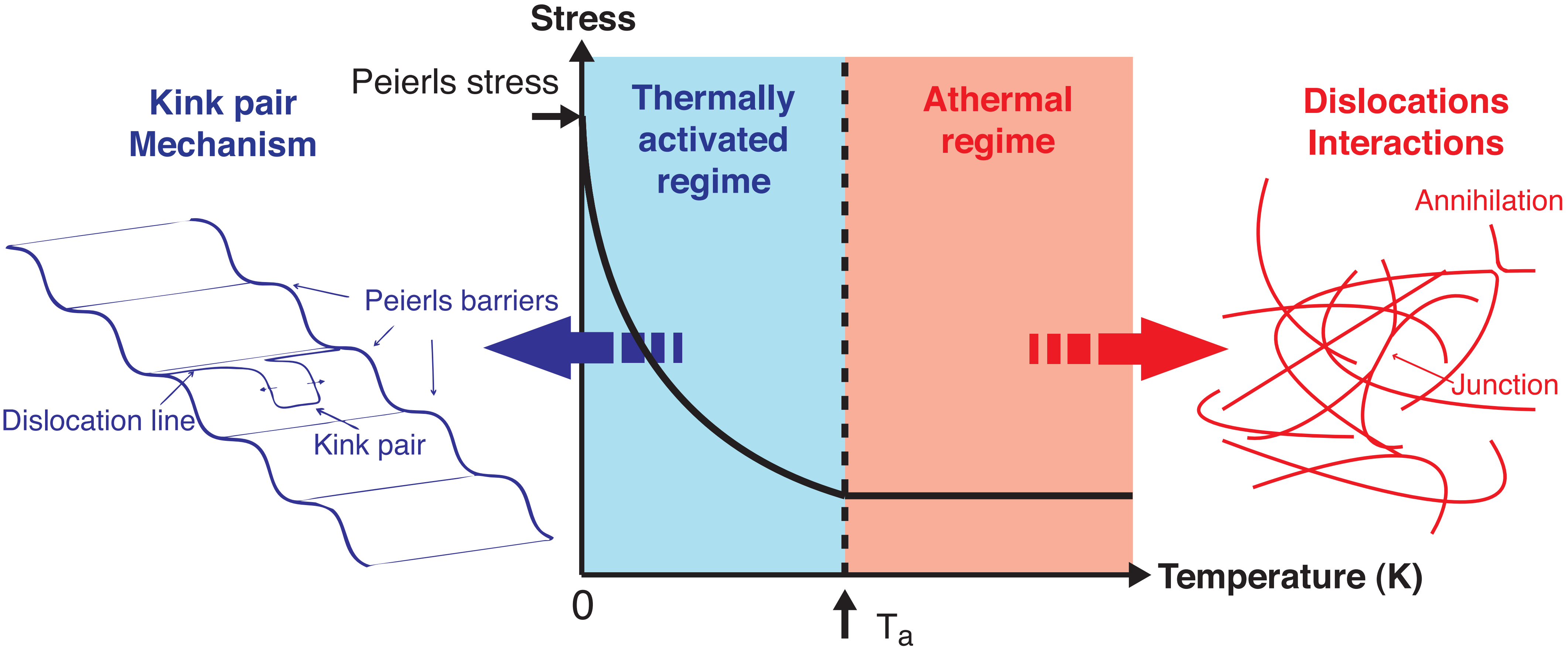


$$v \propto L\exp\Big(f\big(\tau,T\big)\Big)$$

$$\dot{\varepsilon} = \rho.\ b.\ v(\tau) \quad \Rightarrow \quad \eta(\tau) = \tau / \dot{\varepsilon}$$

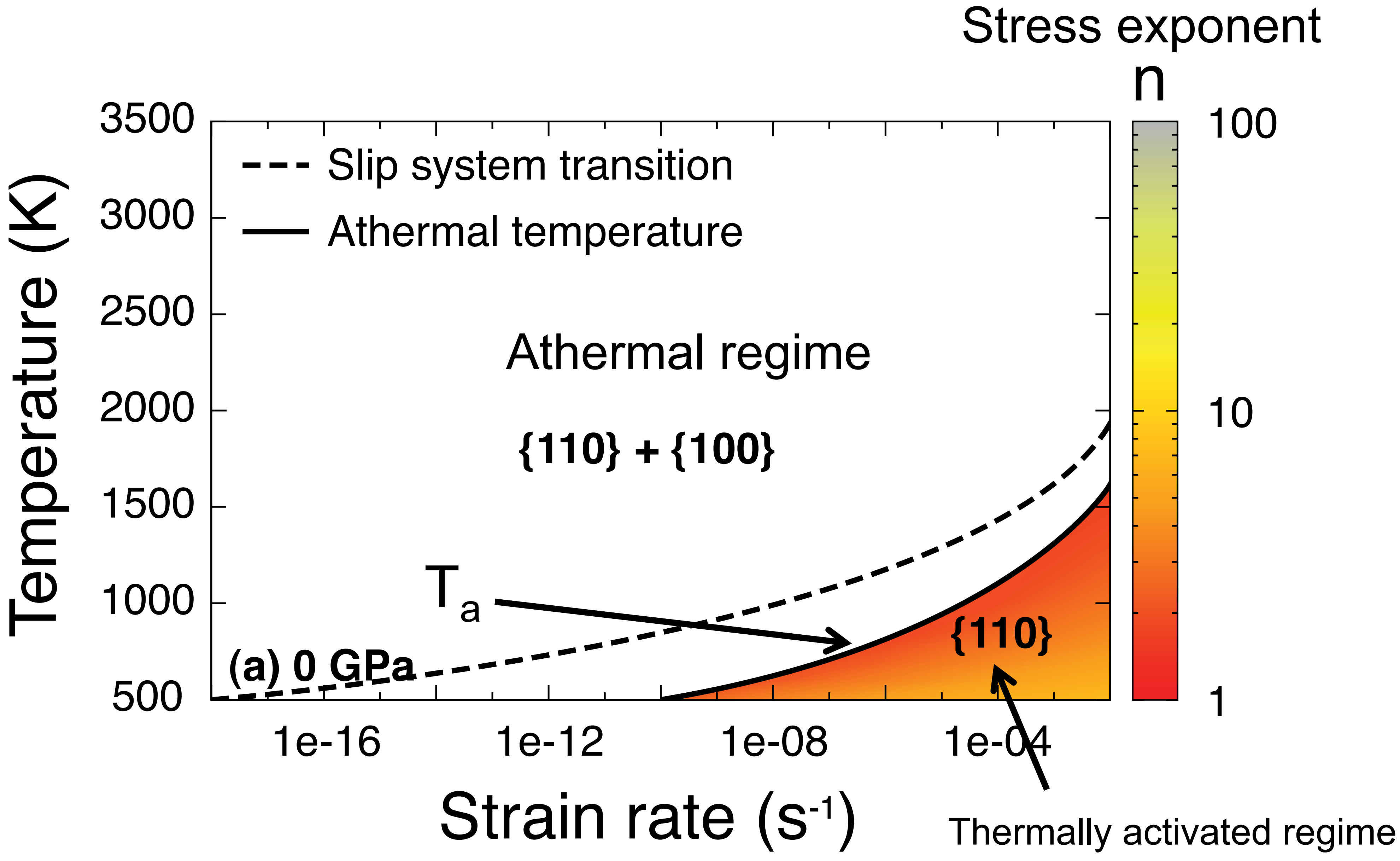
Viscosity

Athermal regime



No temperature dependence
No strain-rate dependence
Flow stress governed by the microstructure: no viscosity !

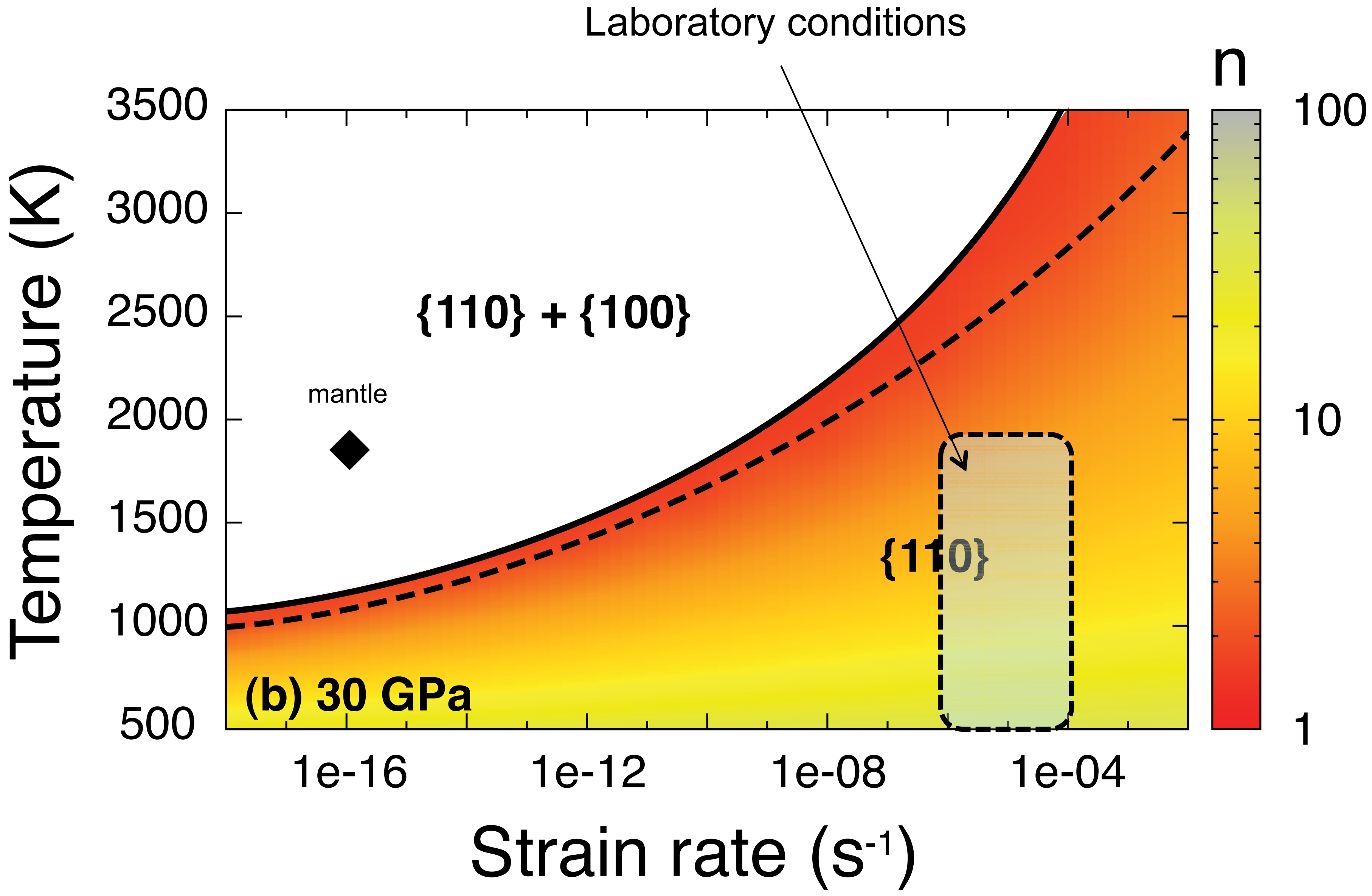
The influence of strain-rate: MgO



Thermally activated regime

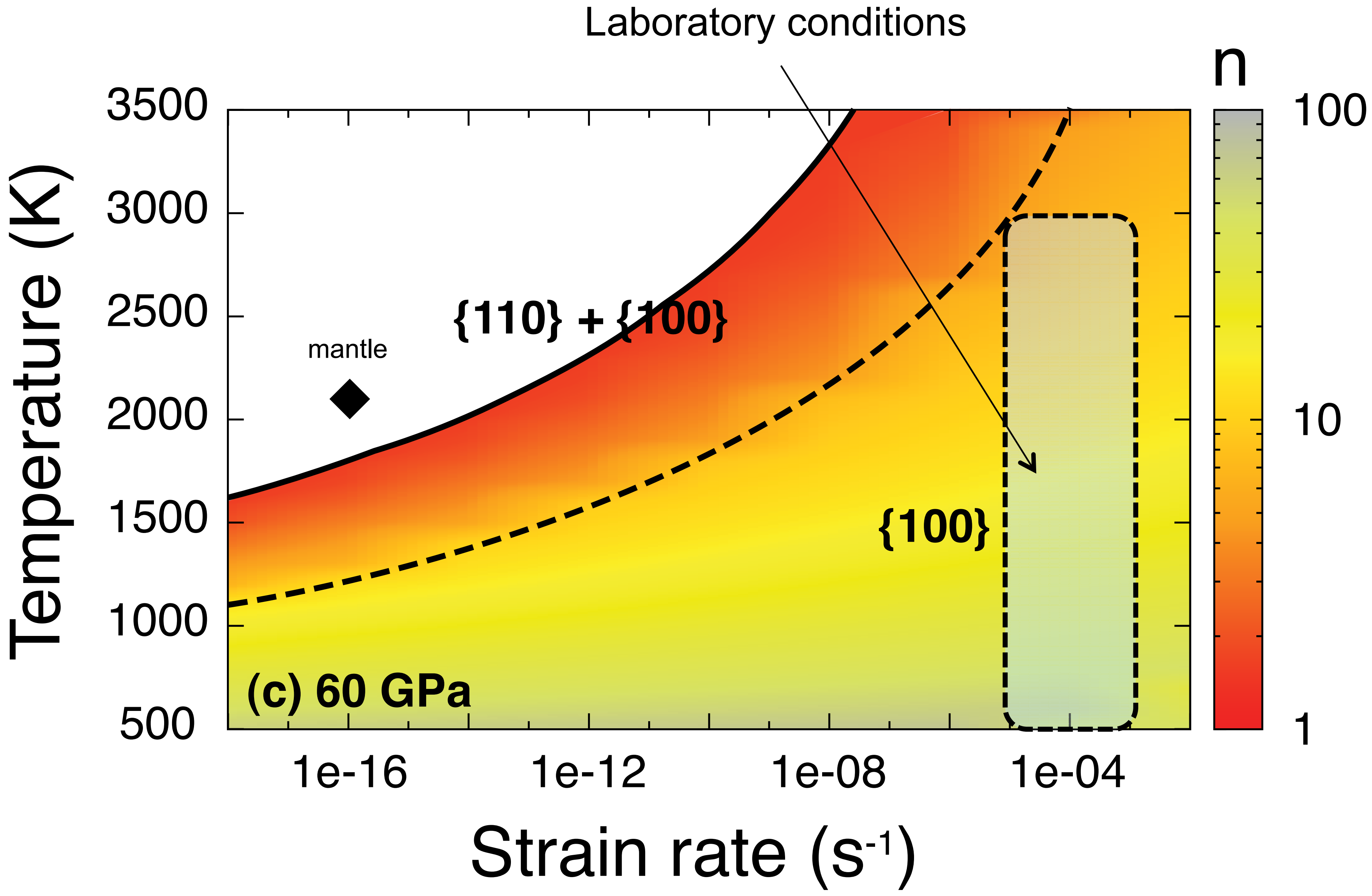
The influence of strain-rate: MgO

ca. 775 km



The influence of strain-rate: MgO

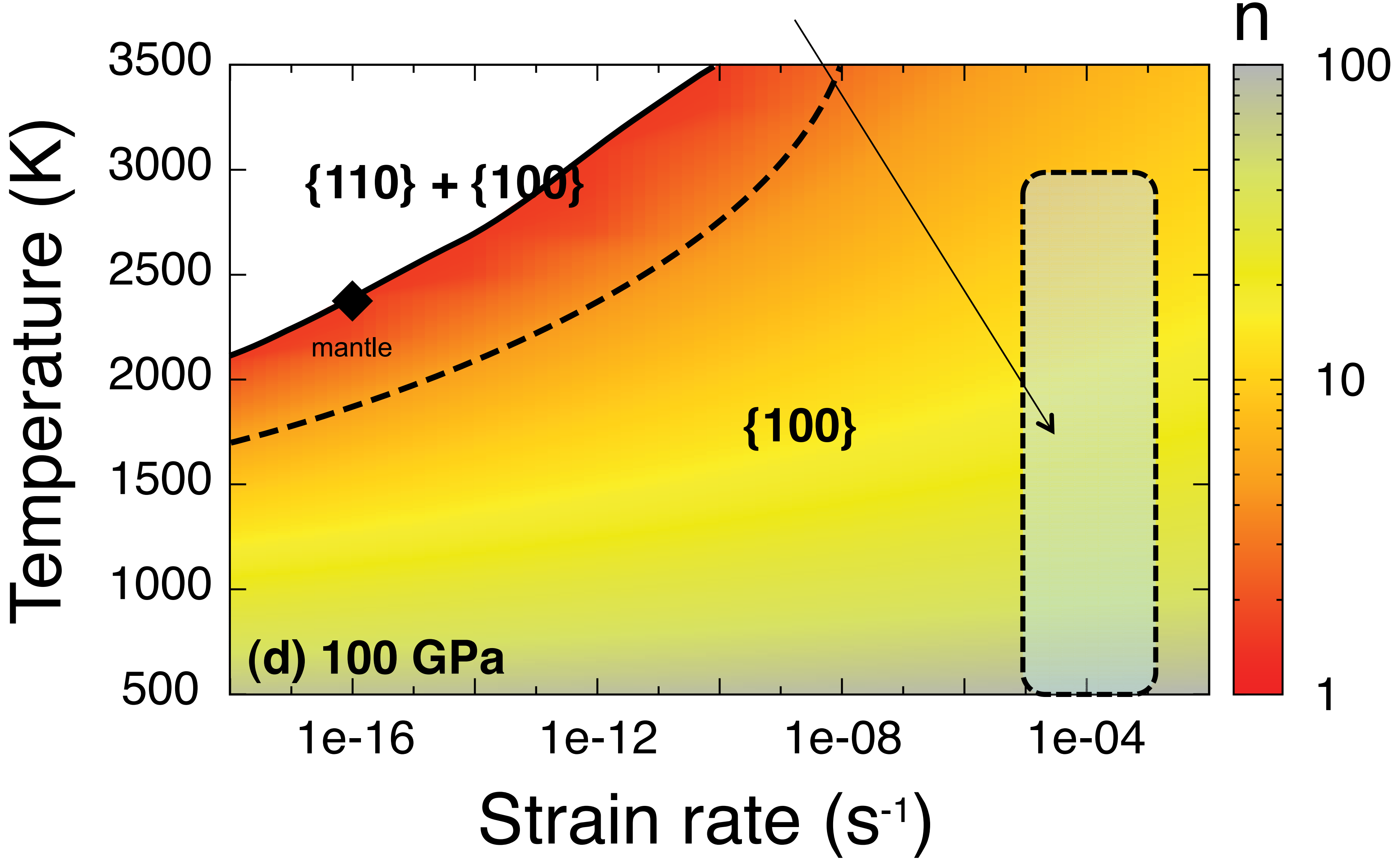
ca. 1500 km



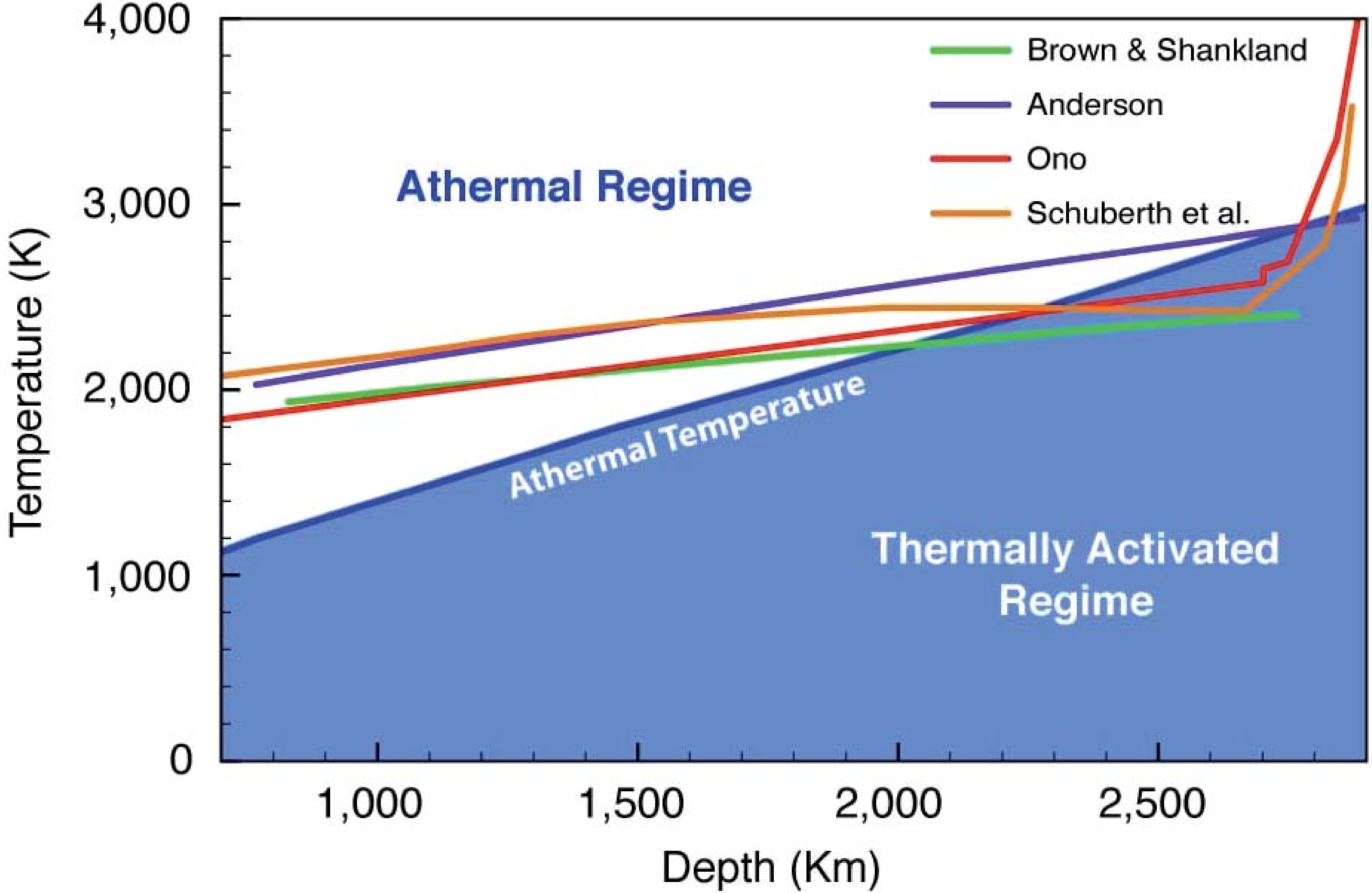
The influence of strain-rate: MgO

ca. 2300 km

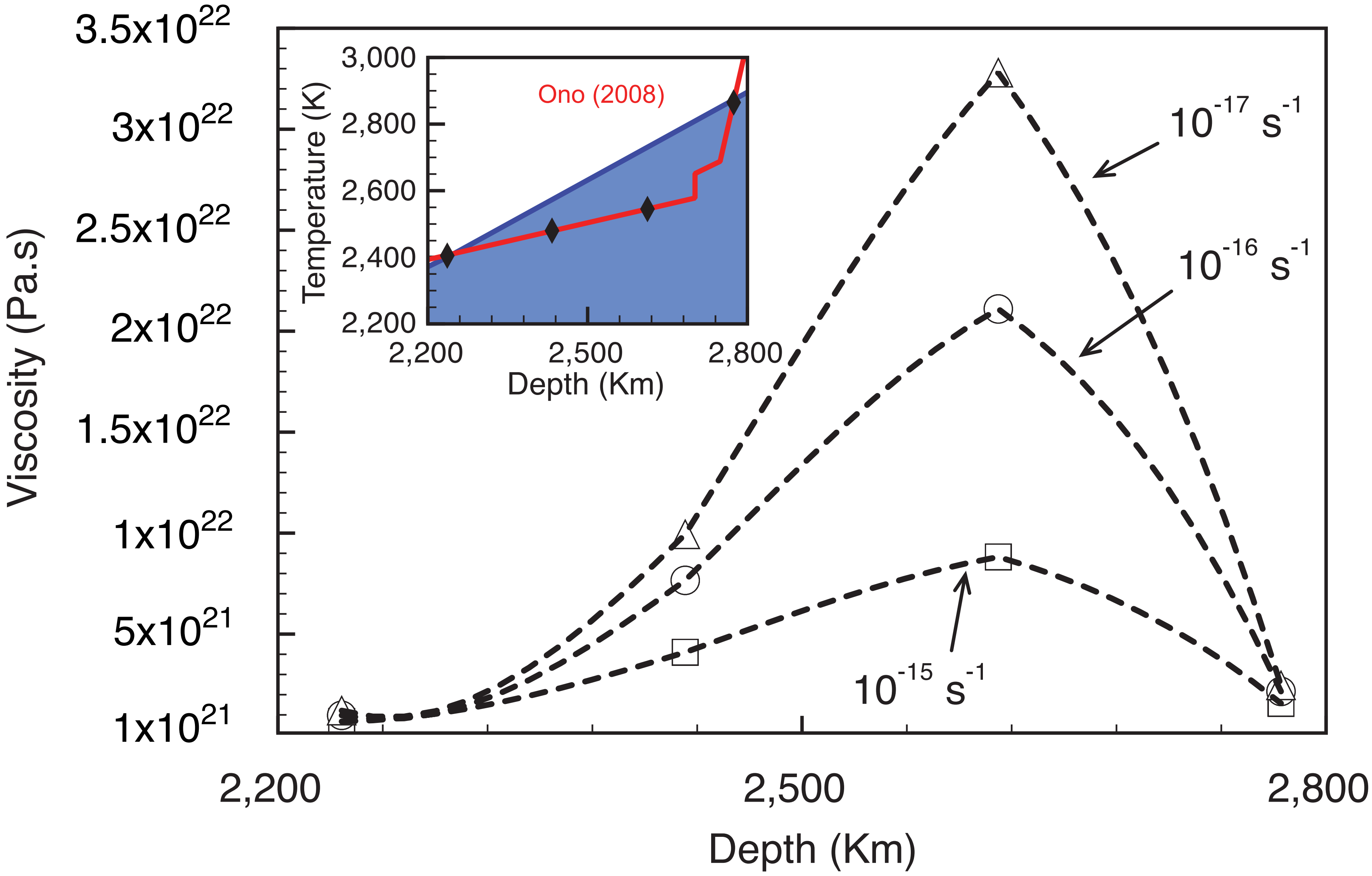
Laboratory conditions



Plasticity of MgO in the mantle



Plasticity of MgO in the mantle



Conclusions

New direction in rheology:

Multiscale numerical modeling

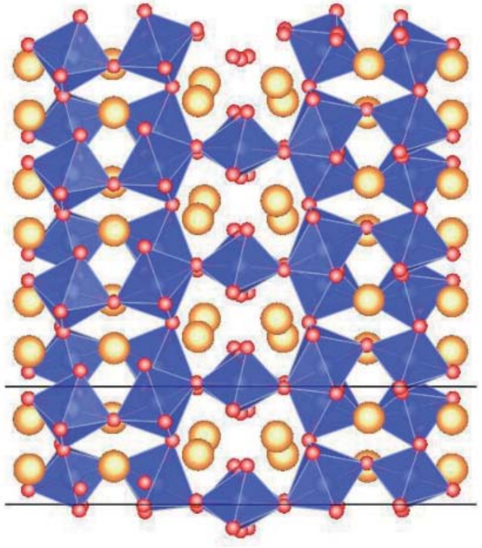
MgO under mantle conditions:

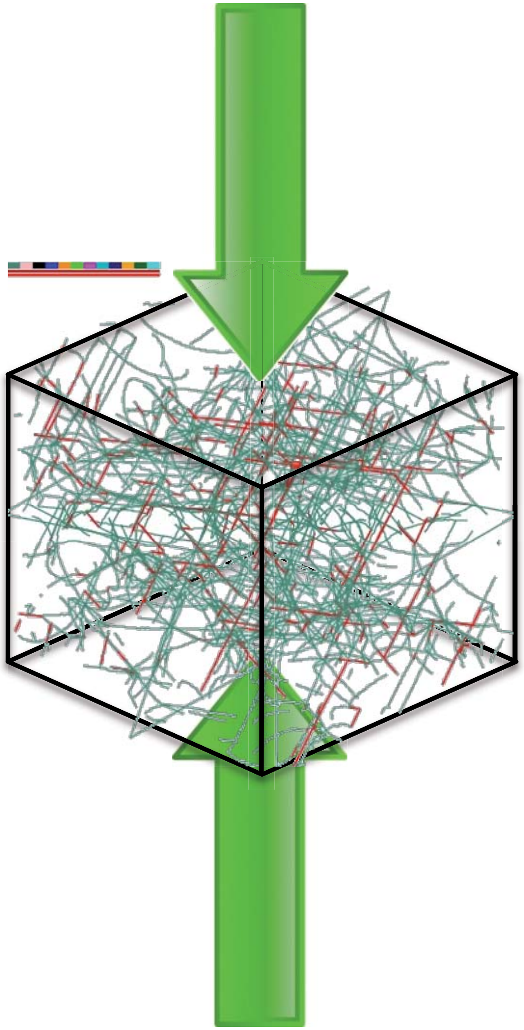
- Change of slip systems under the influence of pressure
- More results (including the influence of strain-rate) have been published already, see Cordier *et al.* (2012) Nature **481**, 177-180

$MgSiO_3$ perovskite under mantle conditions:

- First results on fully atomistic dislocation modelling
- Slip systems inferred from experimental deformation performed at 25 GPa (Cordier *et al.* (2004) Nature, **428**, 837) persist down to CMB pressures

Thank you !





Acknowledgement
This work was supported by funding from the European Research Council
under the Seventh Framework Programme (FP7), ERC grant N°290424 – RheoMan.