Rheology II
Transport properties

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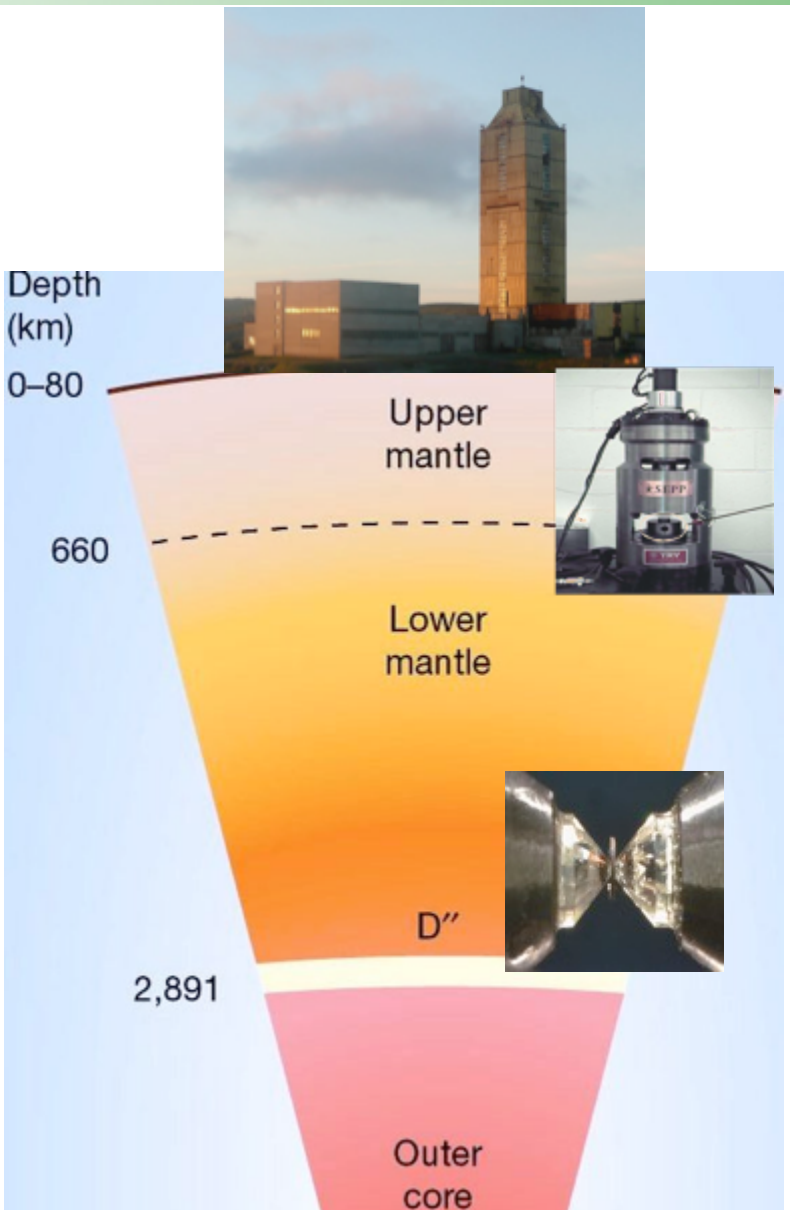
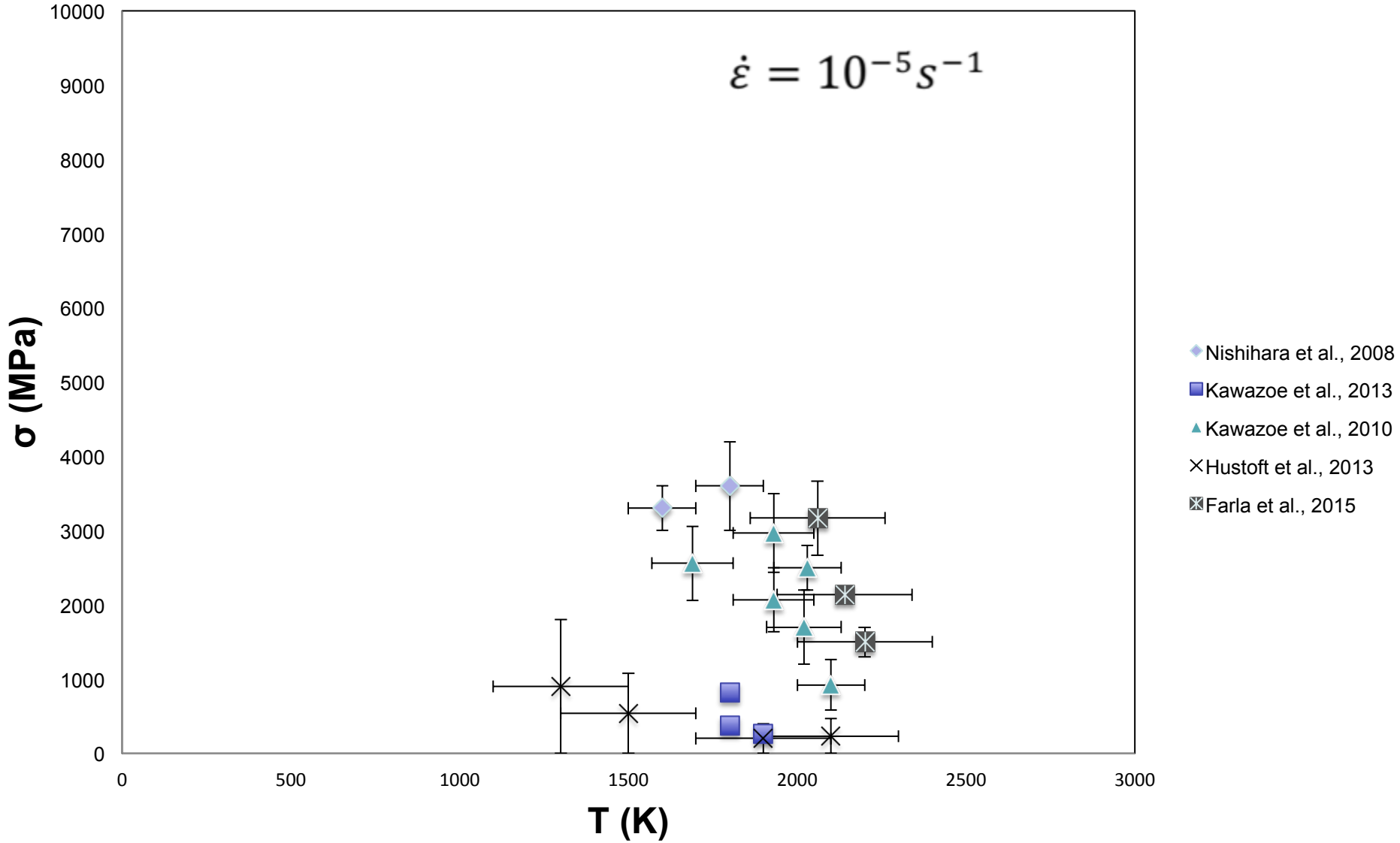
CIDER Summer Program: Flow In the Deep Earth
Santa Barbara CA
July 2016

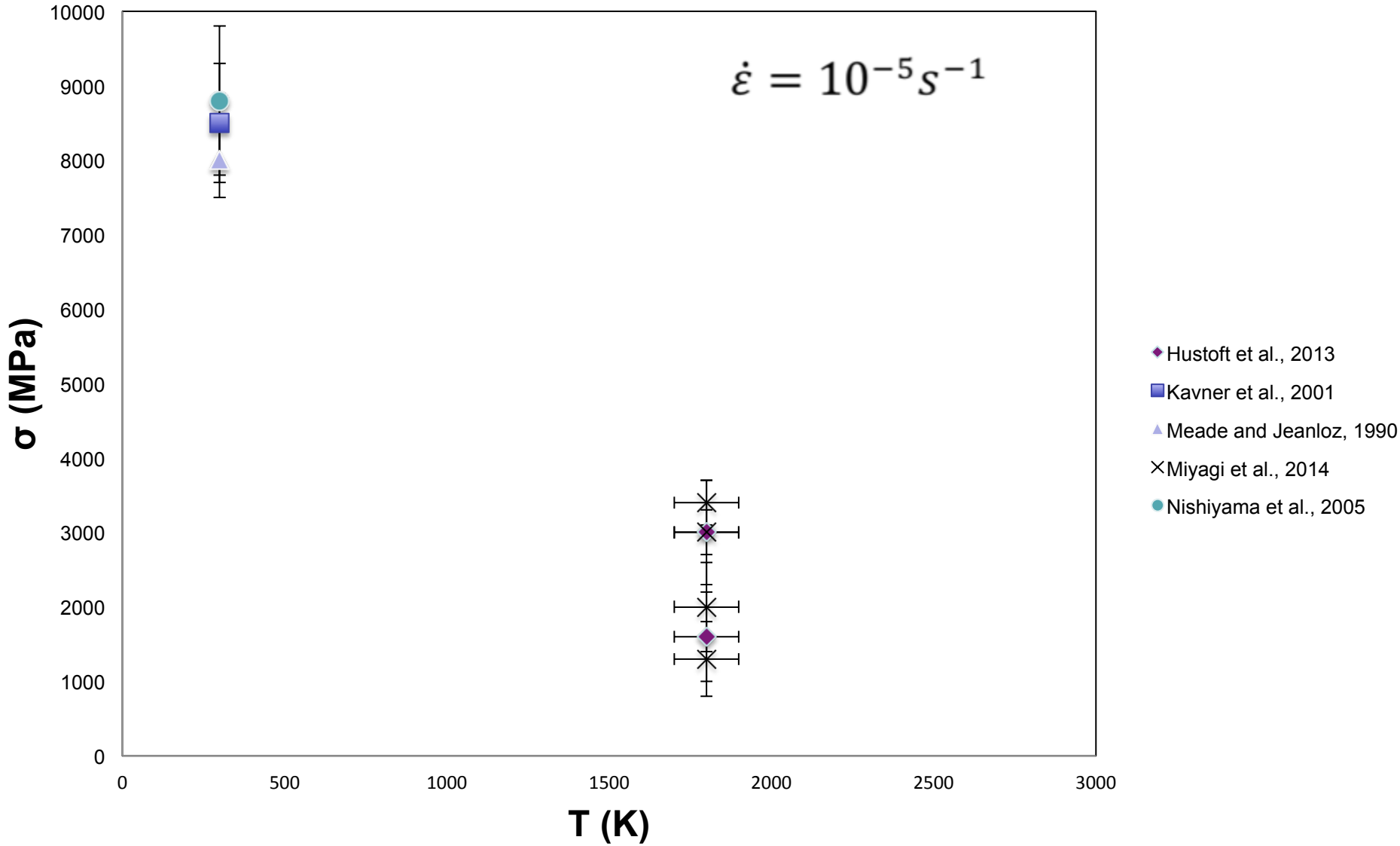
The unreachable Earth



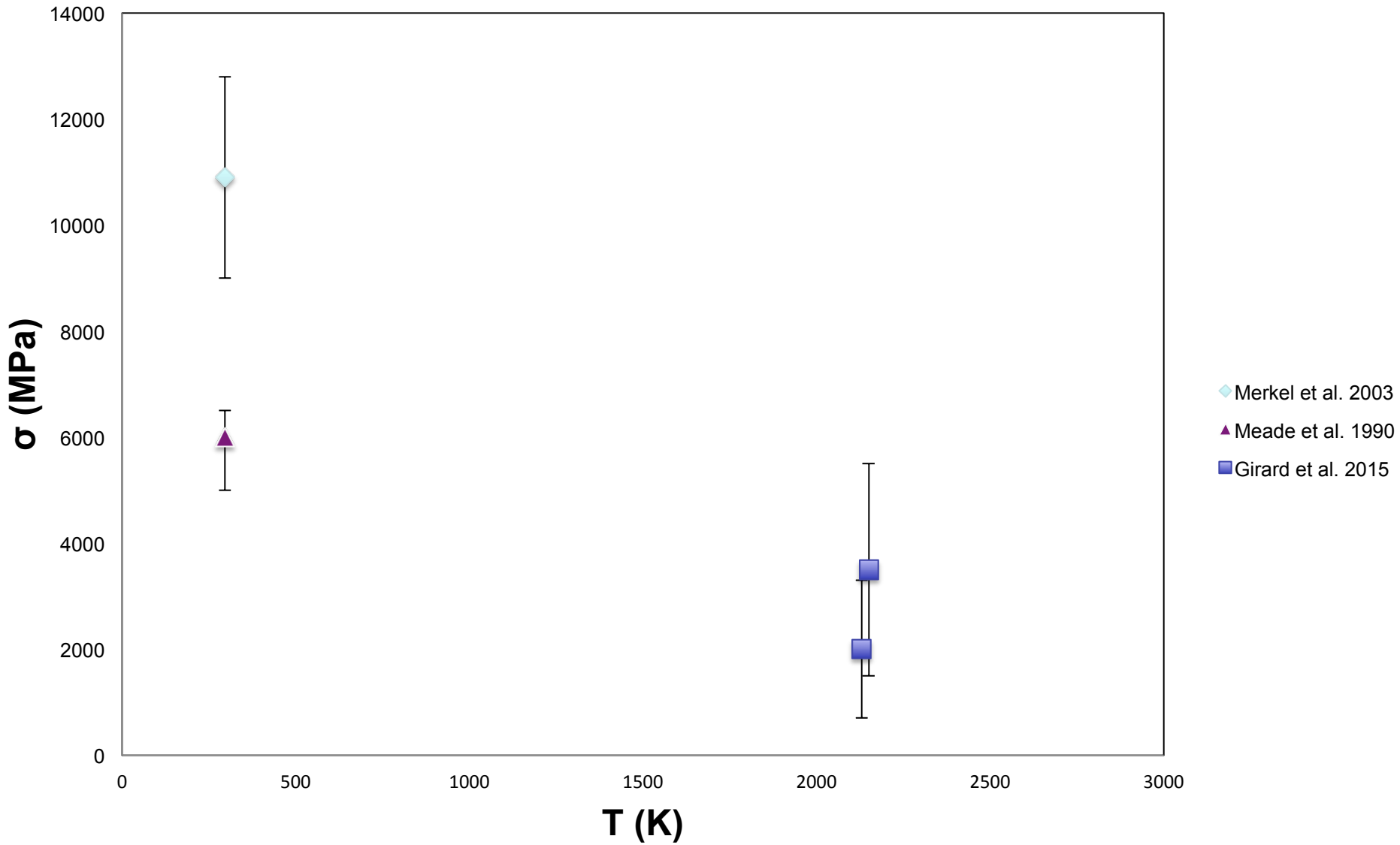
Mechanical properties of wadsleyite



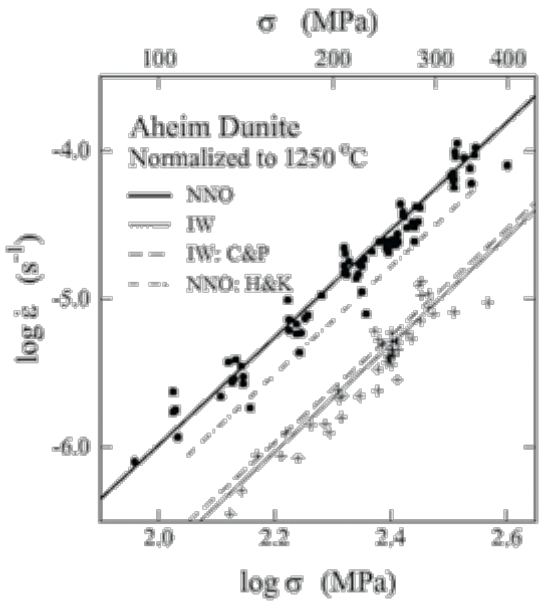
Mechanical properties of ringwoodite



Mechanical properties of bridgmanite



Constitutive equations

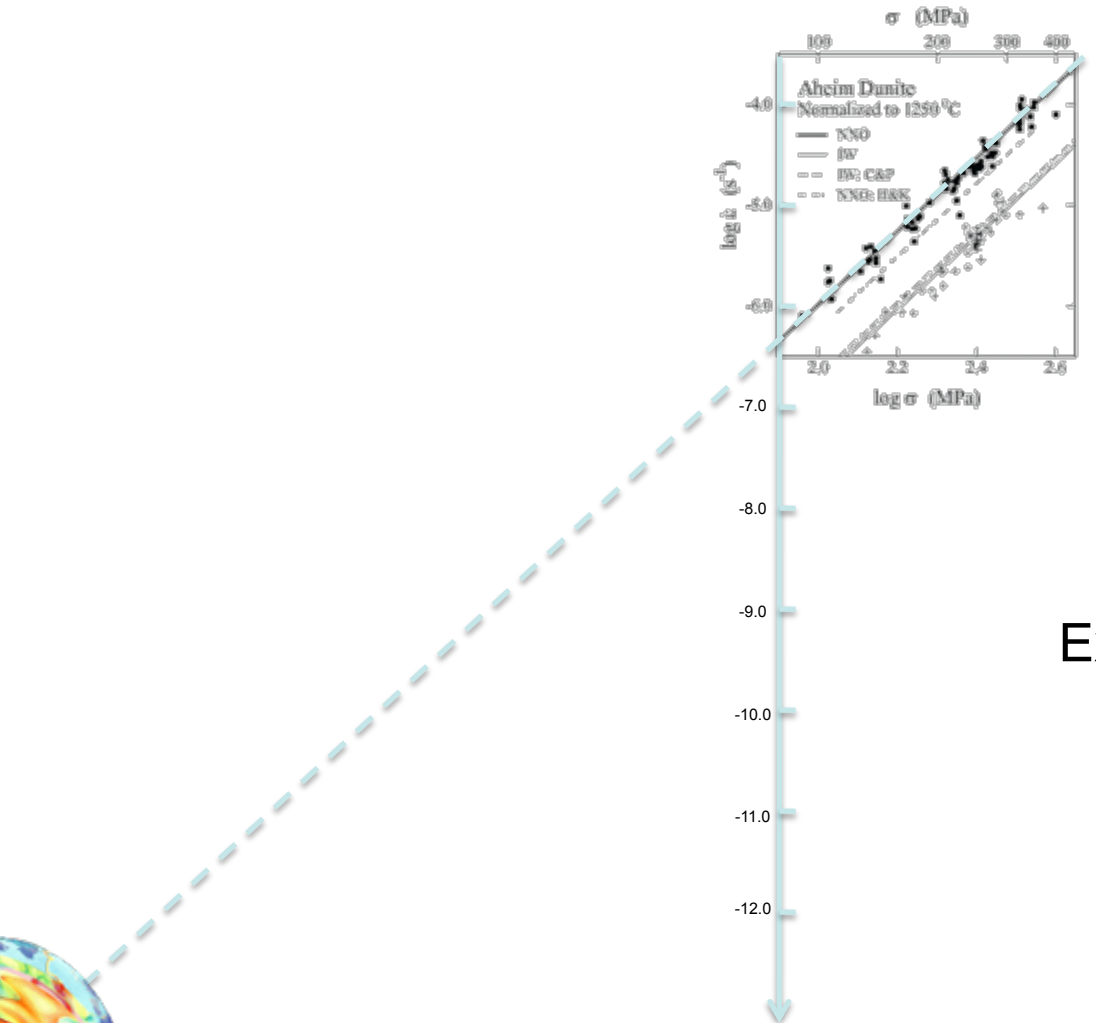


Mackwell, 2008

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

Also need to take high-pressure into account:
Q+PV

Extrapolating to natural timescales



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

Extrapolation to natural conditions

The pitch drop experiment

The University of Queensland pitch drop experiment (started 1927)

Here featuring, Professor John Mainstone (taken in 1990, two years after the seventh drop and 10 years before the eighth drop fell).

Professor John Mainstone died on 23 August 2013, aged 78, after having watched the experiment 52 years

Bitumen $\eta = 2.3\ 10^{11}$ Pa.s

What if….

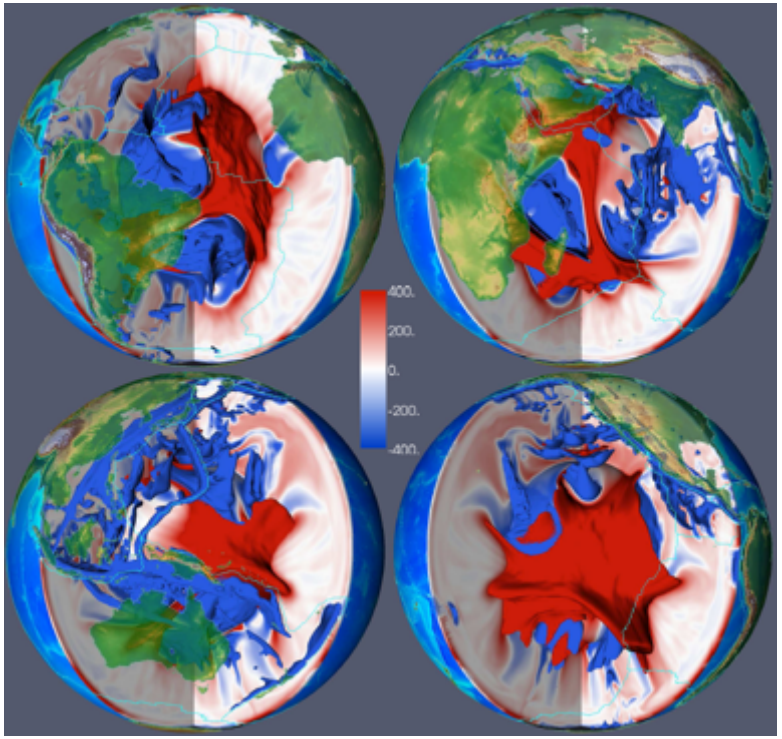
Galileo Galilei (Leyden 1638)

$$\dot{\varepsilon} = 10^{-16} s^{-1}$$

$$\varepsilon = 10^{-6} = 0.0001\% \text{ in 4 centuries}$$

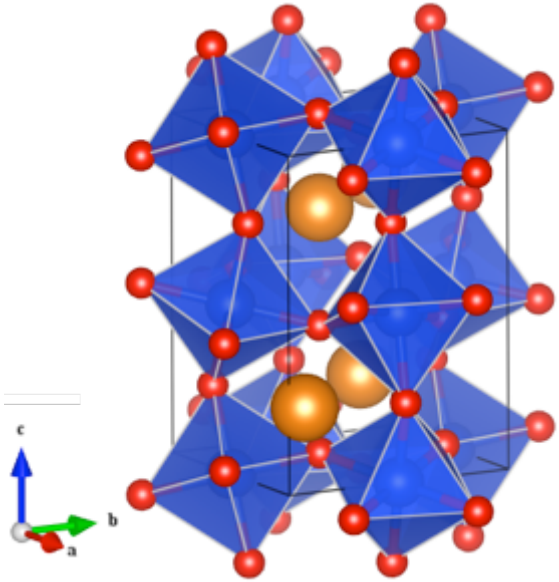
100 nm shortening for a 10 cm sample….

From crystals to mantle flow



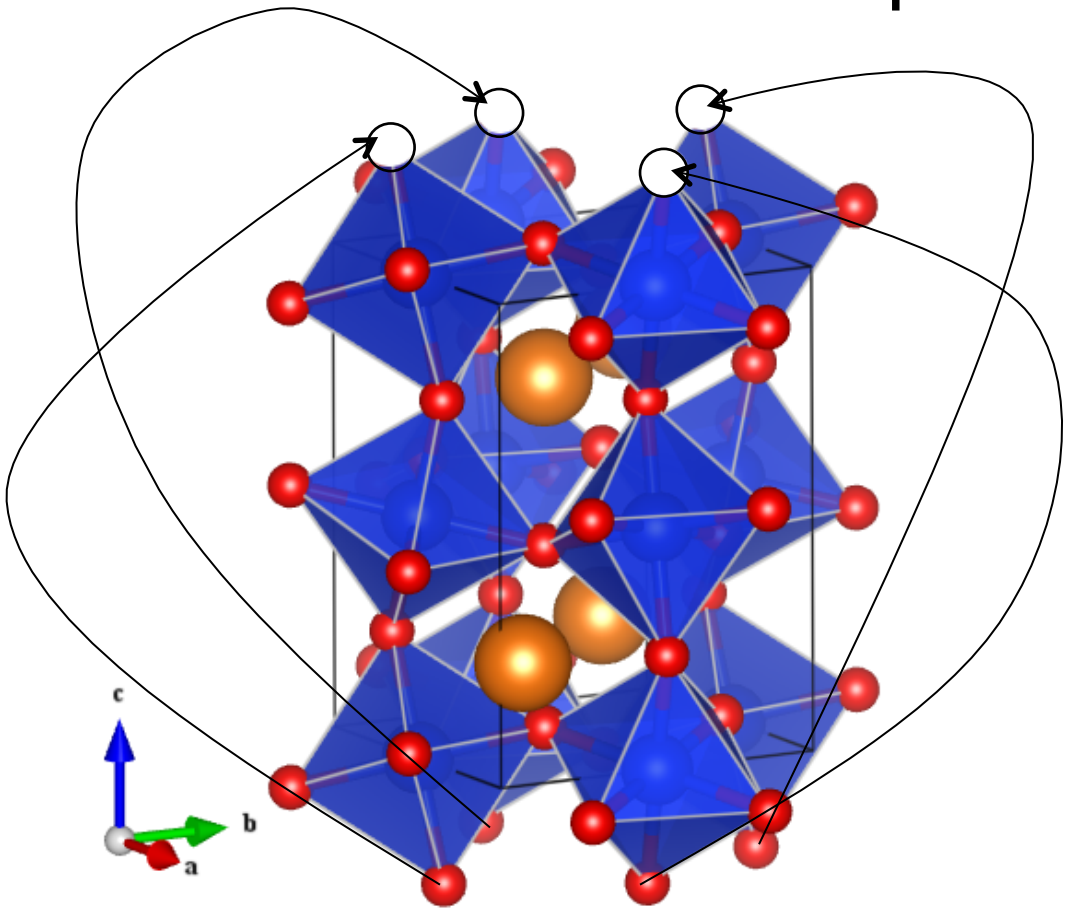
© B. Schuberth

Can we bridge scales ?



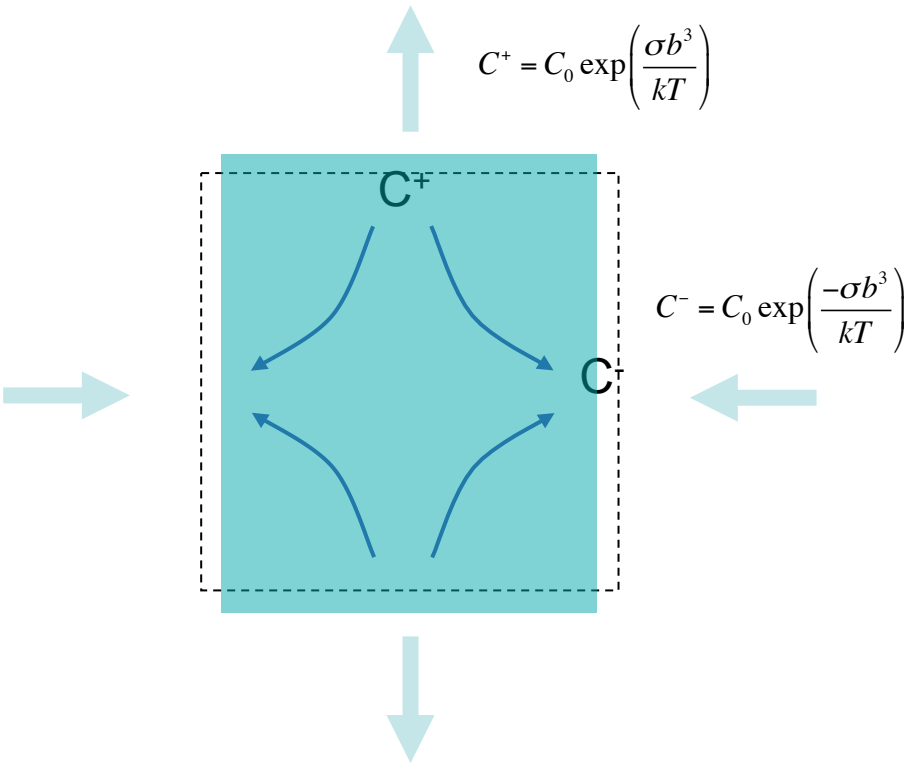
Deforming crystals

transport of matter



Diffusion creep

- Nabarro (1948) - Herring (1950) creep



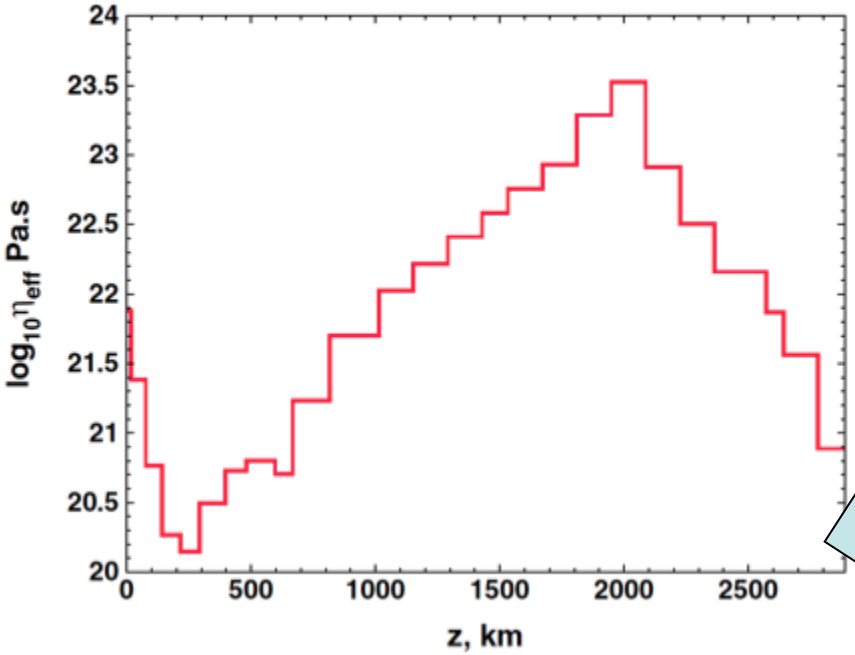
$$J = -D_v grad C \approx \alpha D_v \frac{C^+ - C^-}{d}$$

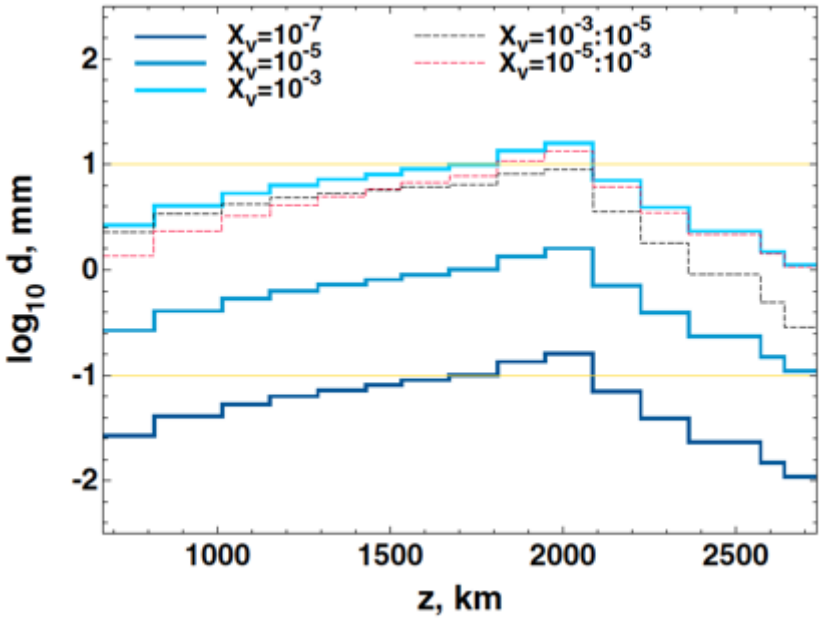
$$\dot{\varepsilon} = \alpha \frac{D_{sd} \sigma \Omega}{d^2 kT}$$

$$\sigma = \frac{d^2 kT}{\alpha D_{sd} \Omega} \dot{\varepsilon}$$

Newtonian

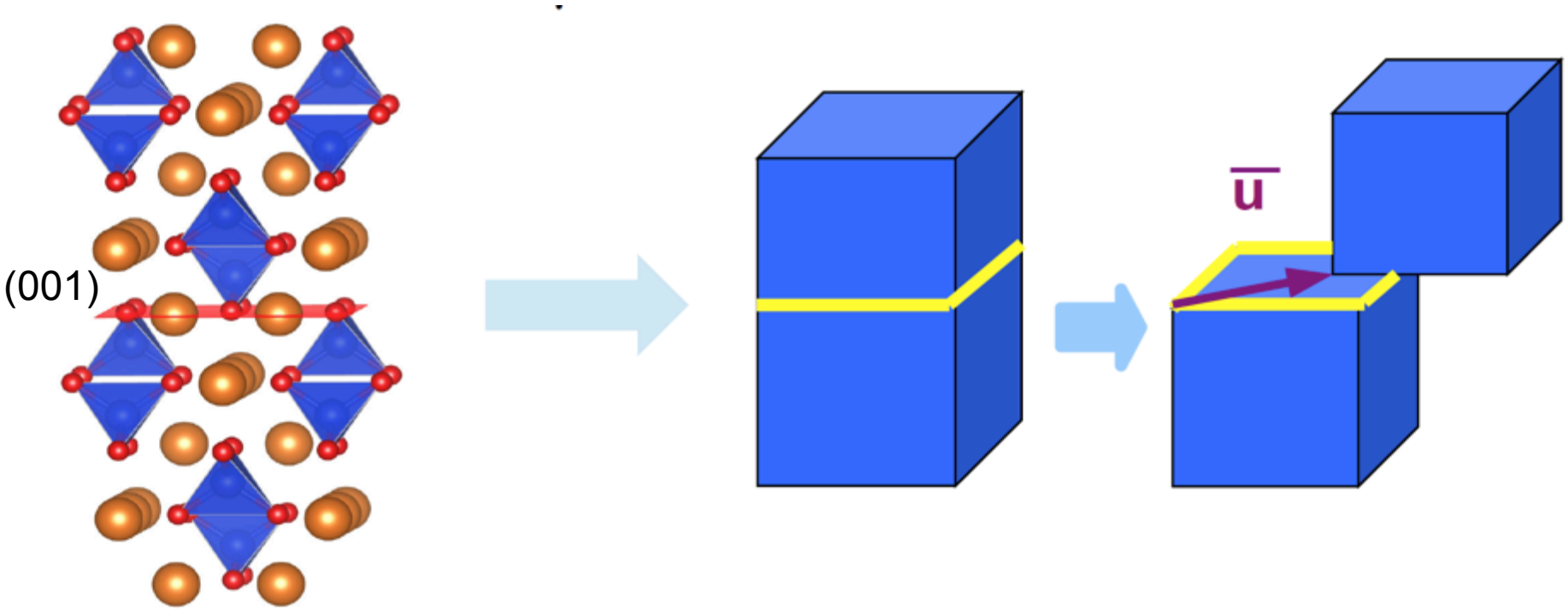
Diffusion creep in the mantle





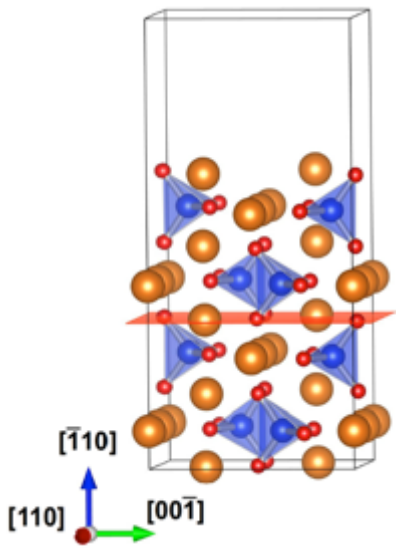
Glišovic et al. (2015)

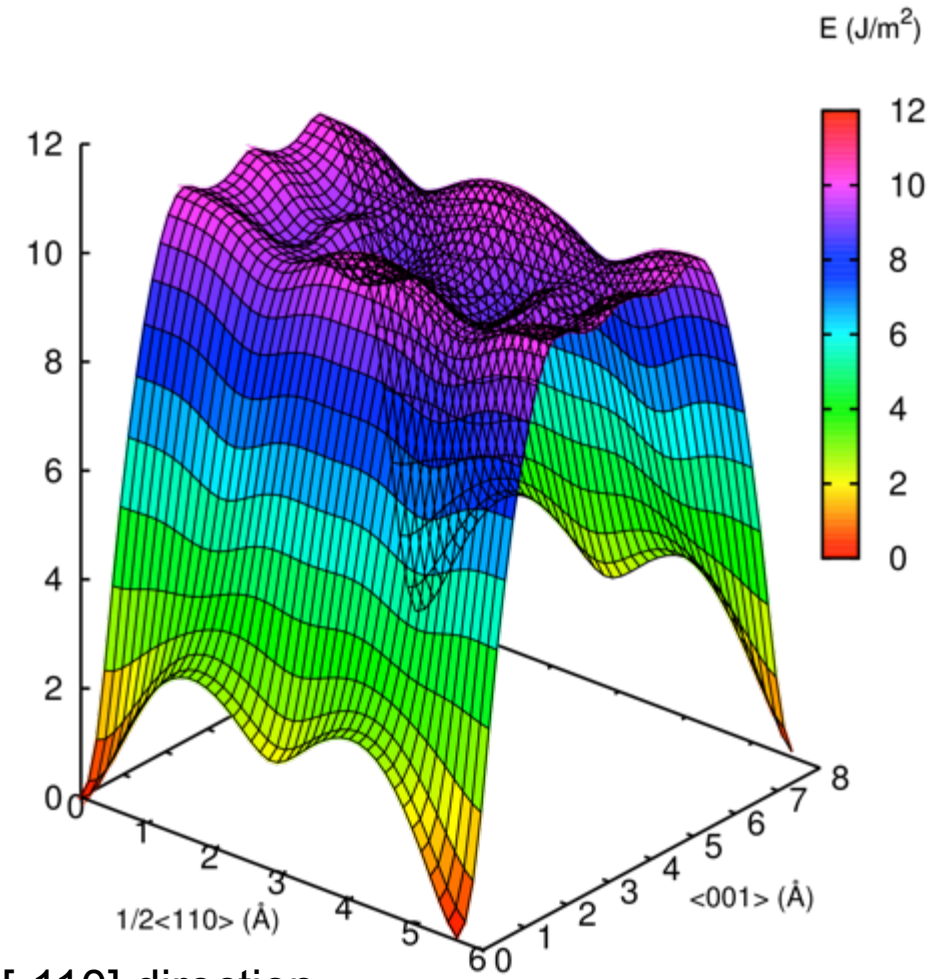
Shearing crystals



Shearing crystals

Ringwoodite (20 GPa)
(110) plane





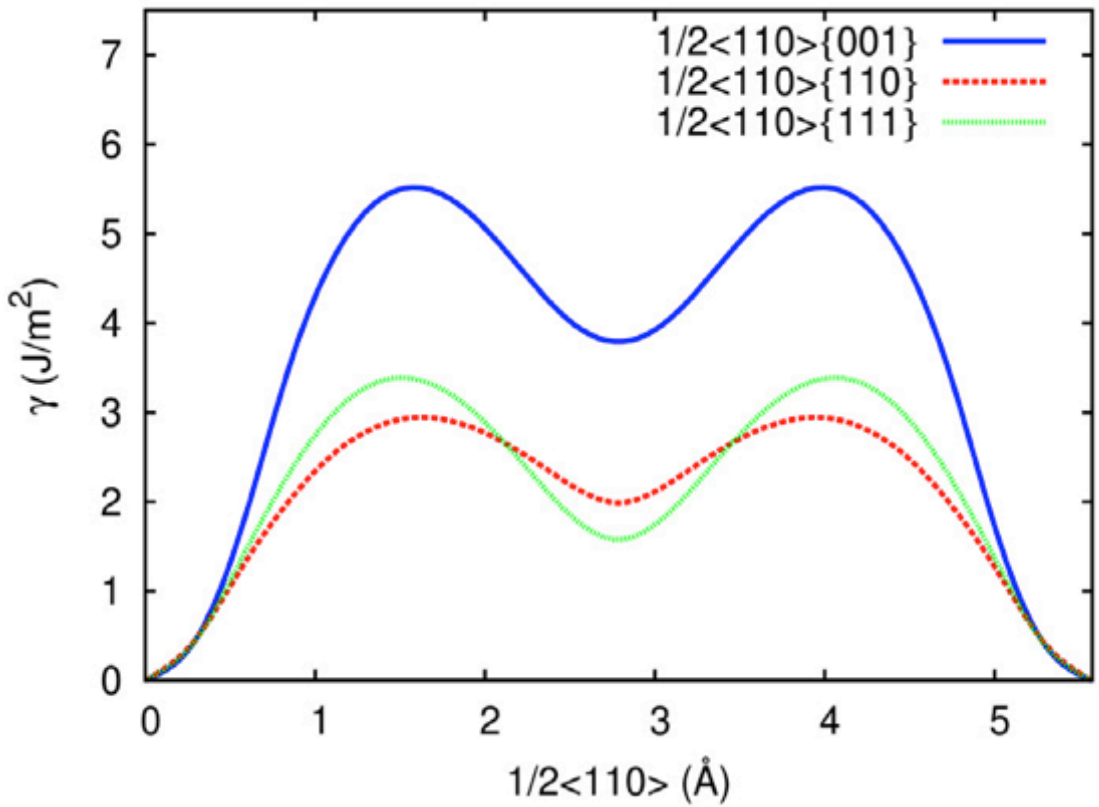
Easy shear path along the ½[-110] direction

Defines the **Burgers vector**

Ritterbex et al. (2015)

Slip systems

Ringwoodite (20 GPa)

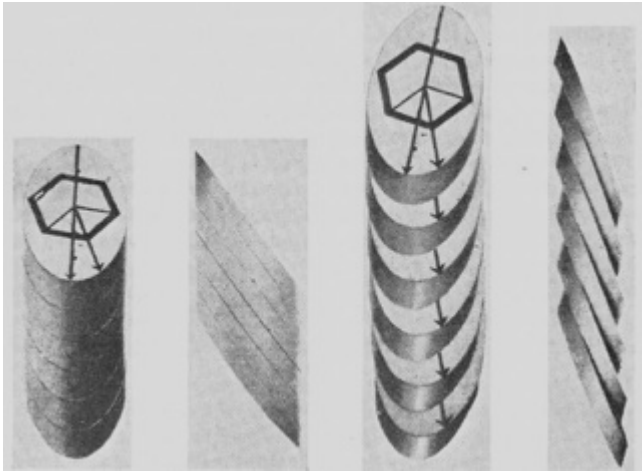


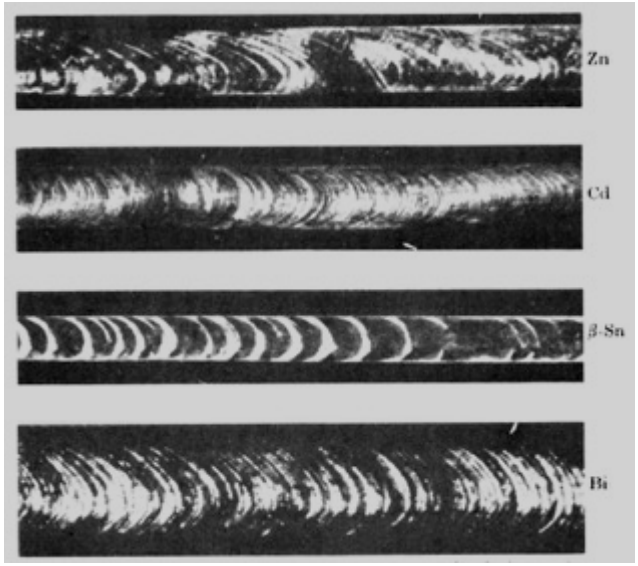
Slip along <110> in: {001}
{110}
{111}

Ritterbex et al. (2015)

We learnt: Slip systems

Plasticity of crystals - Schmid & Boas (1950)





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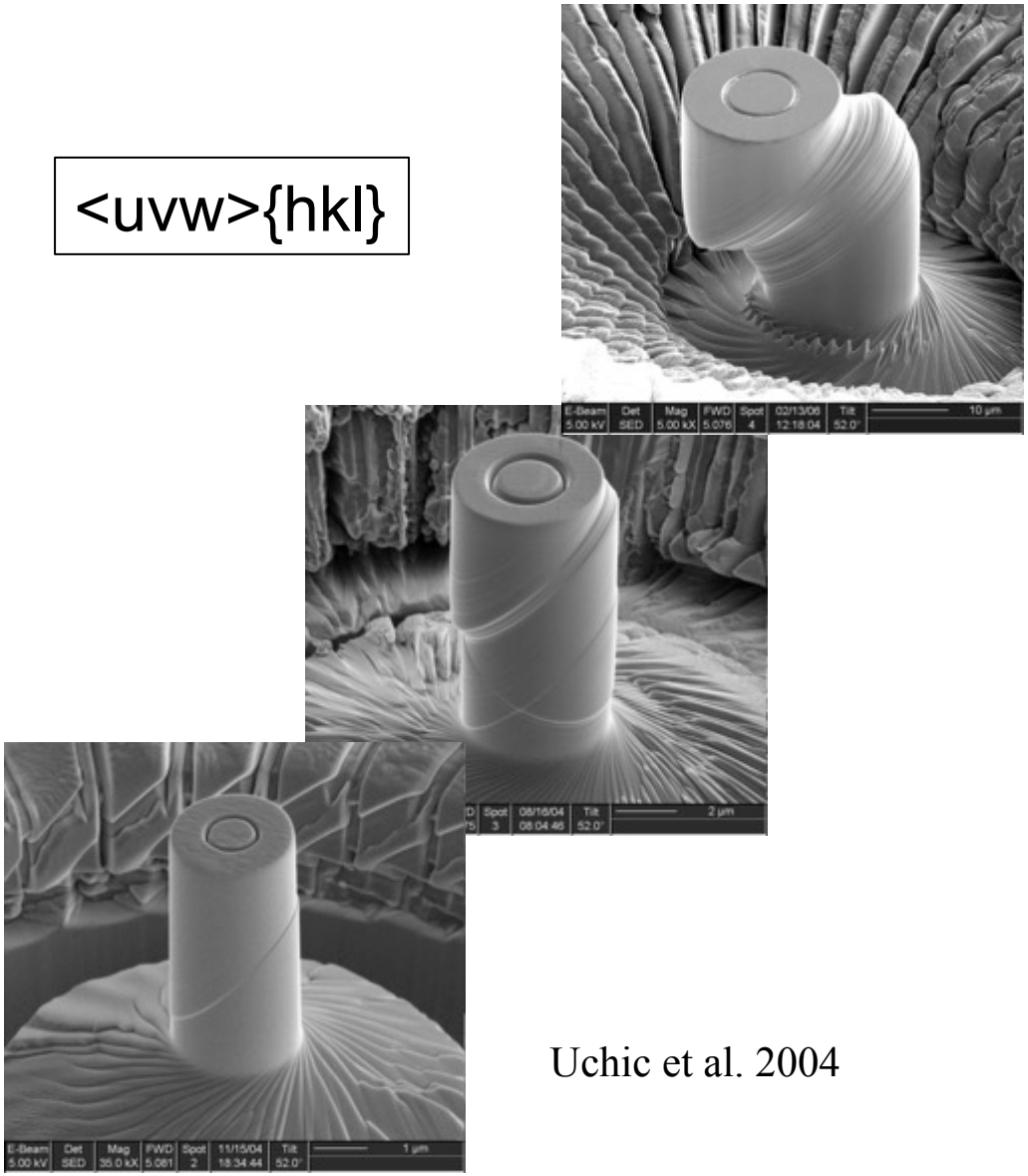
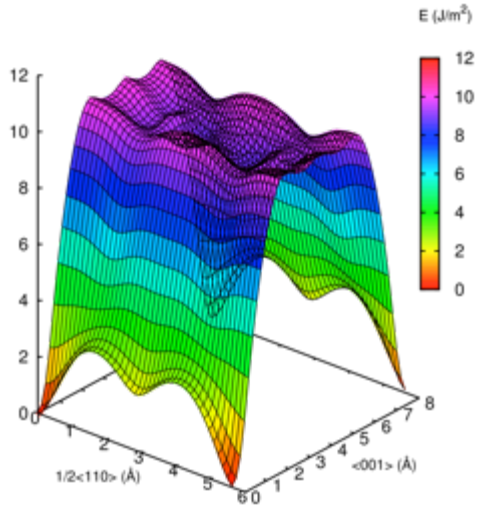


Uchic et al. 2004

We don’t understand: stresses



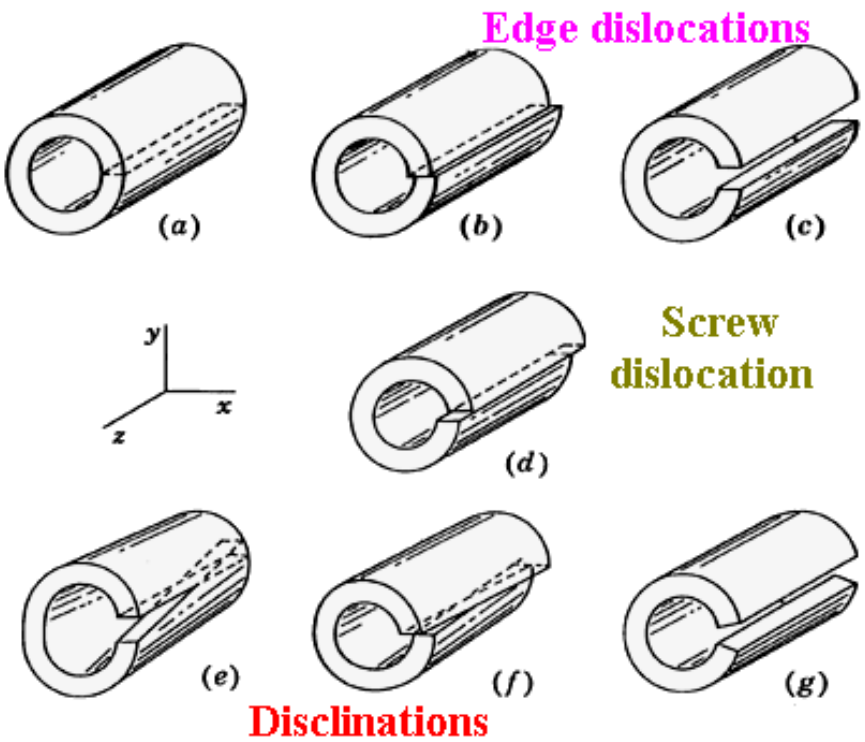
τ_{max}/μ = 0.2-0.3

Two to four orders of magnitude too large

Need for defects: dislocations

The Volterra defects

Vito Volterra (1860-1940)



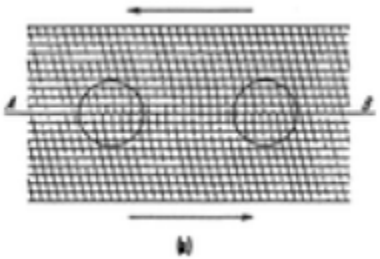
Vito Volterra, Sur les Distorsions des corps élastiques, Gauthier-Villars, Paris, 1960

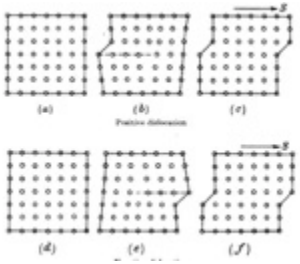
Crystal defects: dislocations

Egon Orowan

Sir Geoffrey Ingram Taylor

Michael Polanyi





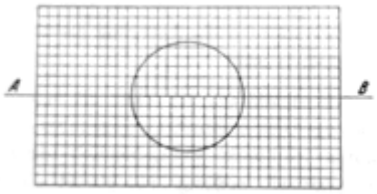
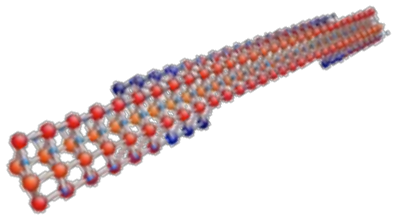


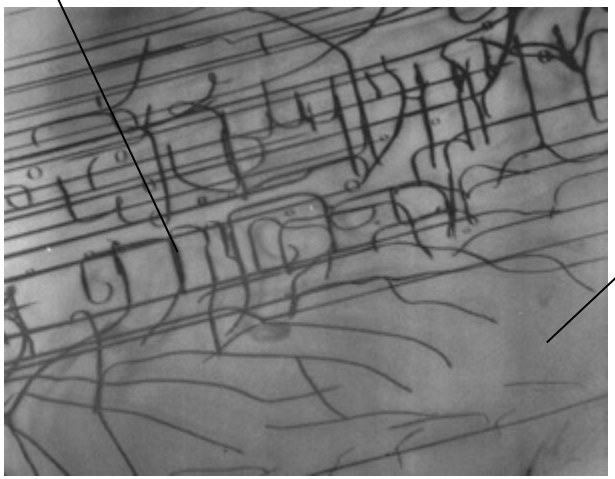
Fig. 1. Schema einer Gitterversetzung.

1934

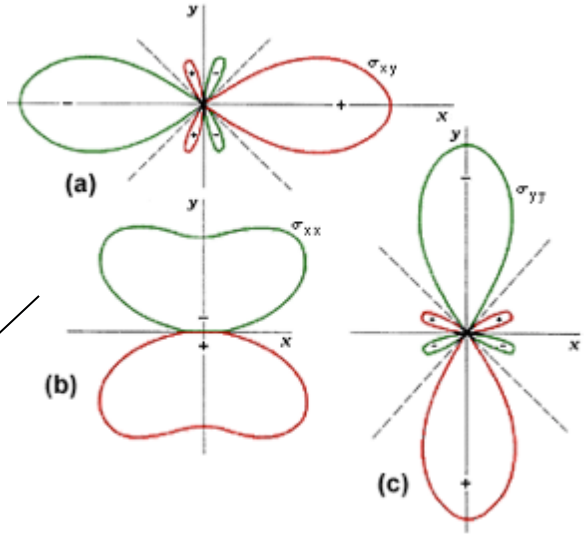
Dislocations duality

Near field: atomistic





Far field: elastic

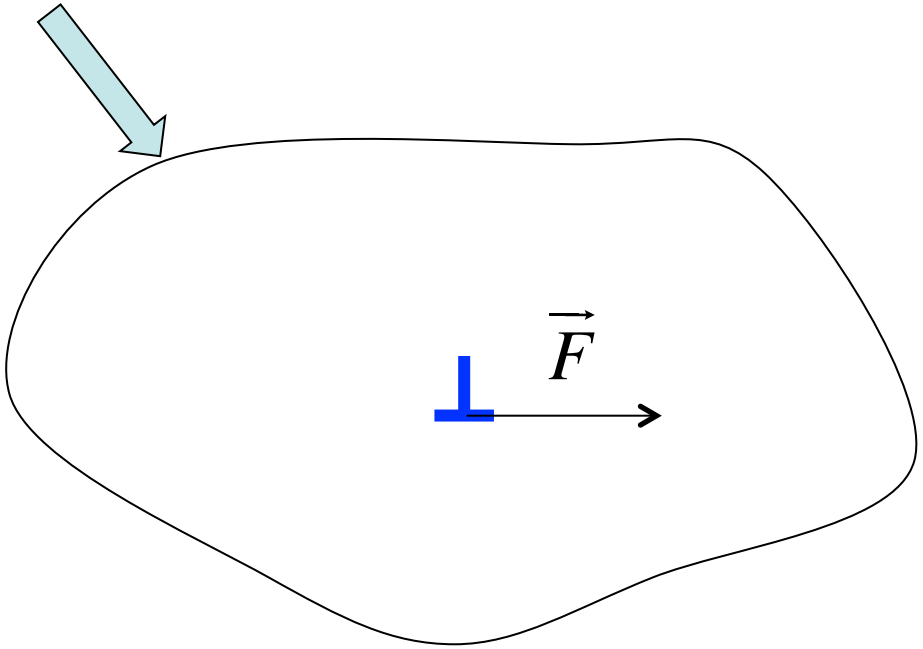


$$\sigma = \frac{\mu b}{2\pi r} f(\theta)$$

Long-range interactions

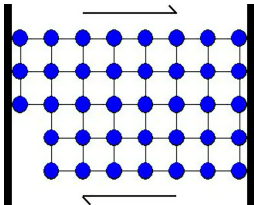
Dislocations respond to stress

External loading $\overline{\overline{\sigma}}$



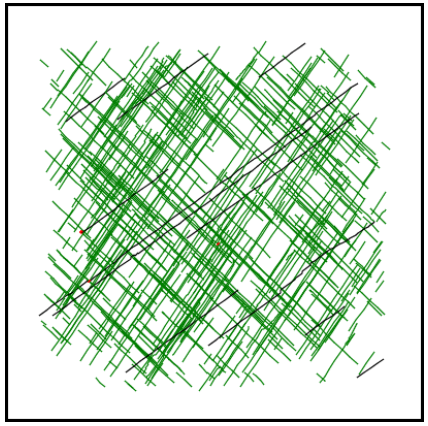
Peach & Koehler (1950) force : $\vec{F} = \overline{\overline{\sigma}}.\vec{b} \times \vec{L}$

velocity $\vec{v}$

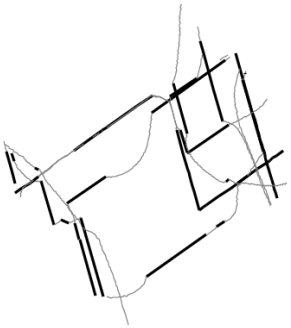


From dislocations to plasticity: the toolbox

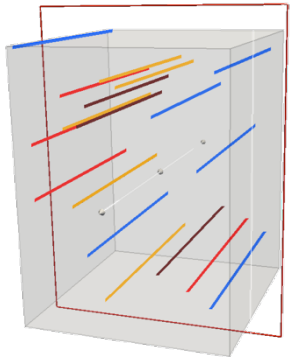
- 3D dislocation dynamics



MgO
J. Amodeo et al.
Mechanics of Materials 71 (2014) 62–73



- 2.5 D dislocation dynamics



Olivine
Boioli et al. (2015)

- Orowan equation

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

Strain rate

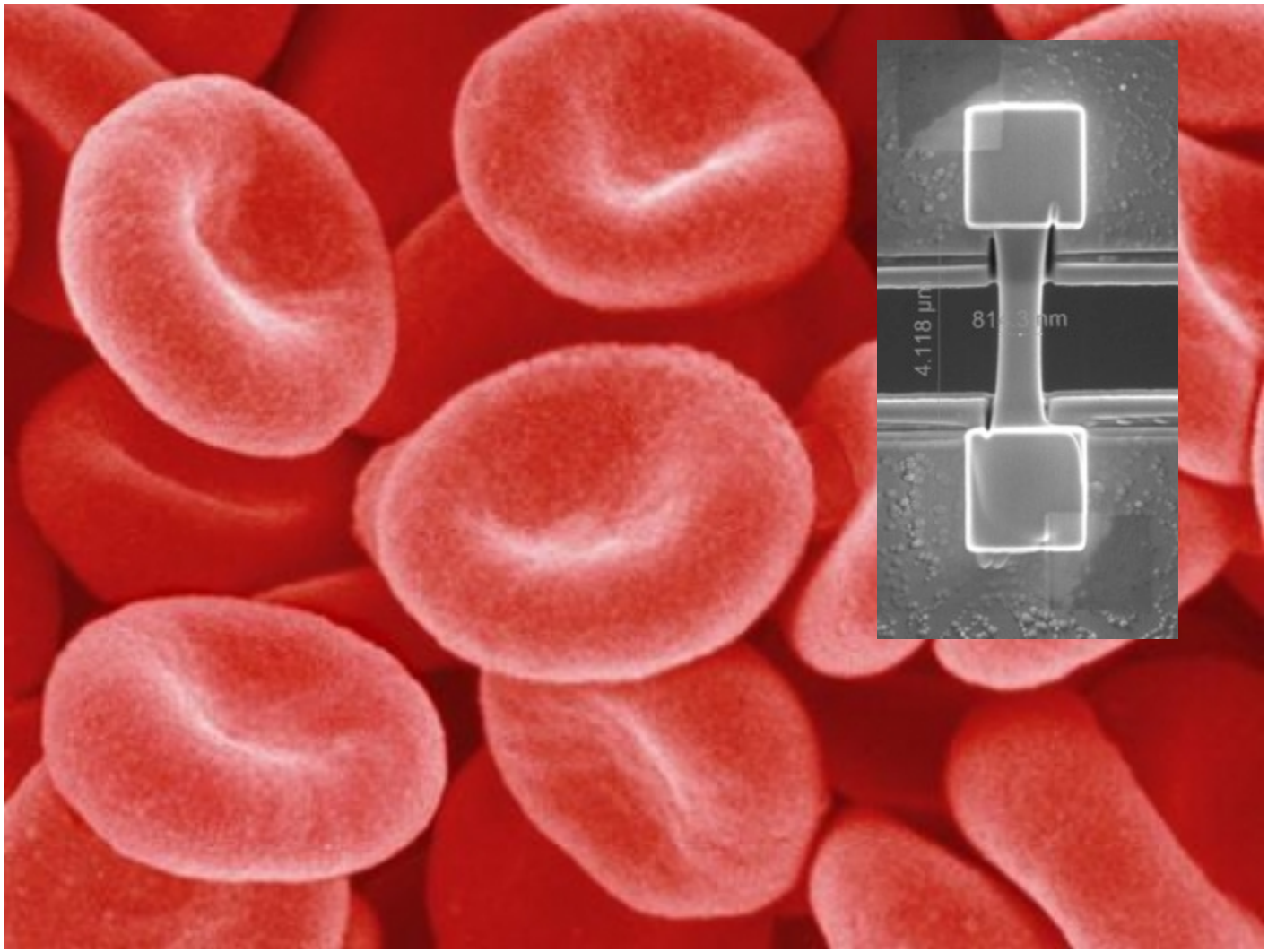
Dislocation density

Burgers vector modulus

Dislocation velocity

Dislocation velocities: can we measure ?

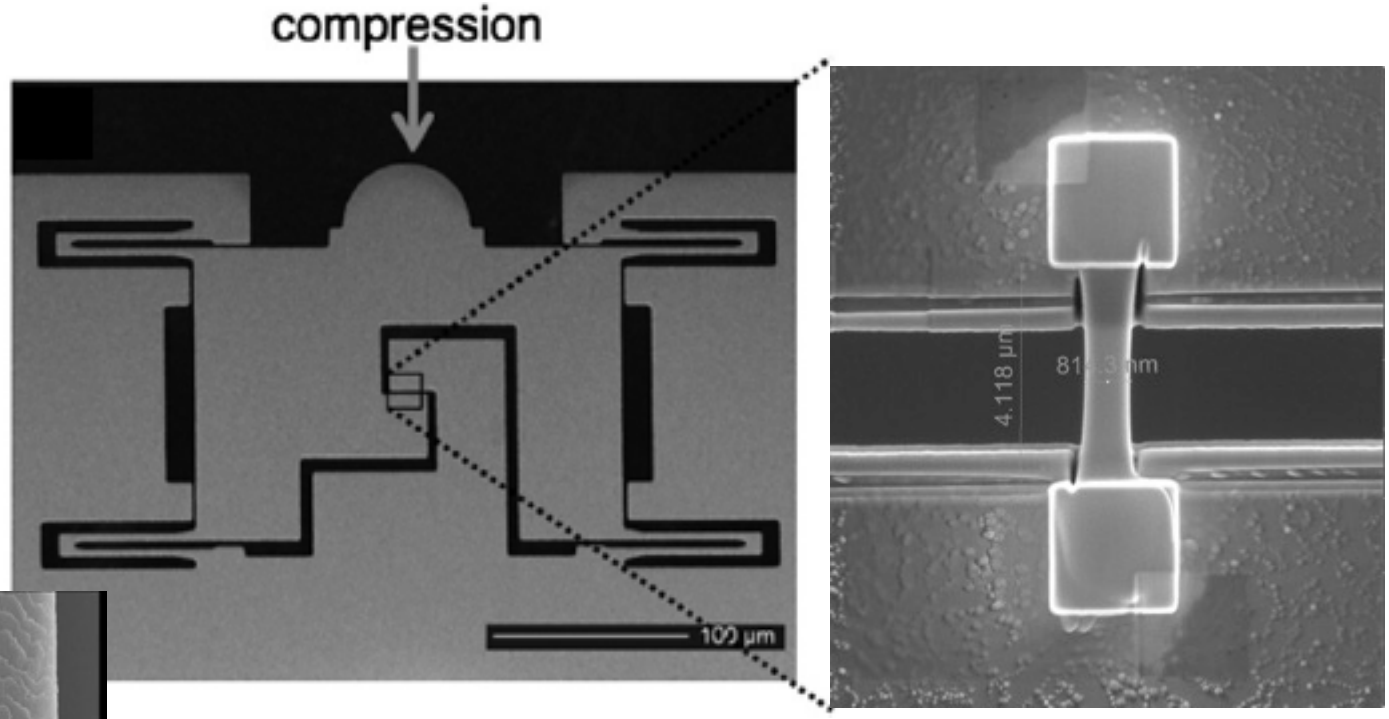
New approack based on nanomechanical testing of olivine in the TEM

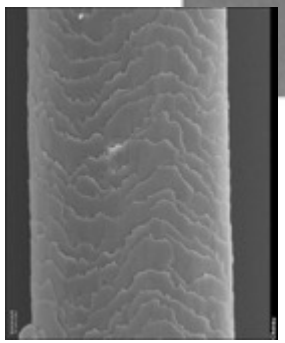


Nanomechanical testing in the TEM

The Push-to-Pull device (Hysitron®)

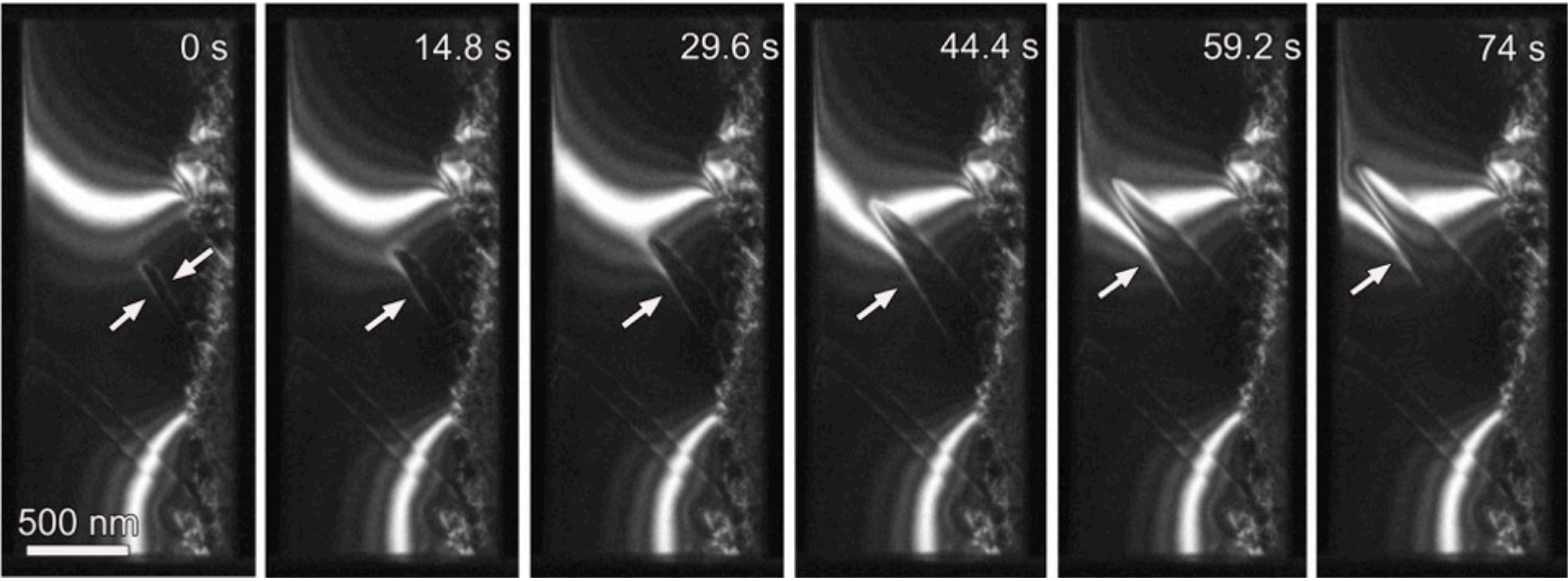
Collaboration with H. Idrissi Antwerpen, Belgium
& C. Bollinger, Bayreuth, Germany



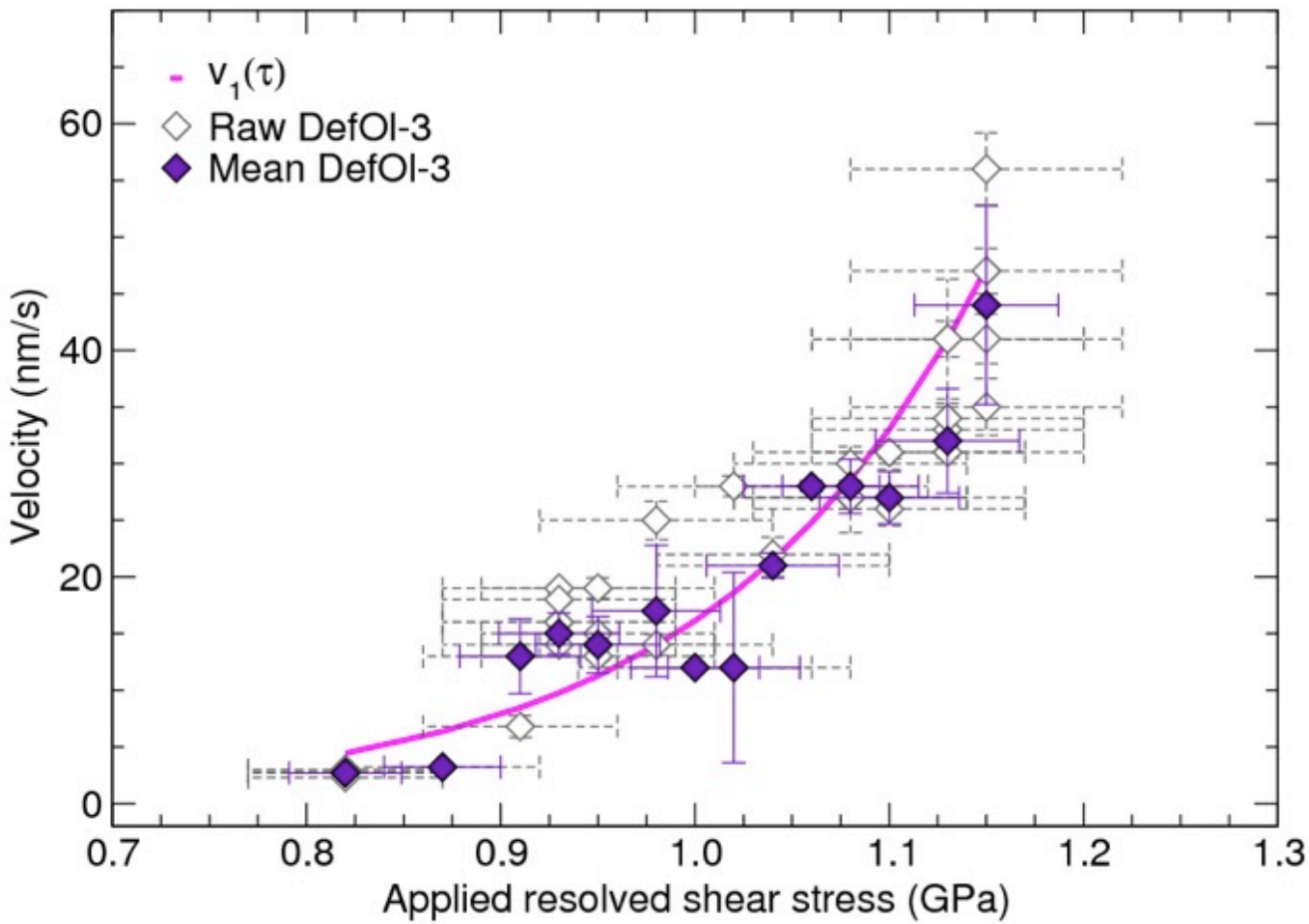


Hair

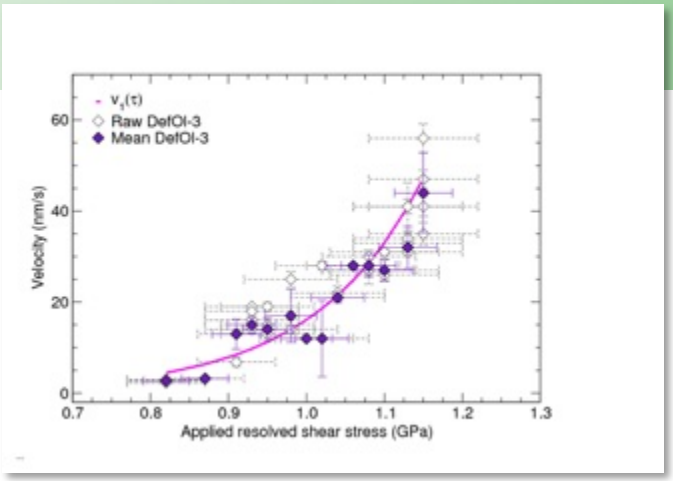
Nanomechanical testing in the TEM

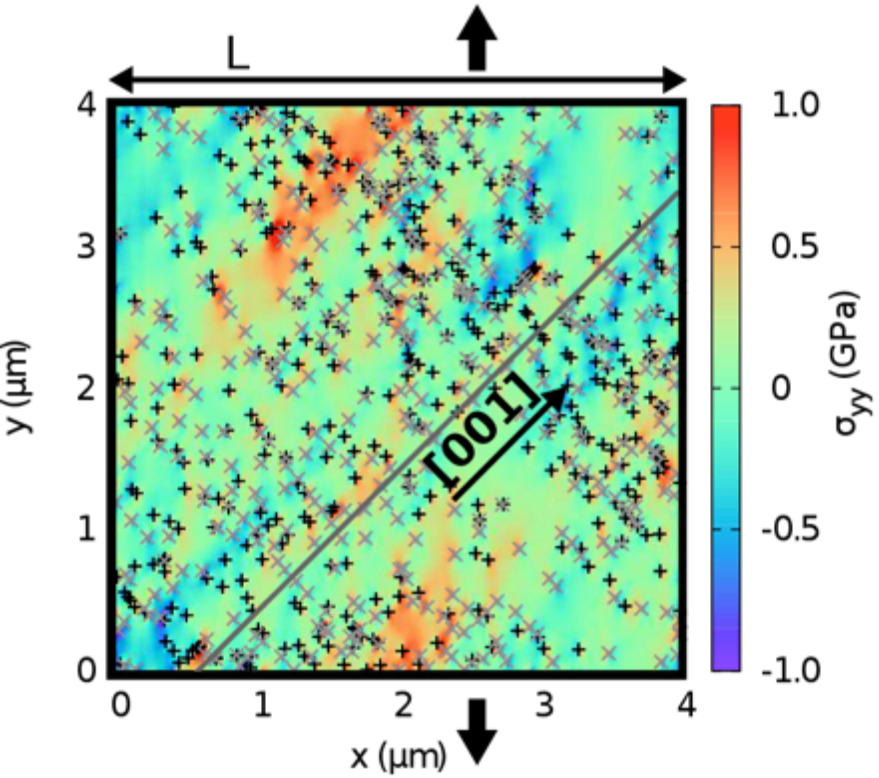


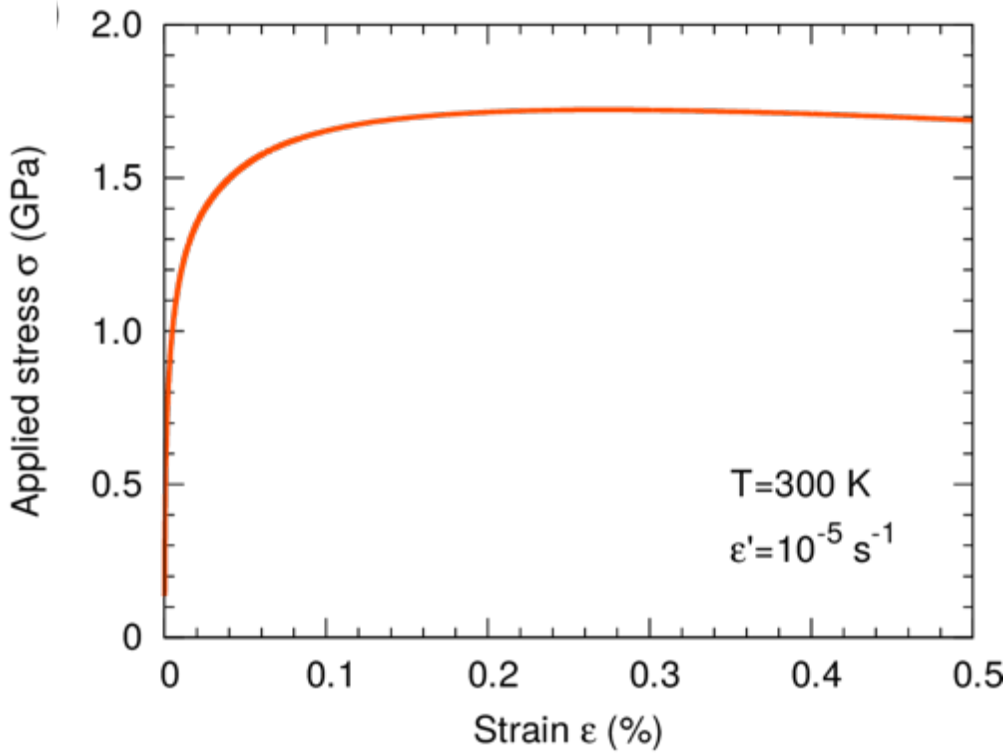
Nanomechanical testing in the TEM



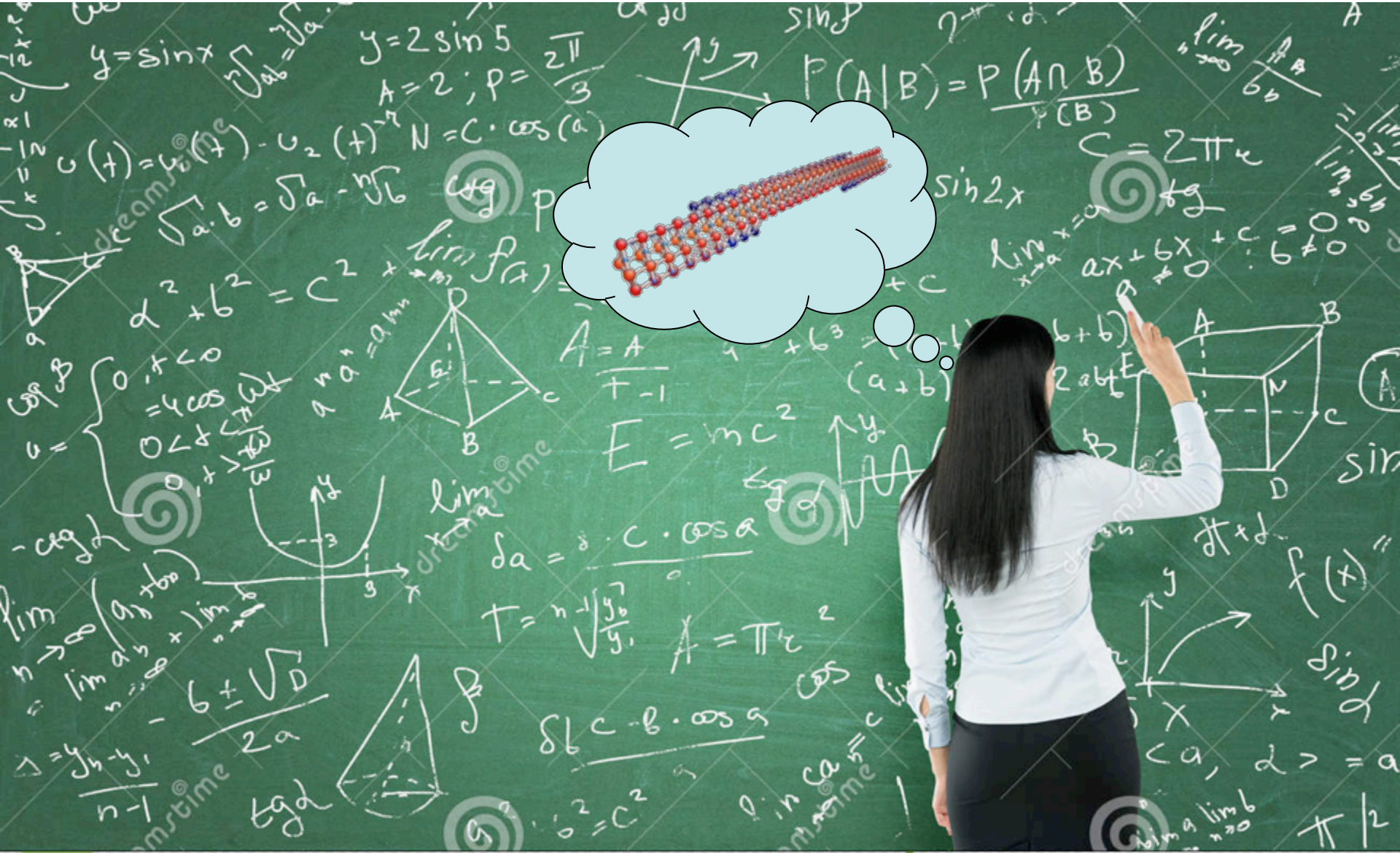
Nanomechanical testing in the TEM







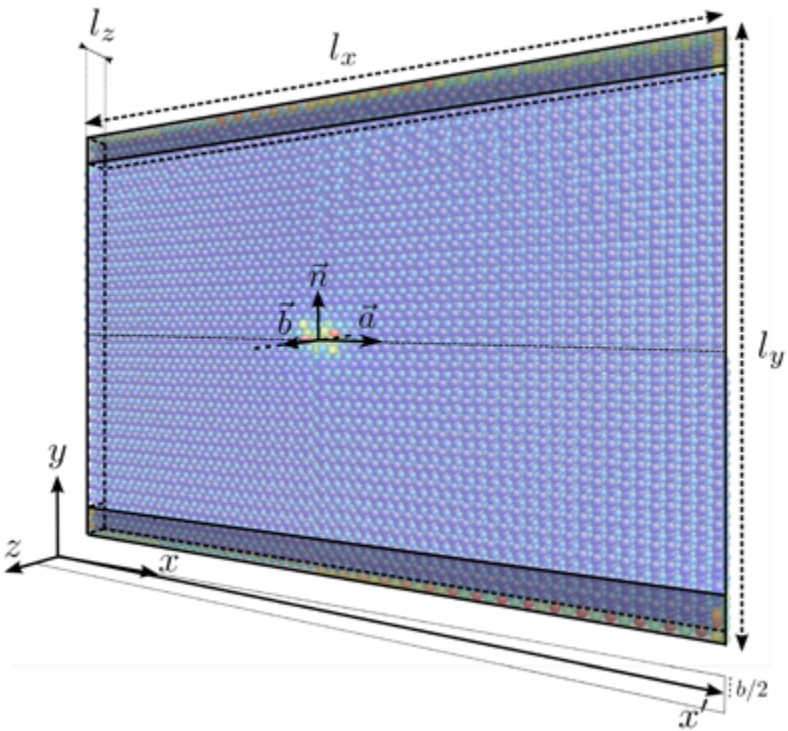
Dislocation velocities: can we calculate ?

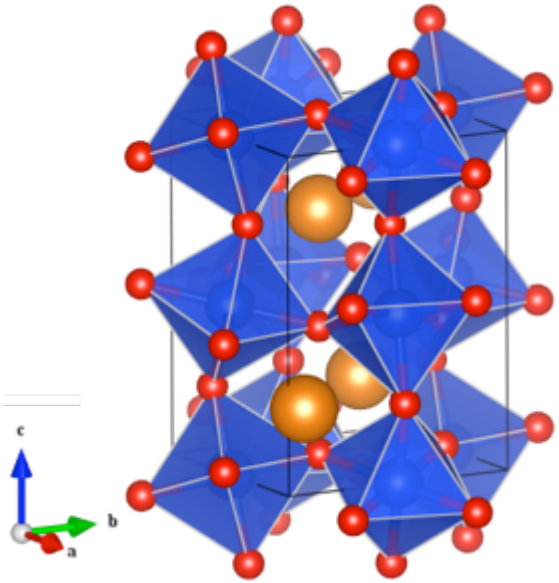


Dislocation core modeling

Perovskite $MgSiO_3$: orthorhombic: 20 atoms / unit cell

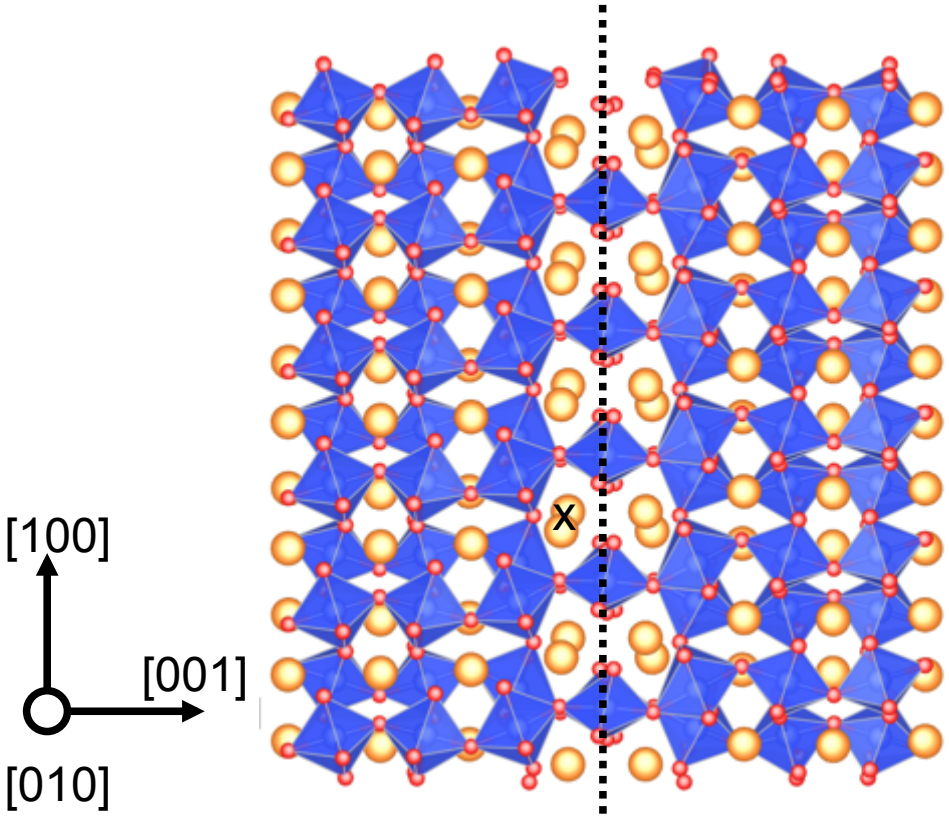
LAMMPS molecular statics
30 000 atoms



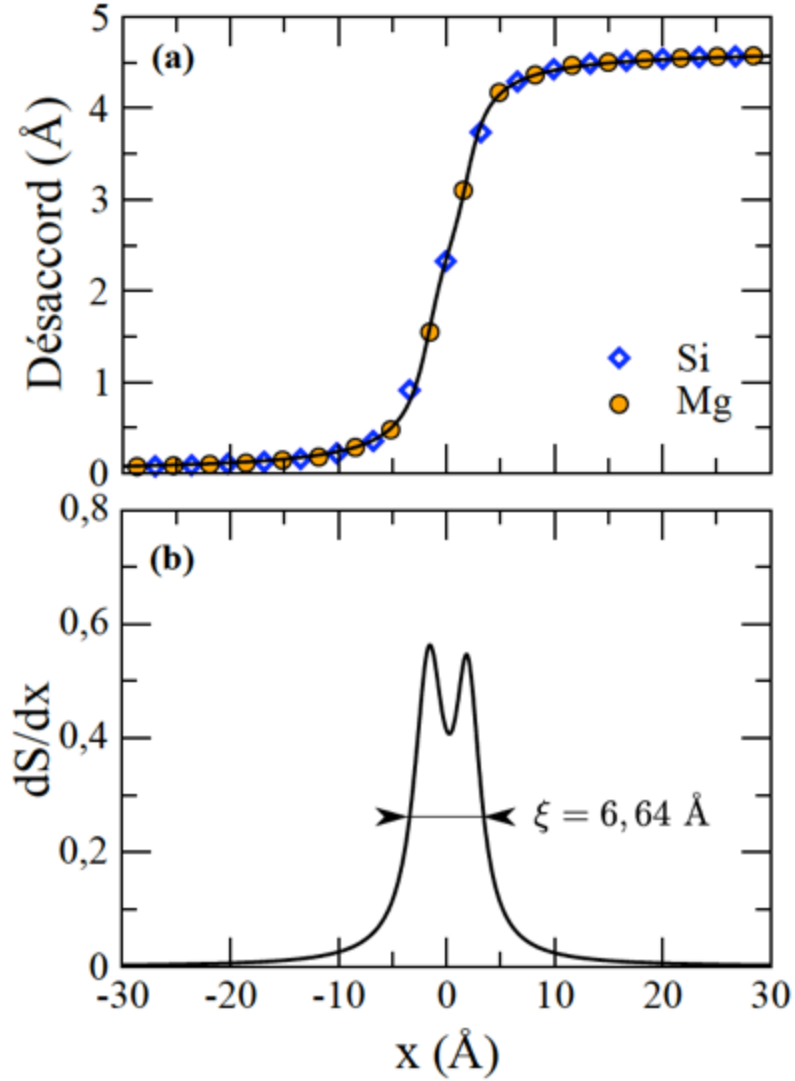


Antoine Kraych's PhD

Atomic structure of dislocations



[100] screw dislocation in bridgmanite at 30GPa

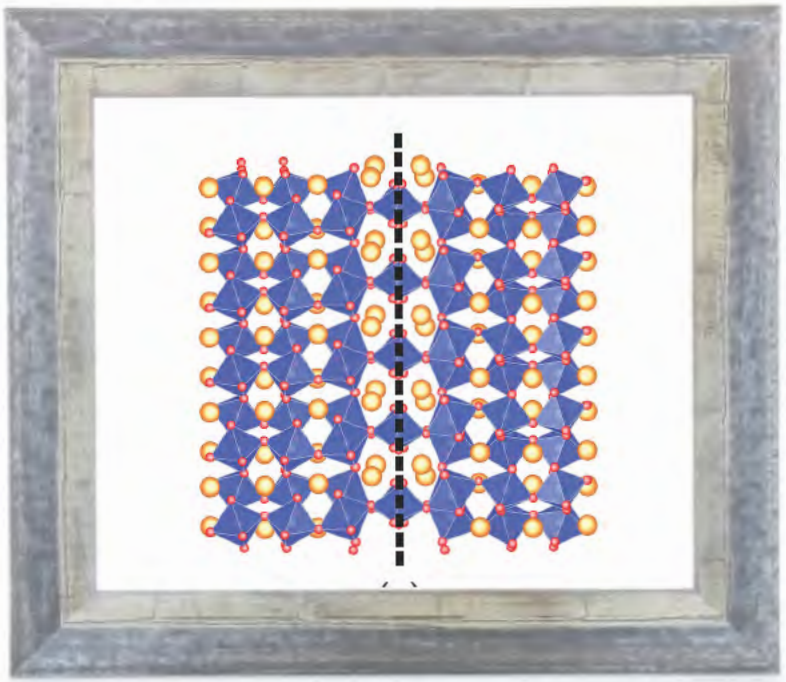


Density of Burgers vector in (010) planes (30GPa)

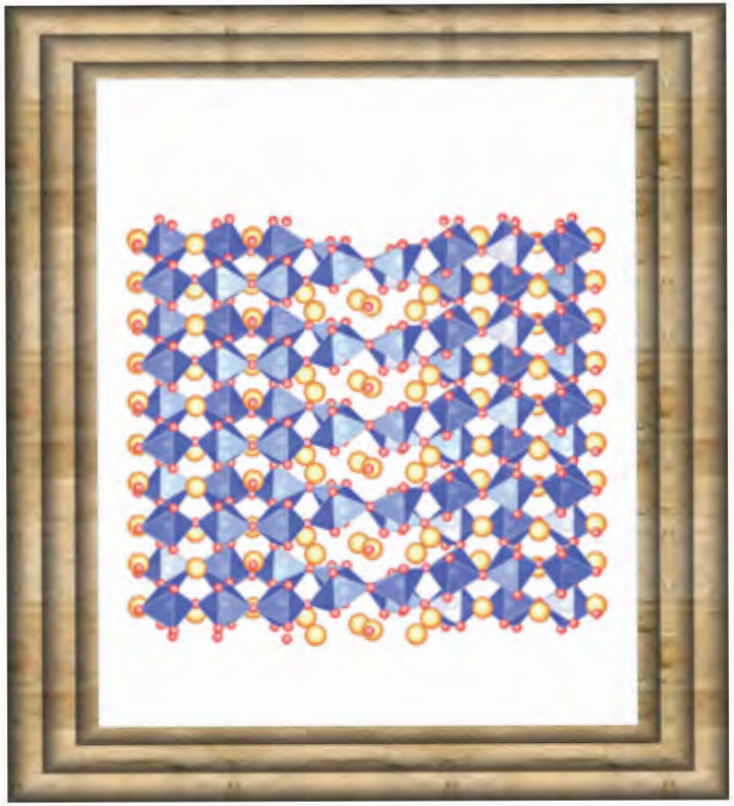
Dislocation position along [001] (Å)

Dislocation gallery

Bridgmanite

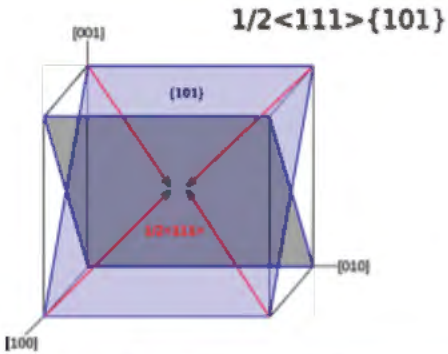


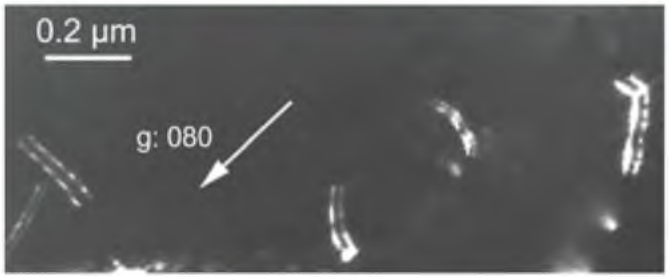
[100](010)



[010](100)

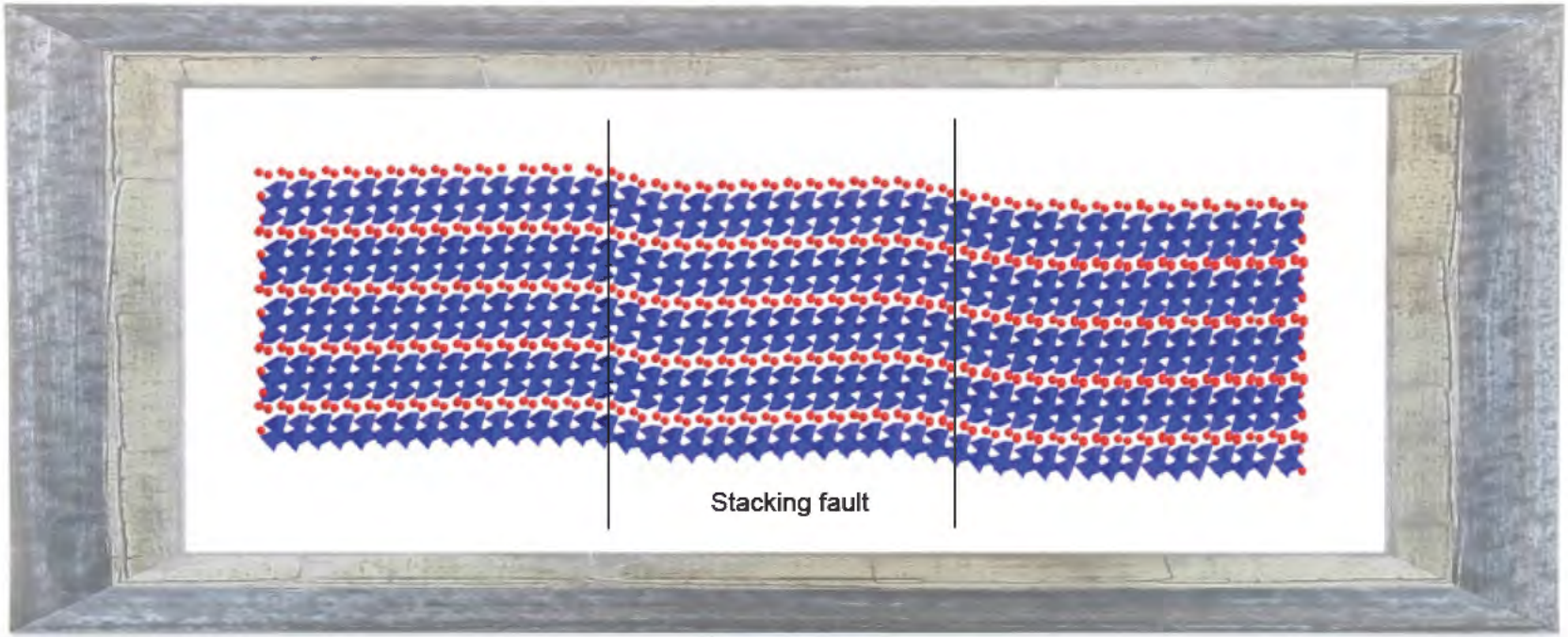
Dislocation gallery





Courtesy E. Thurel

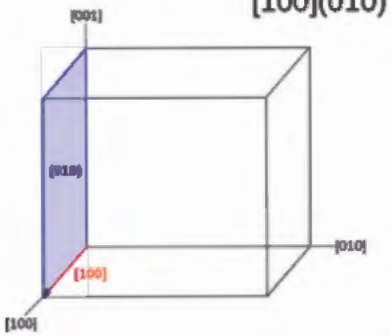
Wadsleyite



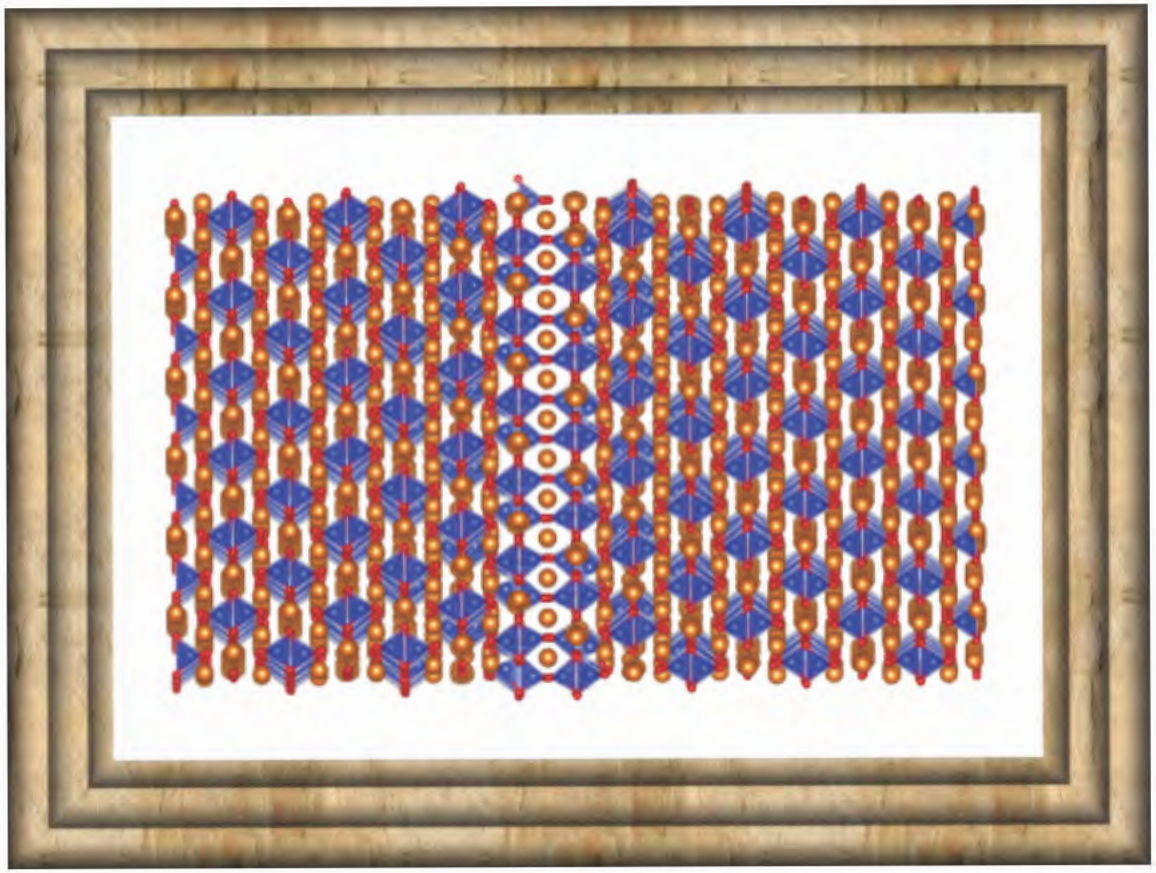
½ [111](101)

Dislocation gallery

[100](010)

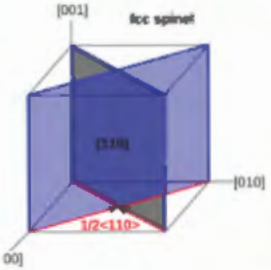


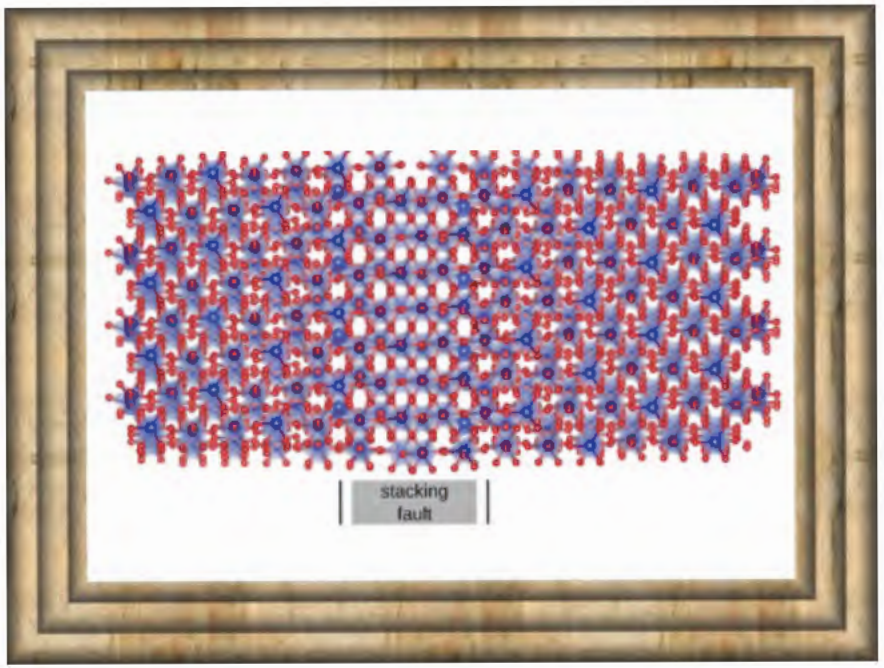
Wadsleyite

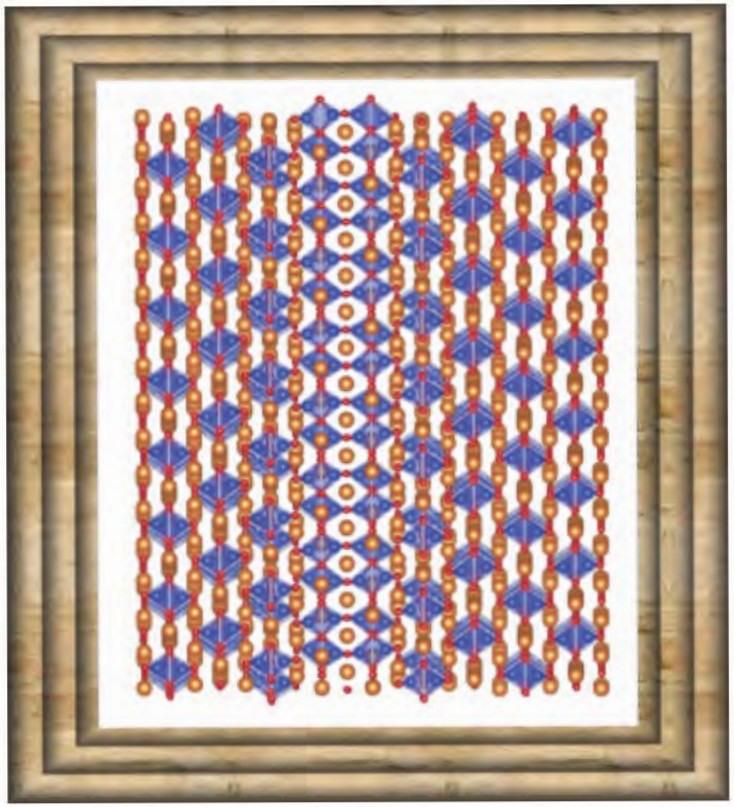


Dislocation gallery

1/2<110>{110}







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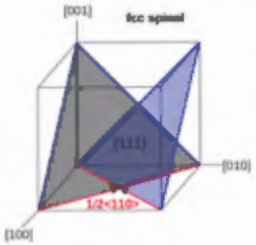
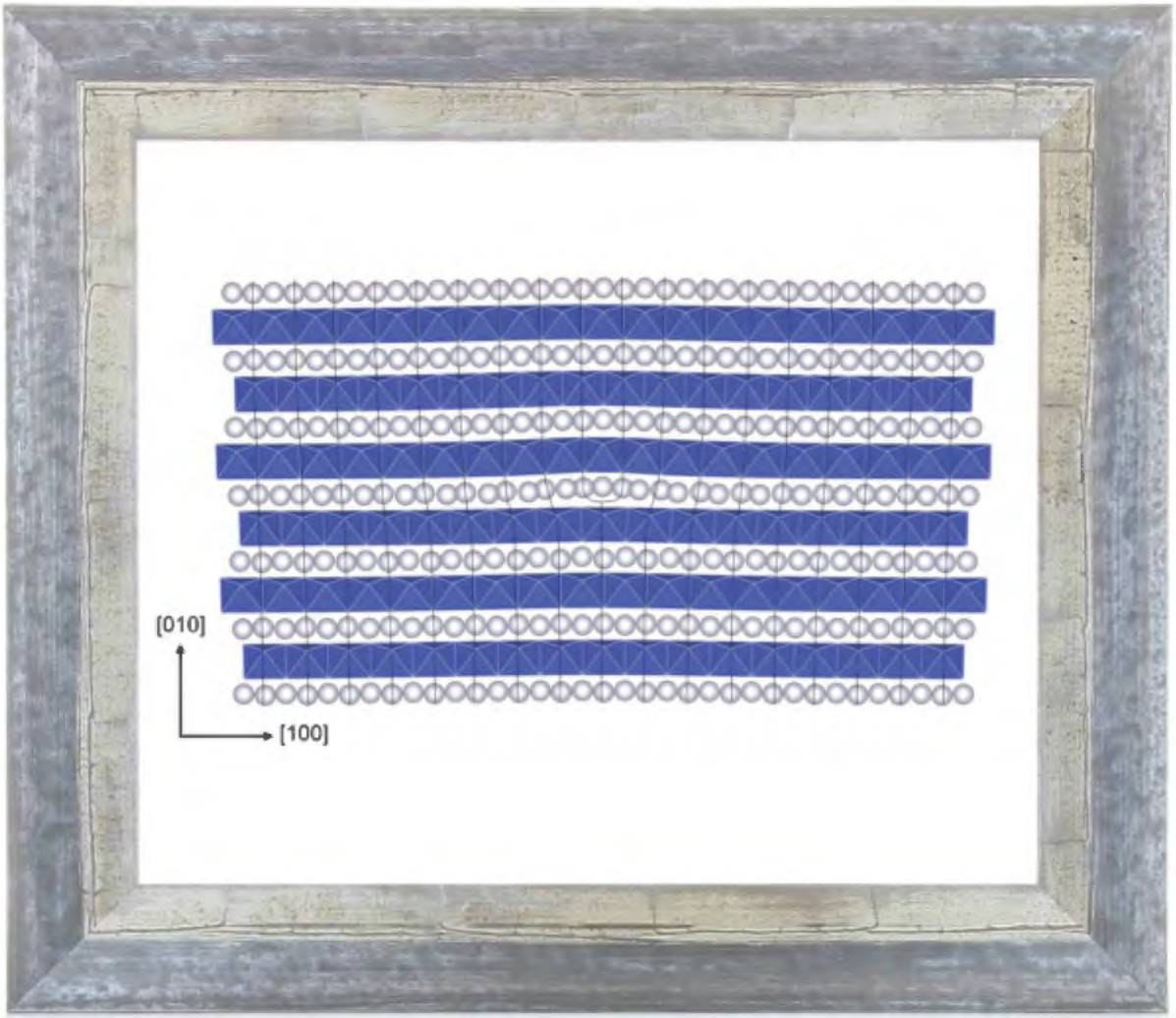


Ringwoodite

Dislocation gallery

Post-perovskite



[100](010)

Stop 2

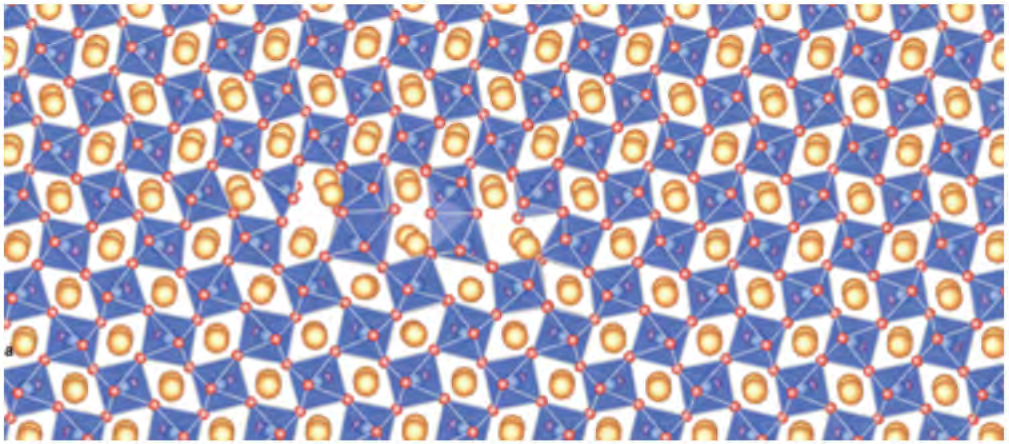
- We know: the « crystallography of defects »

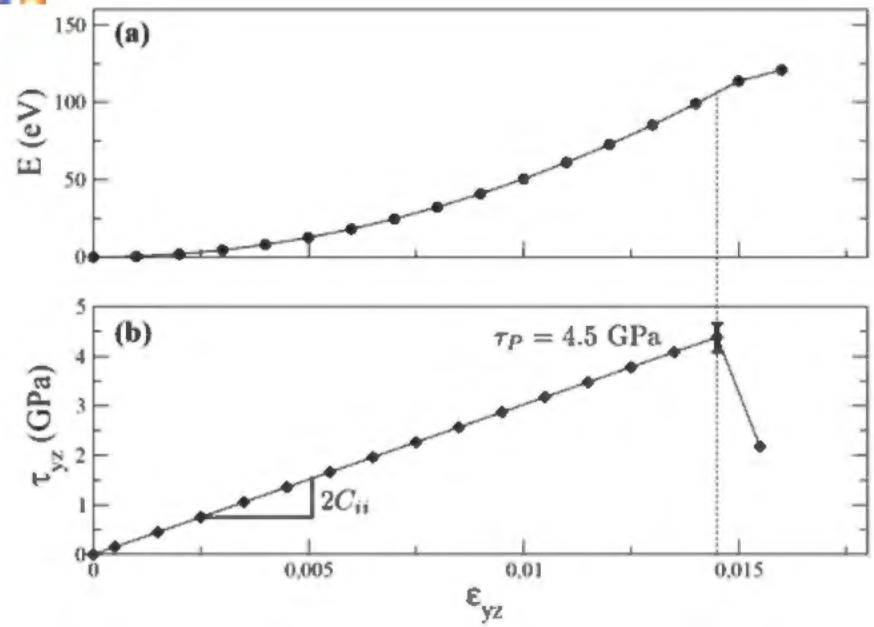
- We don't know: their « dynamics »

Questions:

- Do dislocations move easily when stress is applied ?
- What is their velocity
- How doest it depend on stress ? temperature ?

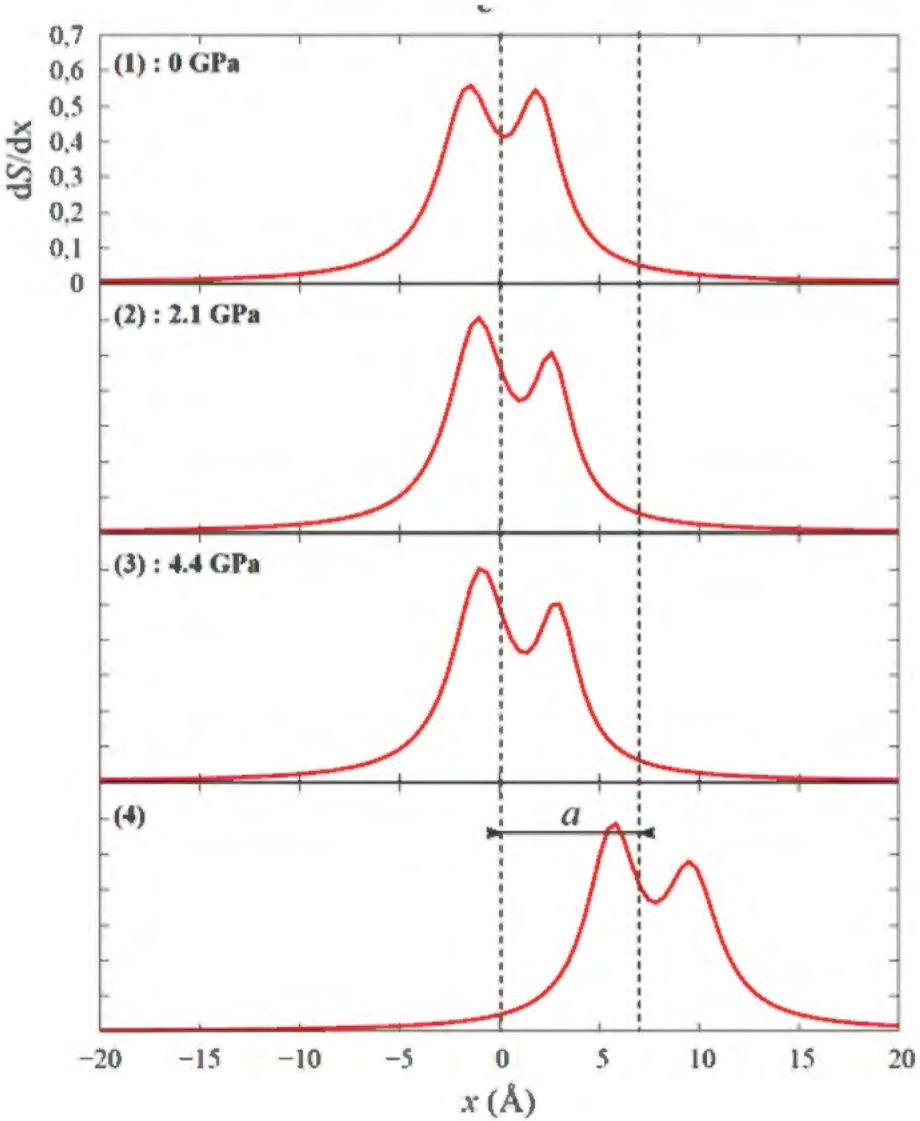
Lattice friction: the brutal force



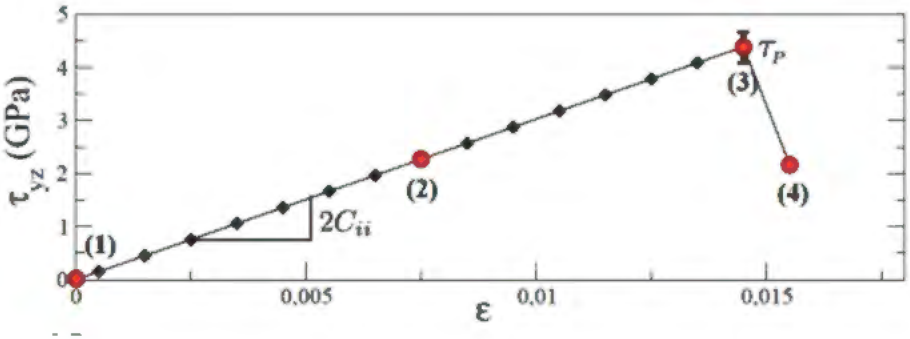


Peierls stress

Lattice friction

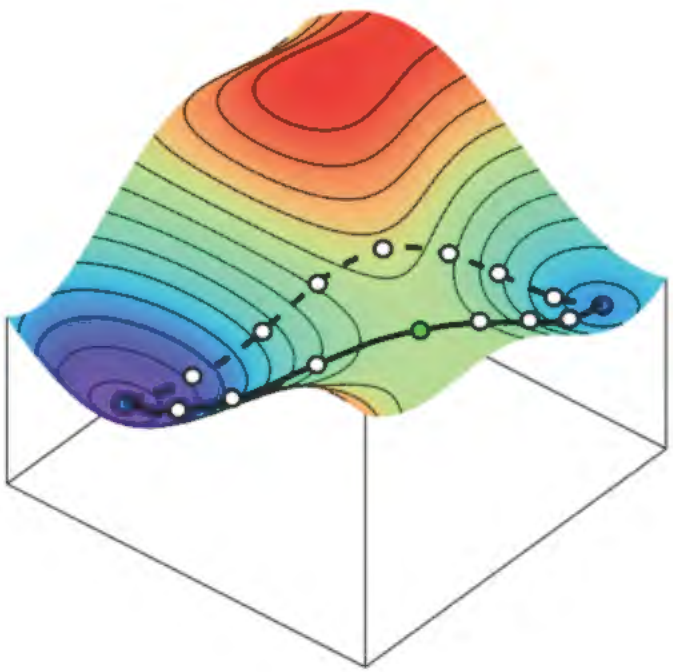


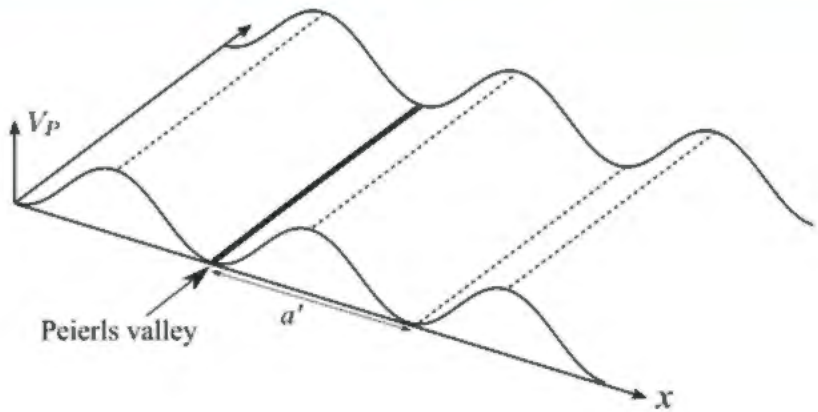
[100](010) in bridgmanite at 30 GPa

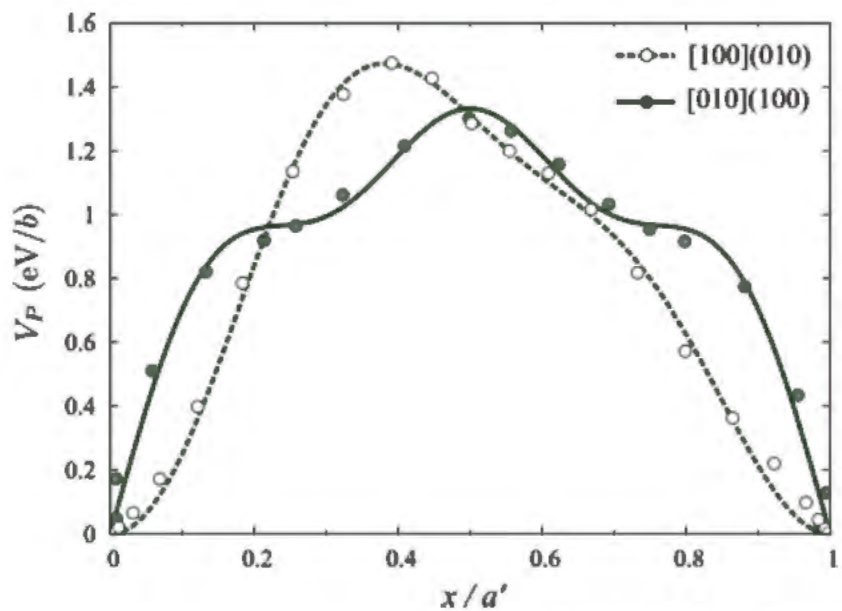


Lattice friction: calculation of the Peierls potential

The "Nudged Elastic Band" (NEB) method
→ energy barrier

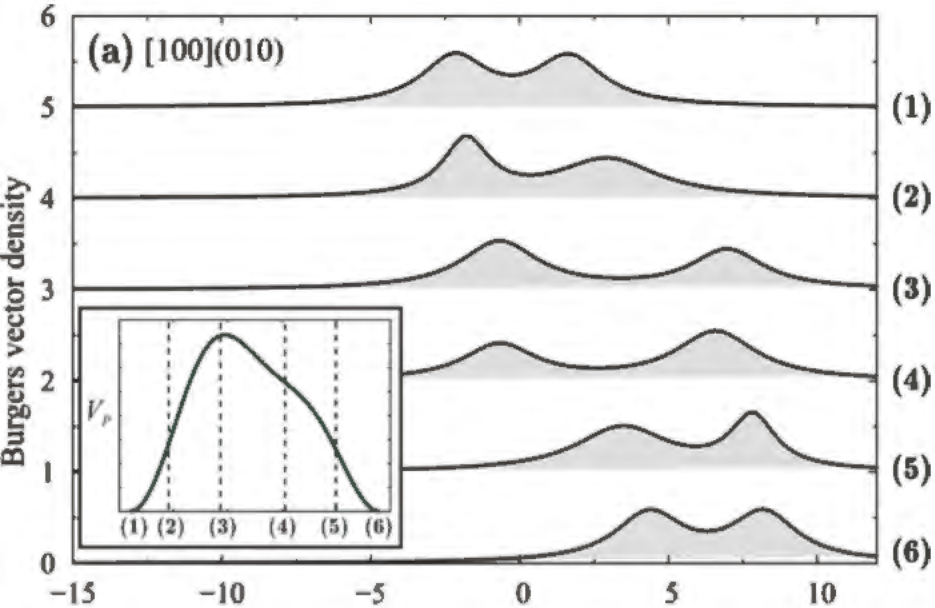


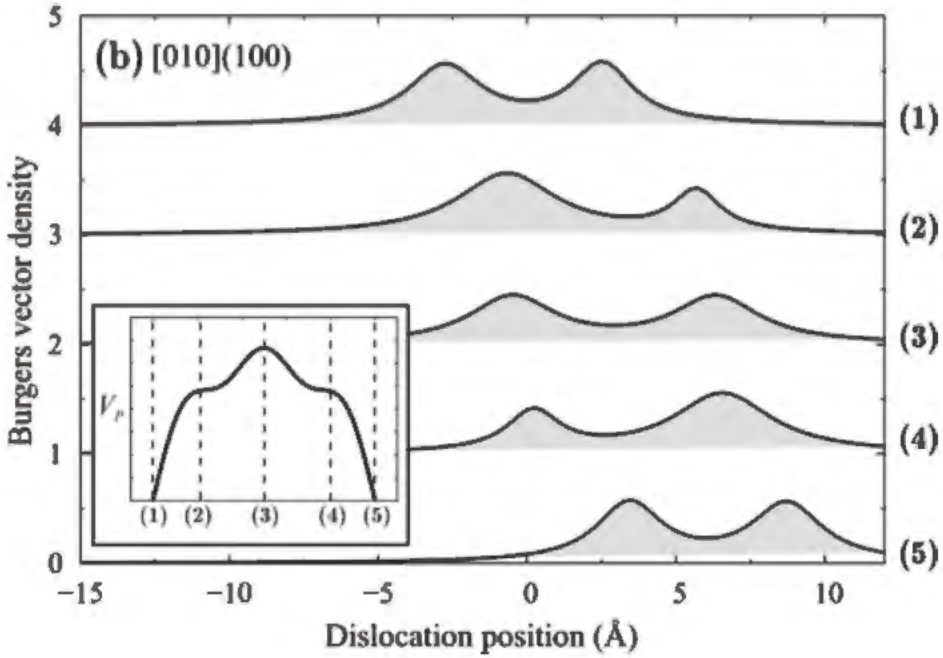




Kraych et al. EPSL in revision

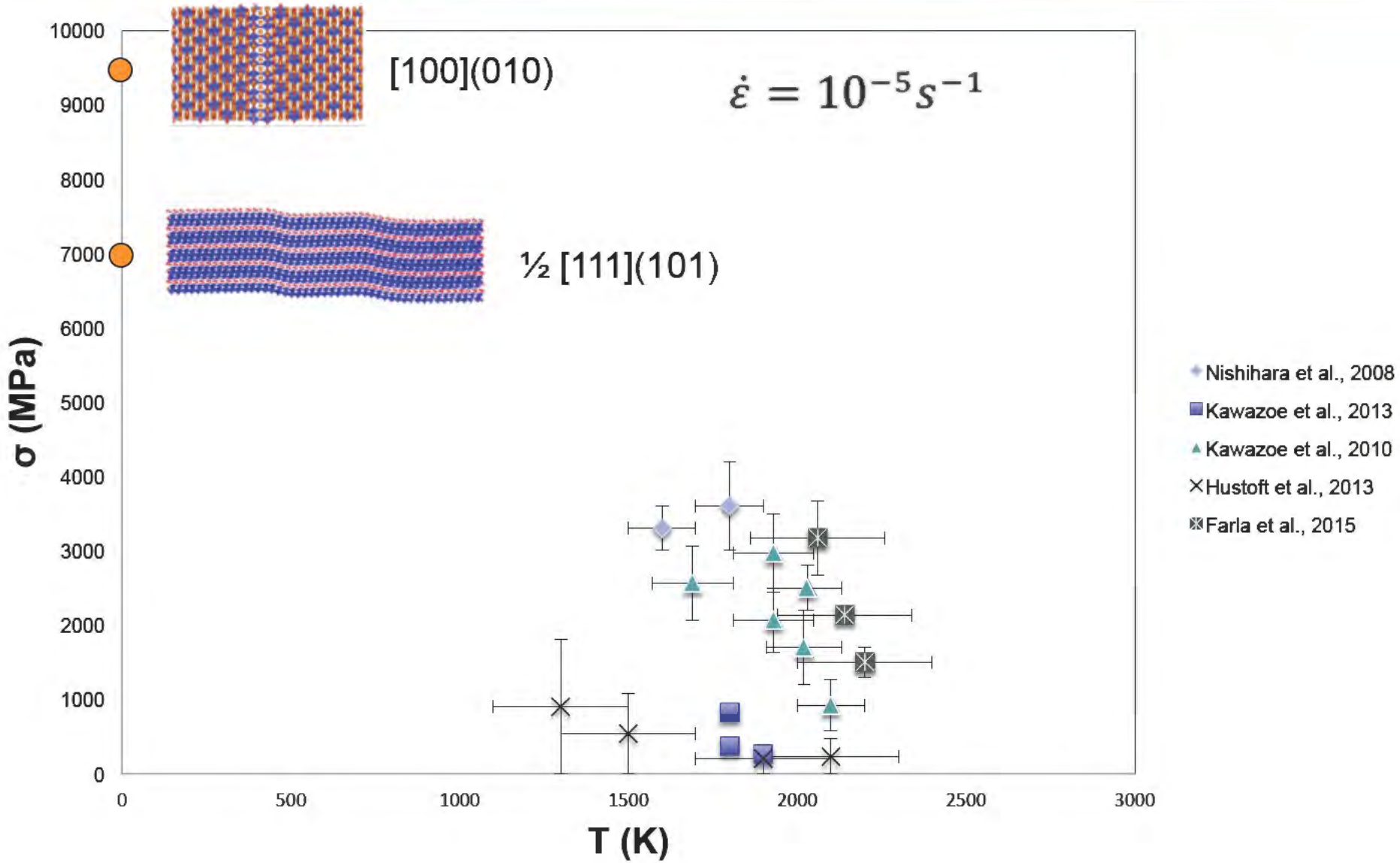
Dislocations: how they move



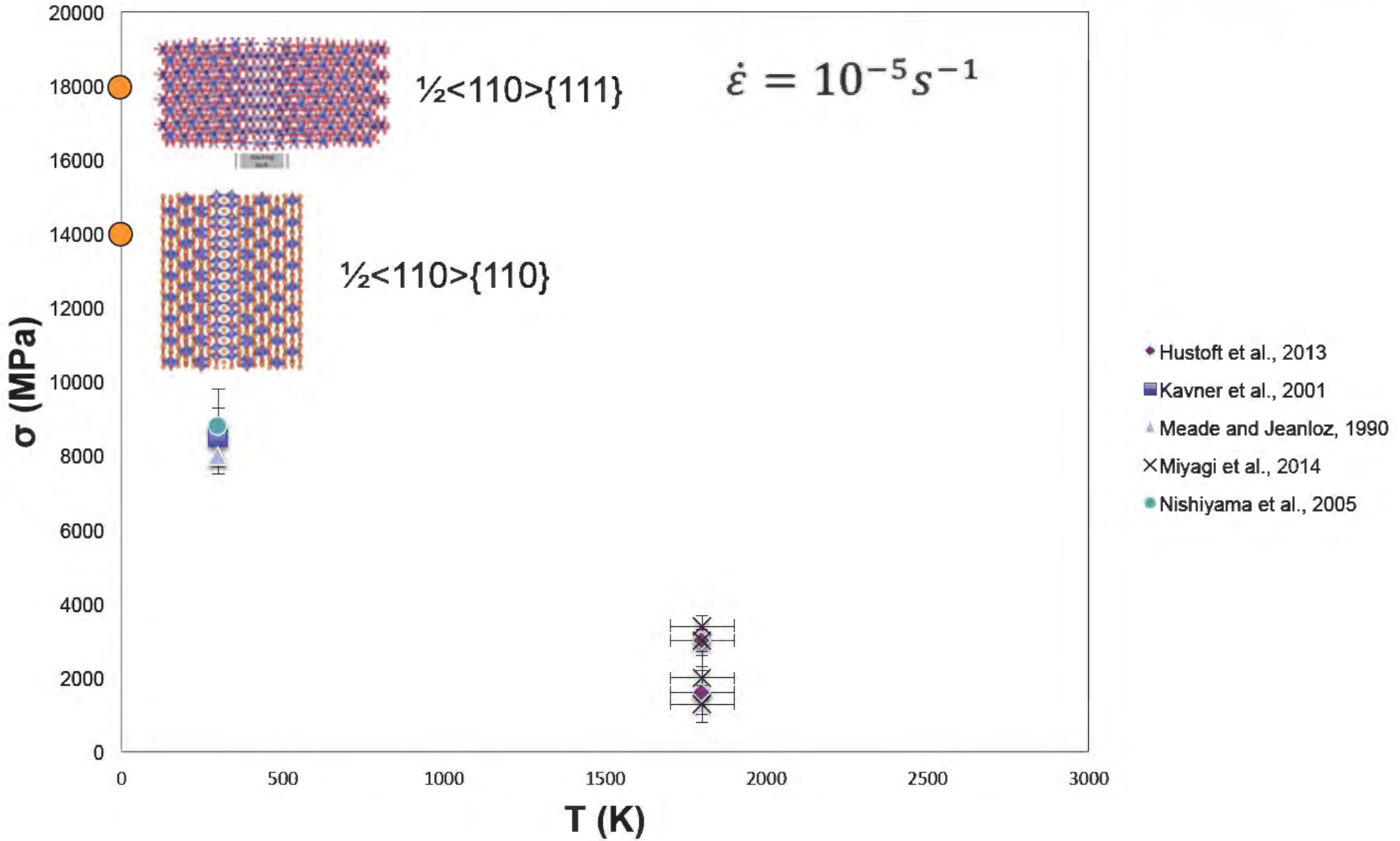


Kraych et al. EPSL in revision

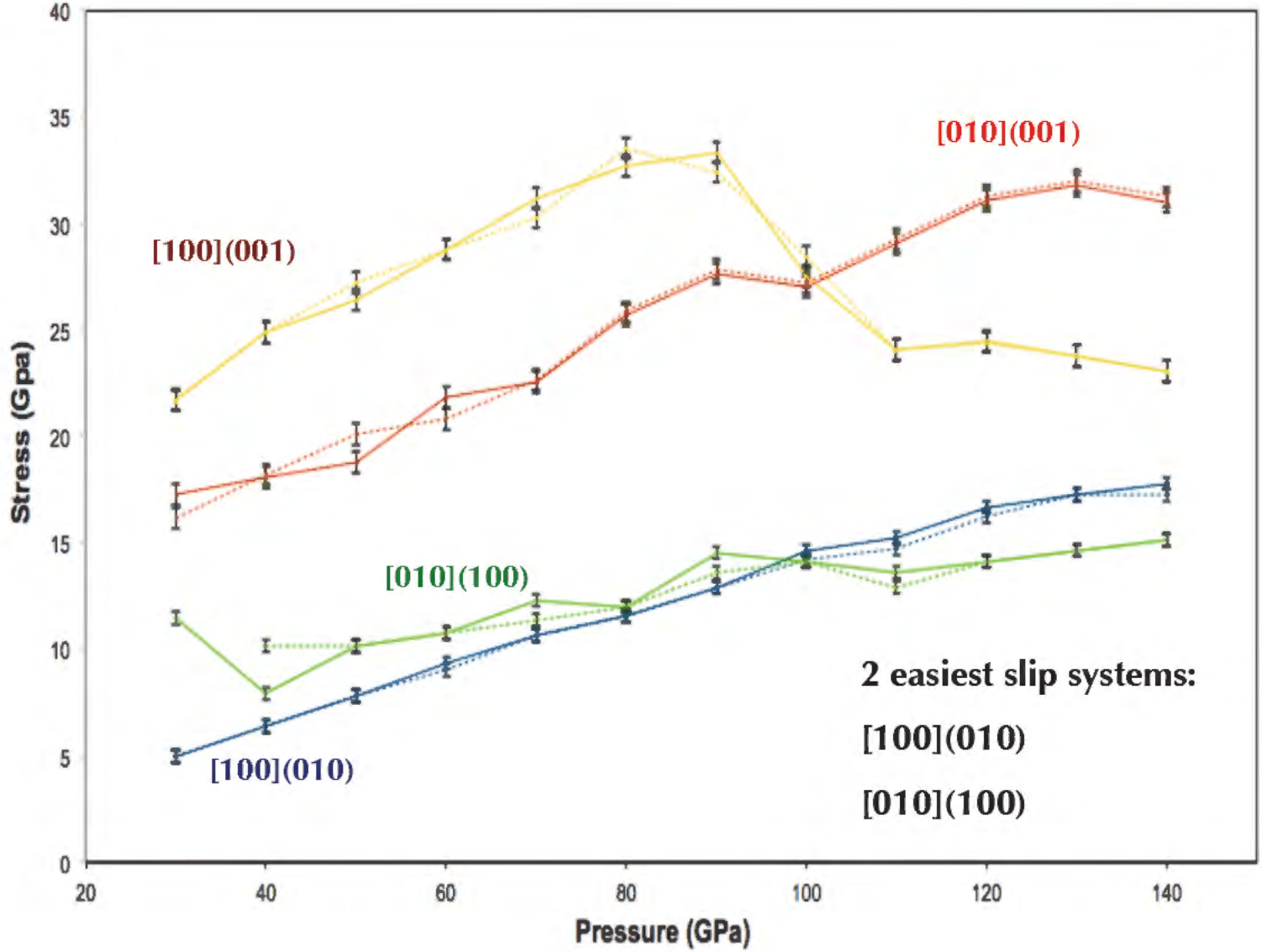
Wadsleyite: Peierls stresses



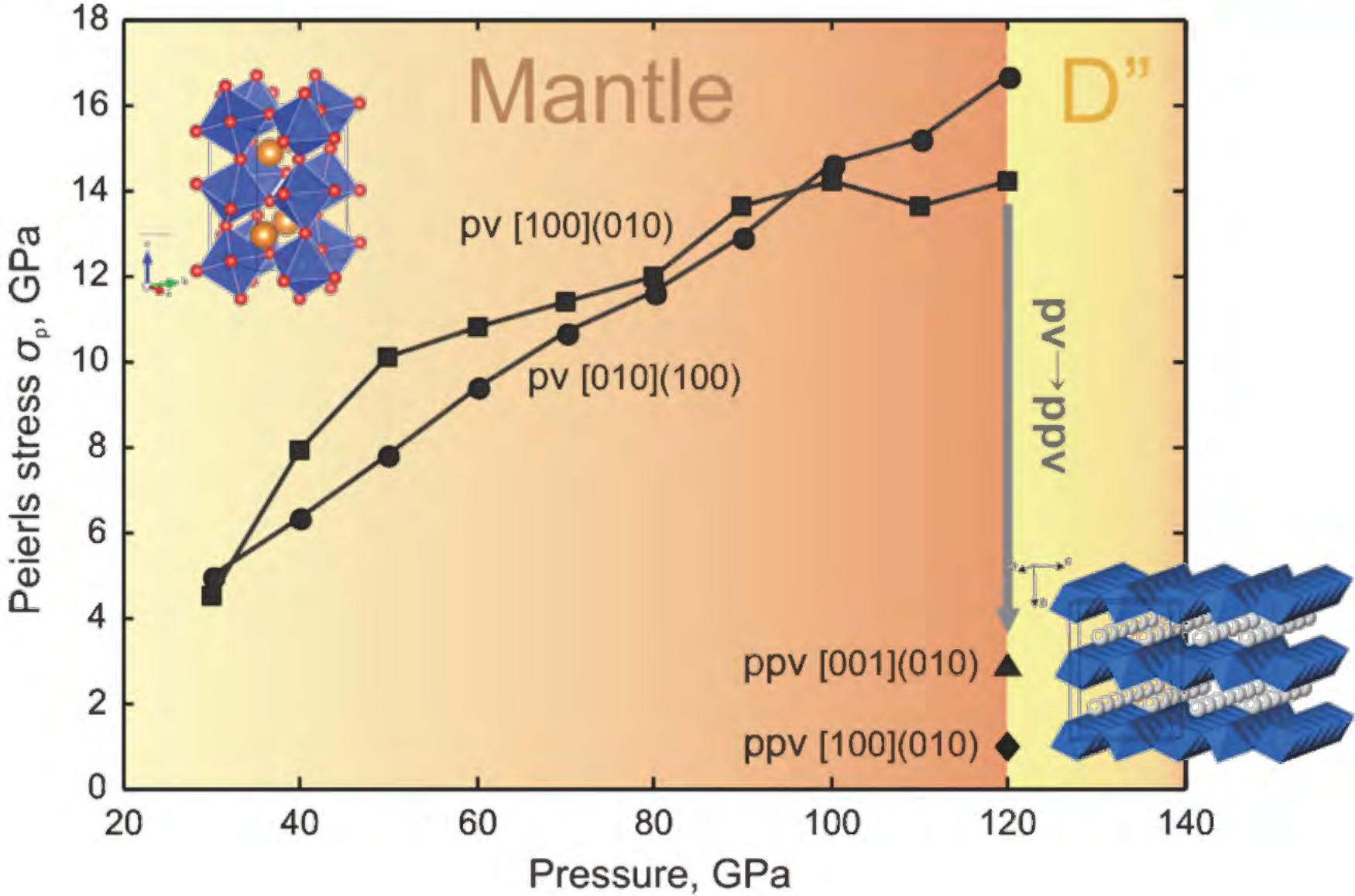
Ringwoodite: Peierls stresses



Lattice friction in $MgSiO_3$ Perovskite

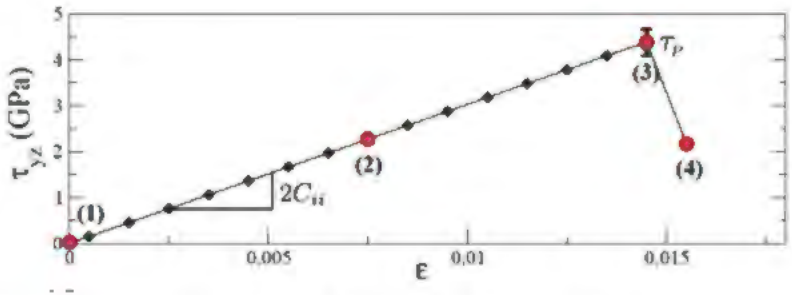


Lattice friction in $MgSiO_3$: from bridgmanite to post-perovskite

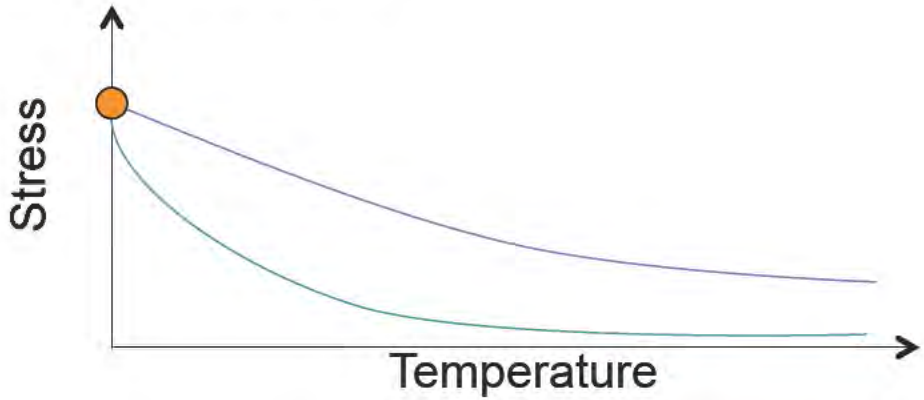


Stop 3

- We know: the intrinsic resistance that the crystal opposes to dislocation motion: the Peierls stress



- We don't know: how temperature helps to overcome this lattice friction

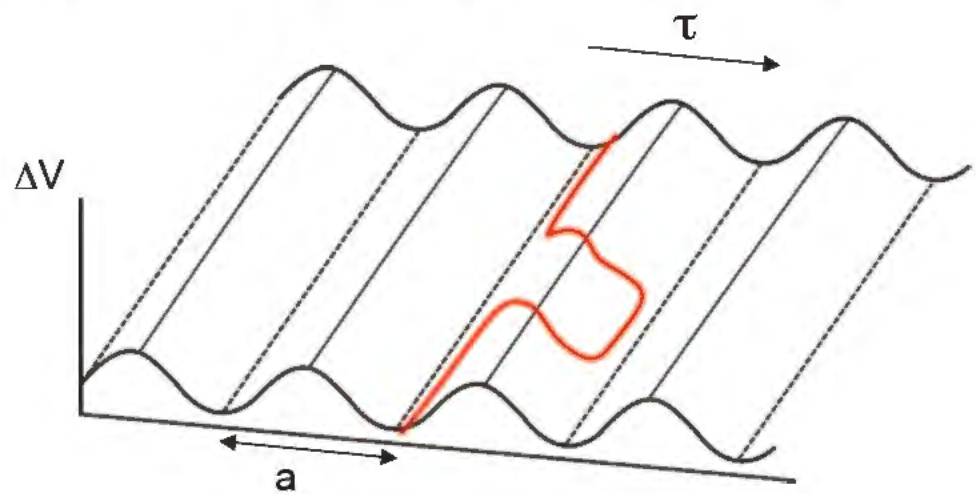


Modeling dislocation mobility

- Core structure
- Peierls Potential

Stress assisted thermal activation : (τ,T)

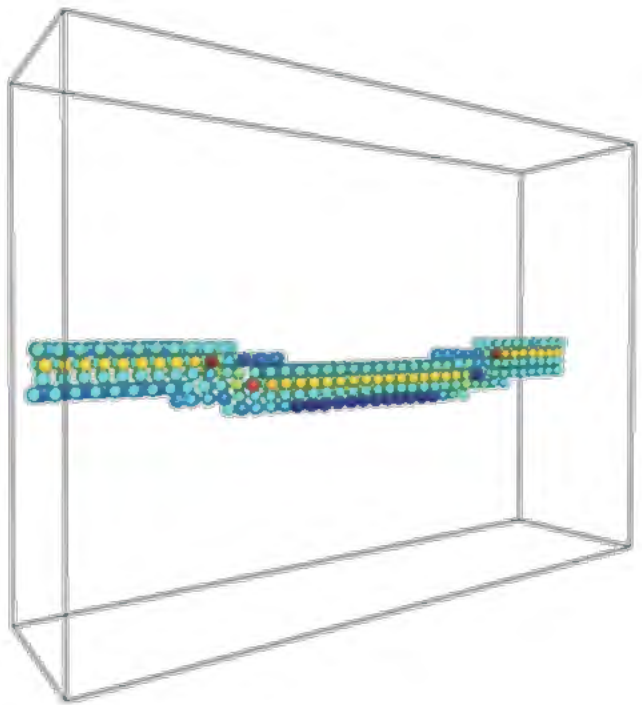
Kink pair mechanism :

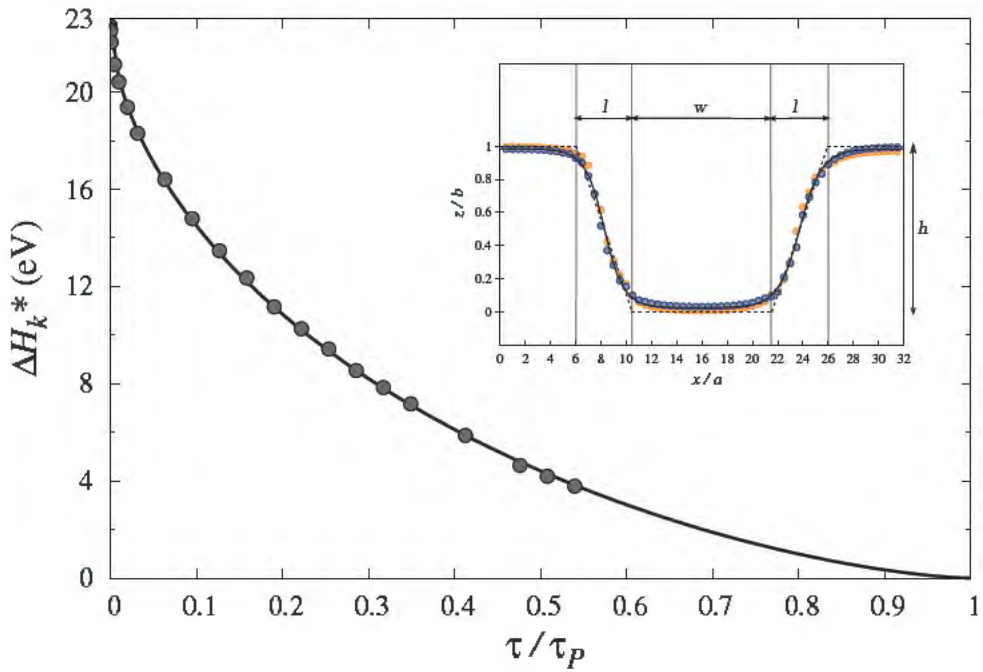


Modeling rare events:

Wadsleyite; 1700K, 1 GPa: 100ps

$MgSiO_3$ perovskite: kink pair mechanism



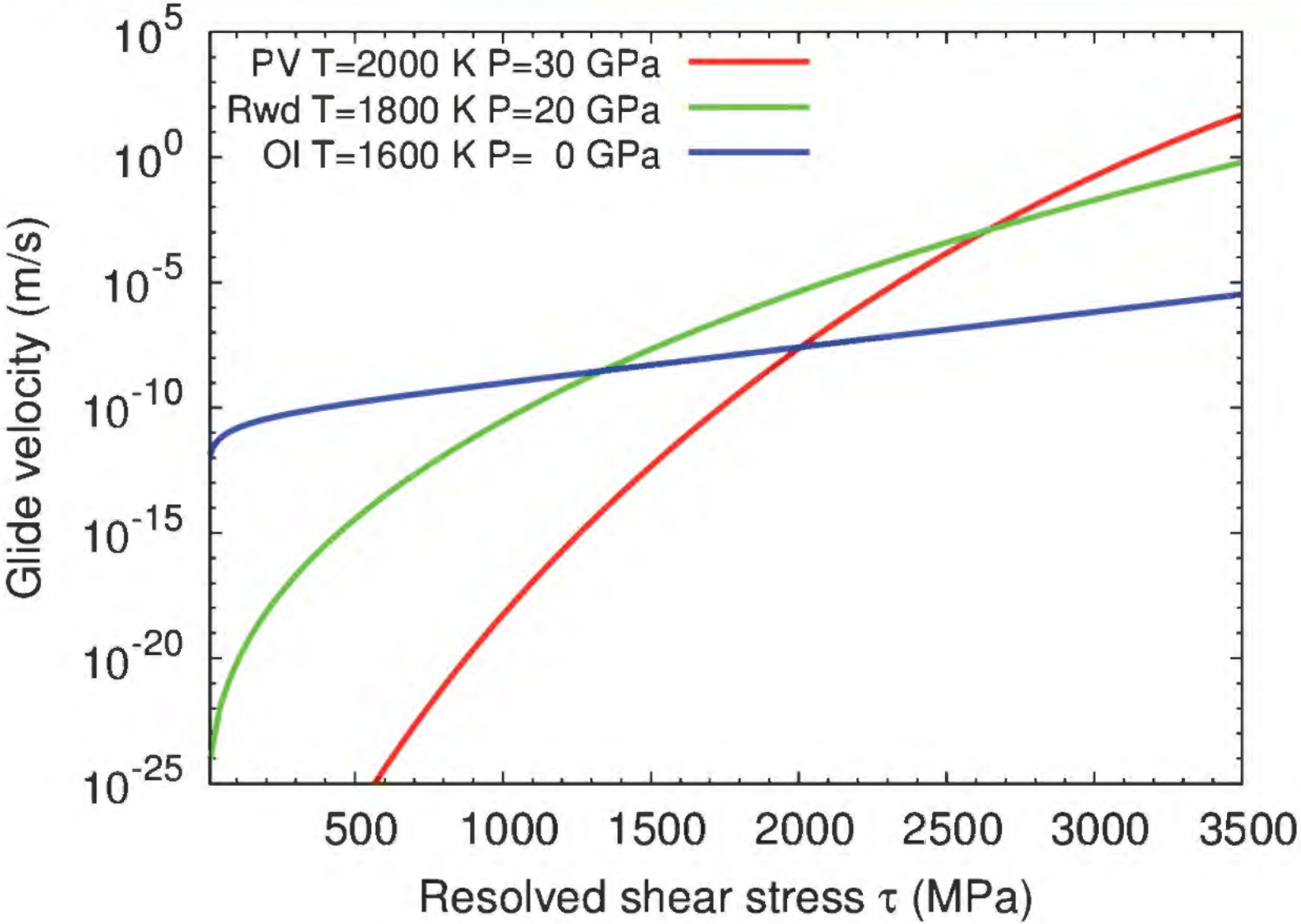


Transient state theory

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

Antoine Kraych's PhD

Dislocation velocities



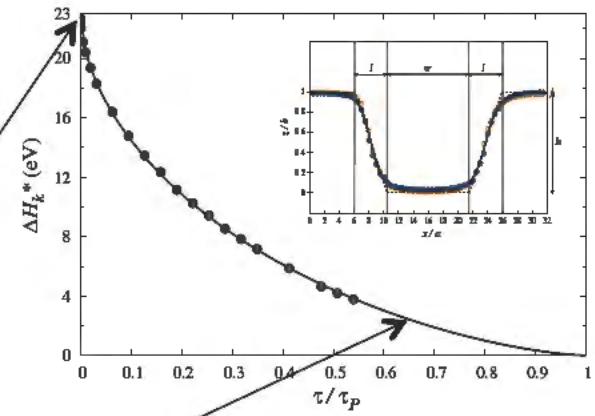
From dislocations to plasticity: a practical example

Orowan equation $\dot{\varepsilon} = \rho\, b\, v(\tau, T)$

Kraych et al. EPSL submitted

$$v(\tau, T) = v_0 exp\left(\frac{-\Delta H^*(\tau)}{kT}\right)$$

$$\Delta H^*(\tau) = 2H_k\left(1 - \left(\frac{\tau}{\tau_p}\right)^p\right)^q$$

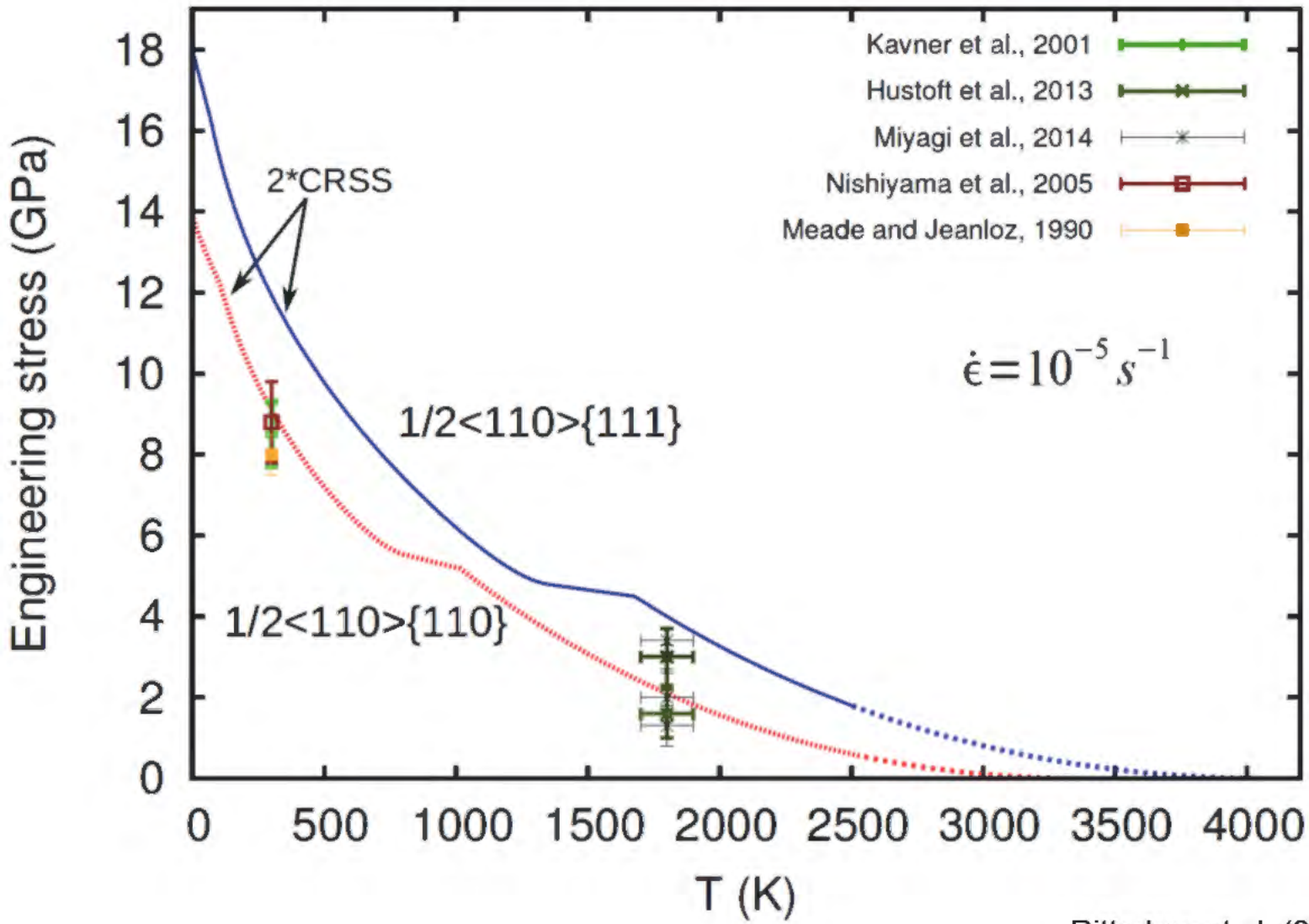


$$\tau = \tau_p\left(1 - \left(C\frac{T}{H_k}\right)^{1/q}\right)^{1/p}$$

$$C = \frac{k}{2}\ln\left(\frac{v_D a' b^2}{2w^{*2}}\frac{\sqrt{\rho}}{\dot{\varepsilon}}\right)$$

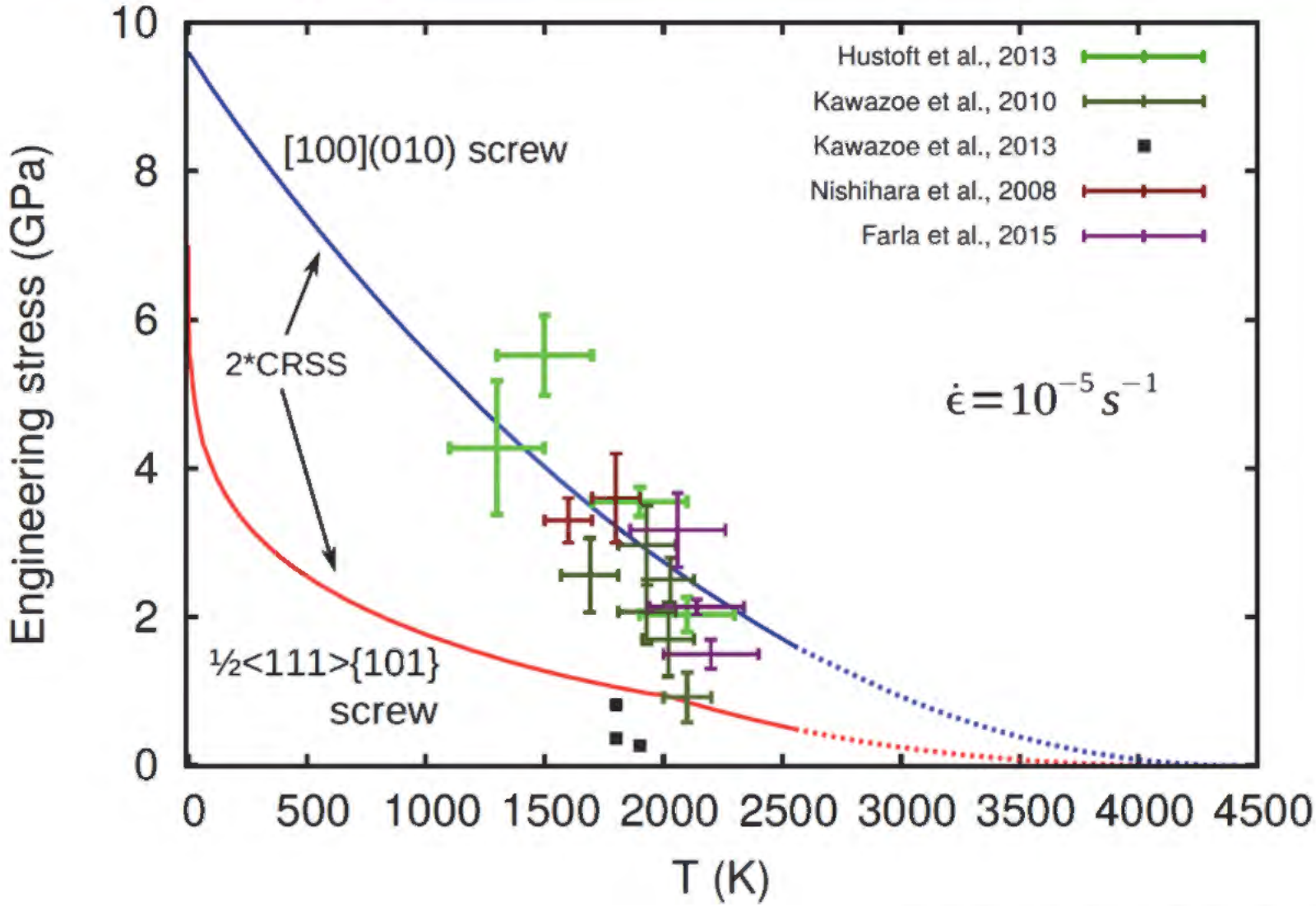
The strain rate is here

Dislocation Glide in Ringwoodite (20 GPa)



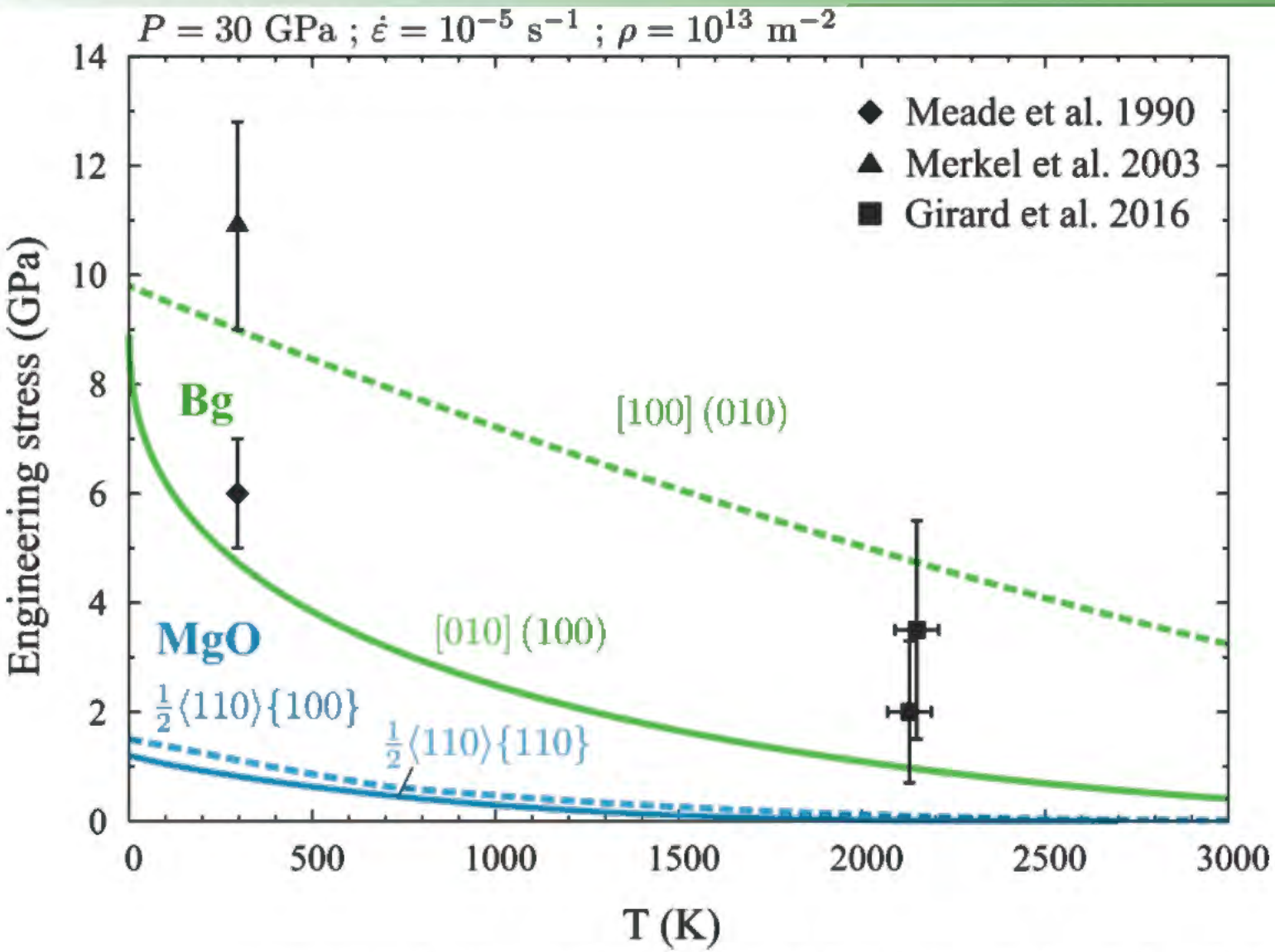
Ritterbex et al. (2015) PEPI

Dislocation Glide in Wadsleyite (15 GPa)



Ritterbex et al. Am. Mineralogist in press

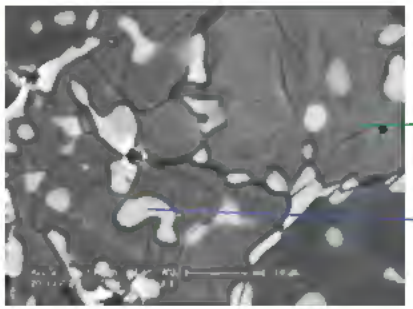
$MgSiO_3$ perovskite (30 GPa)

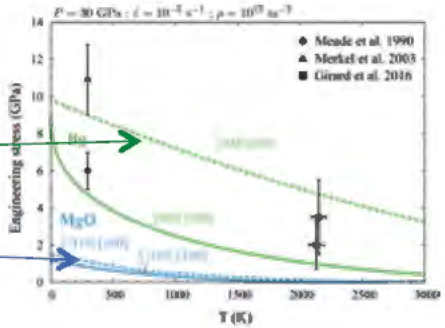


Krayc h et al. EPSL submitted – Results on MgO from Amodeo et al. Phil. Mag. 2012

Stop 4

- We know: the intracrystalline flow properties of major high pressure minerals





Courtesy J. Girard

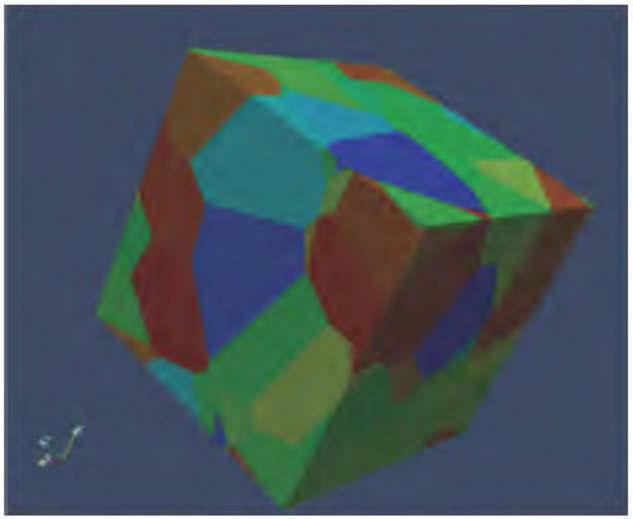
- We don’t know the mechanical properties of the « rock »

From the grain to the aggregate

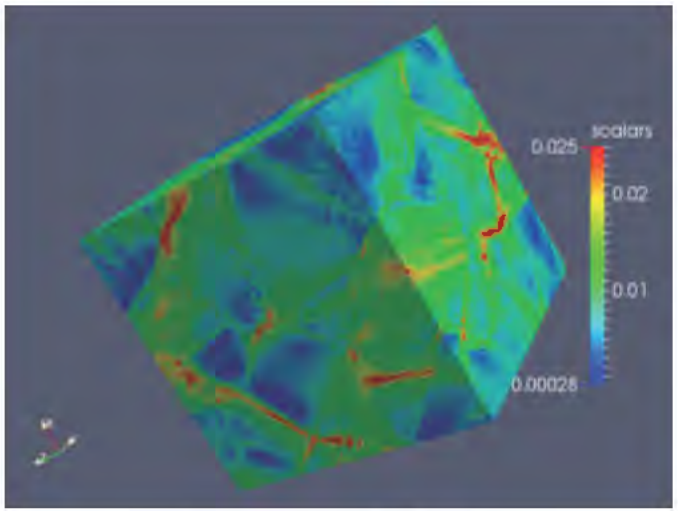
Collaboration with O. Castelnau & K. Derrien
ENSAM, Paris

- Visco Plastic Self Consistent modelling

- Finite Elements modelling



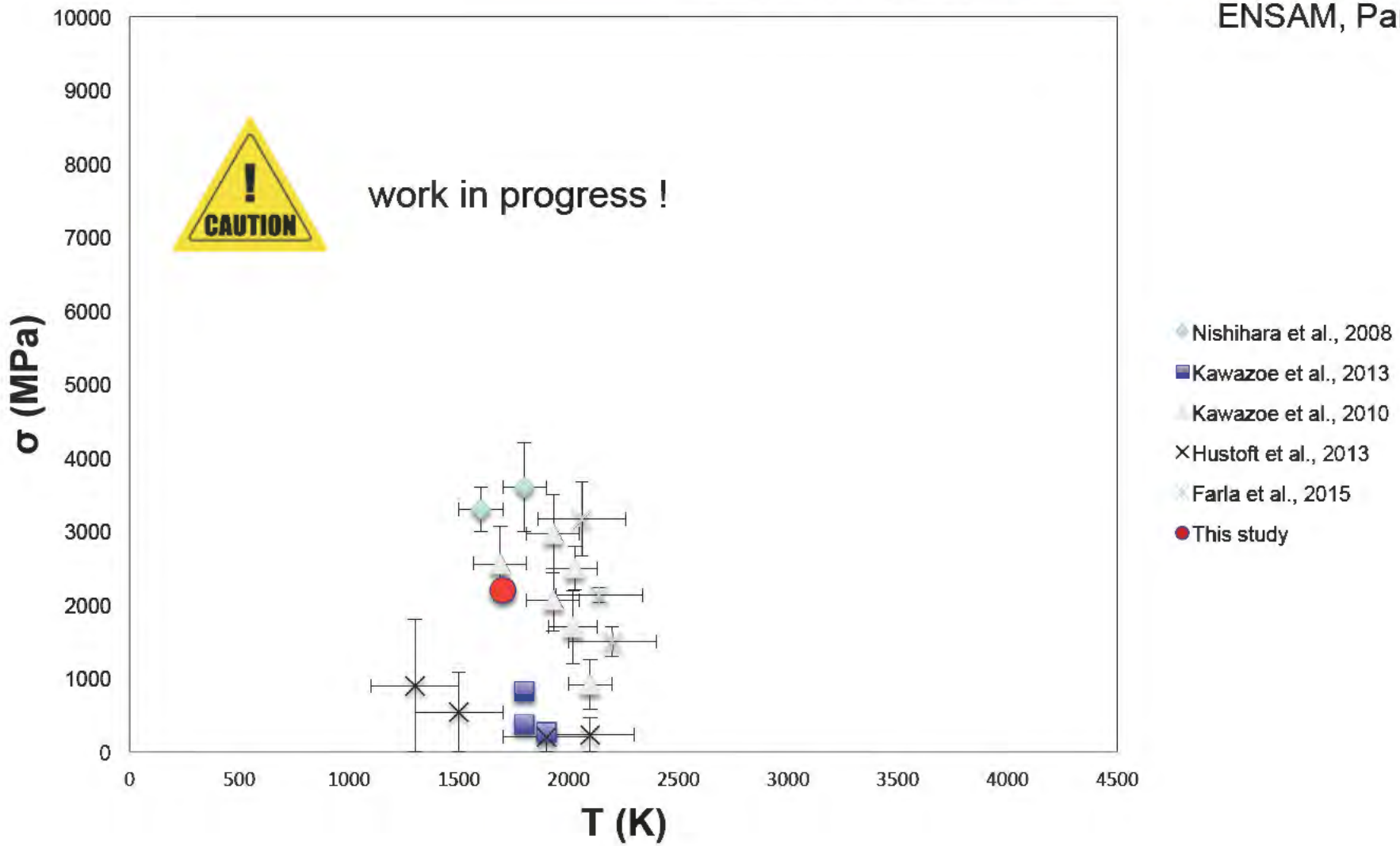
Building an aggregate



Equivalent strain

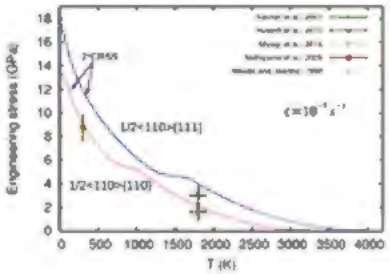
From the grain to the aggregate

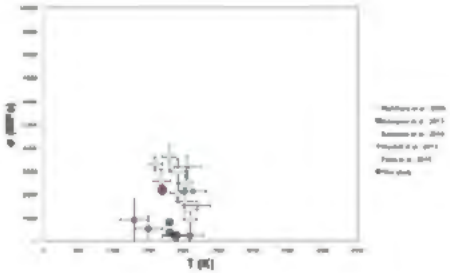
Collaboration with O. Castelnau & K. Derrien
ENSAM, Paris



Stop 5

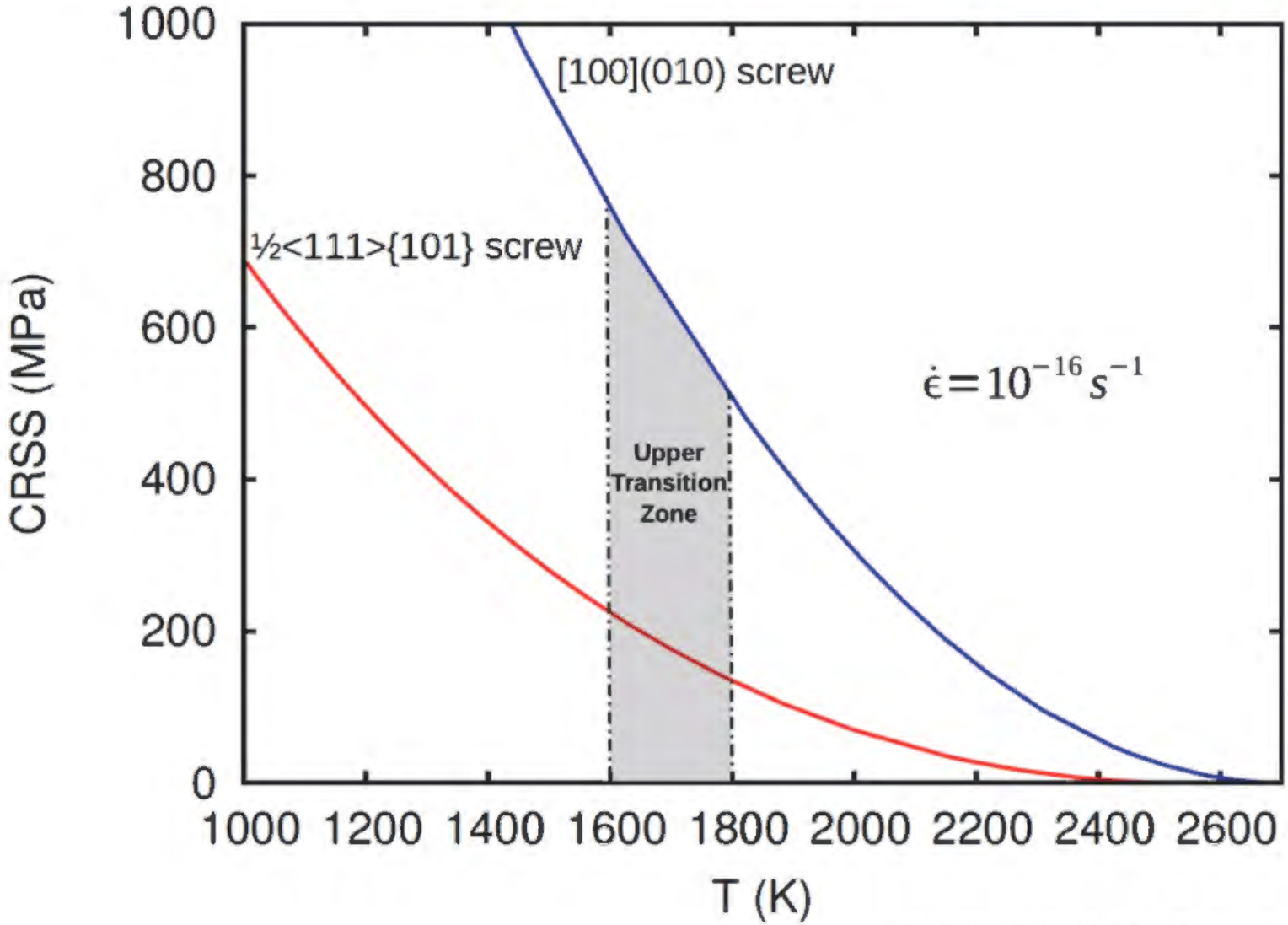
- We can model (and we agree with) mechanical data obtained in laboratory conditions





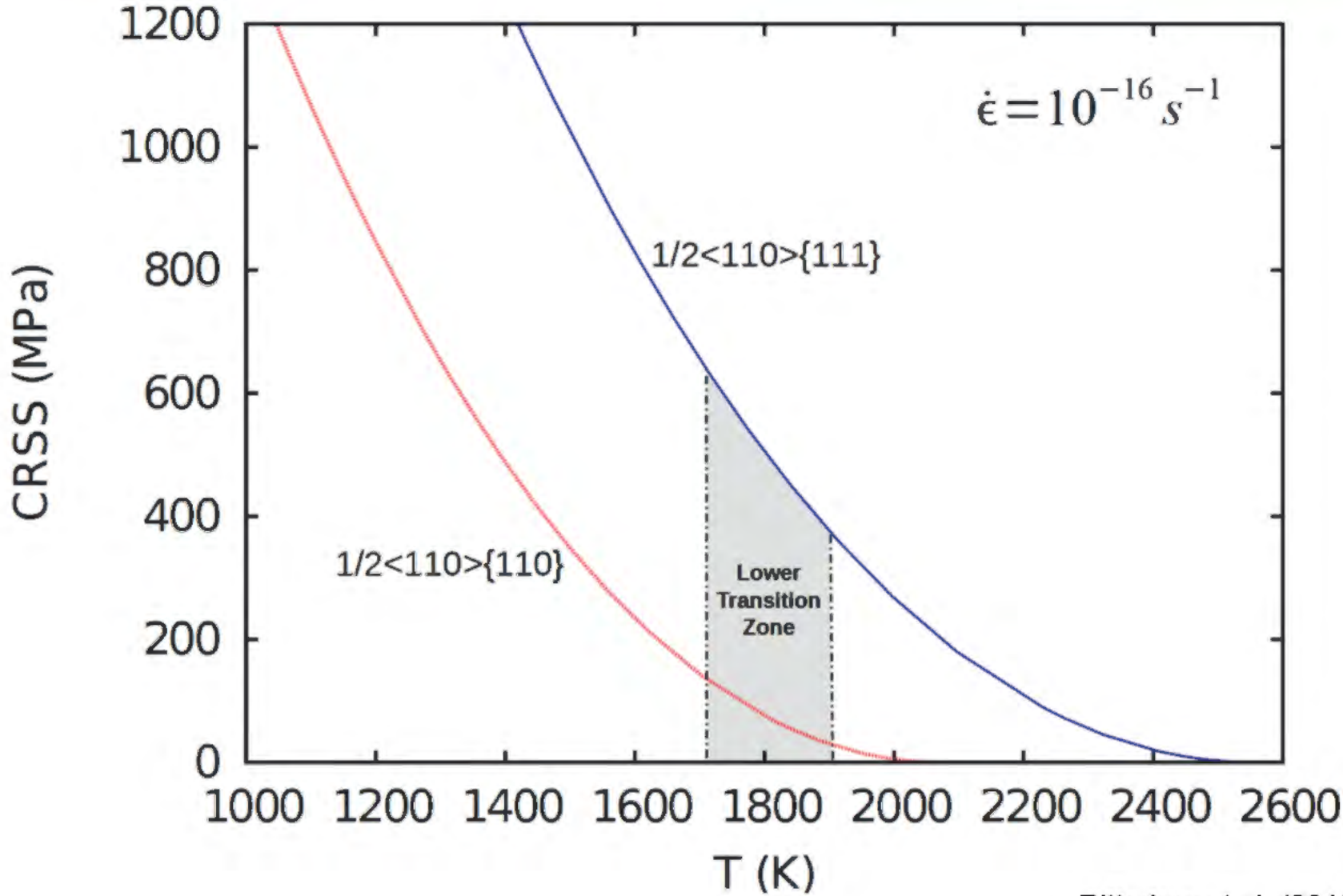
- But we can do the same at mantle strain-rates (no extrapolation !)

Dislocation Glide in Wadsleyite (15 GPa)



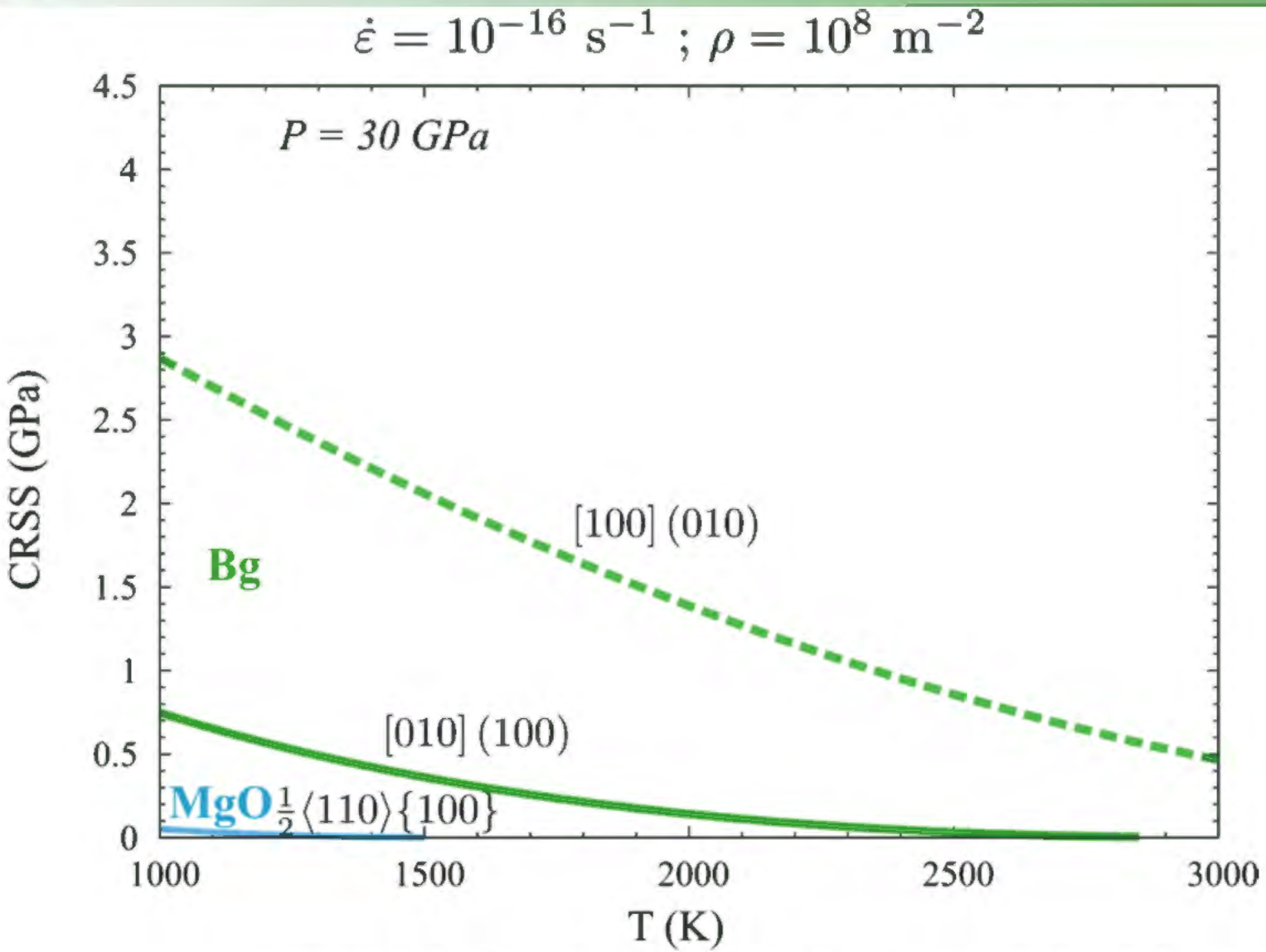
Ritterbex et al. Am. Mineralogist in press

Dislocation Glide in Ringwoodite (20 GPa)



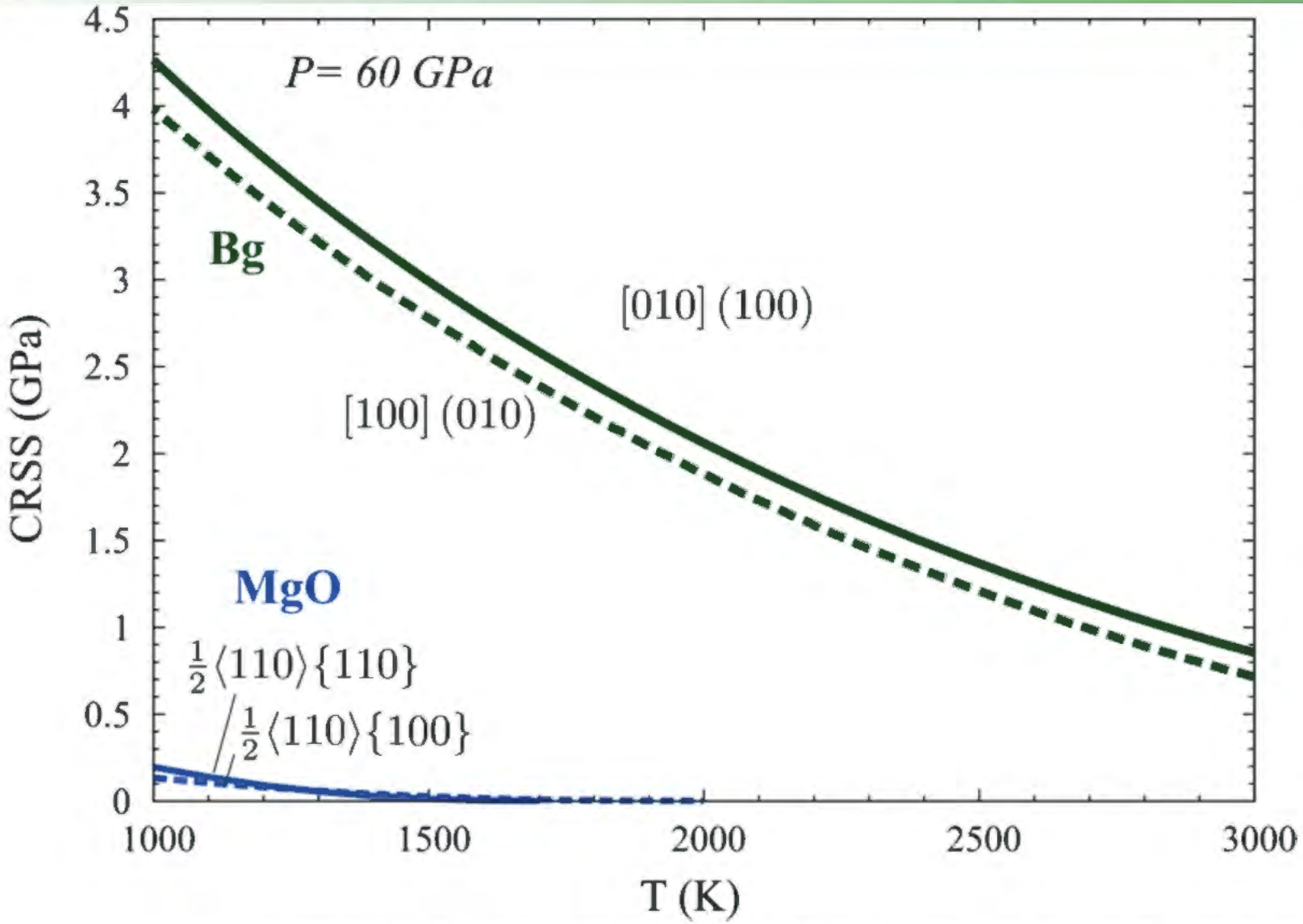
Ritterbex et al. (2015) PEPI

$MgSiO_3$ perovskite (30 GPa)



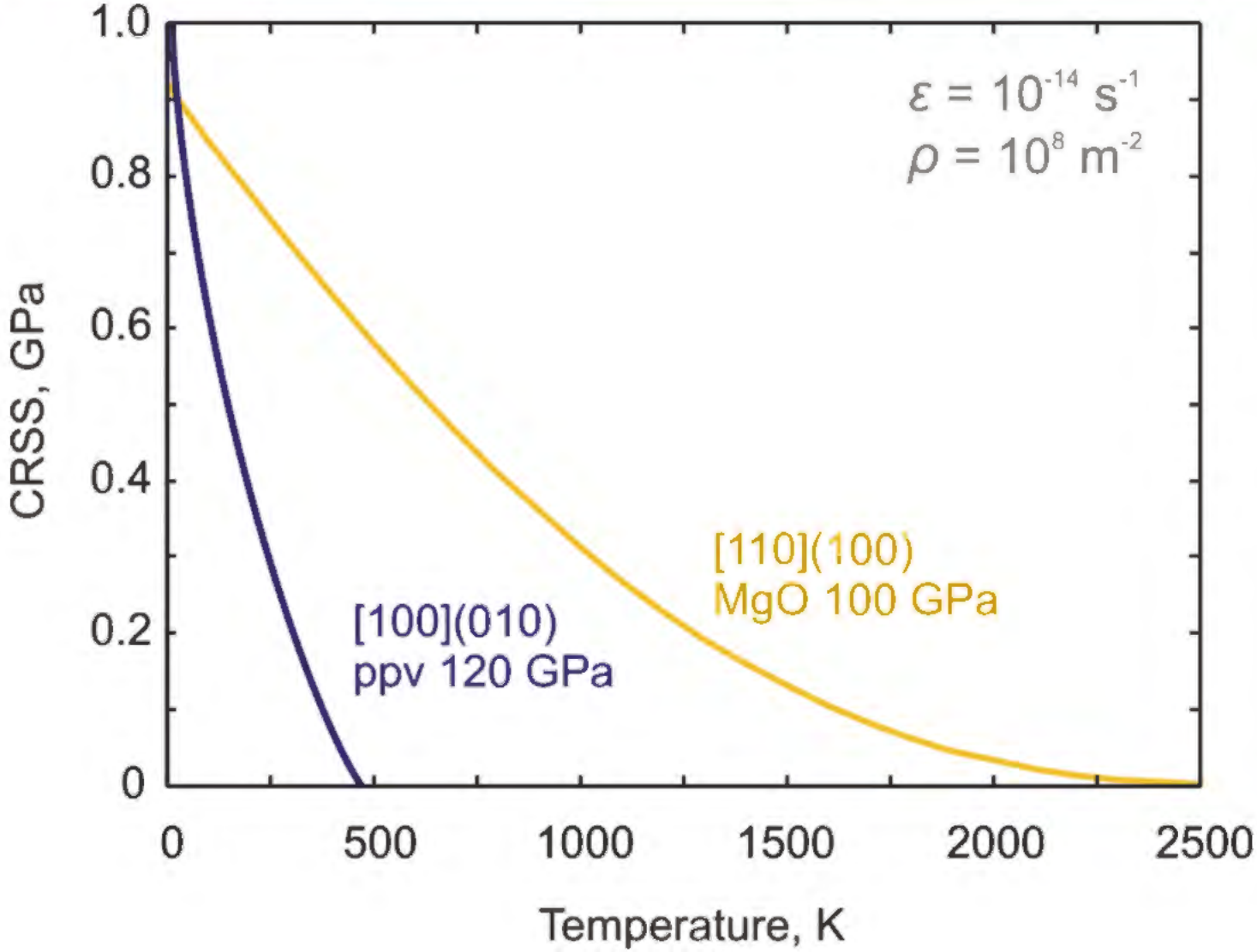
Krayc h et al. EPSL submitted – Results on MgO from Amodeo et al. Phil. Mag. 2012

$MgSiO_3$ perovskite (60 GPa)



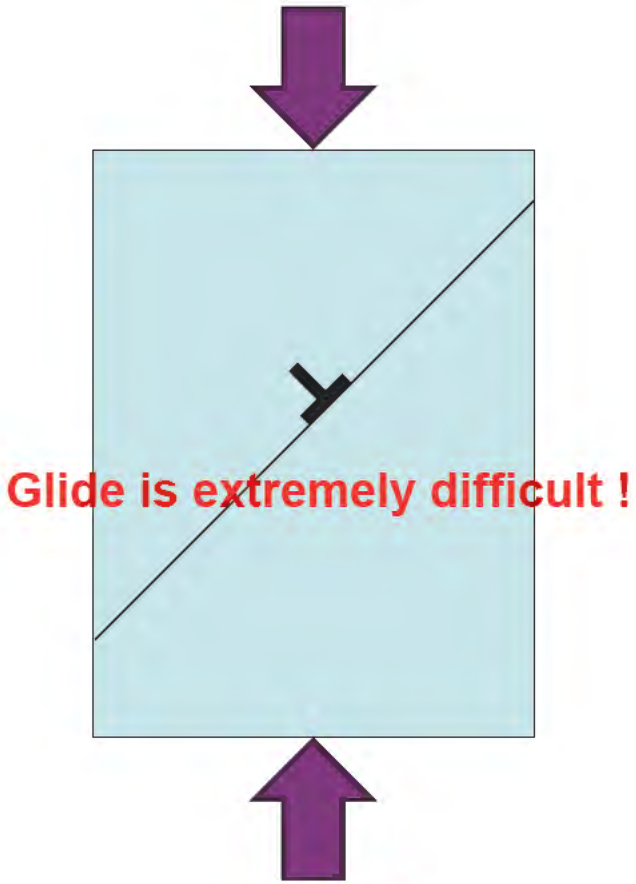
Krayc h et al. EPSL submitted – Results on MgO from Amodeo et al. Phil. Mag. 2012

$MgSiO_3$ post-perovskite (120 GPa)

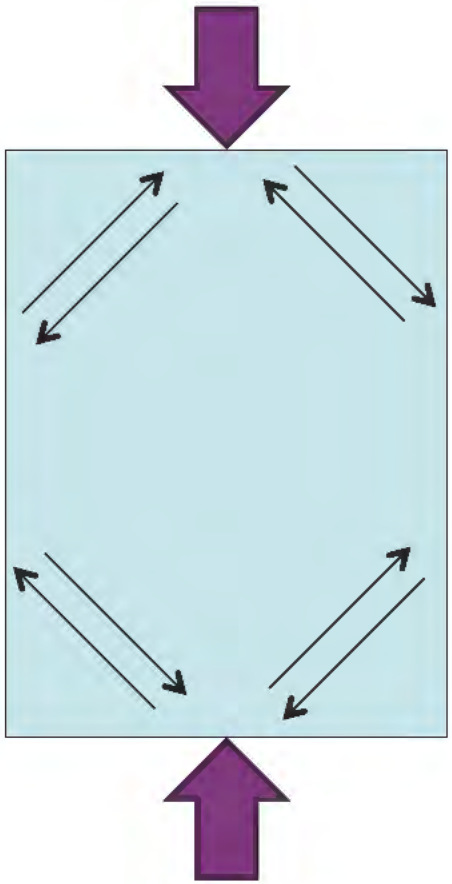


A. Goryaeva in prep

Which mechanism ?



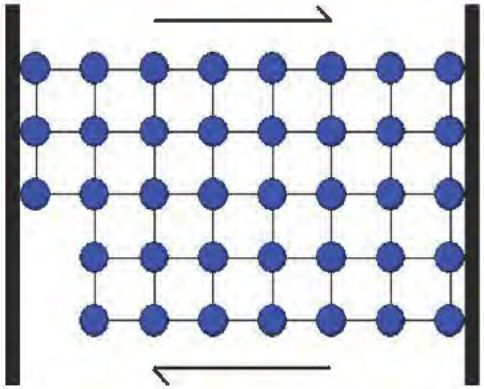
~~Dislocation creep~~



Diffusion creep ?

Stop 6

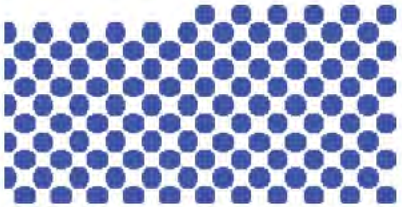
- We understand, model, quantify dislocation glide



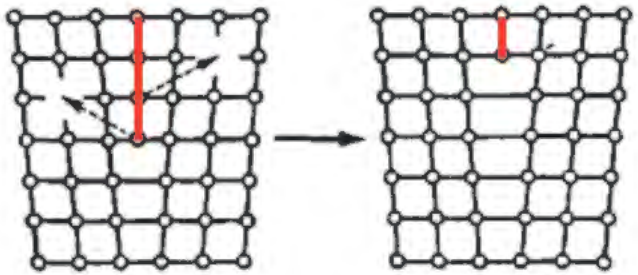
- But creep in the mantle would involve glide and climb !

What is climb ?

- Point defects (vacancies) diffuse toward the dislocations



- They are absorbed (or emitted)

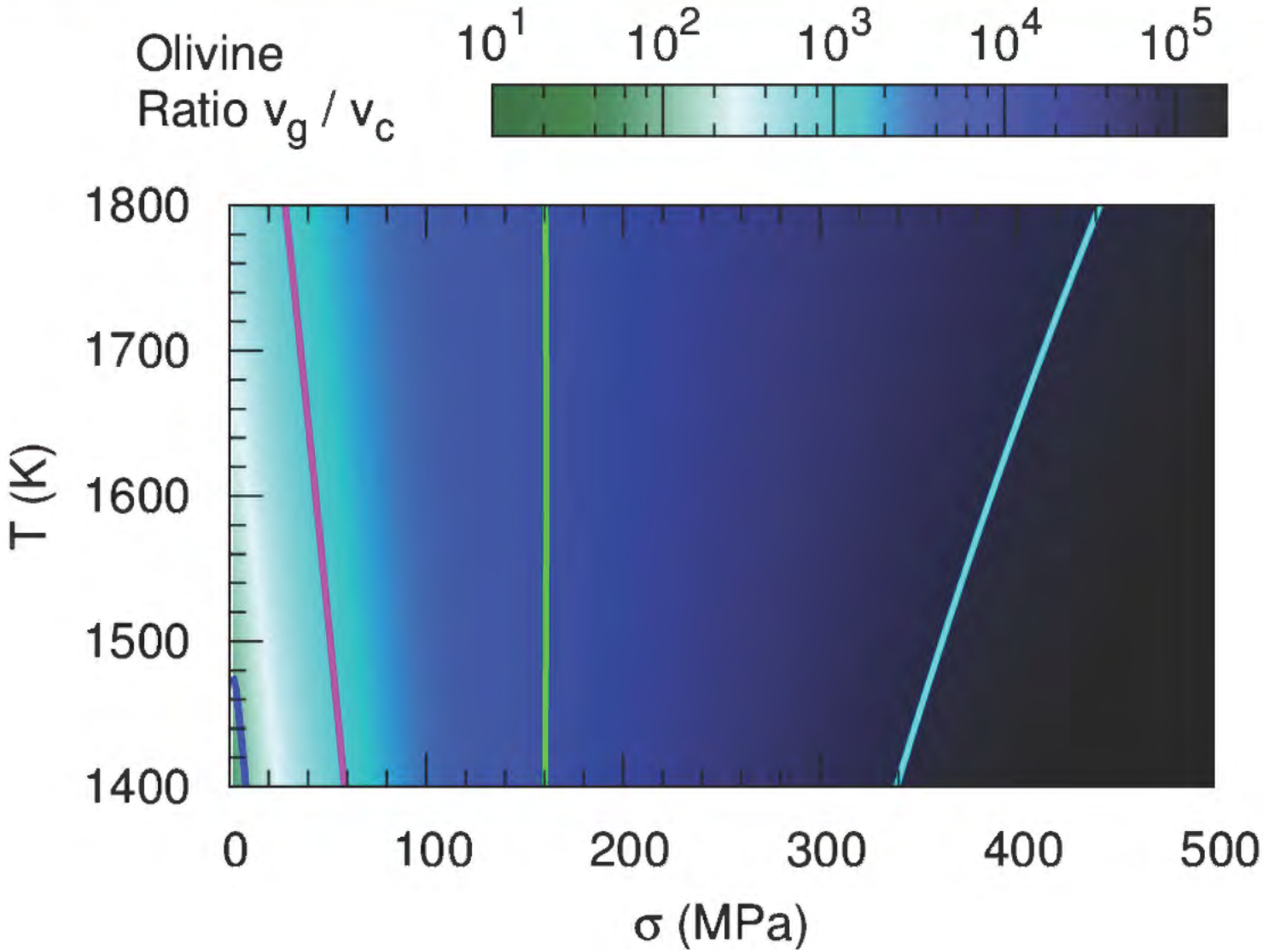


The dislocation moves away from its glide plane

$$v_{climb} = \frac{2\pi}{\ln R/r_c} \frac{D_{Si}{}^{sd}}{b} \left(\exp\left(\frac{\tau\Omega}{kT}\right) - 1 \right)$$

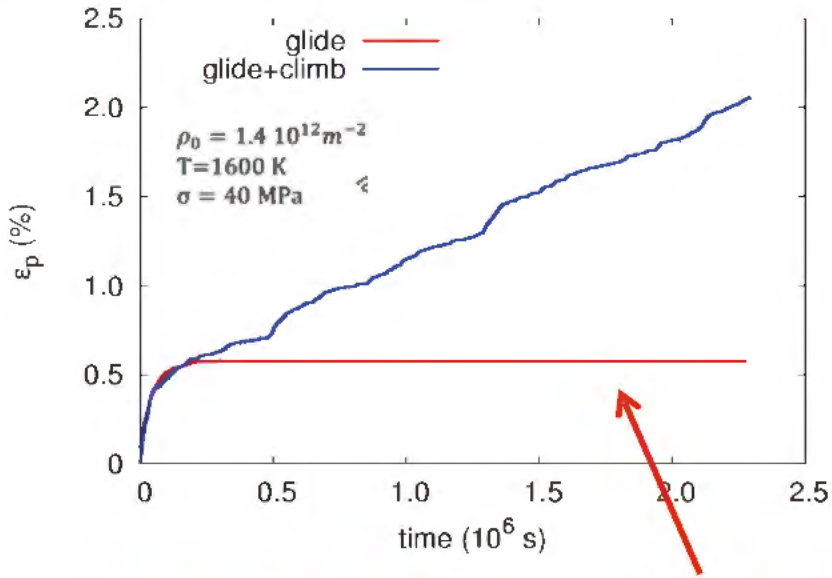
Interplay between glide and climb

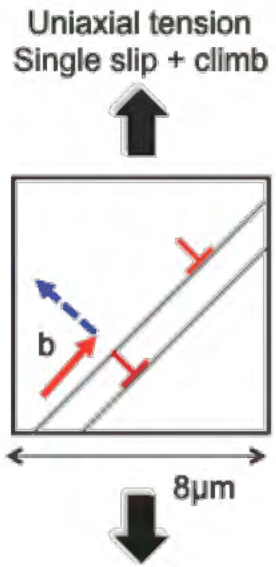
[100] dislocations

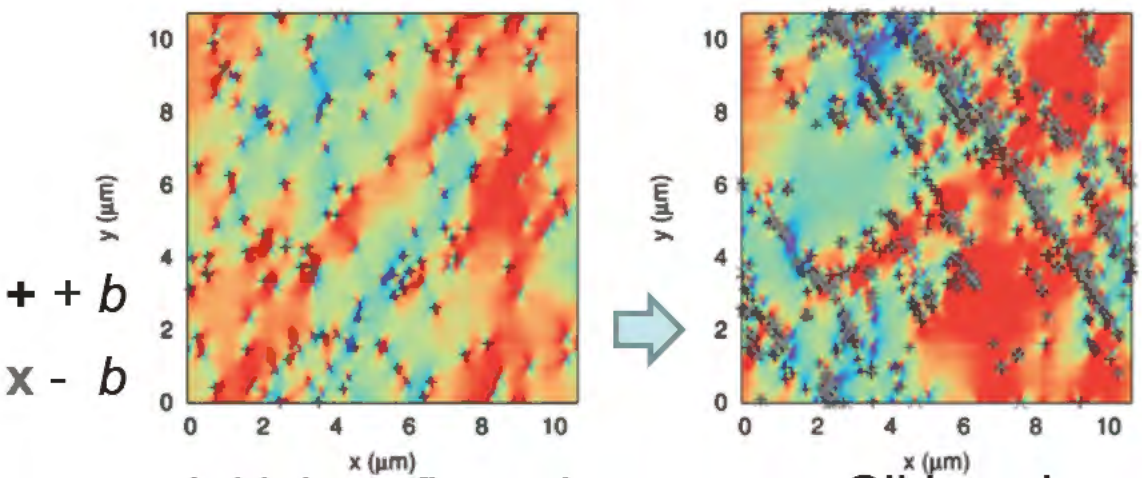


Interplay between glide and climb

[100] dislocations







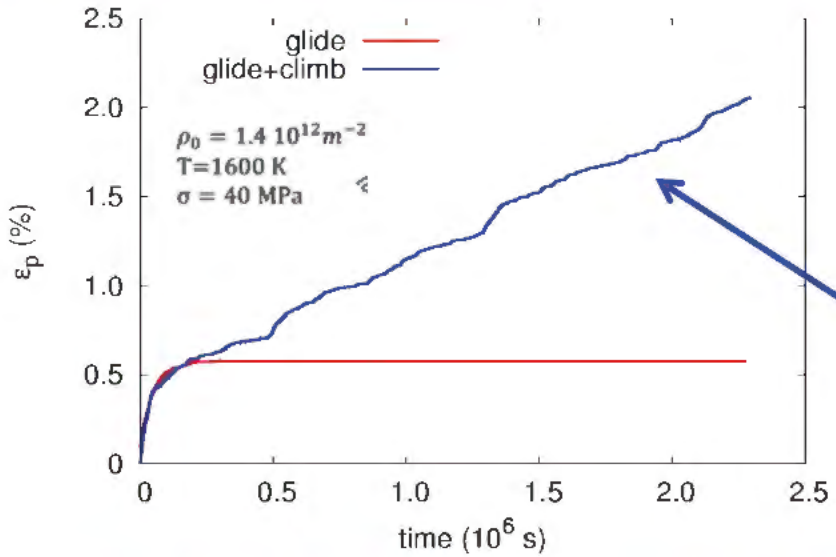
Initial configuration

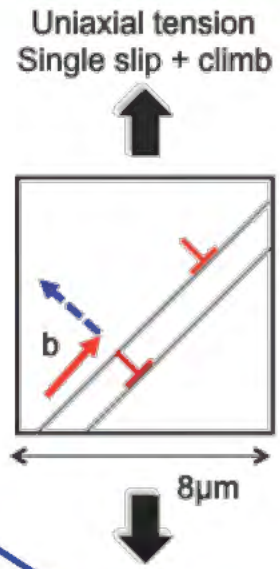
Glide only

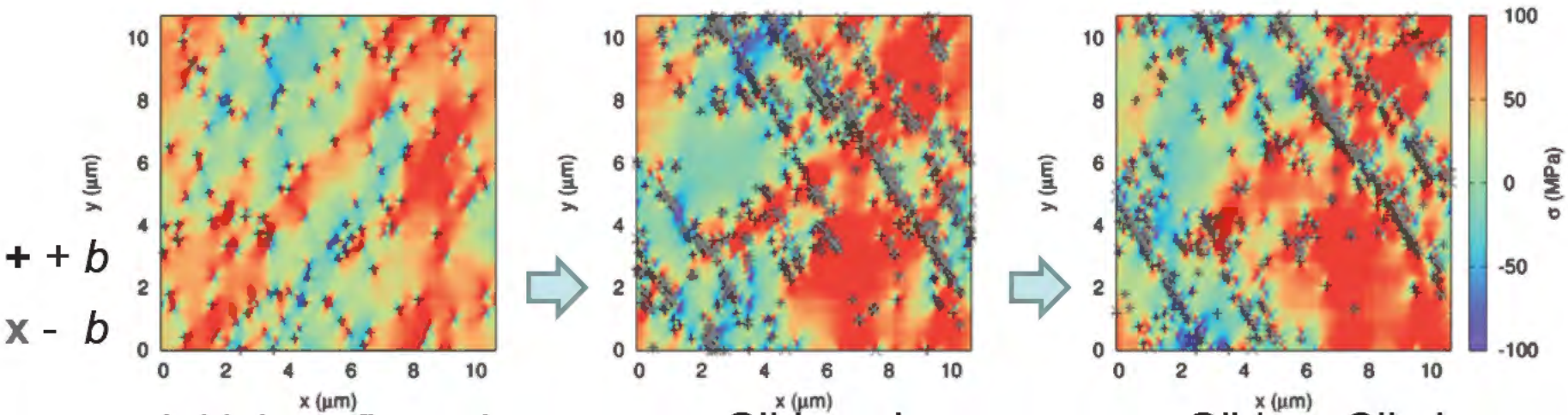
Boioli et al. Phys Rev B 2015

Interplay between glide and climb

[100] dislocations

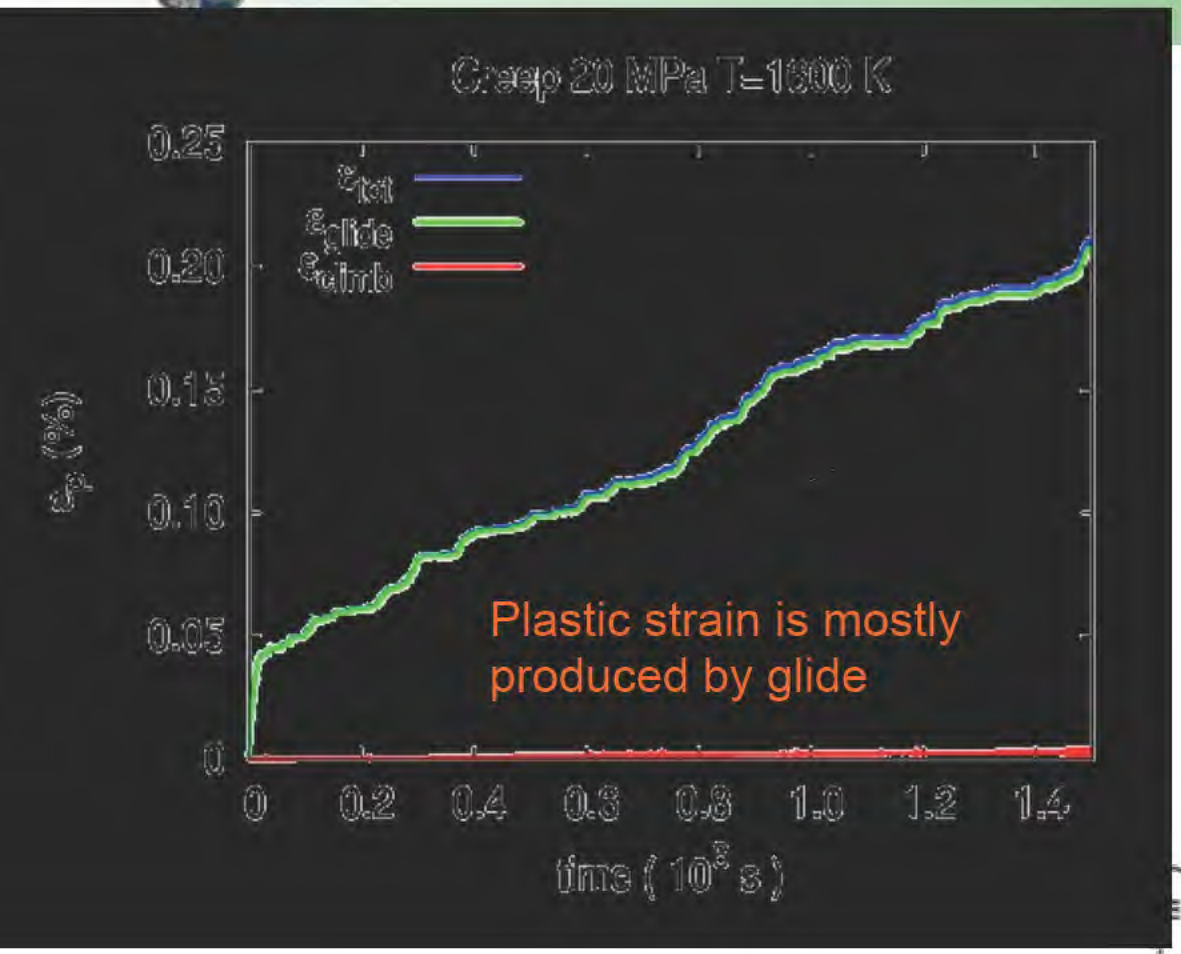


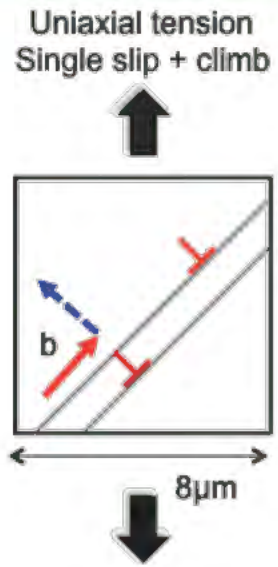


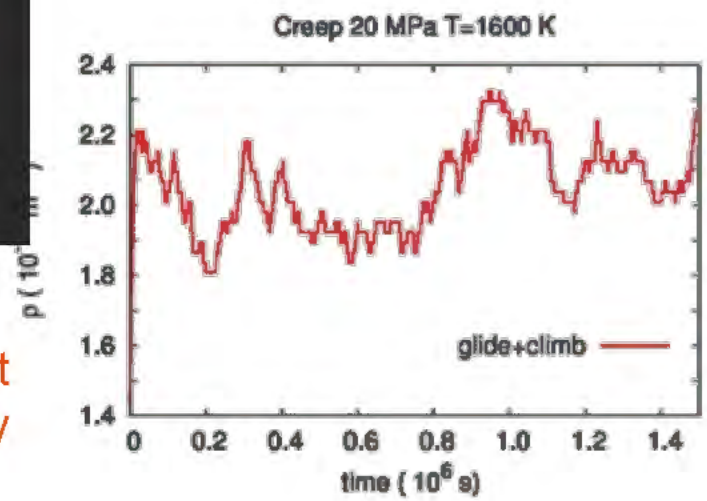


Interplay between glide and climb

[100] dislocations



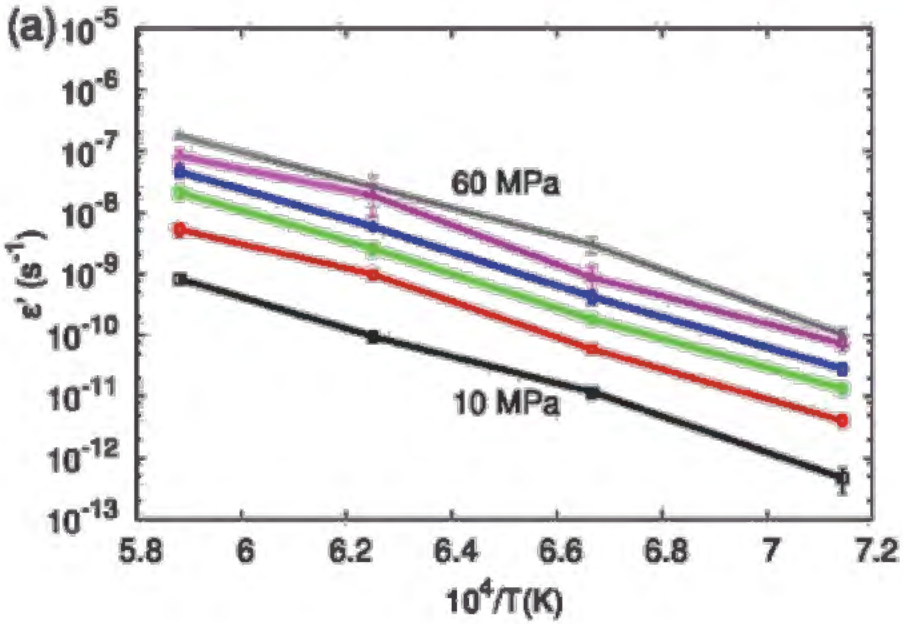




At steady state: nearly constant dislocation density

Boioli et al. Phys Rev B 2015

Activation enthalpy



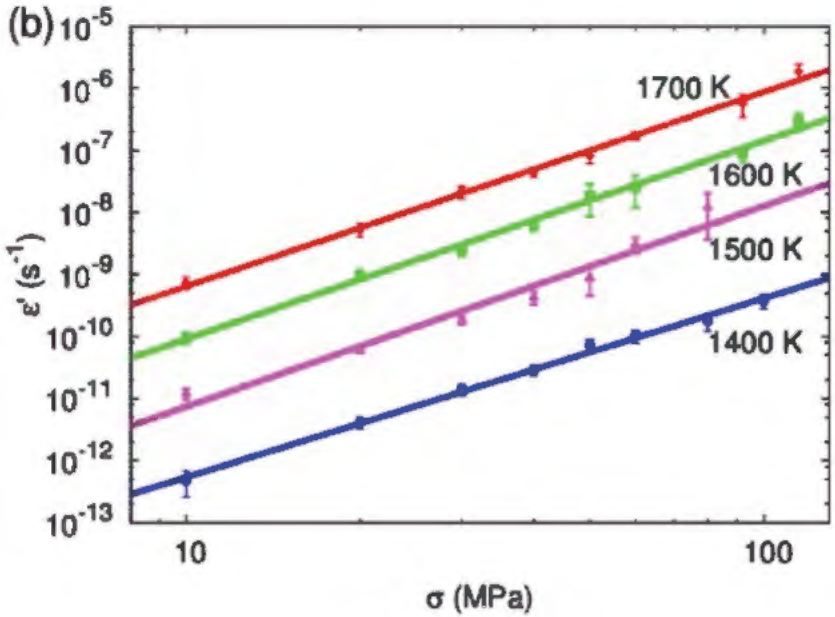
	glide	creep	diffusion
(eV)	5.7	4.7	4.25

Durinck et al.
Am. Min. (2007)

Fei et al. Earth Planet. Sci. Lett. 345,95 (2012)
Fei et al. Nature 498 (2013)

Boioli et al. Phys Rev B 2015

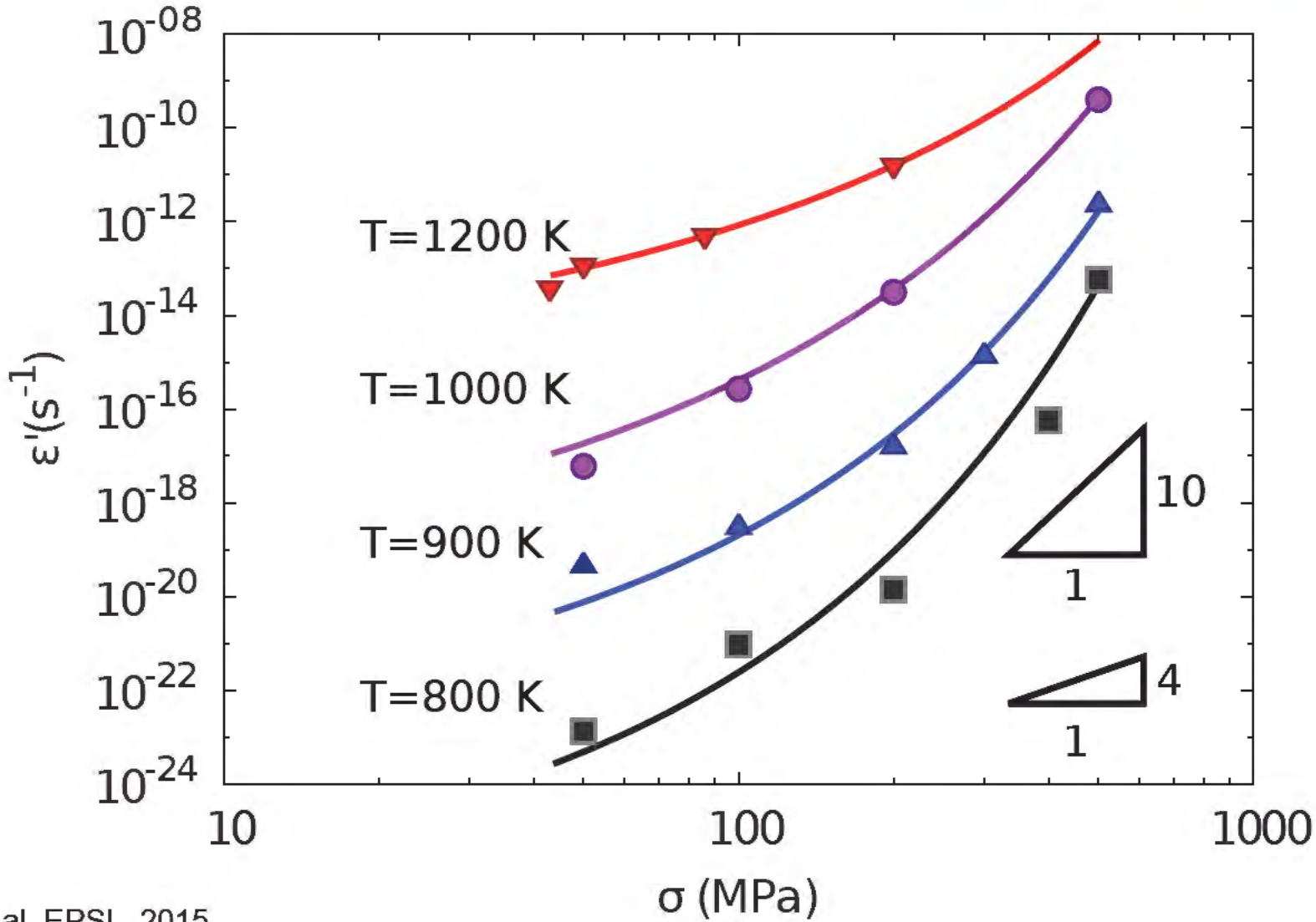
Stress exponent



T(K)	1700	1600	1500	1400
	3.1	3.2	3.2	2.9

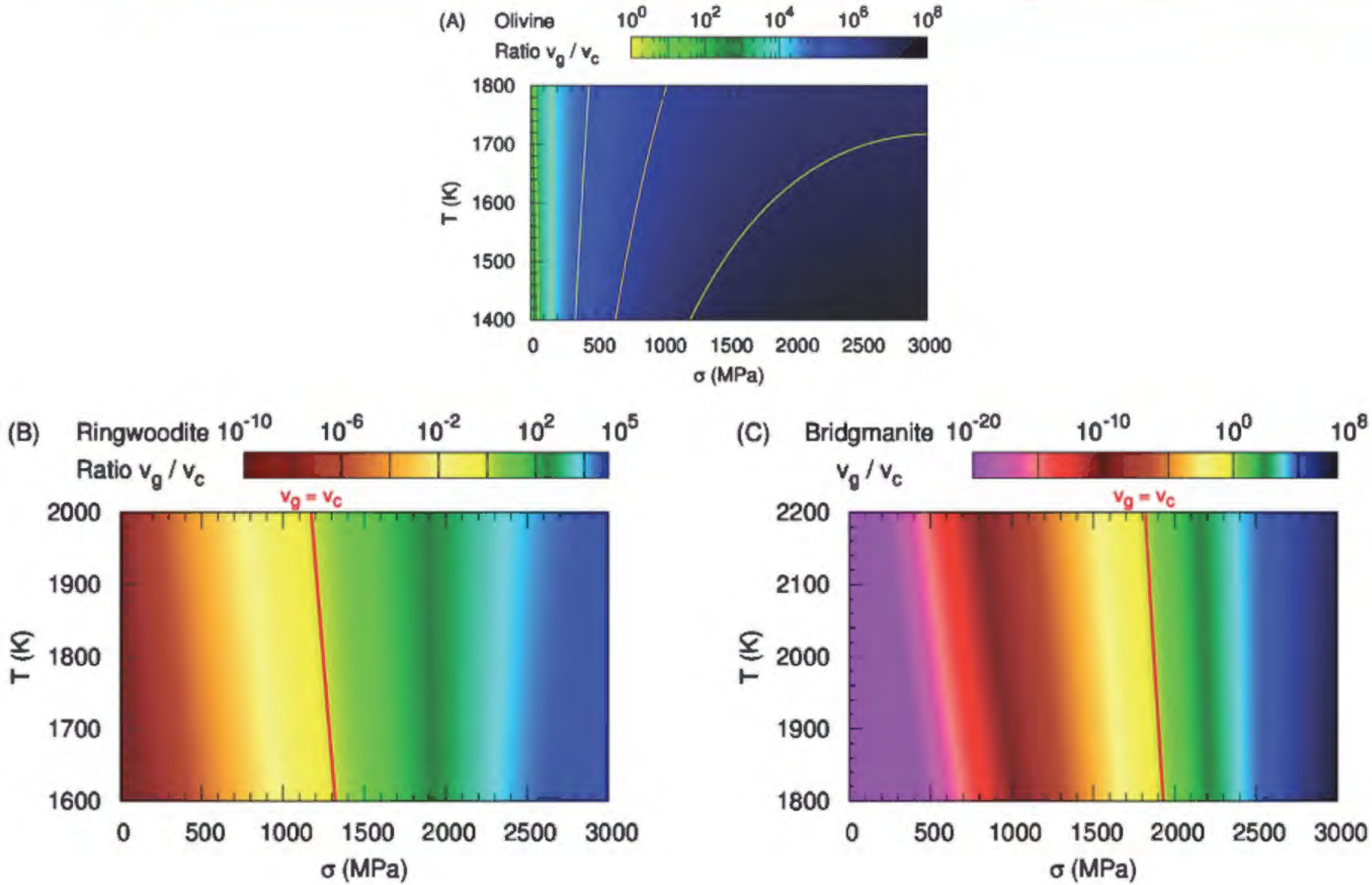
Boioli et al. Phys Rev B 2015

Olivine rheology at low temperature [001] glide

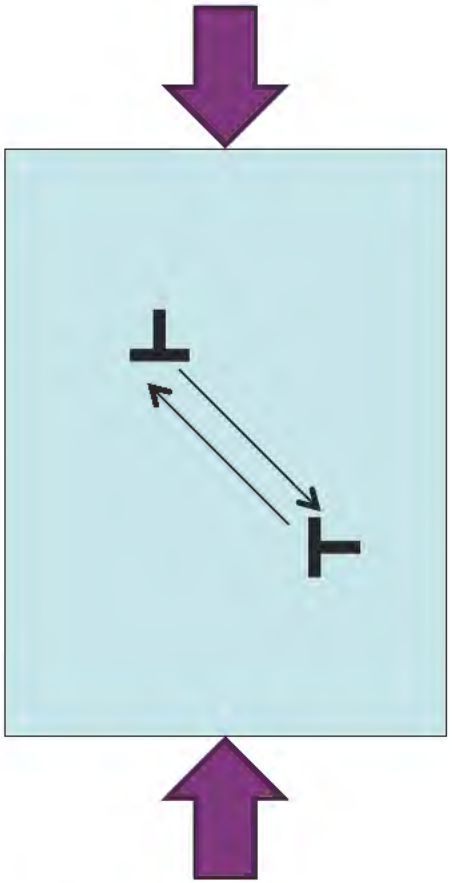


Boioli et al. EPSL 2015

Creep in the lower mantle



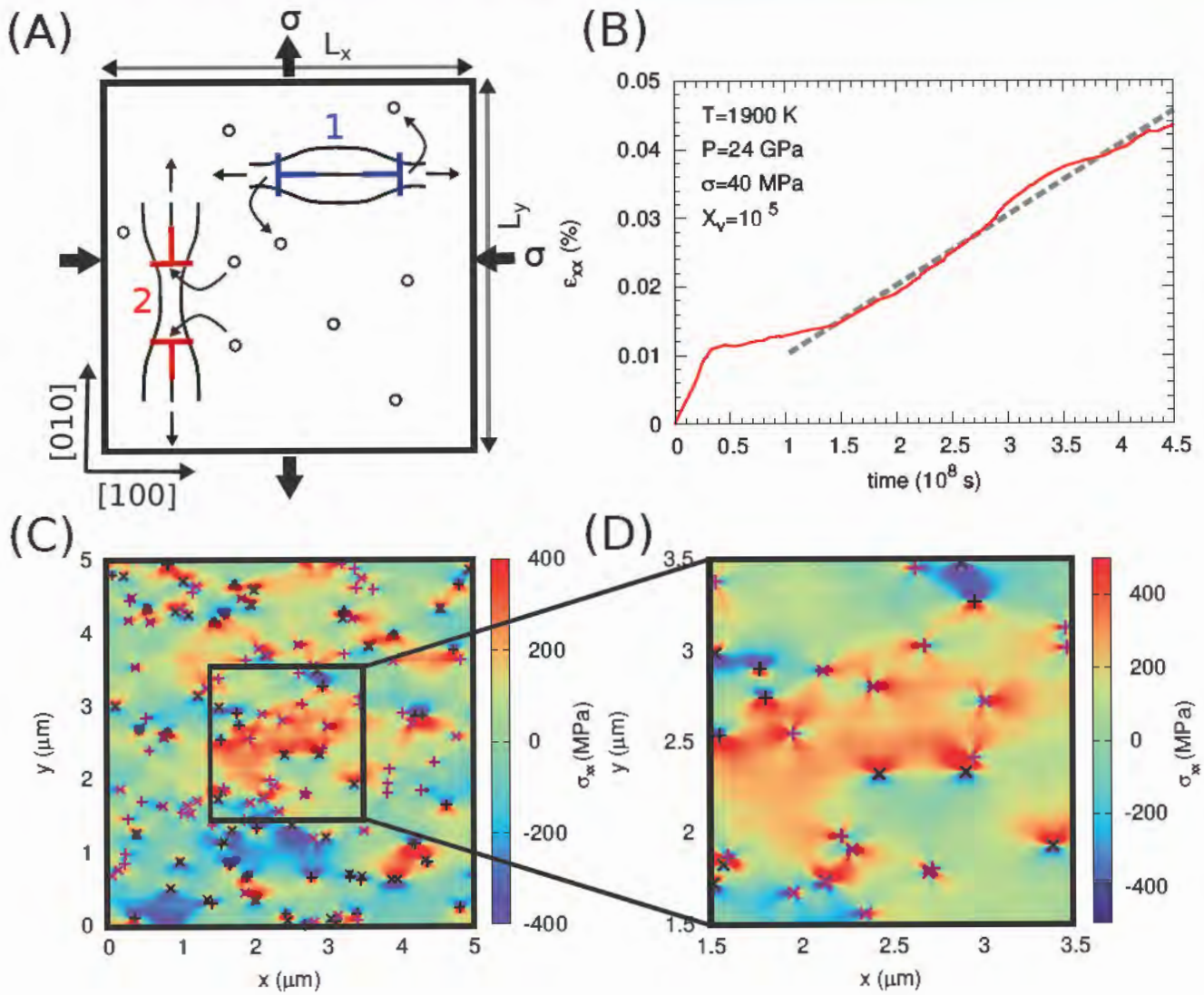
Introducing pure climb creep



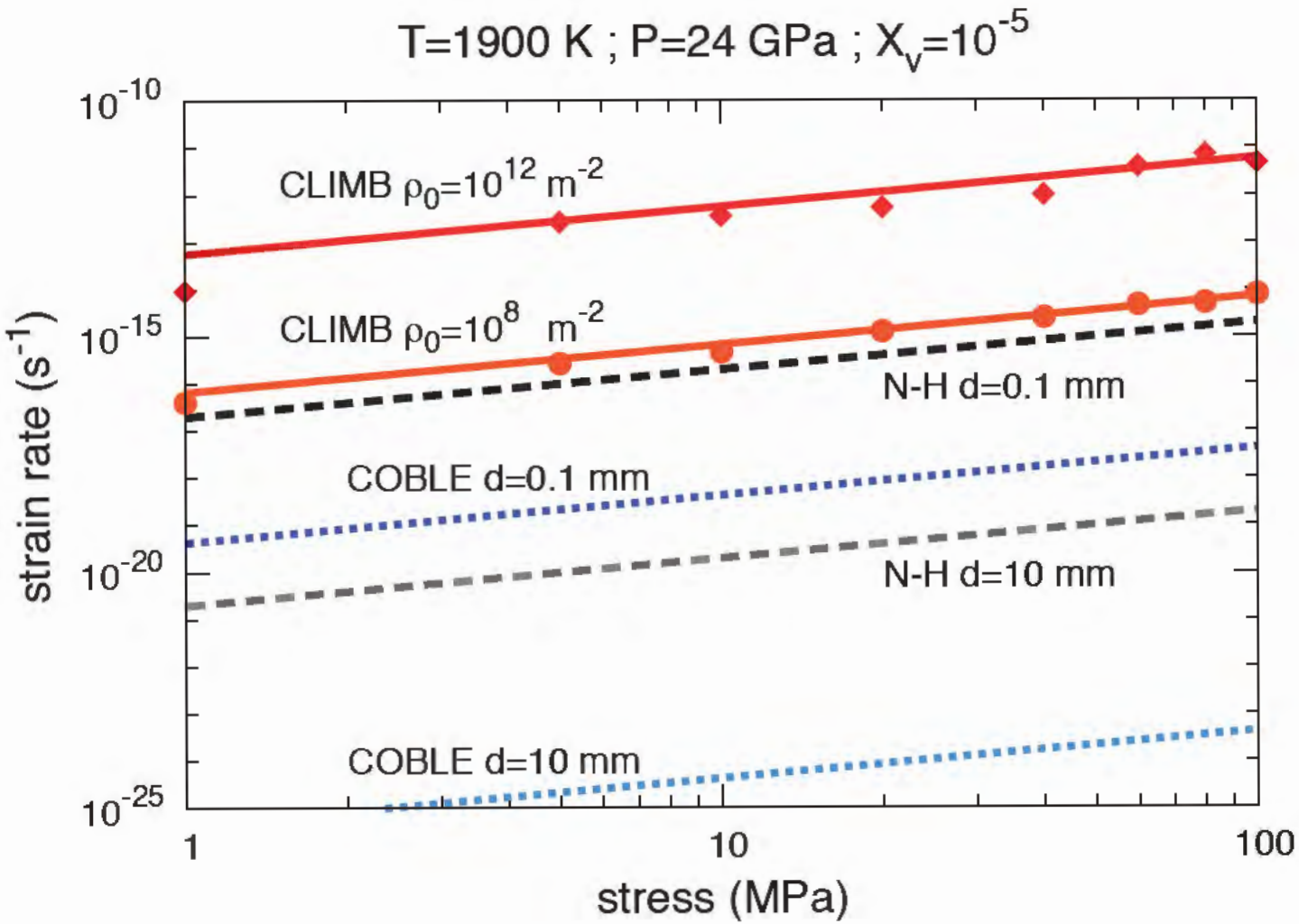
Pure climb creep

- Strain is produced by dislocation ***climb***
- Dislocations act as sources and sinks of point defects (vacancies)
- Dislocations exchange vacancies
- The characteristic diffusion length is determined by the dislocation density

Modelling pure climb creep

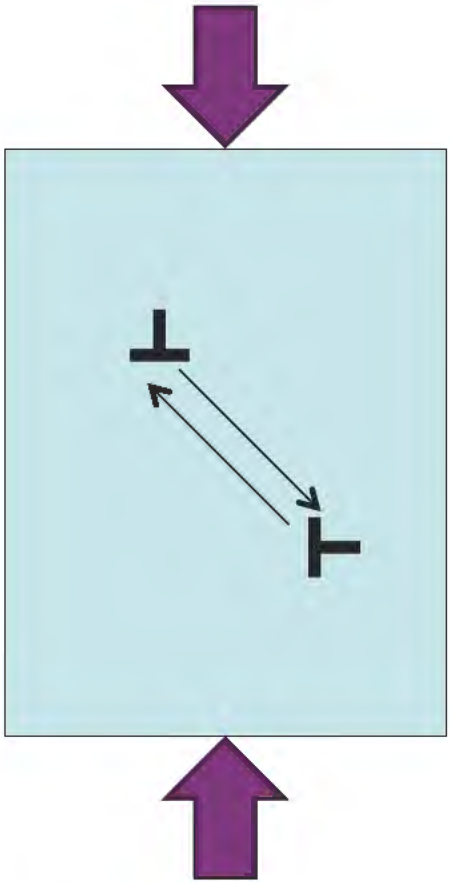


Modelling pure climb creep in bridgmanite



Pure climb creep:

A very important mechanism for planetary interiors rheology



Pure climb creep

A few facts:

- Strain is produced by dislocation ***climb***
- Strain is not produced by shear: no crystal preferred orientations
- No grain size dependence
- Controlled by diffusion, but rheology *may not* be linear

Stop 7

- Diffusion creep ✓
- Dislocation creep ✓
- Pure climb creep ✓

- What about grain boundaries ?

Toward a more general elastic field theory

Collaboration with C. Fressengeas & V. Taupin, Metz

Displacement field: $\vec{u}$

Total distortion tensor: $\overline{\overline{U}} = grad\ \vec{u}$

Cauchy stress: $\overline{\overline{\sigma}} = \overline{\overline{\overline{\overline{C}}}} : \overline{\overline{\varepsilon}}$

Equilibrium condition $\boldsymbol{div}\ \overline{\overline{\sigma}} = 0$

Energy: $E_{Cauchy} = \frac{1}{2}\sigma_{ij}\varepsilon_{ij}$

Rotation vector: $\vec{\omega} = -\frac{1}{2}\overline{\overline{\omega}} : \overline{\overline{\overline{\overline{X}}}}$

Curvature tensor: $\overline{\overline{\kappa}} = grad\ \vec{\omega}$

Couple stress tensor: $\overline{\overline{M}} = \overline{\overline{\overline{\overline{A}}}} : \overline{\overline{\kappa}}$

Equilibrium condition $\boldsymbol{div}\ \overline{\overline{M}} = 0$

Energy: $E_{couple} = \frac{1}{2}M_{ij}\kappa_{ij}$

Toward a more general elasto-plastic field theory

Compatibility equations: $curl\ \overline{\overline{U}} = 0$ $\qquad$ $curl\ \overline{\overline{\kappa}} = 0$

<u>Incompatible elasto-plasticity</u>:

Nye's dislocation density tensor:

$$\overline{\overline{\alpha}} = curl\ \overline{\overline{U}}_e = -curl\ \overline{\overline{U}}_p$$

Disclination density tensor:

$$\overline{\overline{\theta}} = curl\ \overline{\overline{\kappa}}_e = -curl\ \overline{\overline{\kappa}}_p$$

Burgers vector: closure defect obtained by integrating the incompatible elastic distortions along a circuit *C*

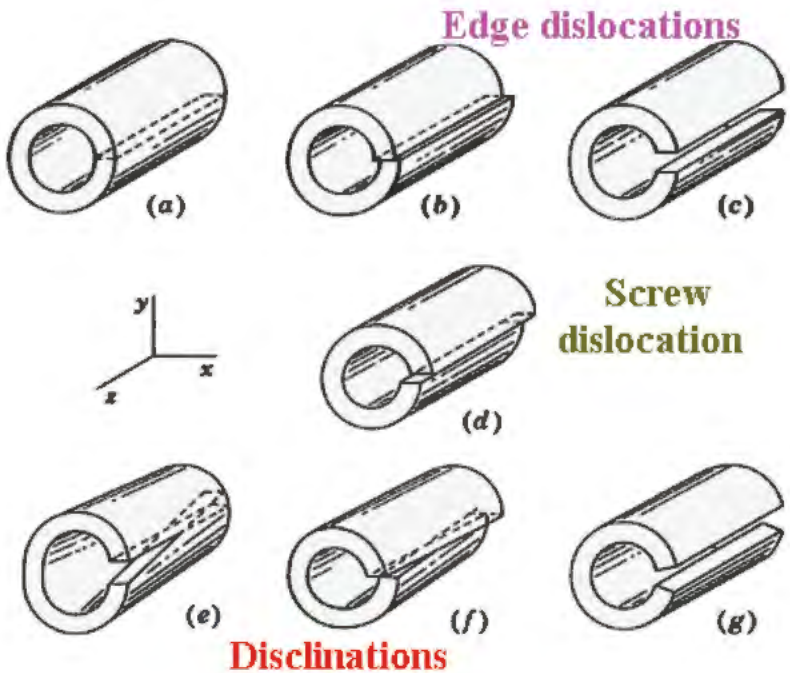
$$\mathbf{b} = \int_C \overline{\overline{U}}_e . \overrightarrow{dr} = \int_S \overline{\overline{\alpha}} . \vec{n}\, dS$$

Frank vector: closure defect obtained by integrating the incompatible elastic curvature along a circuit *C*

$$\vec{\Omega} = \int_C \overline{\overline{\kappa}}_e . \overrightarrow{dr} = \int_S \overline{\overline{\theta}} . \vec{n}\, dS$$

Toward a more general elasto-plastic field theory

$$curl\ \overline{\overline{\kappa}} = 0$$



Disclination density tensor:

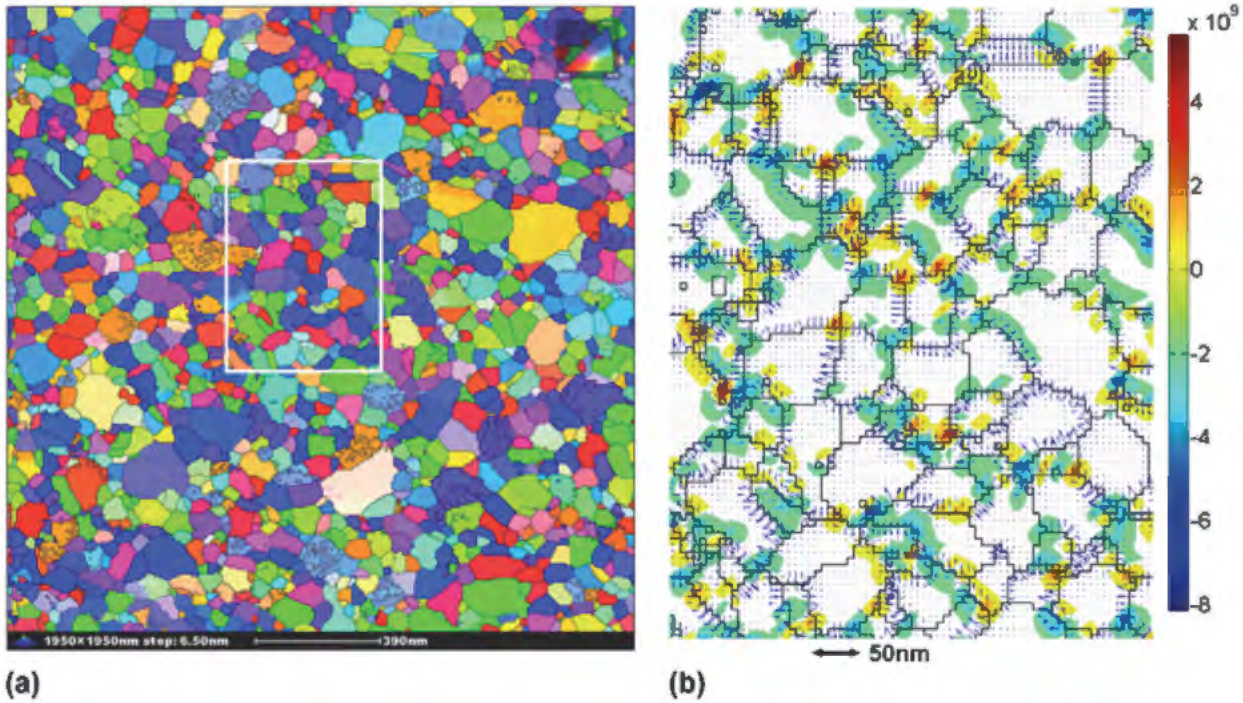
$$\overline{\overline{\theta}} = curl\ \overline{\overline{\kappa}}_e = -curl\ \overline{\overline{\kappa}}_p$$

Frank vector: closure defect obtained by integrating the incompatible elastic curvature along a circuit *C*

$$\vec{\Omega} = \int_C \overline{\overline{\kappa}}_e . \vec{dr} = \int_S \overline{\overline{\theta}} . \vec{n}\, dS$$

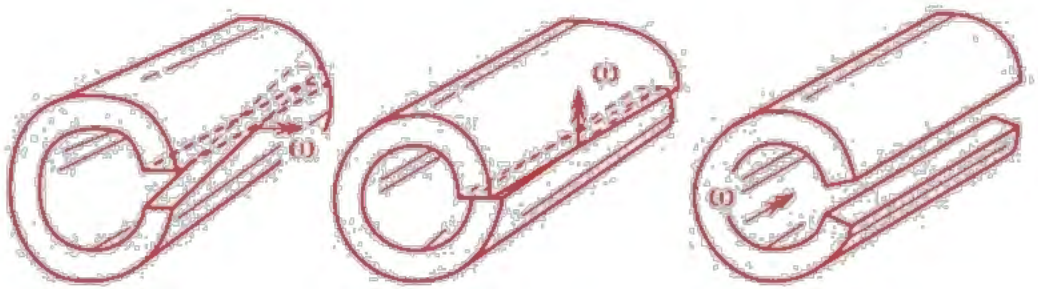
You remember ?

Disclinations



Disclinations were recently evidenced in metals, here Al

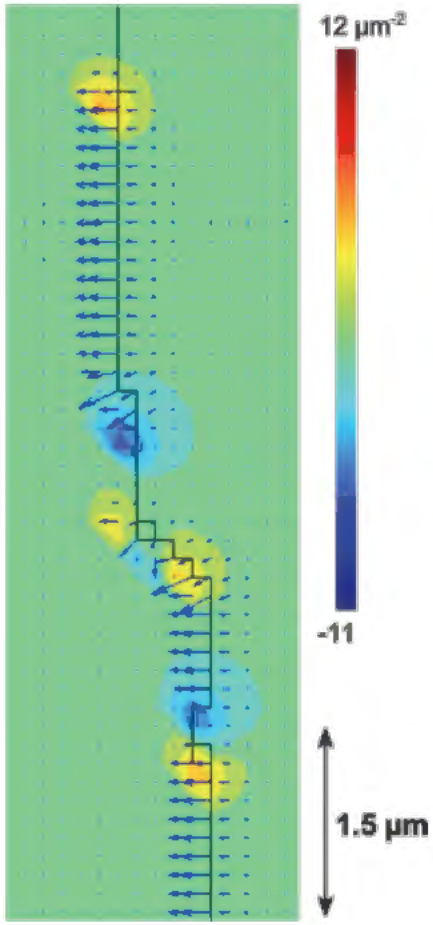
Beausir & Fressengeas (2013)



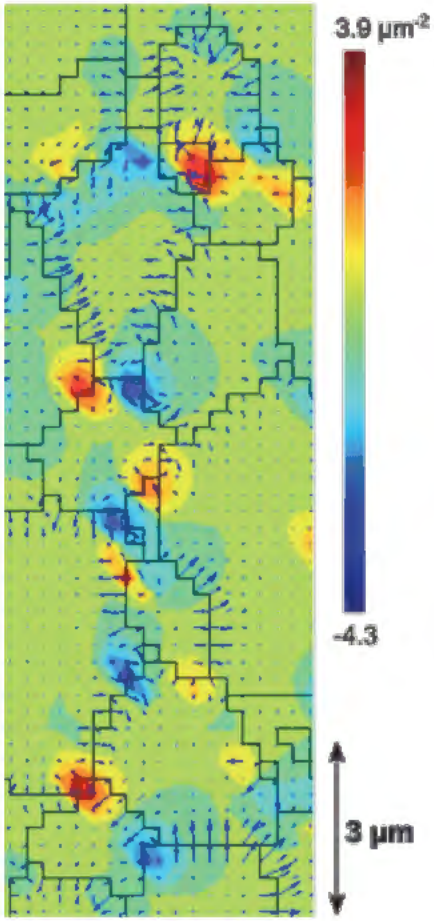
Disclinations

Dislocation and disclinations analysis by EBSD

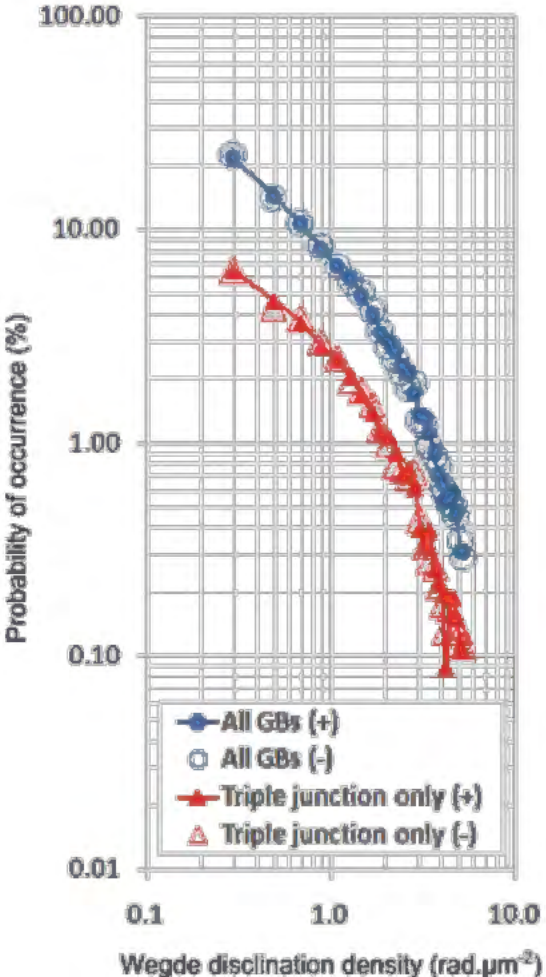
OOM – naturally deformed mylonitic harzburgite from the Oman ophiolite (Sumail massif)



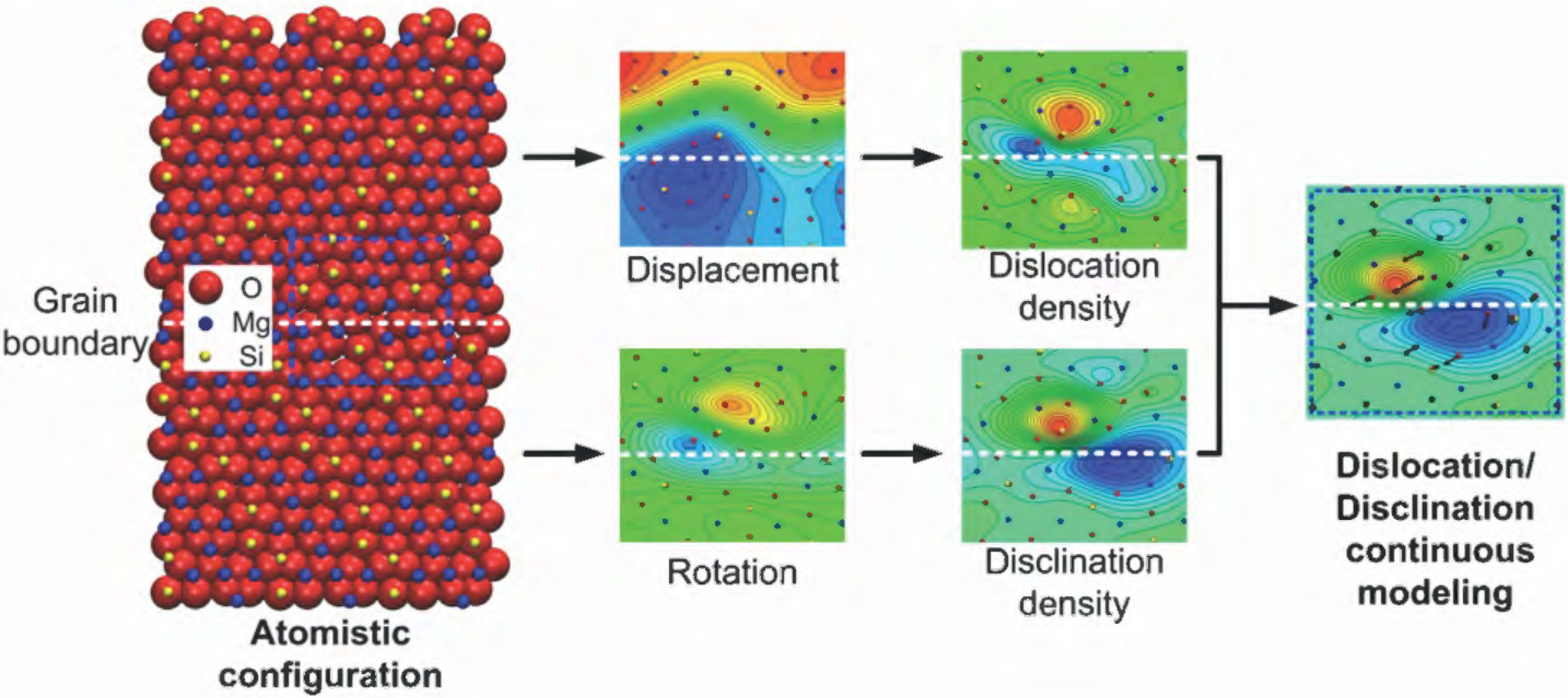
T0548
Experimentally deformed at 1200°C



Cordier et al. Nature 2014



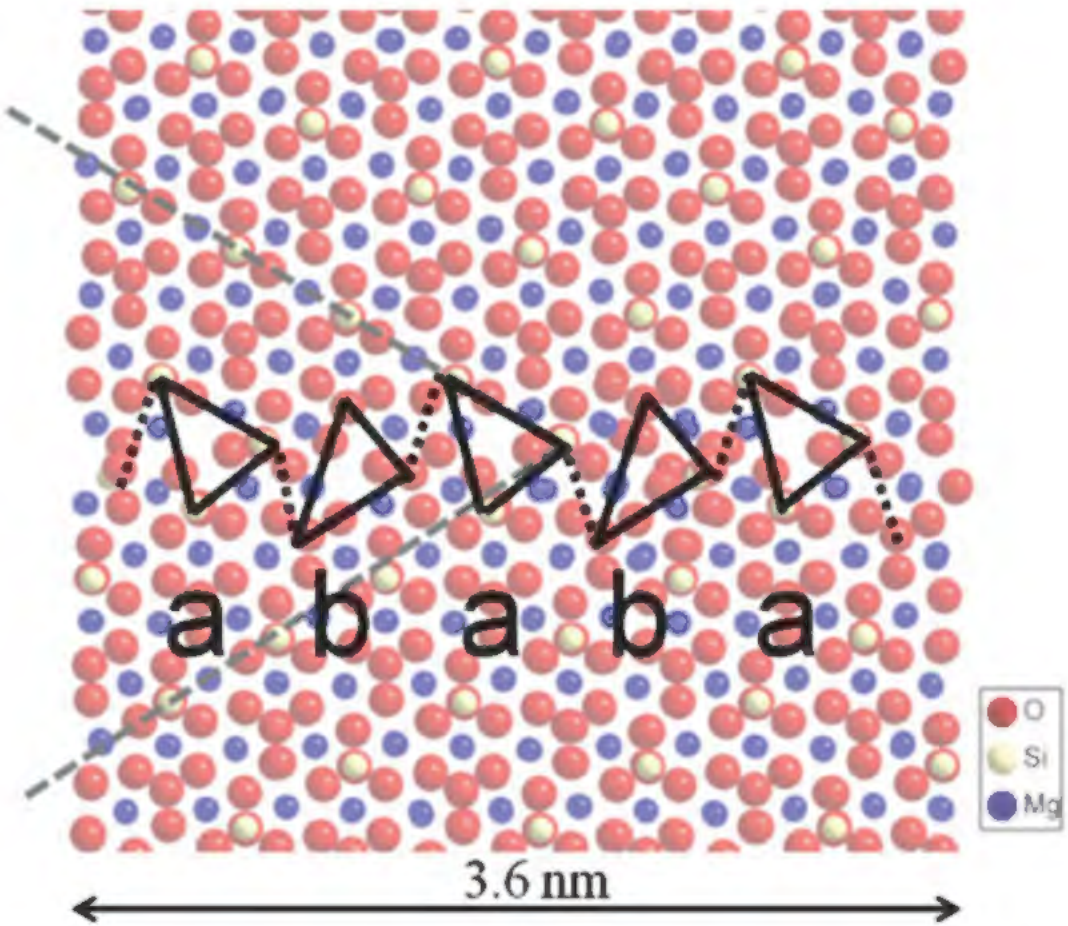
Grain boundary modeling based on disclinations



Sun et al. IJP 2016

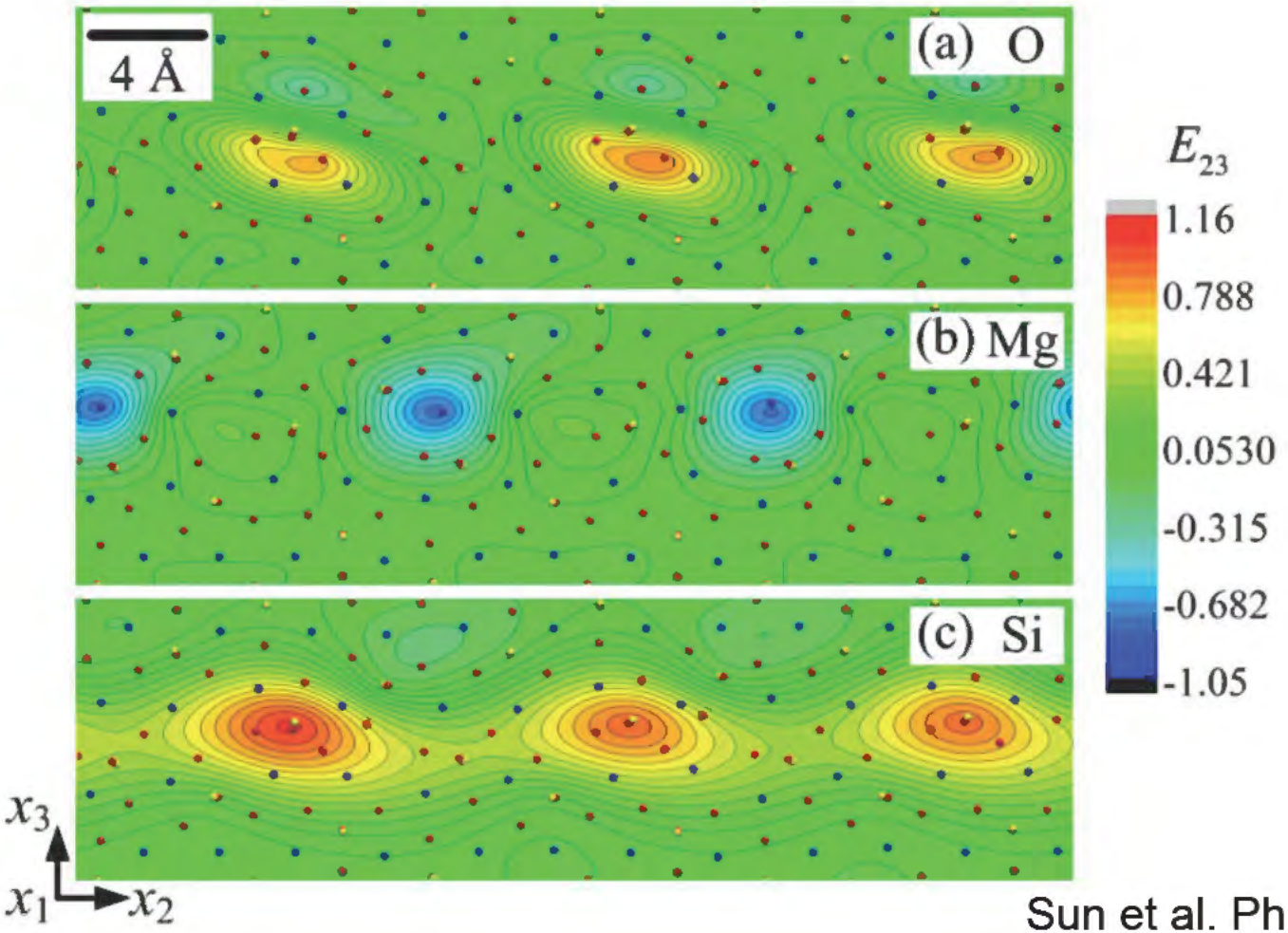
Grain boundary modeling based on disclinations

Forsterite: (011)/[100] tilt grain boundary with misorientation 60.80° (coll S. Jahn)



Grain boundary modeling based on disclinations

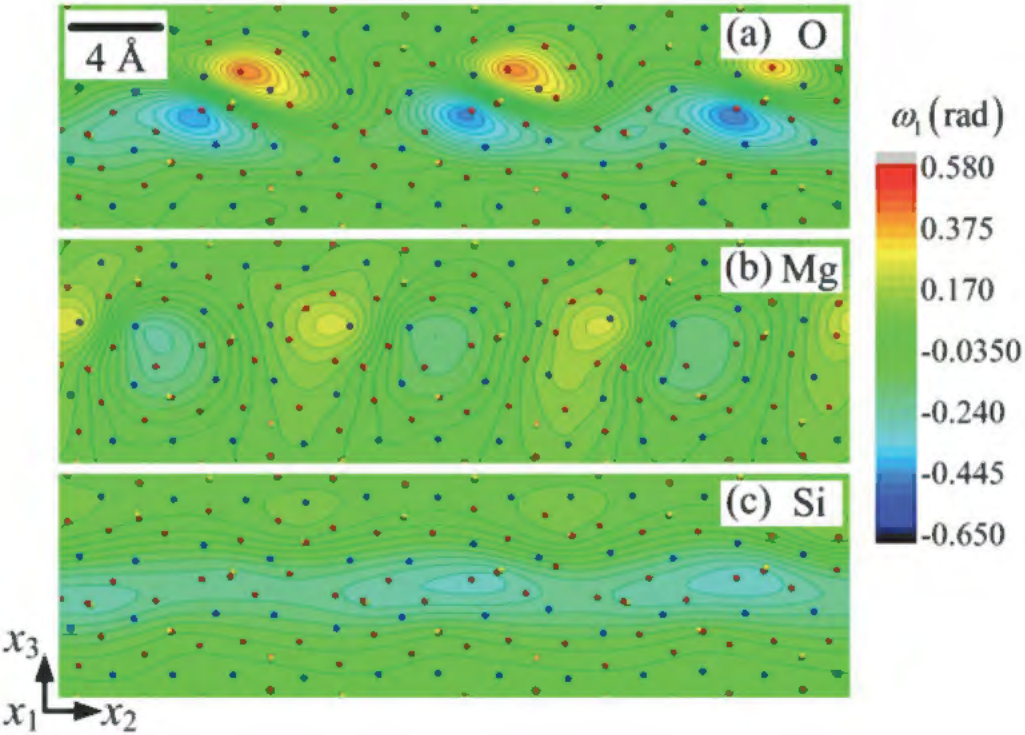
Forsterite: (011)/[100] tilt grain boundary with misorientation 60.80° (coll S. Jahn)

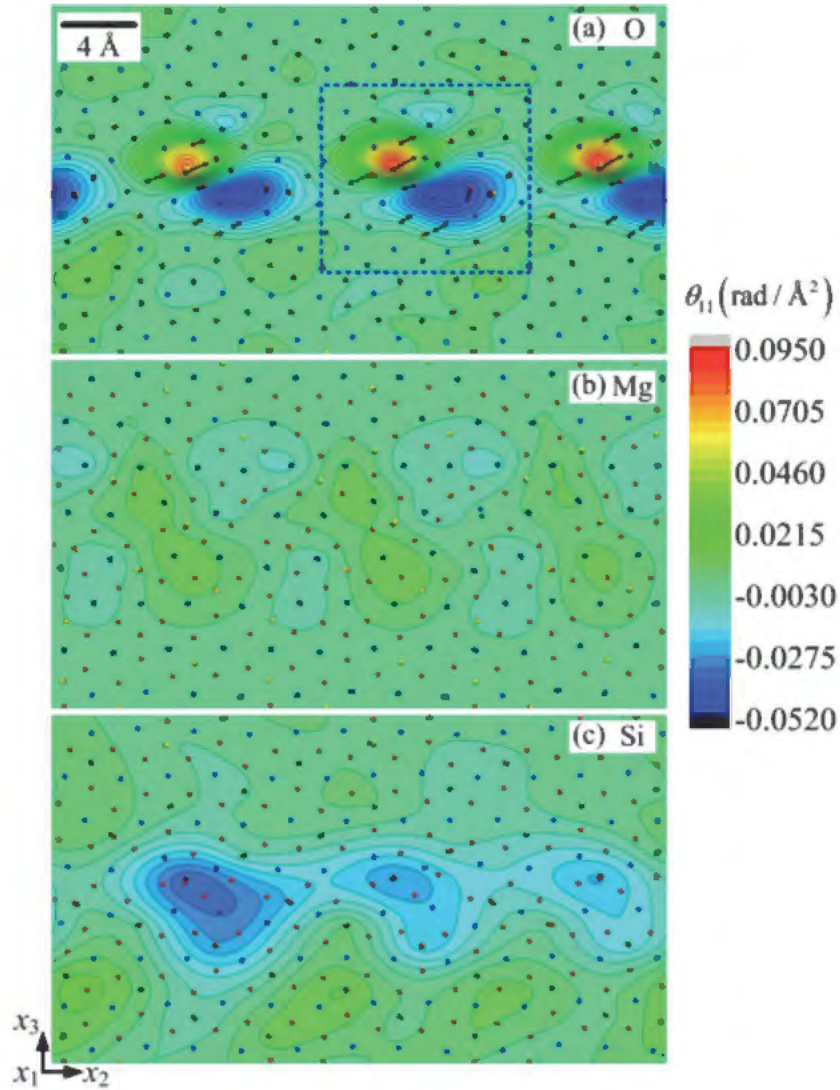


Sun et al. Phil Mag 2016

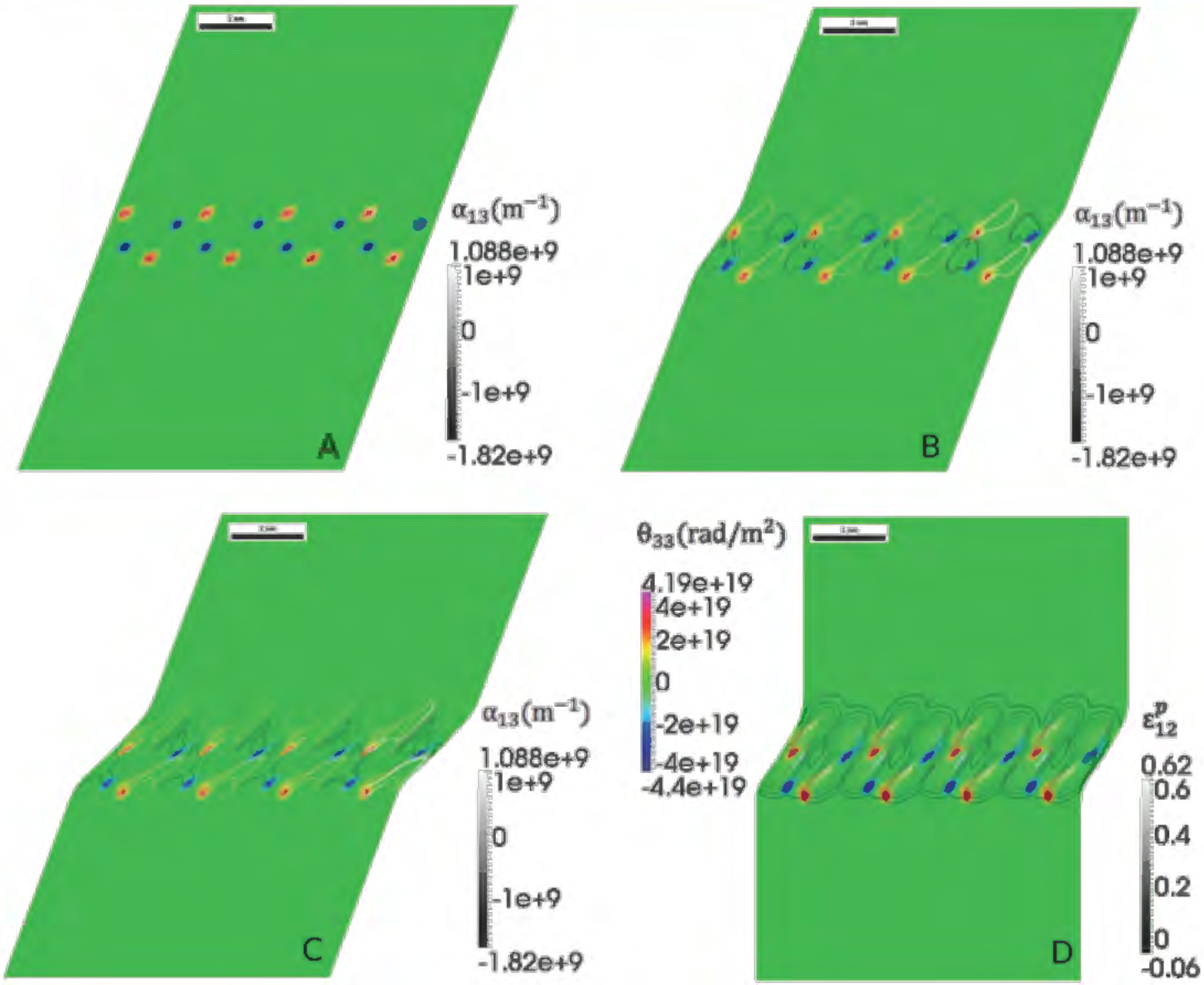
Grain boundary modeling based on disclinations

Forsterite: (011)/[100] tilt grain boundary with misorientation 60.80° (coll S. Jahn)

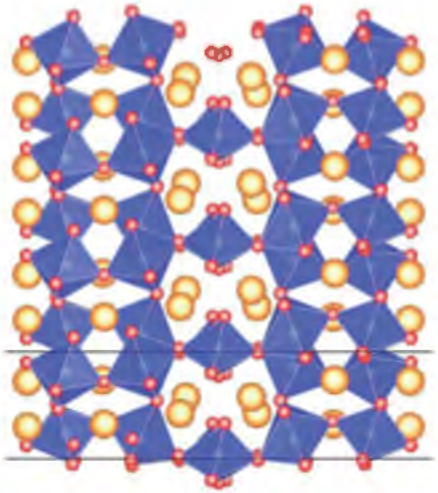


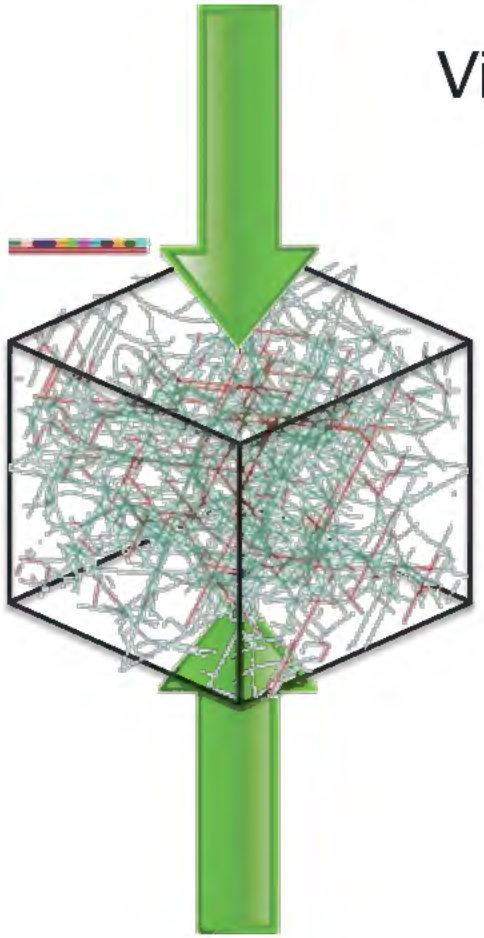


Shear –coupled boundary migration



Final stop : Thank you !





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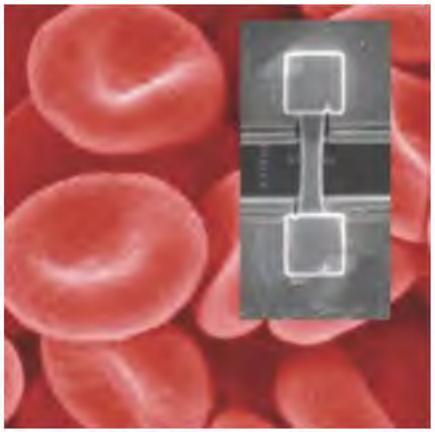

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