What Numerical Modelling Tells Us About Dislocation Creep in Earth Mantle

Philippe Carrez

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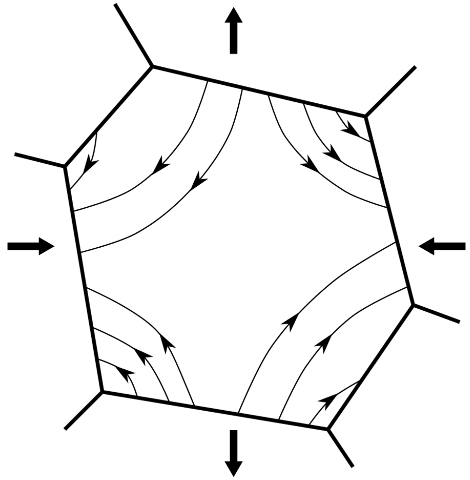
Various creep mechanisms (dependant on temperature, stress, …)



Diffusion creep

Bulk diffusion (Nabarro-Herring creep)

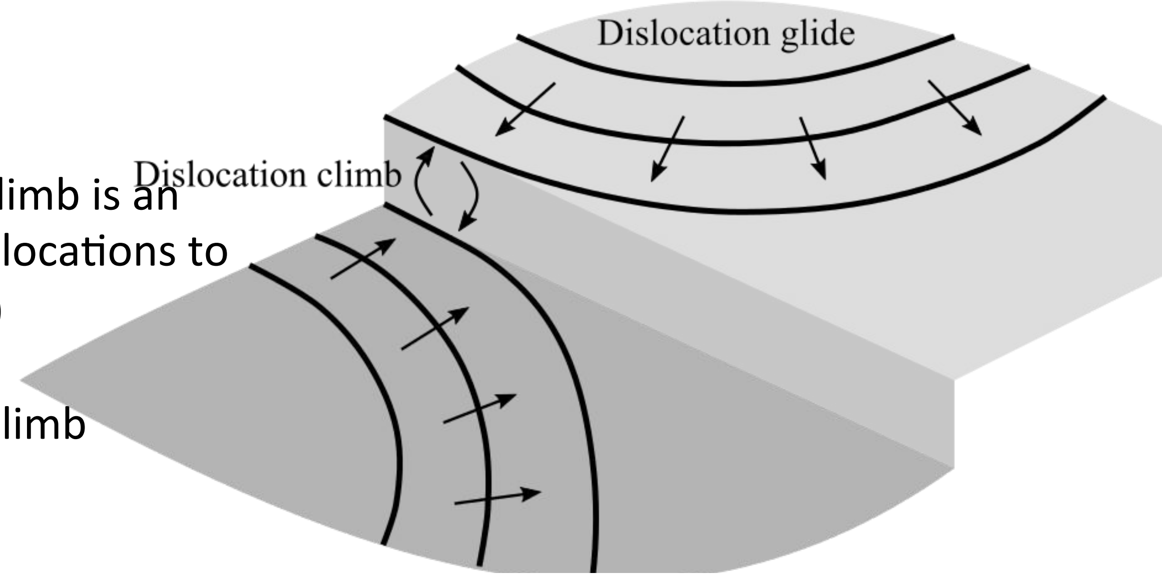
Grain boundary diffusion (Coble creep)

Dislocation creep

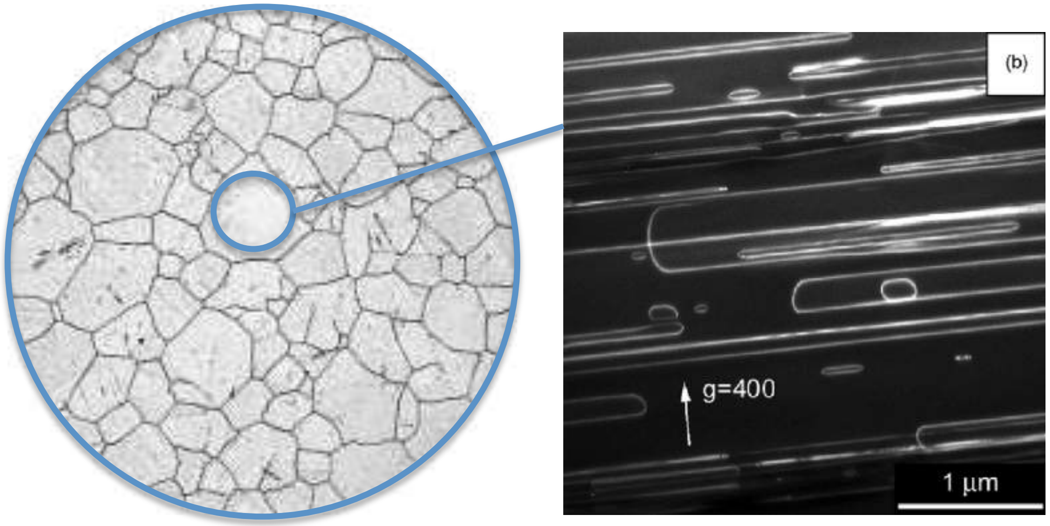
dislocation glide

Climb-assisted glide — here the climb is an enabling mechanism, allowing dislocations to get around obstacles (Weertman)

Climb —strain accomplished by climb

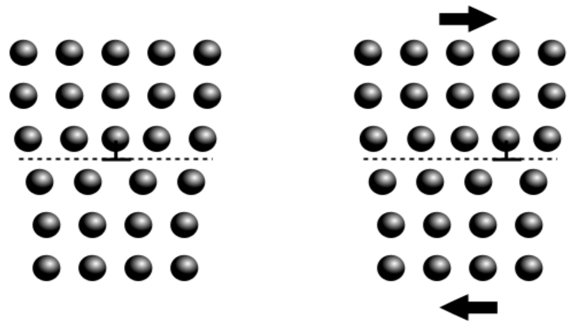


A few words about dislocation

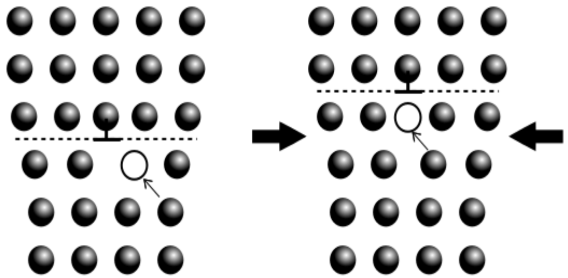


Olivine (P. Raterron)

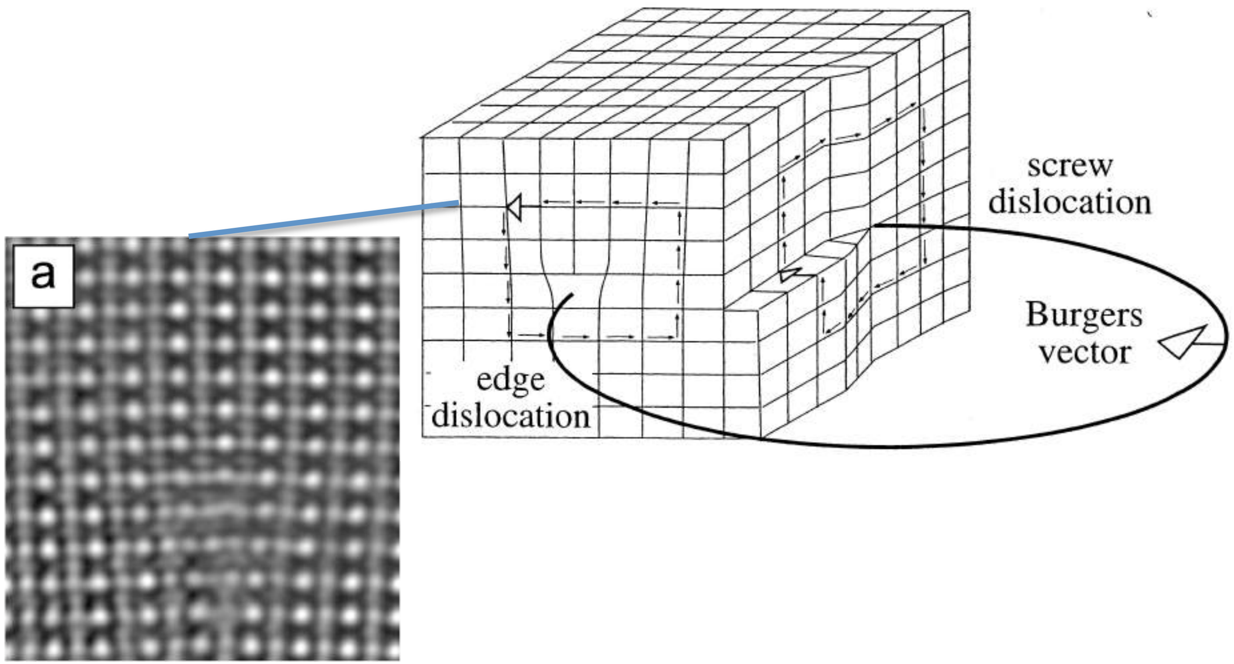
Glide



Climb



Jia et al. 2005



Various creep mechanisms (dependant on temperature, stress, …)

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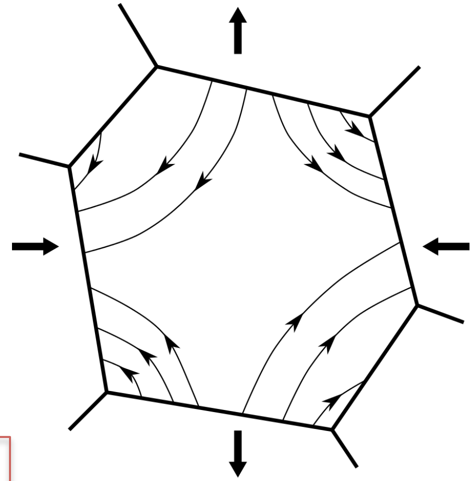

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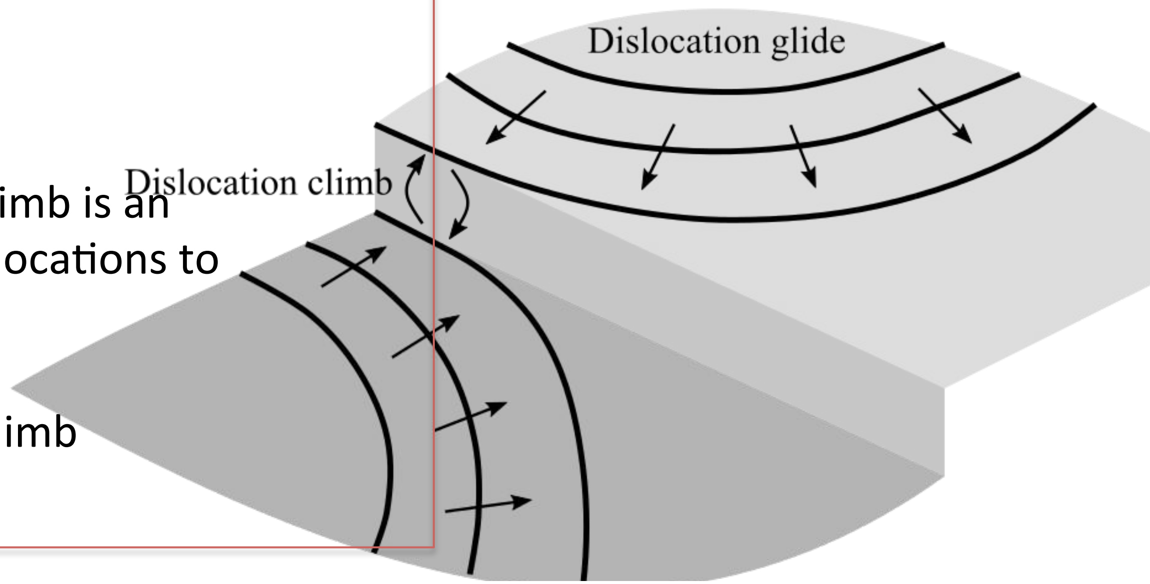
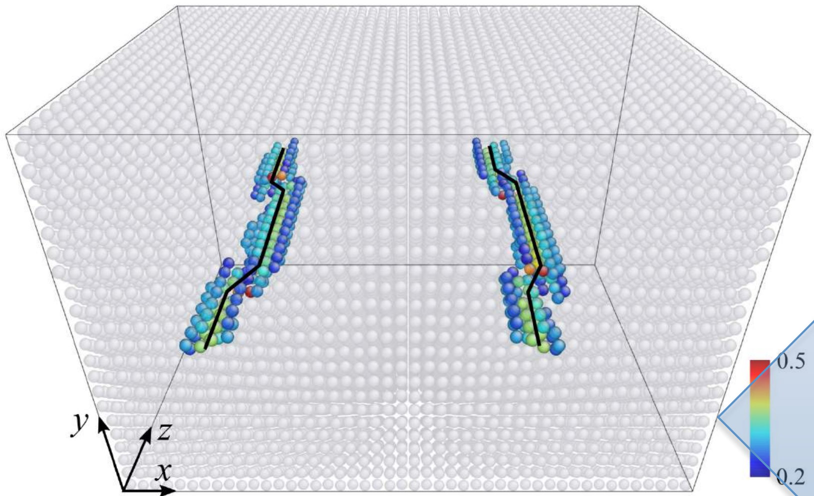
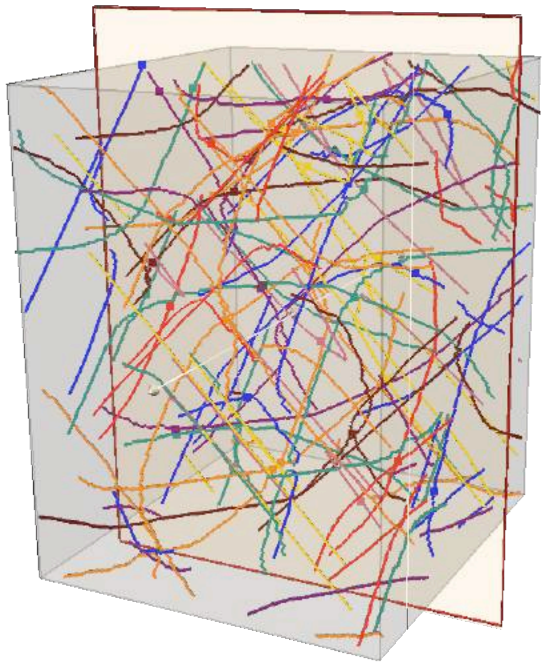


Multi-Scale model of dislocation creep

Atomistic calculations



Dislocation Dynamic (DD) simulation



◦ dislocation core properties
(effect of high Pressure)
◦ Dislocation mobility
(effect of temperature on glide velocity)

Mesoscale simulation (grain scale)
-> Collective behavior

Introduction of Climb (Steady state conditions, Constant vacancy concentration)

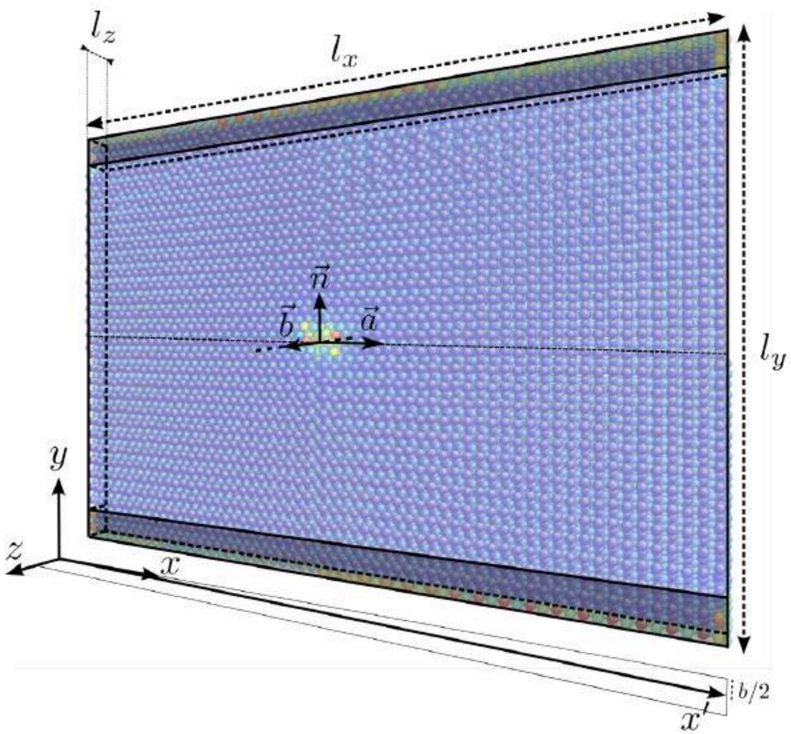
-> Rheological law (strain rate vs stress)

Computational details for atomic scale calculations

Atomistic calculations performed with LAMMPS using a classical pairwise potential

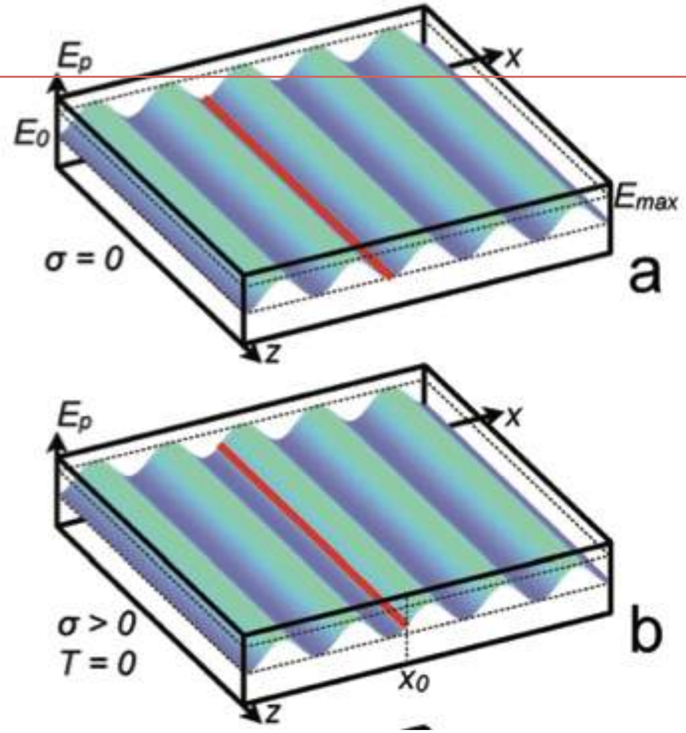
$$U_{ij}(R_{ij}) = \frac{z_i z_j}{R_{ij}} + b_{ij} \exp\left(-\frac{R_{ij}}{\rho_{ij}}\right) - \frac{c_{ij}}{R_{ij}^6}$$

R_{ij} interatomic distance and z_i charge



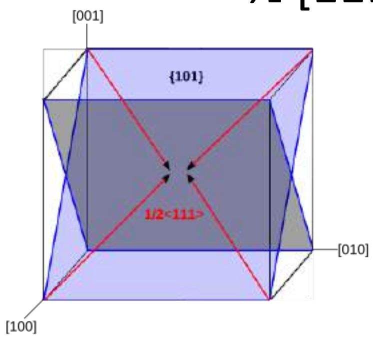
Atomic arrangement of atoms in the vicinity of the defect => Core structure

Peierls potential Vp (eV/Angs) and associated Peierls stress

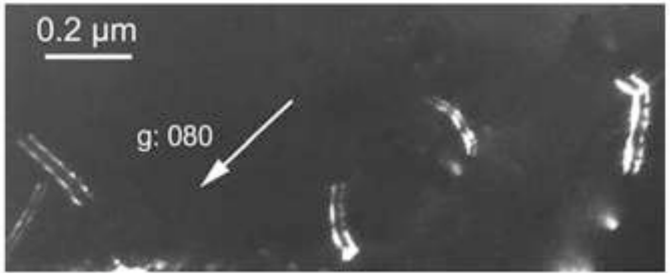


Dislocation in wadsleyite (15 GPa)

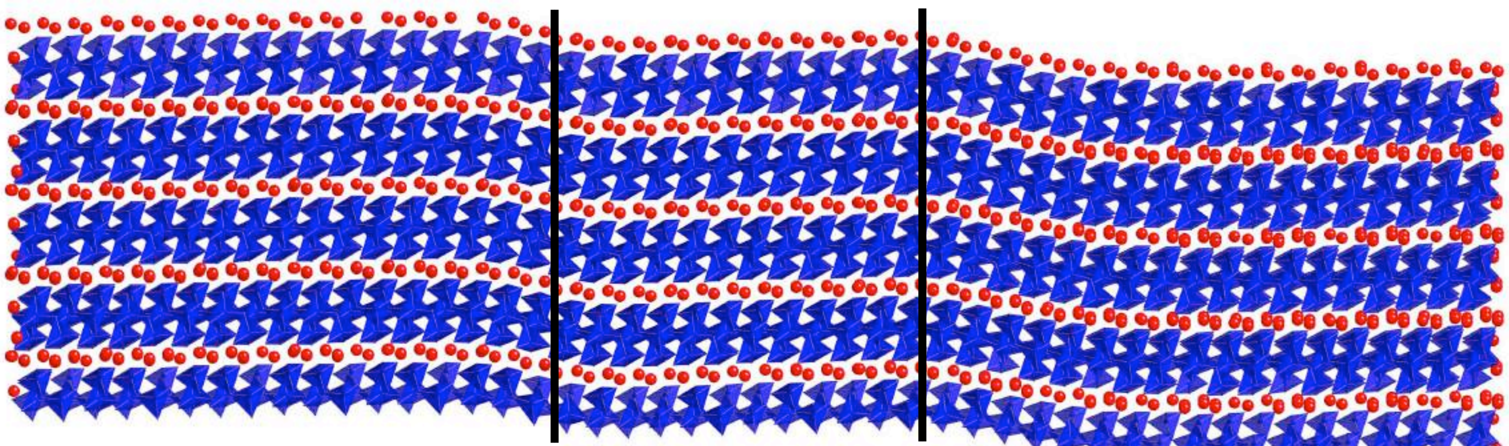
½ [111](101)



[111



Courtesy E. Thurel

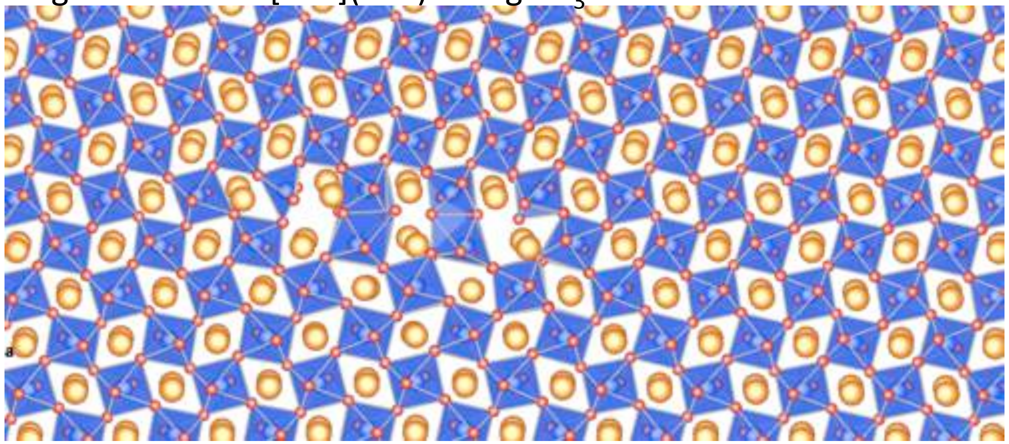


Stacking fault

Ritterbex et al. Am. Min. 2016

Dislocation core structure and Peierls stress

Edge dislocation [010](100) in $MgSiO_3$



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Acta Materialia 79 (2014) 117–125
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Atomic core structure and mobility of [100](010) and [010](100) dislocations in $MgSiO_3$ perovskite

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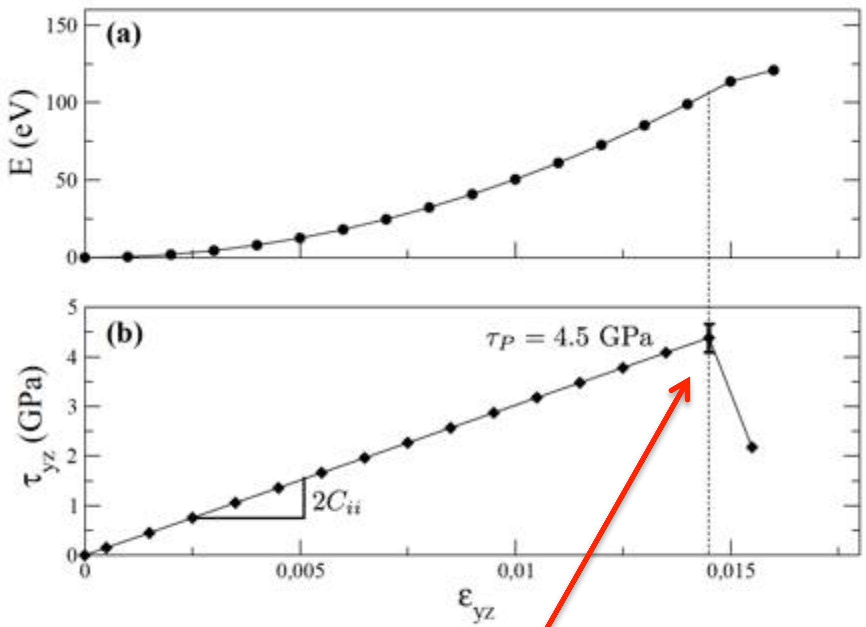
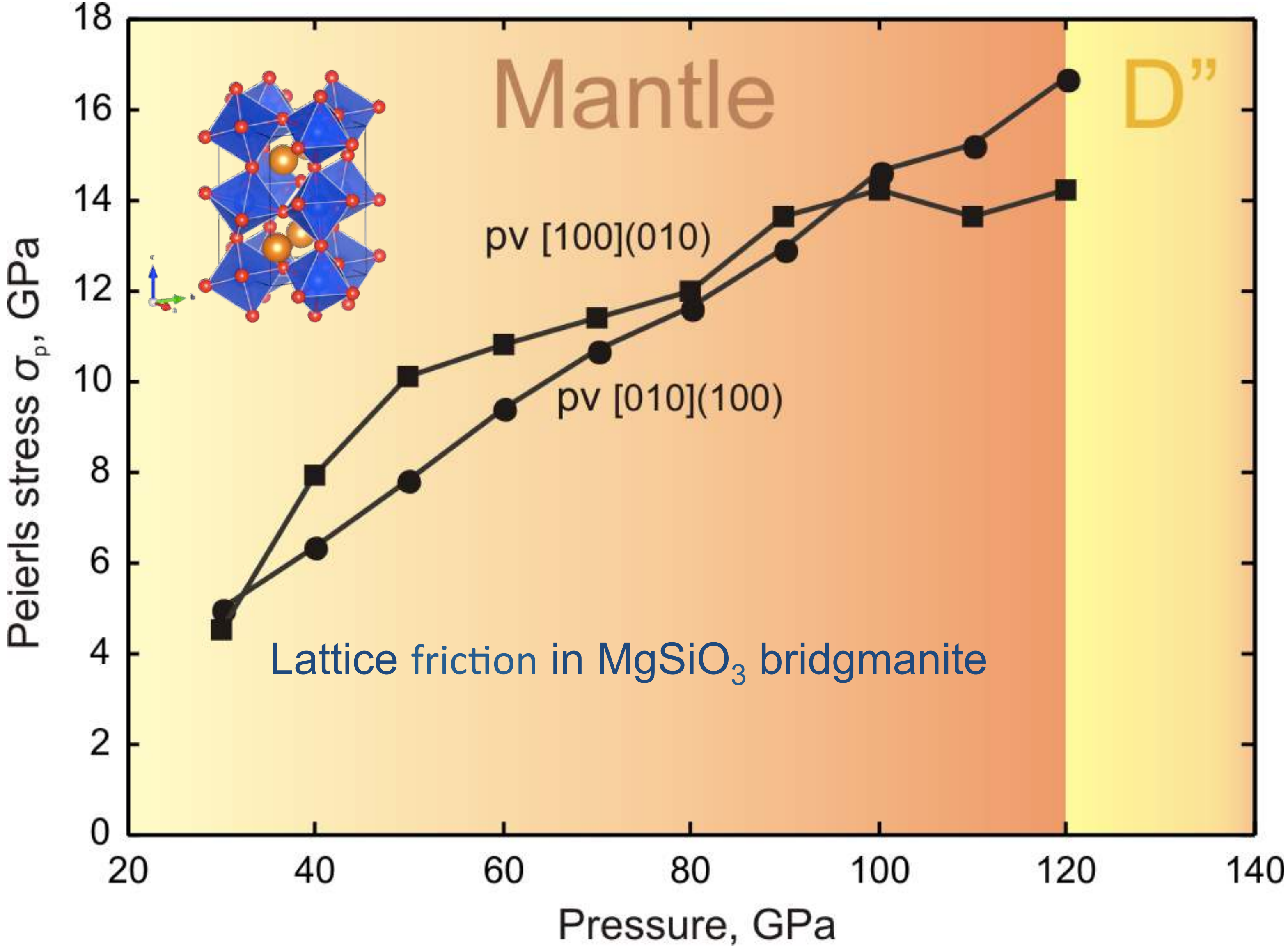
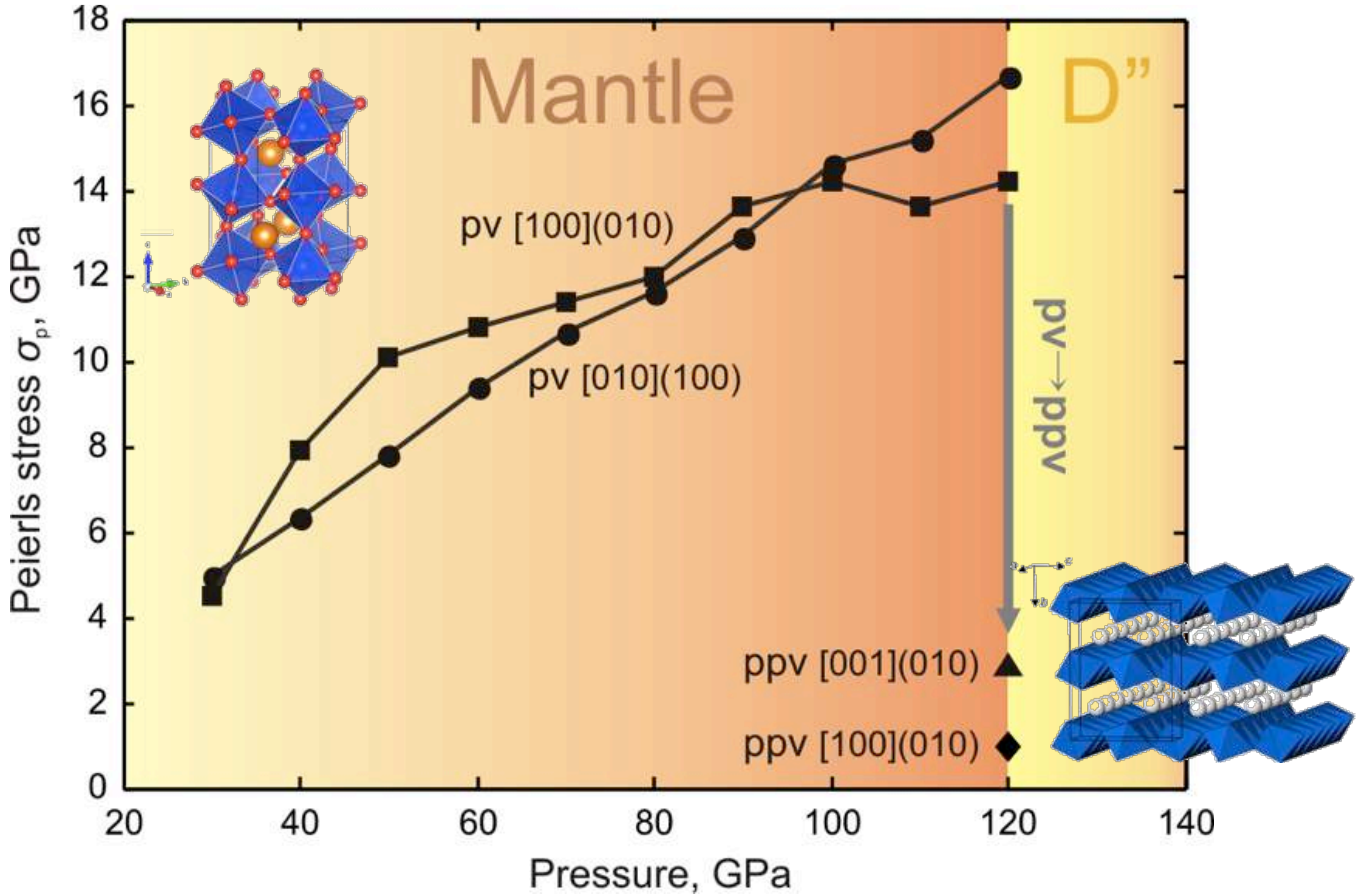


Peierls stress

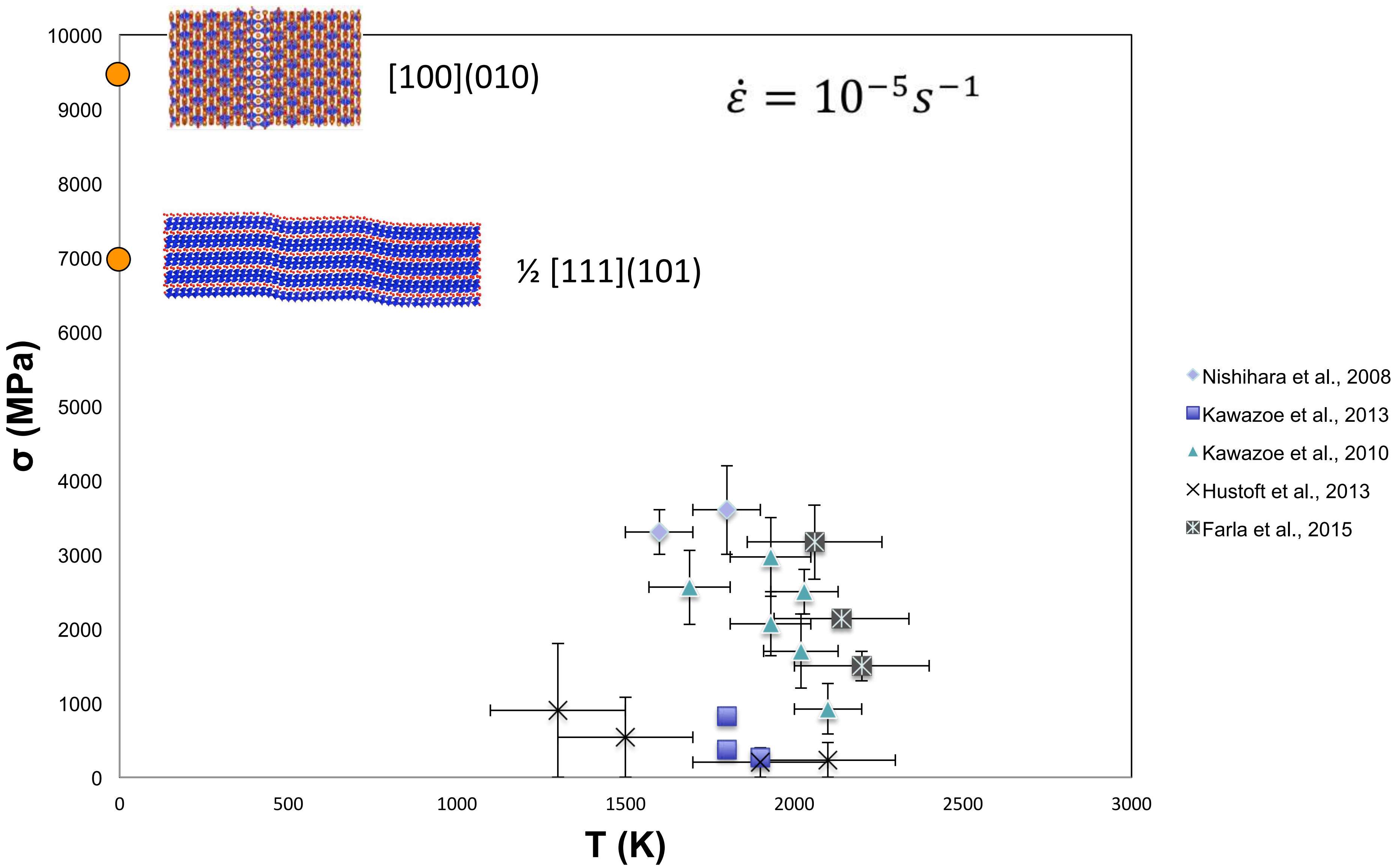
Effect of Pressure on lattice friction: Peierls stress versus Pressure



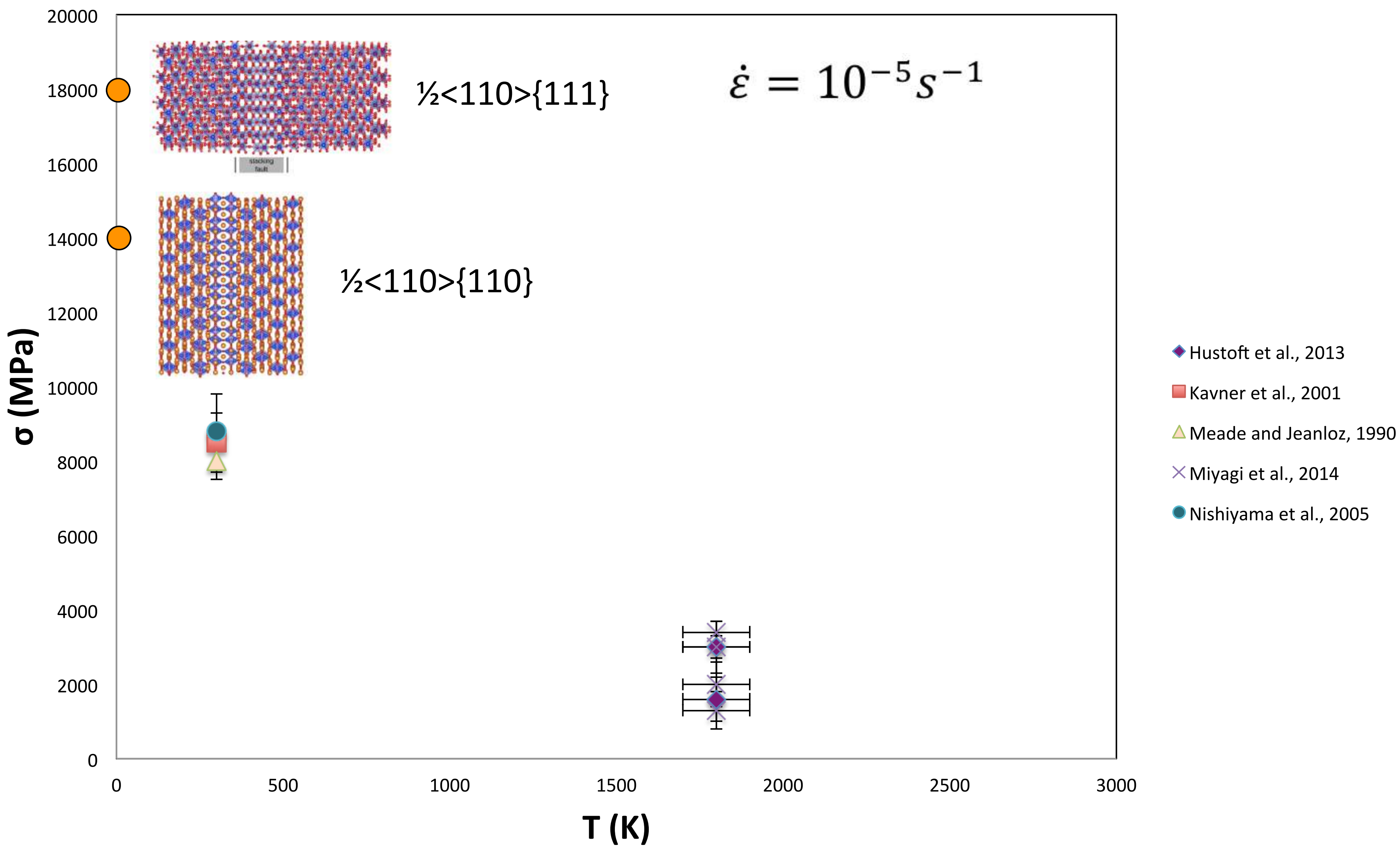


Mantle
D"
pv [100](010)
pv [010](100)
pv→ppv
ppv [001](010)
ppv [100](010)
Peierls stress σ_p, GPa
Pressure, GPa
0
2
4
6
8
10
12
14
16
18
20
40
60
80
100
120
140

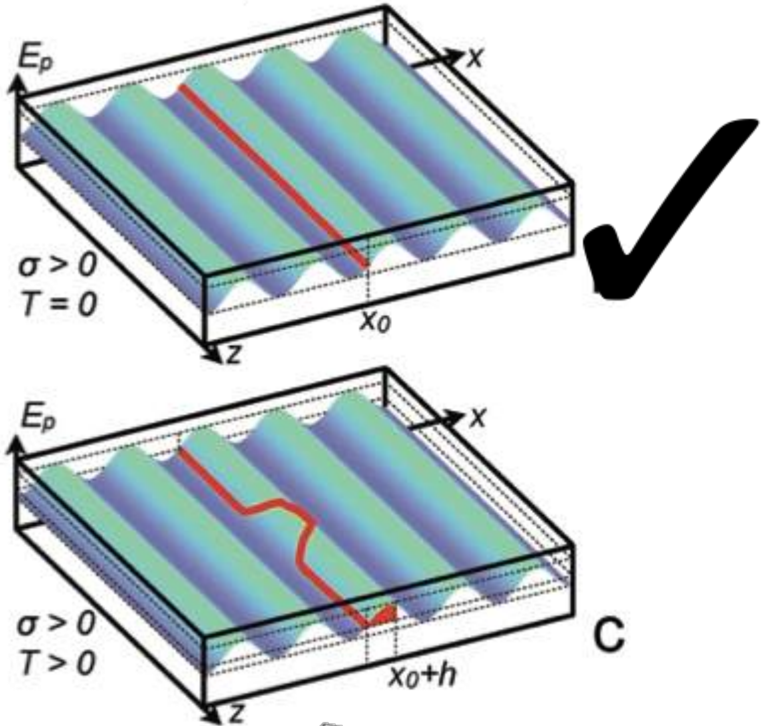
Comparison with experimental data: Wadsleyite Peierls stresses



Comparison with experimental data: Ringwoodite Peierls stresses



Thermally activated glide velocity



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KINK PAIR NUCLEATION AND CRITICAL SHEAR STRESS

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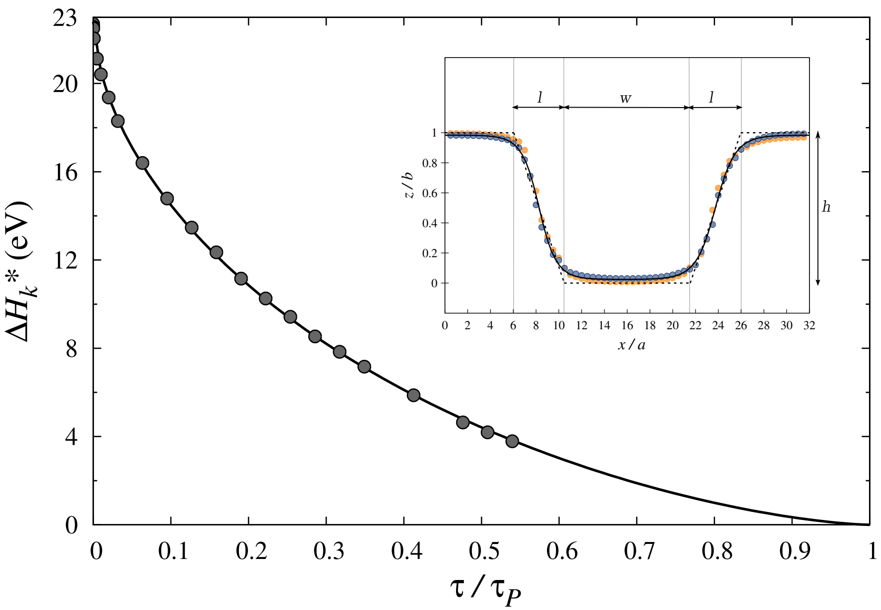
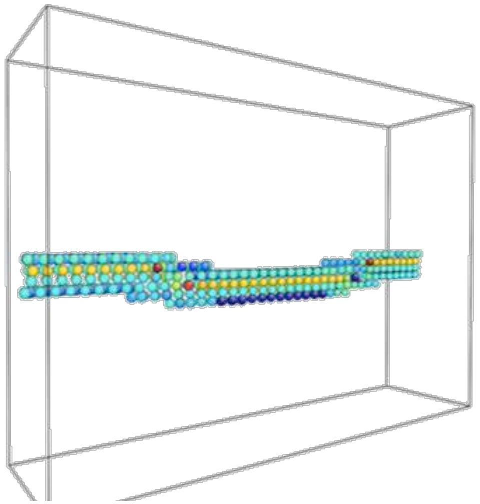
[3]Institute of Industrial Science, University of Tokyo, Roppongi, Minato-ku, Tokyo 106, Japan

$$\Delta H_k = \Delta E_{\rm elas} + \Delta W_P - W_\tau$$





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

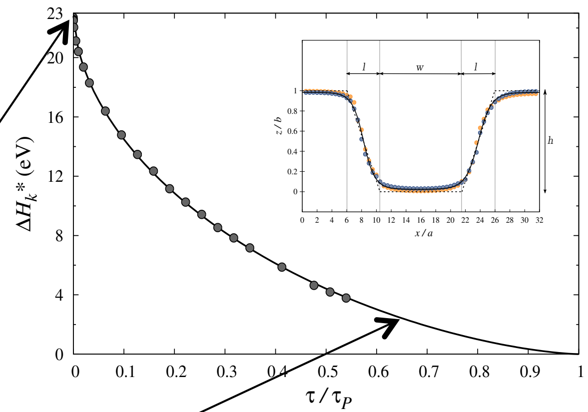
From dislocations to plasticity: a practical example

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

Kraych et al. EPSL 2016

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

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

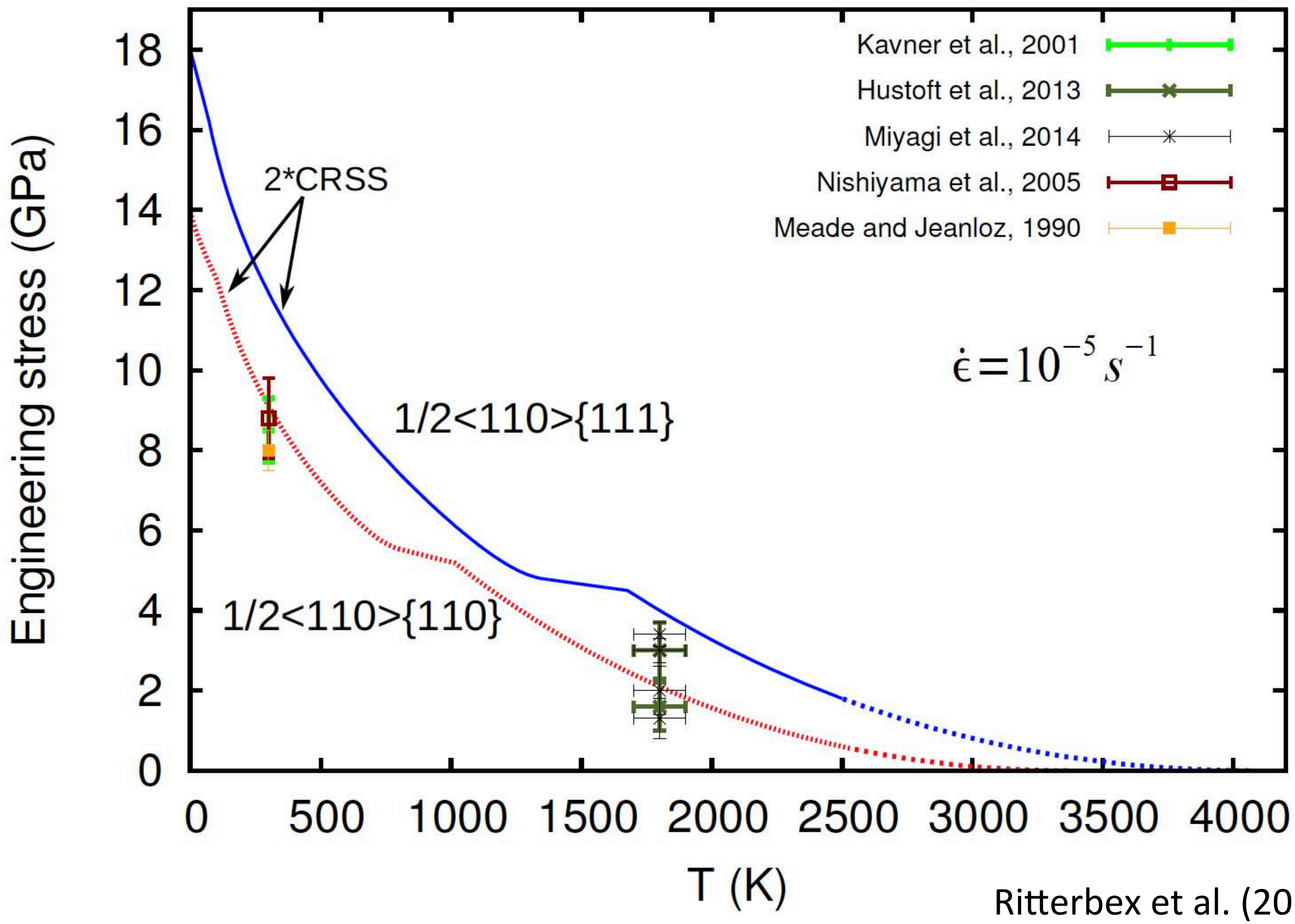


$$\tau = \tau_p\left(1-\left(C\frac{T}{H_k}\right)^{1/q}\right)^{1/p}$$

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

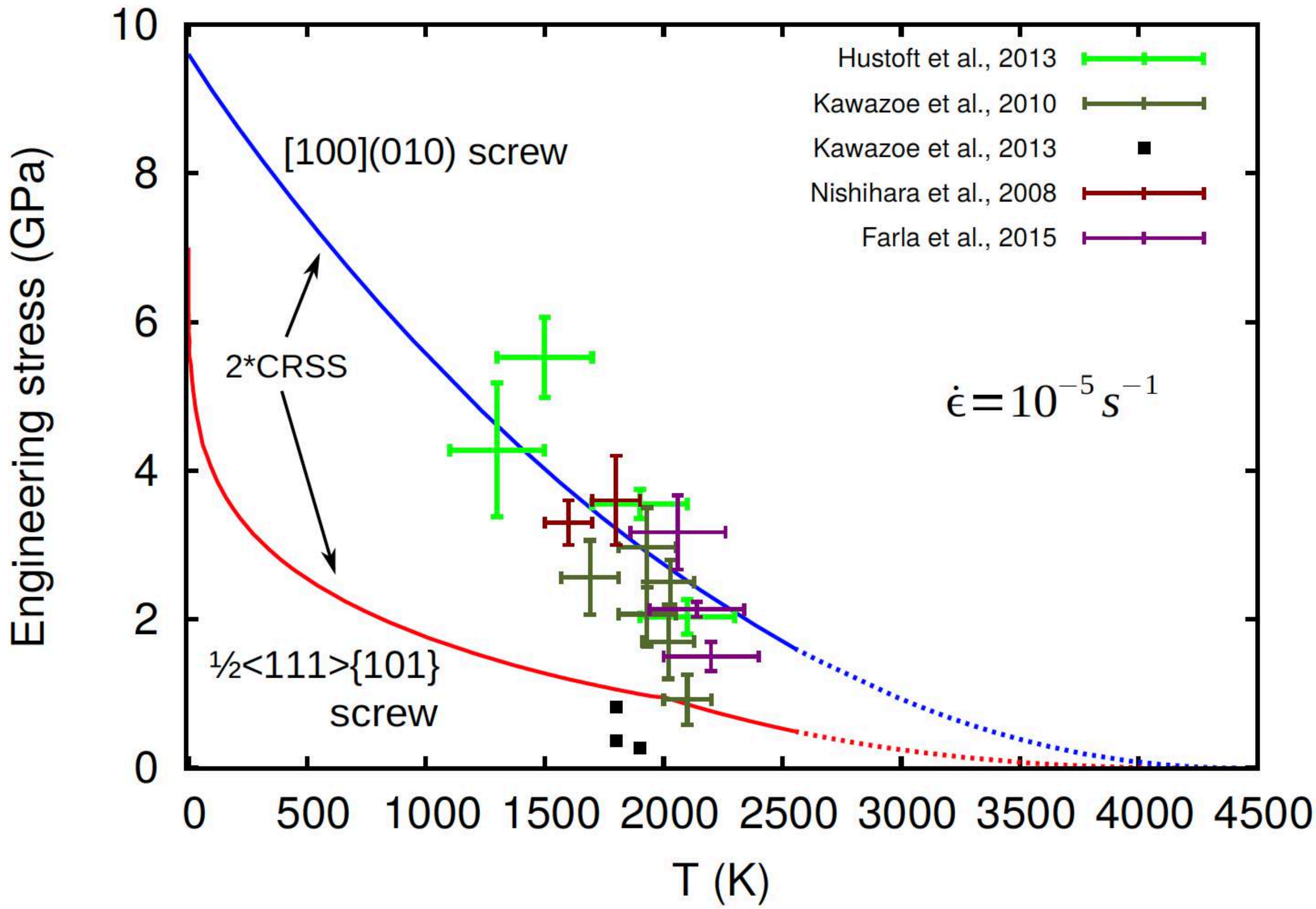
The strain rate is here

Comparison with experimental data: Ringwoodite (20 GPa)



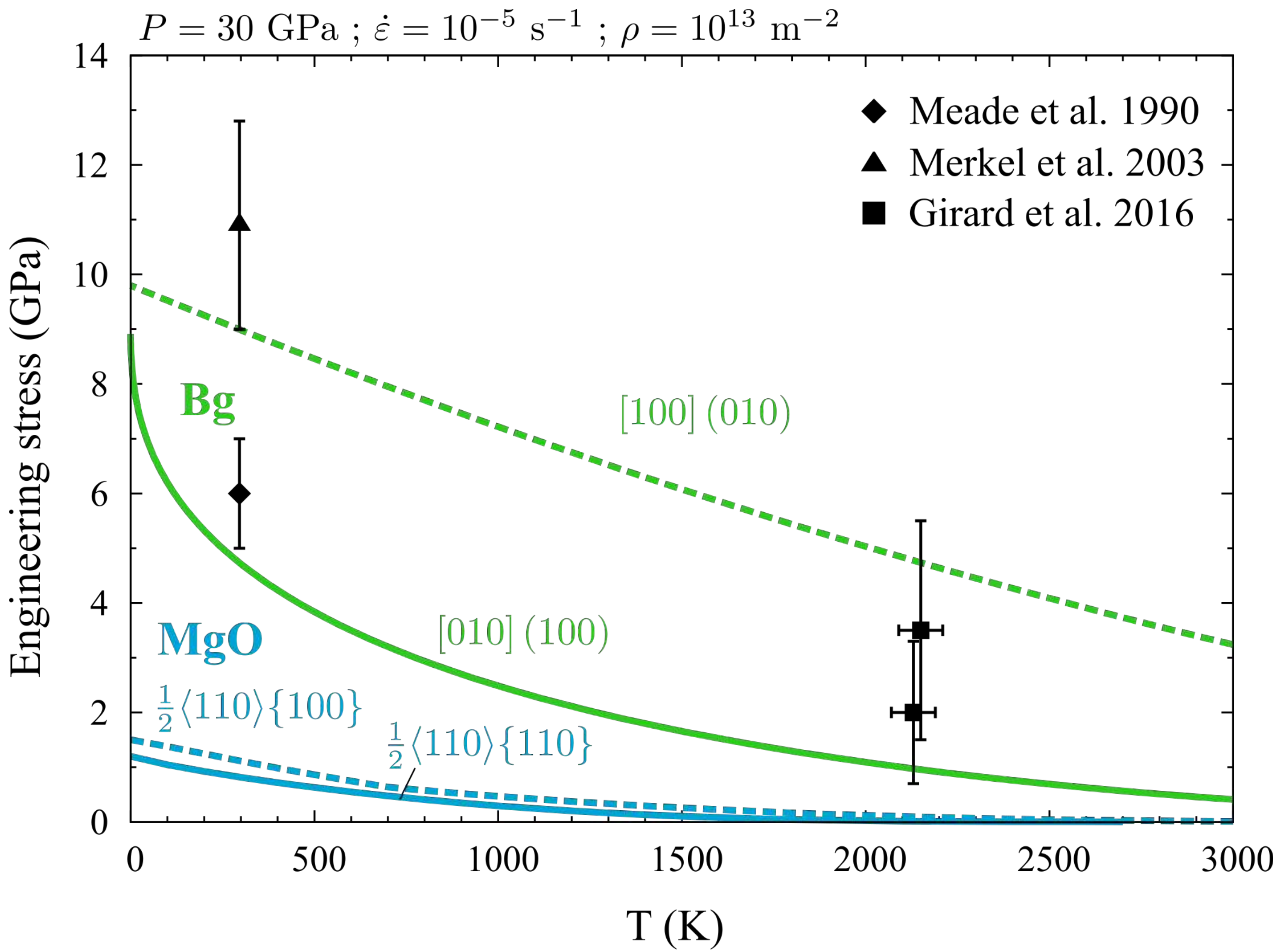
Ritterbex et al. (2015) PEPI

Dislocation glide in wadsleyite (15 GPa)



Ritterbex et al. Am. Mineralogist (2016)

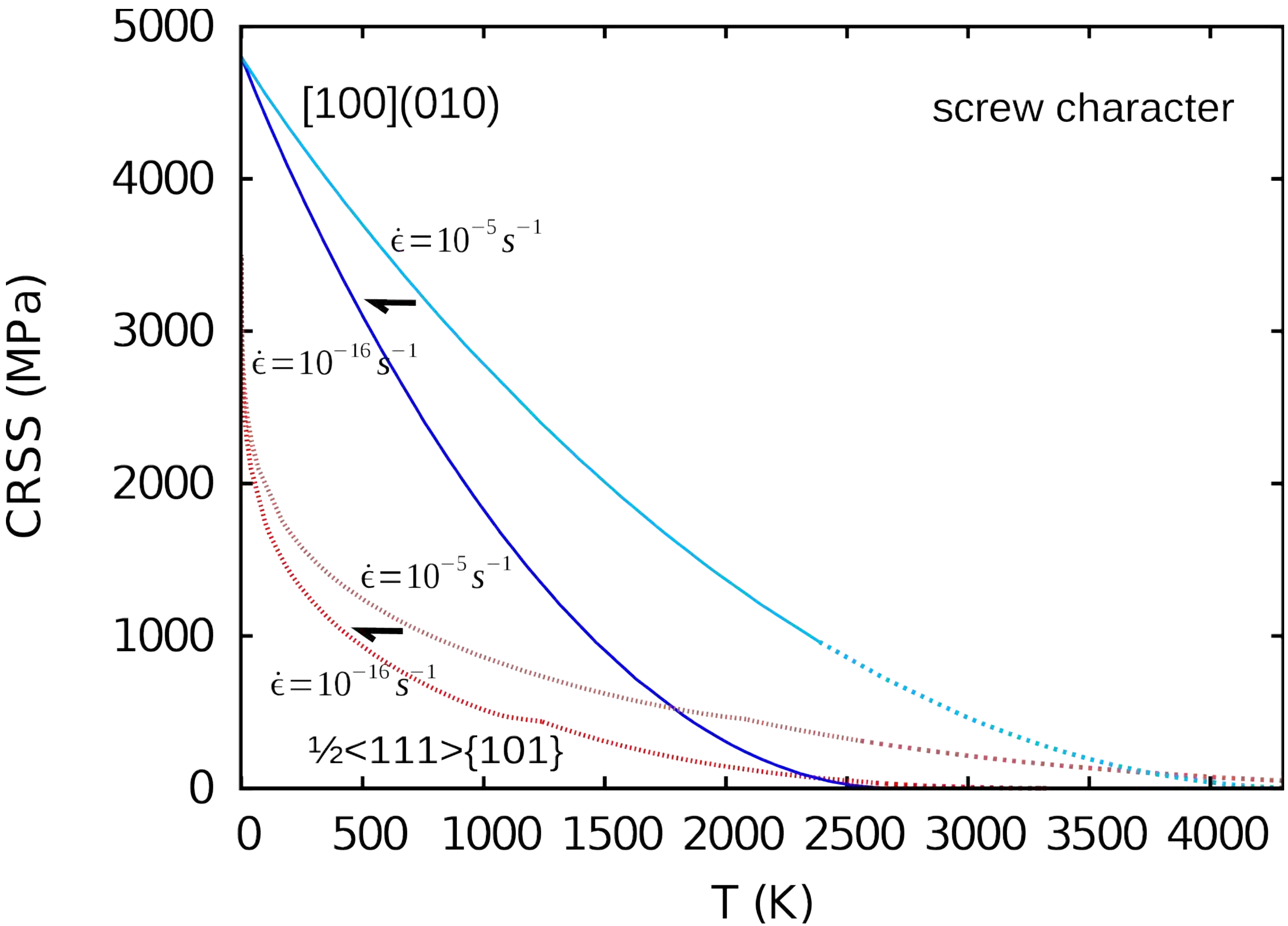
Dislocation glide in bridgmanite (30 GPa)



Kraych et al. (2016) EPSL – Results on MgO from Amodeo et al. Phil. Mag. 2012

Dislocation glide in wadsleyite: from the lab to the mantle

Decreasing strain rate shifts CRSS to lower stress values



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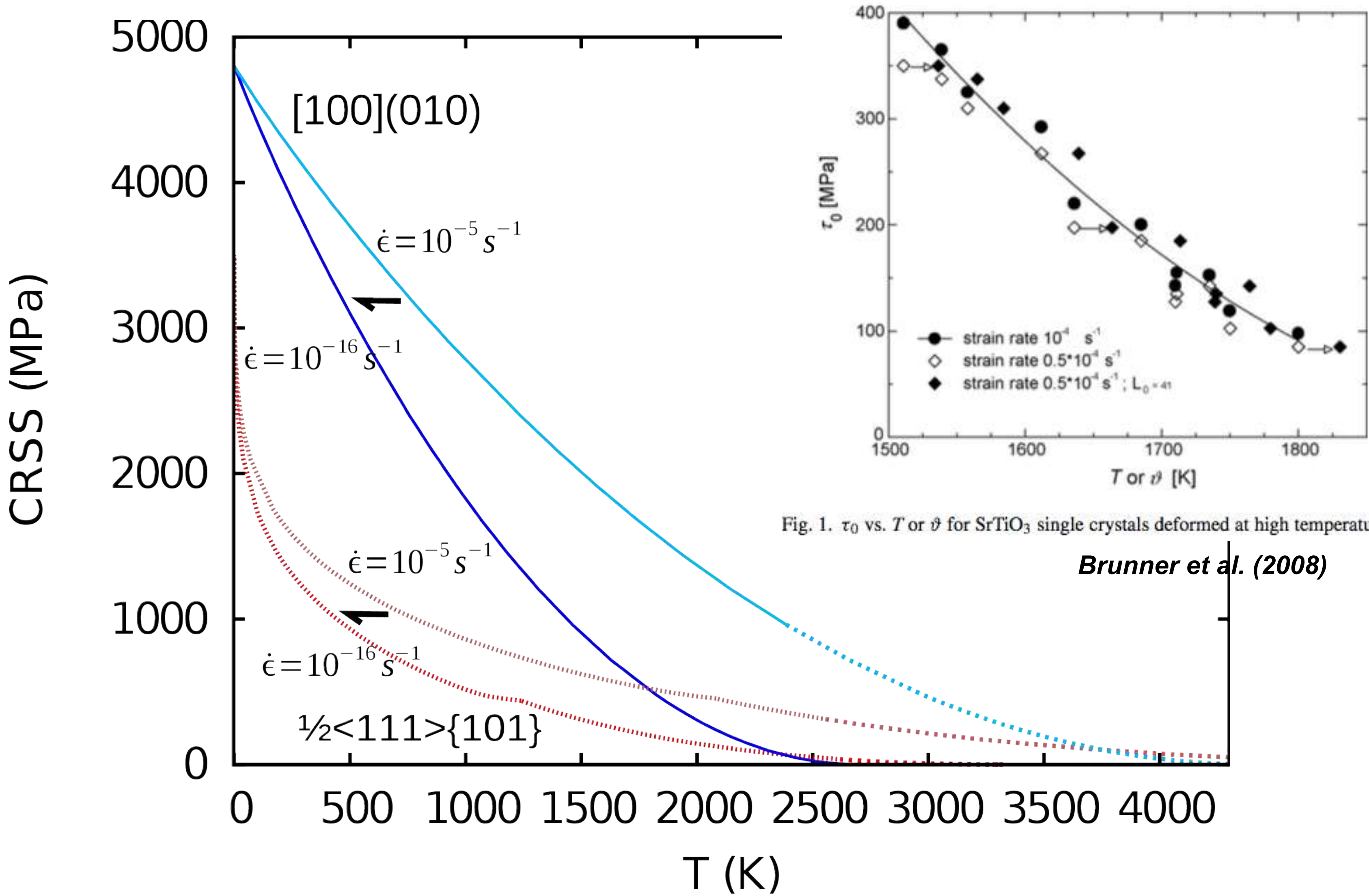
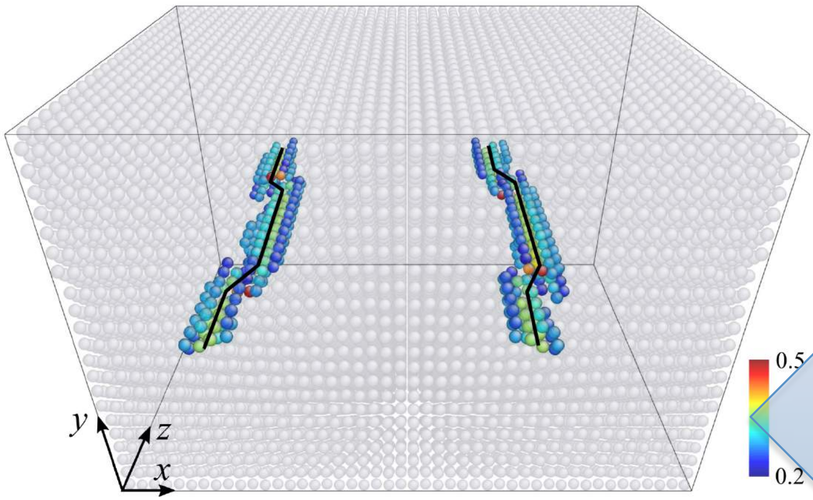


Fig. 1. τ_0 vs. T or ϑ for $SrTiO_3$ single crystals deformed at high temperatures.

Brunner et al. (2008)

Multi-Scale model of dislocation creep

Atomistic calculations of dislocation core properties



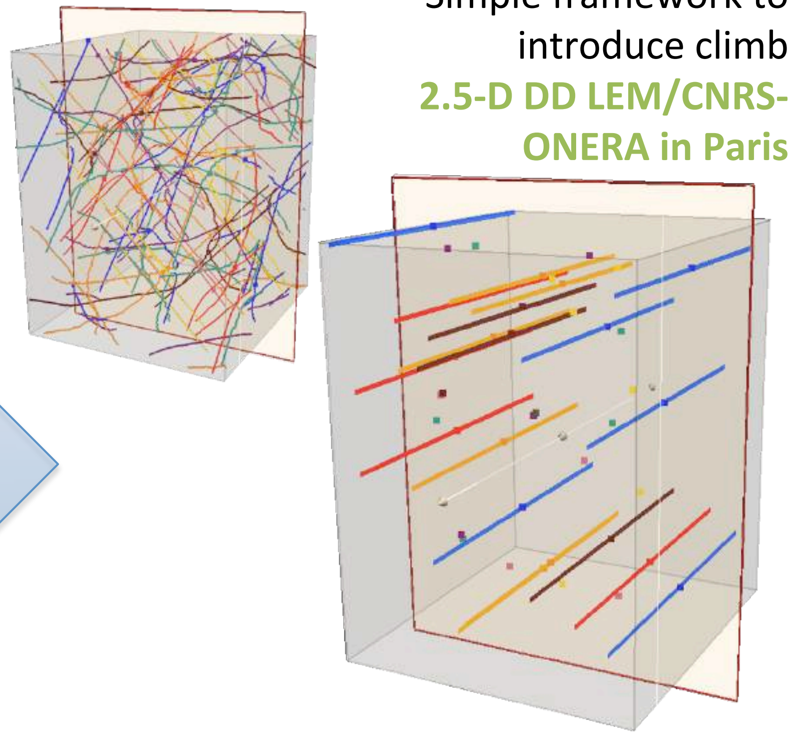
Thermally activated glide velocity

✓

Dislocation Dynamic (DD) simulation

Simple framework to introduce climb

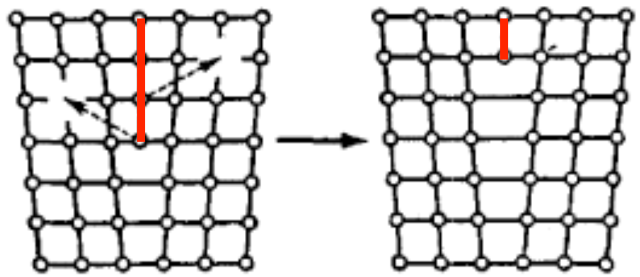
2.5-D DD LEM/CNRS-ONERA in Paris



Climb velocity

Climb velocity in Dislocation Dynamics simulations

- Point defects (vacancies) diffuse toward the dislocations
- They are absorbed (or emitted)

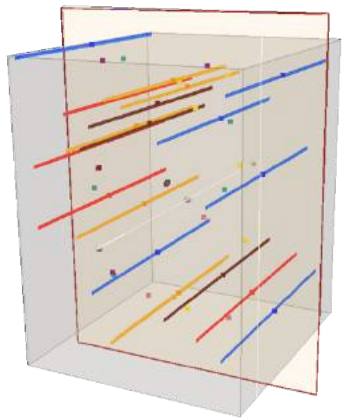


The dislocation moves away from its glide plane

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

Steady state conditions

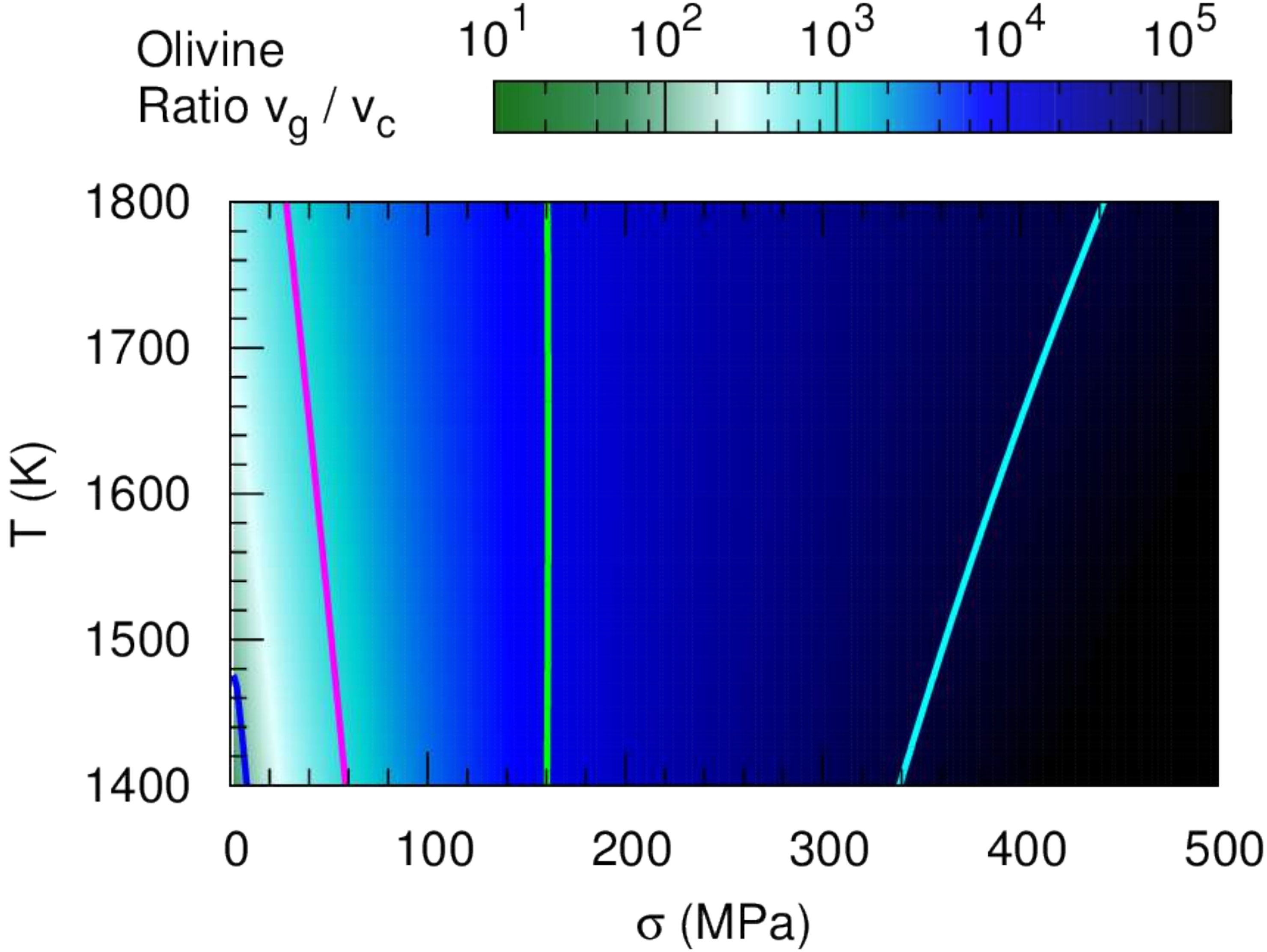
Constant vacancy concentration



(see Mordehai et al. Phil. Mag. 2008 or Keralavarma et al. 2012)

Interplay between glide and climb

[100] dislocations



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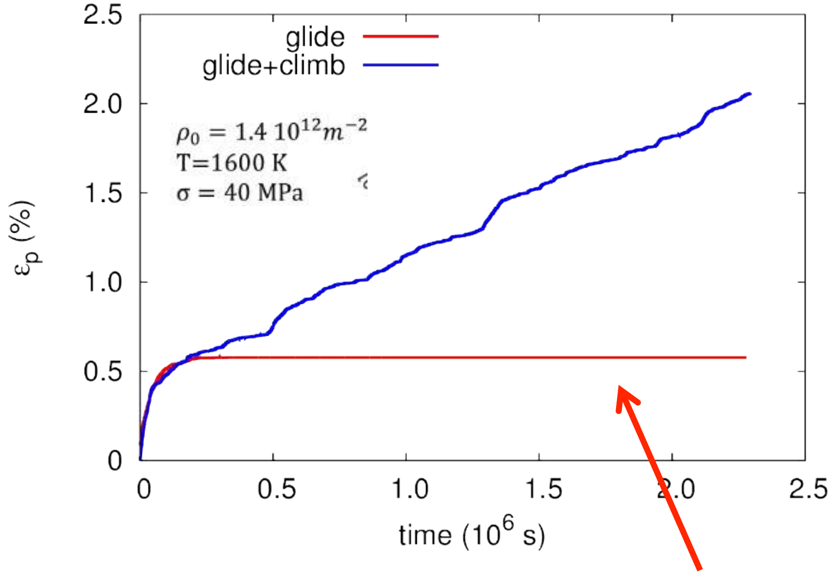
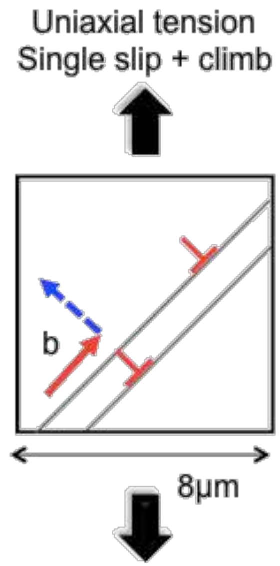
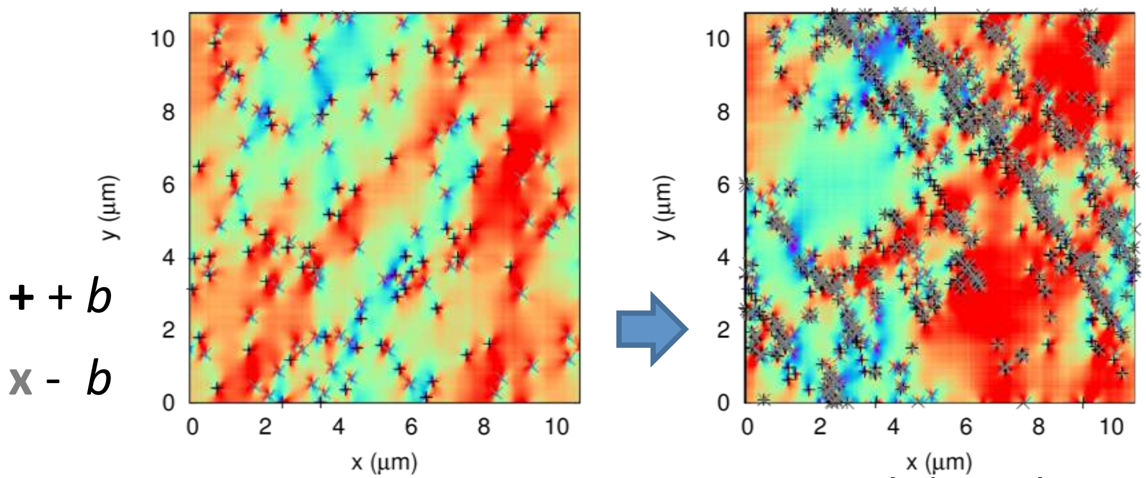






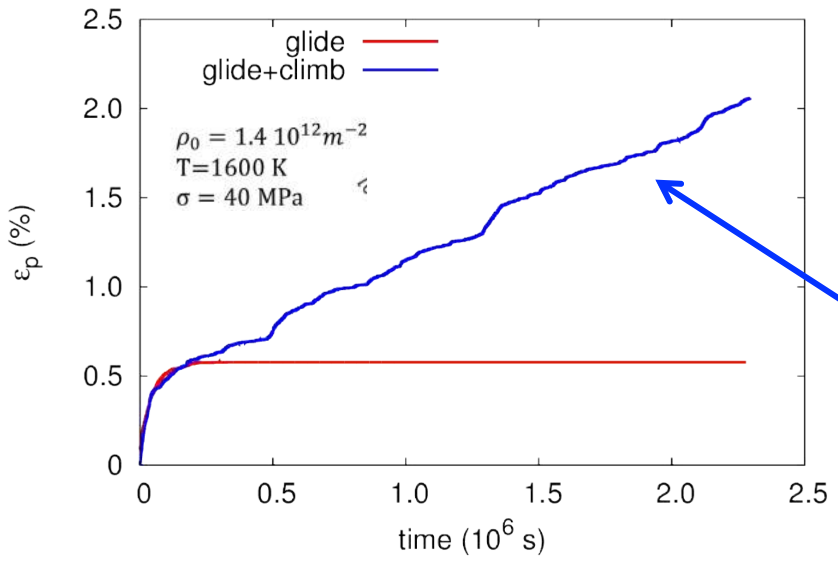
Initial configuration

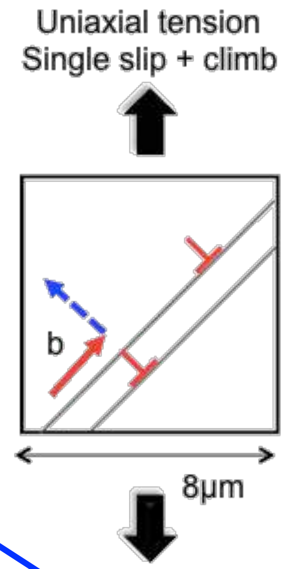
Glide only

Boioli et al. Phys Rev B 2015

Interplay between glide and climb

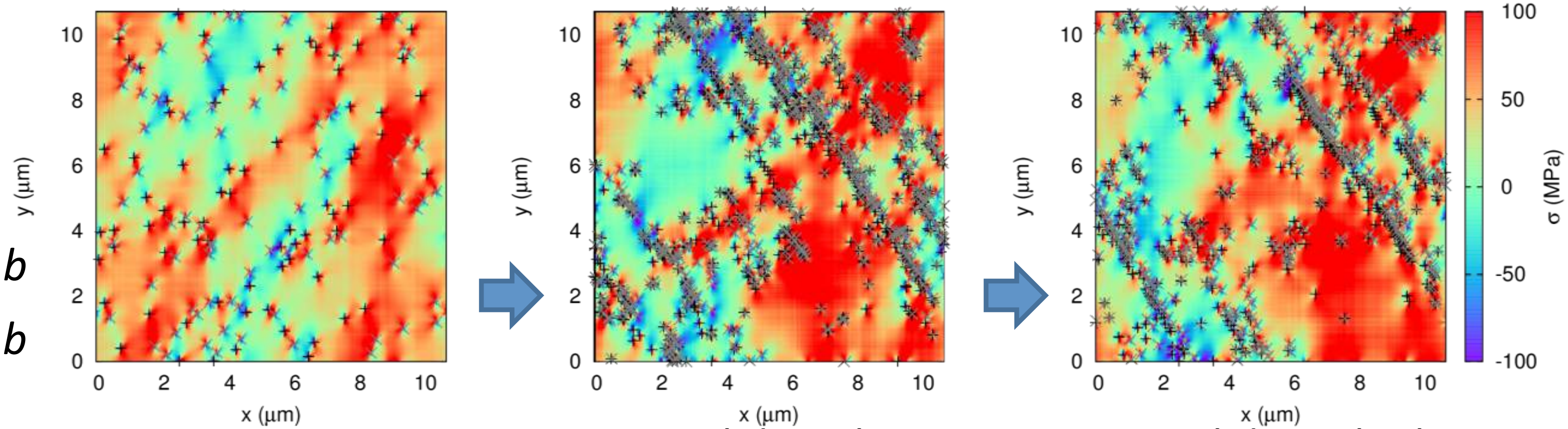
[100] dislocations





+ + *b*

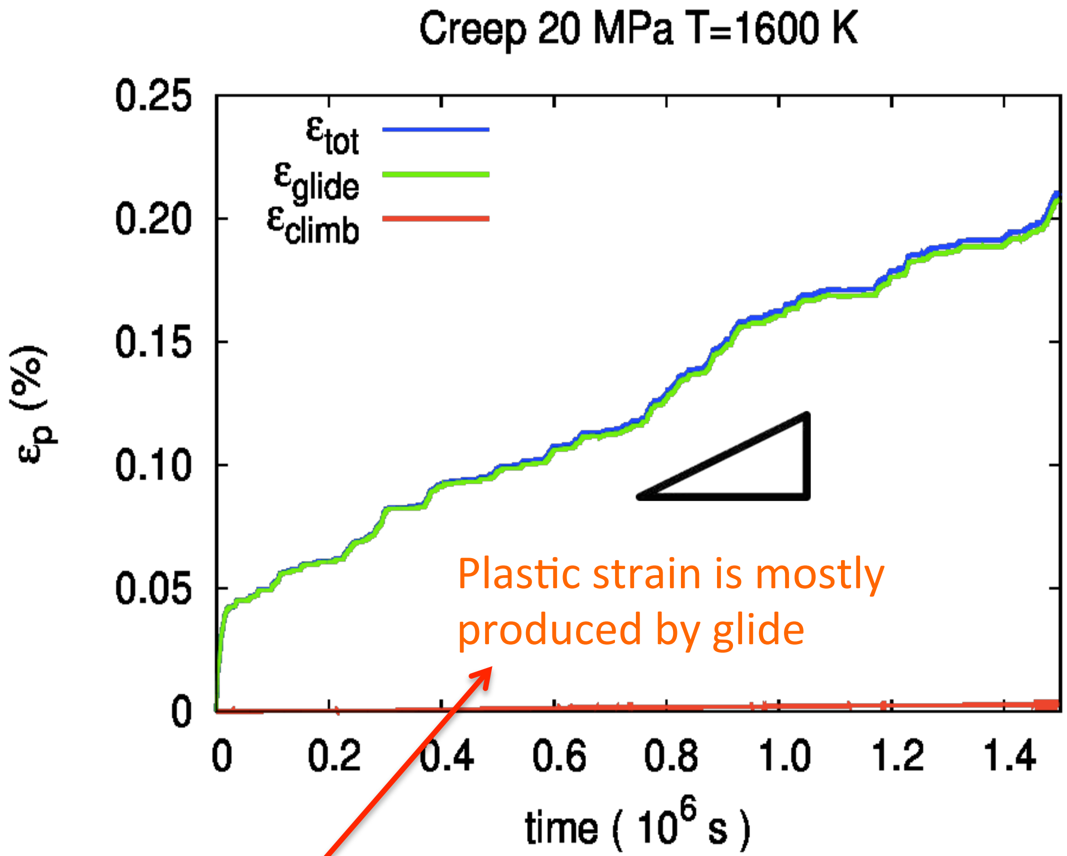
x - *b*



Initial configuration   Glide only   Glide + Climb

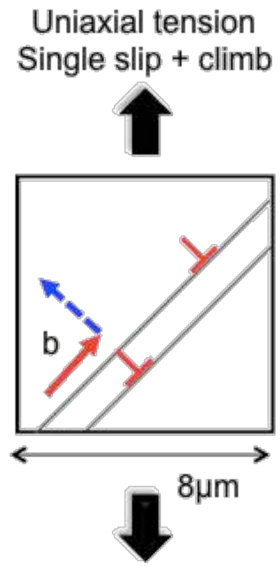
Interplay between glide and climb

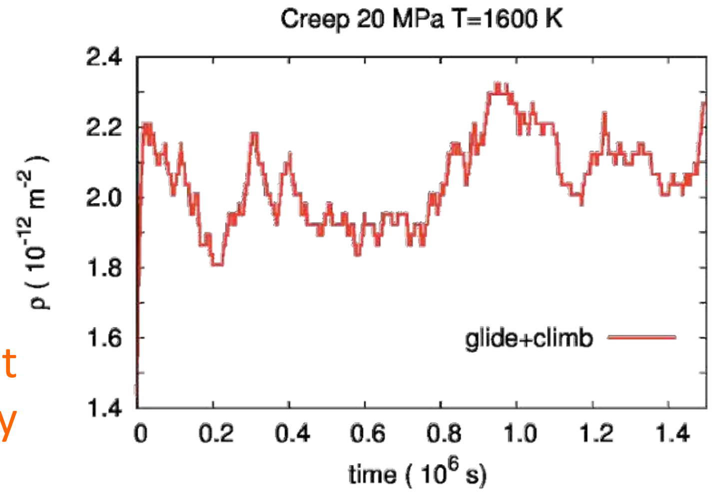
[100] dislocations



Plastic strain is mostly produced by glide

Weertman creep

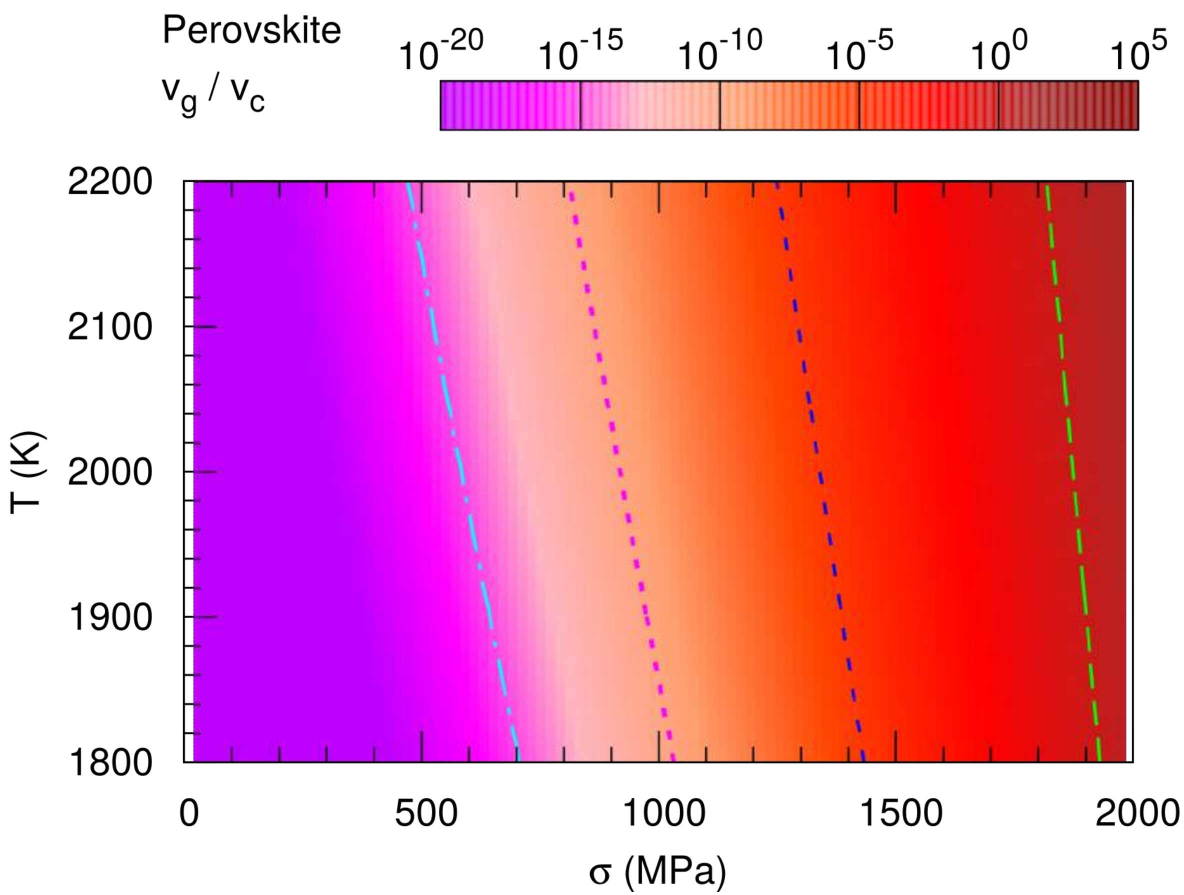




At steady state: nearly constant dislocation density

Boioli et al. Phys Rev B 2015

Glide versus Climb in $MgSiO_3$ perovskite as a function of Stress and Temperature



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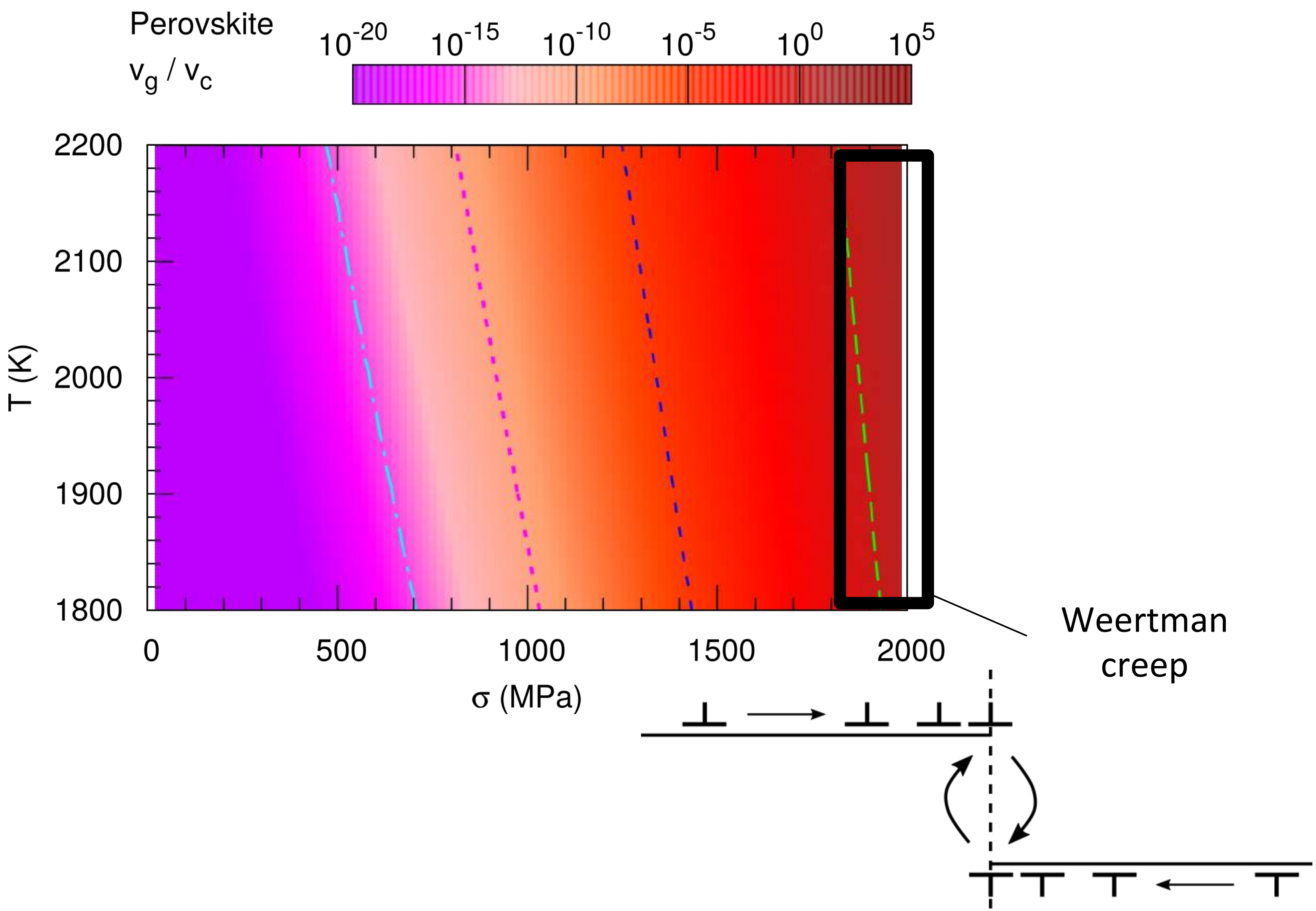

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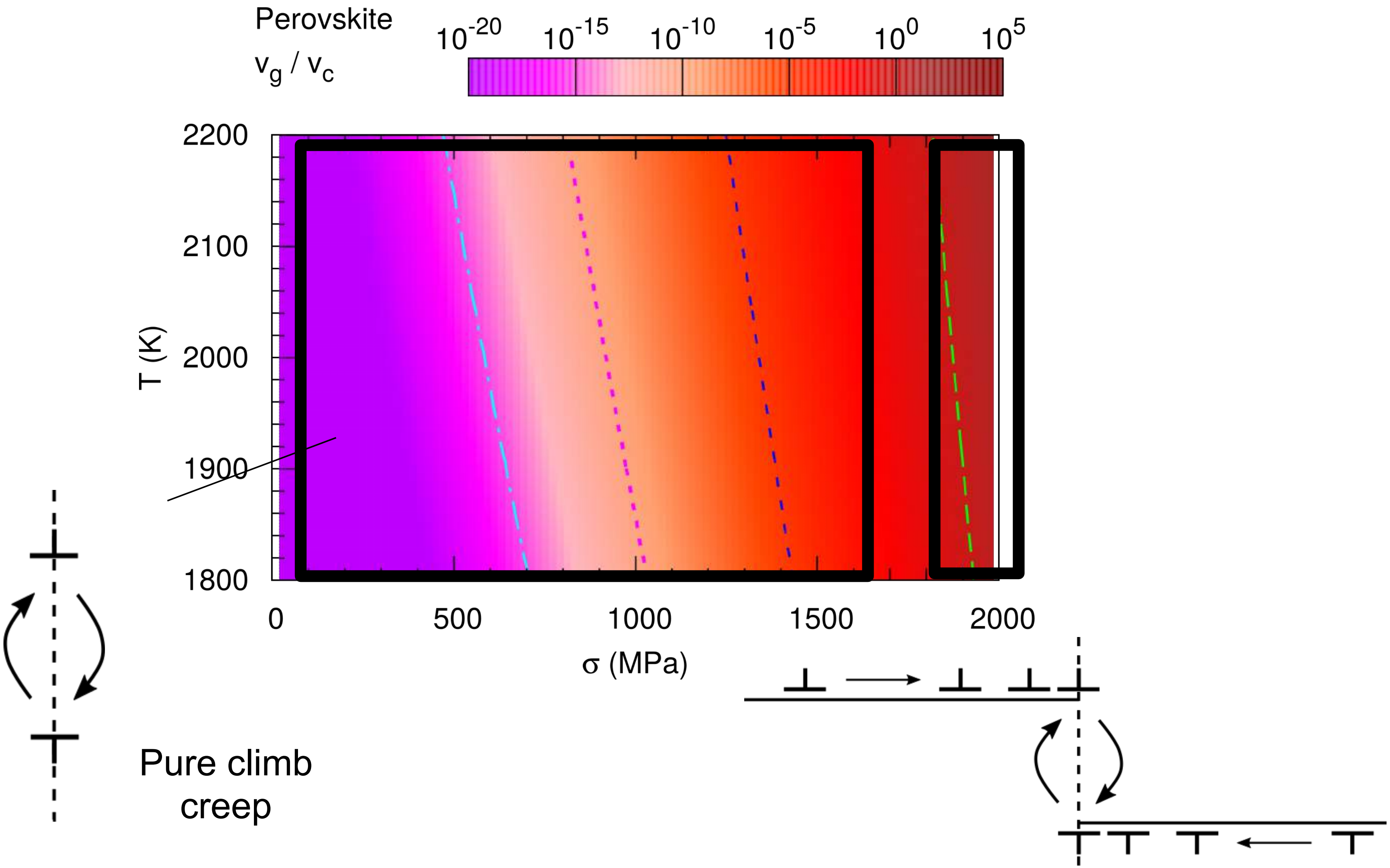
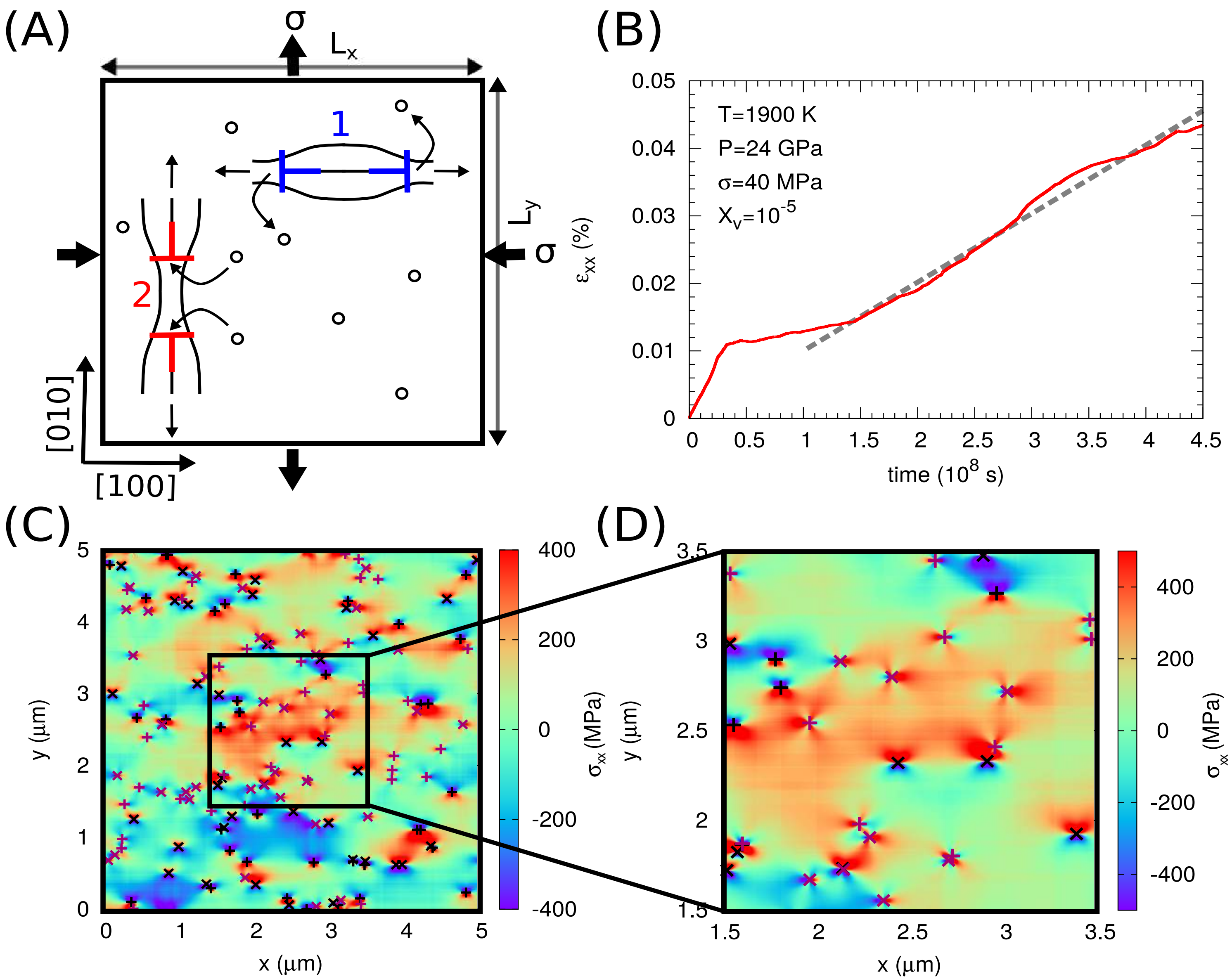


2.5 DD simulations of pure climb creep



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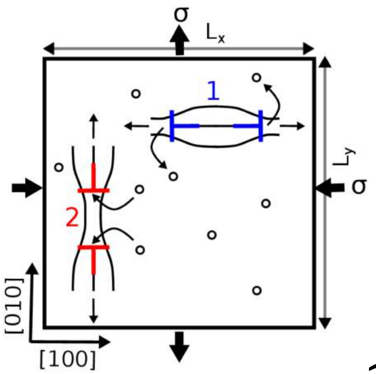
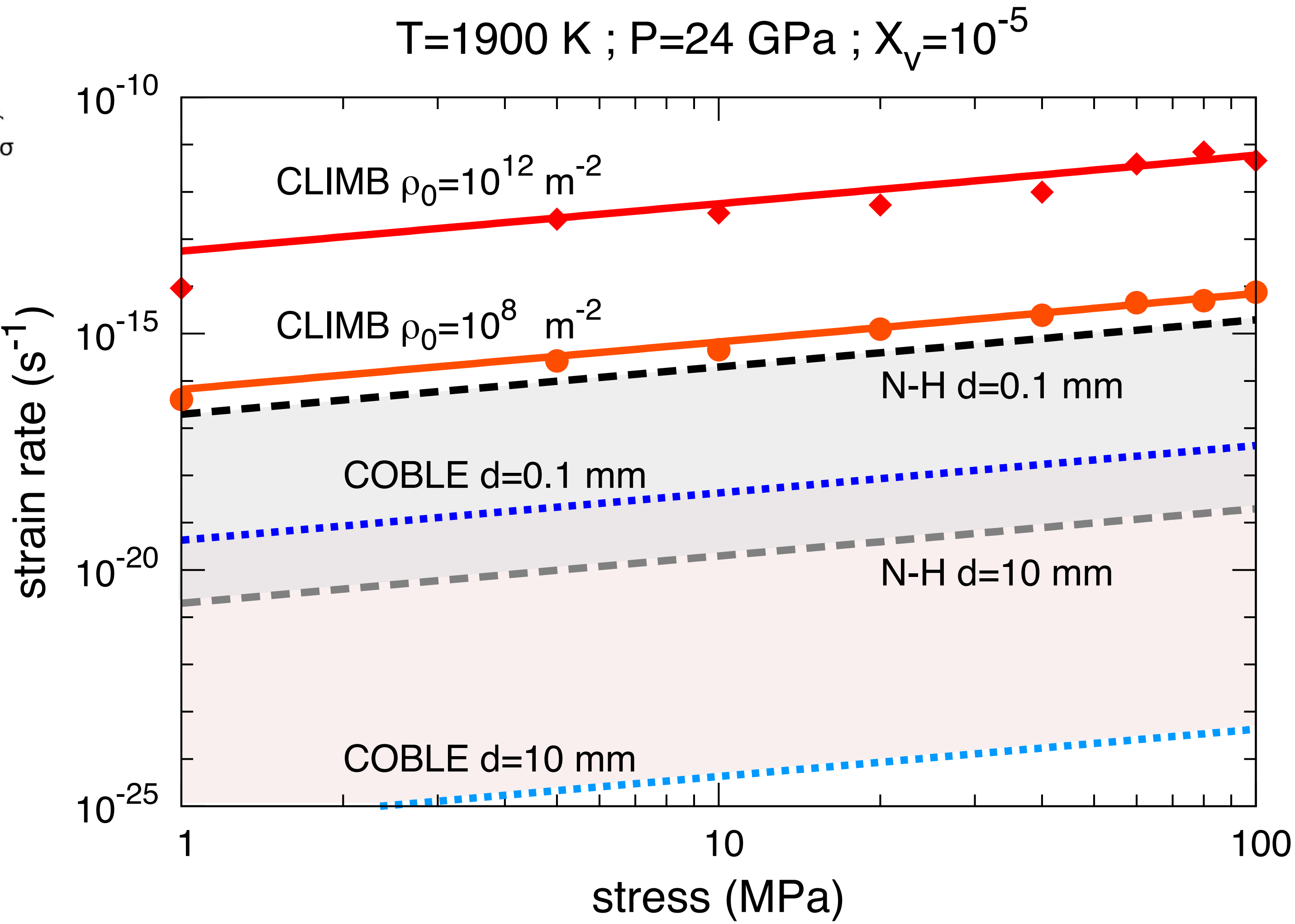
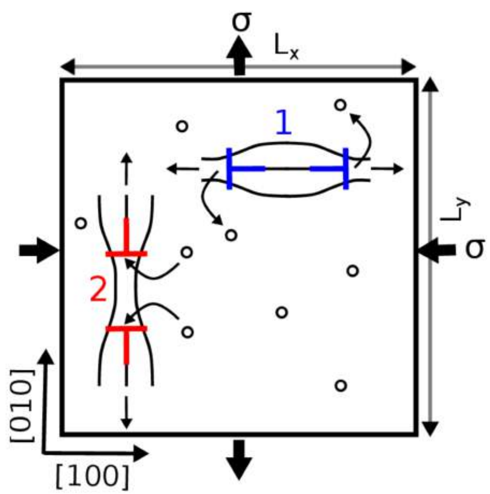




d > 0,1 mm → Pure climb creep > NH creep

Pure climb creep:

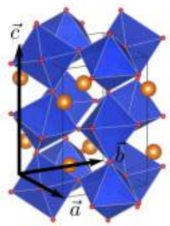
A very important mechanism for planetary interiors rheology



A few facts:

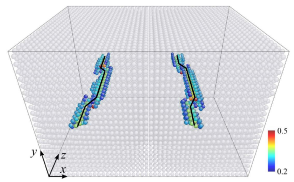
- Strain is produced by dislocation ***climb***
- Strain is not produced by shear: no crystal preferred orientations
- No grain size dependence
- Controlled by diffusion, but rheology *may not* be linear

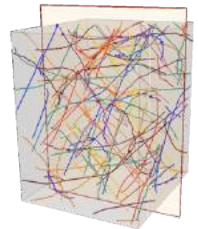
Conclusions



We develop a multi-scale model of dislocation creep in high pressure mineral

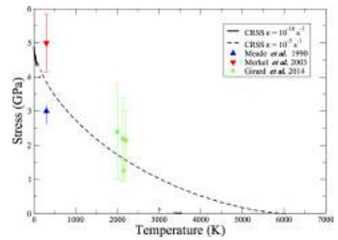
- Combining atomic scale and meso-scale DD simulations



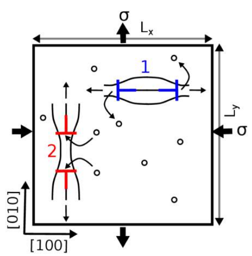


- Calculated glide properties are found in agreement with experiments

- Confirm that at relatively low stress glide is highly prohibited



- Creep may involves pure climb (grain size > a few mm)

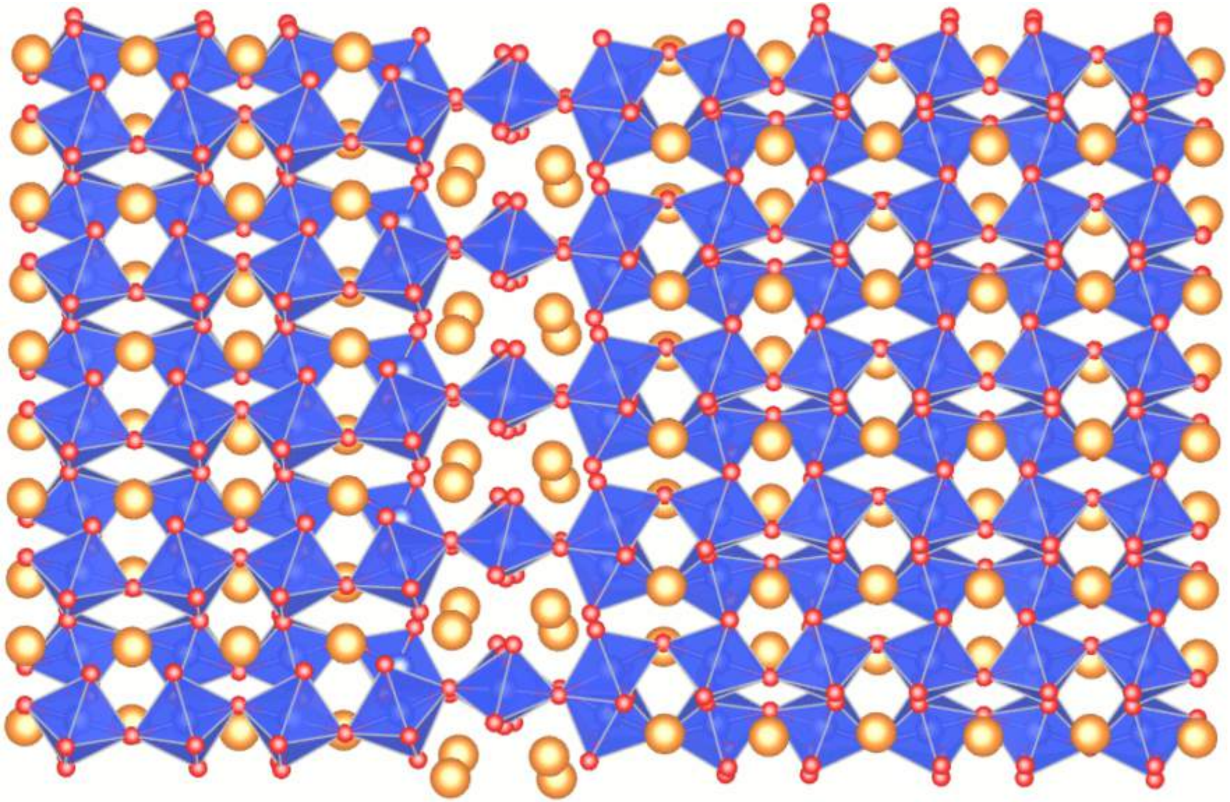


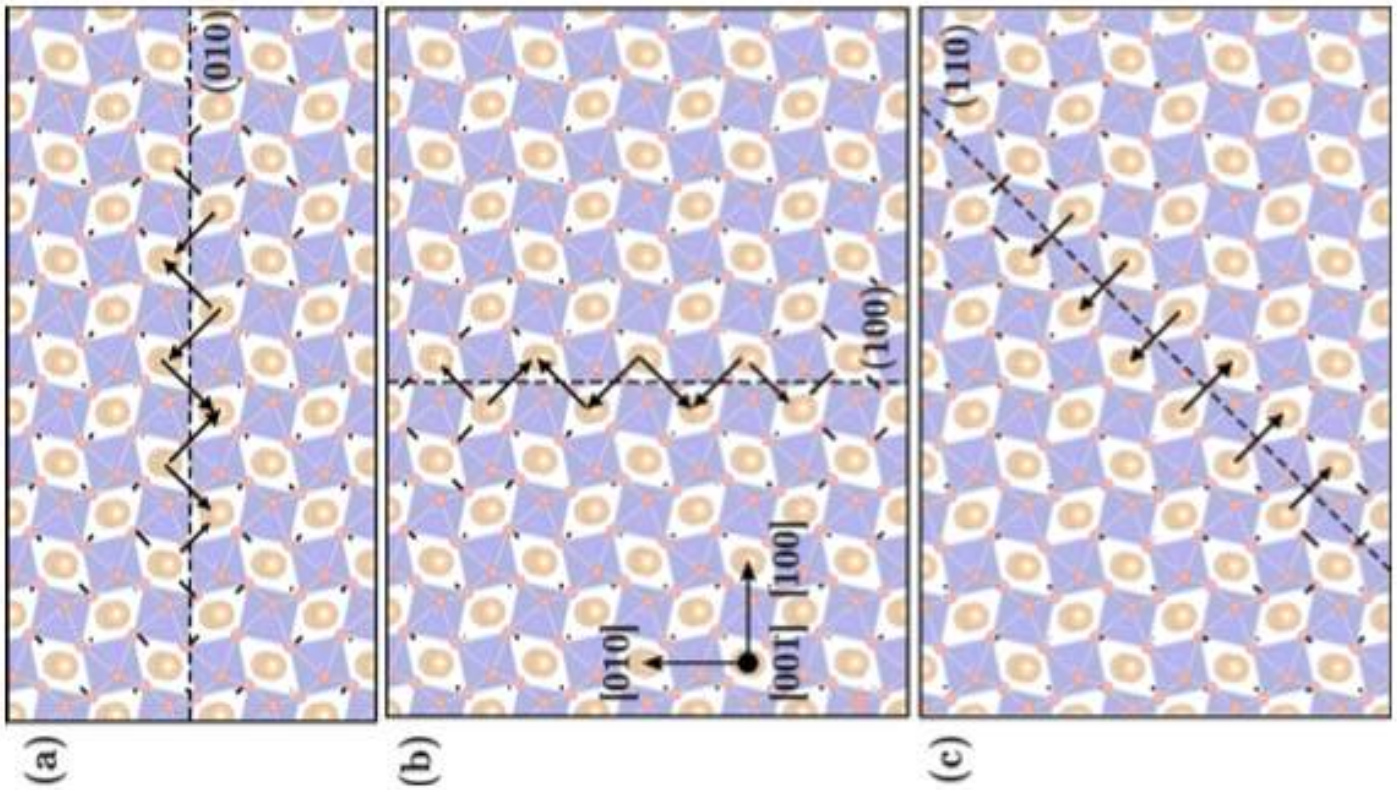
Thanks for your attention

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

www.rheoman.eu

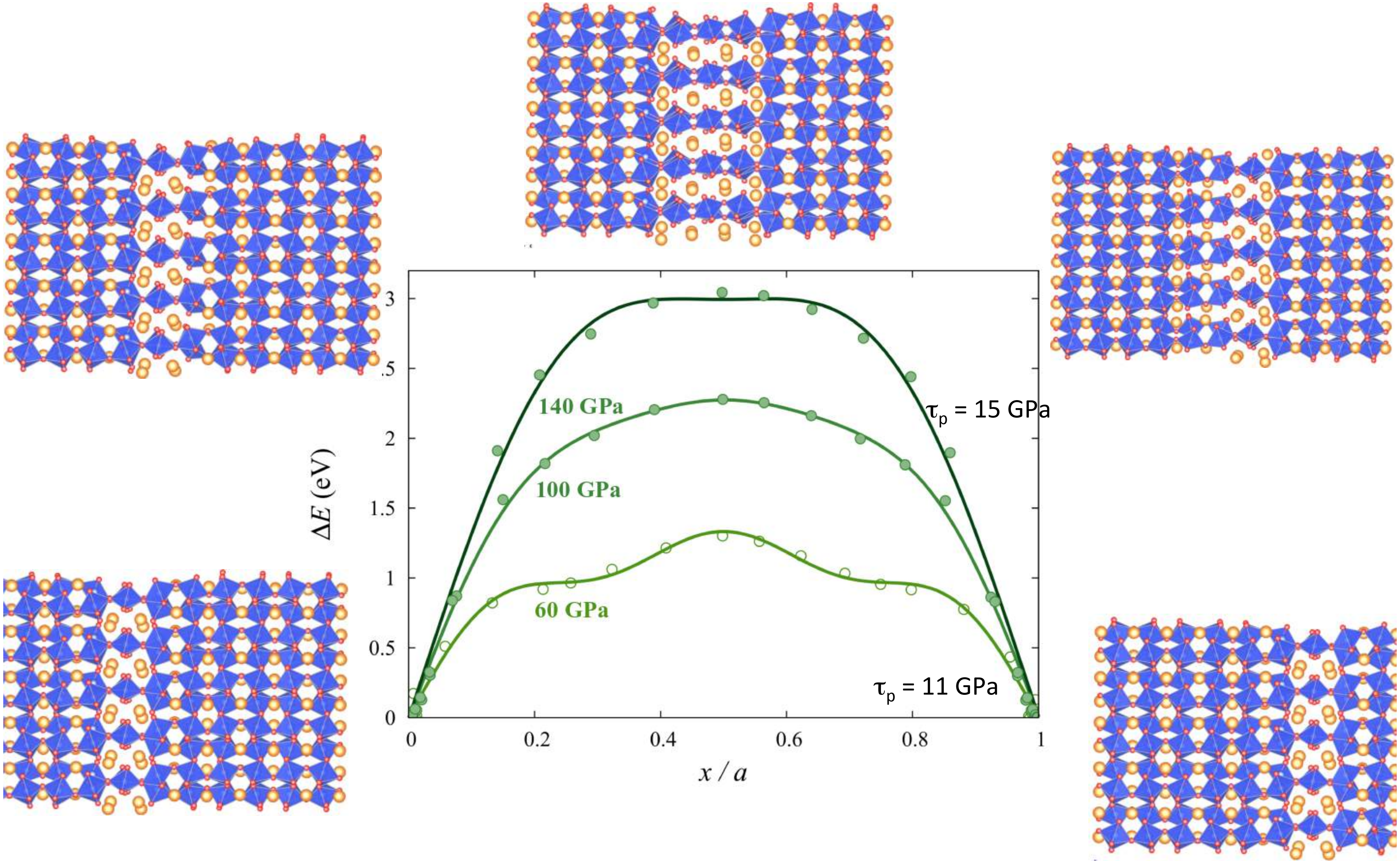
atomistic calculation of thermally activated glide velocity



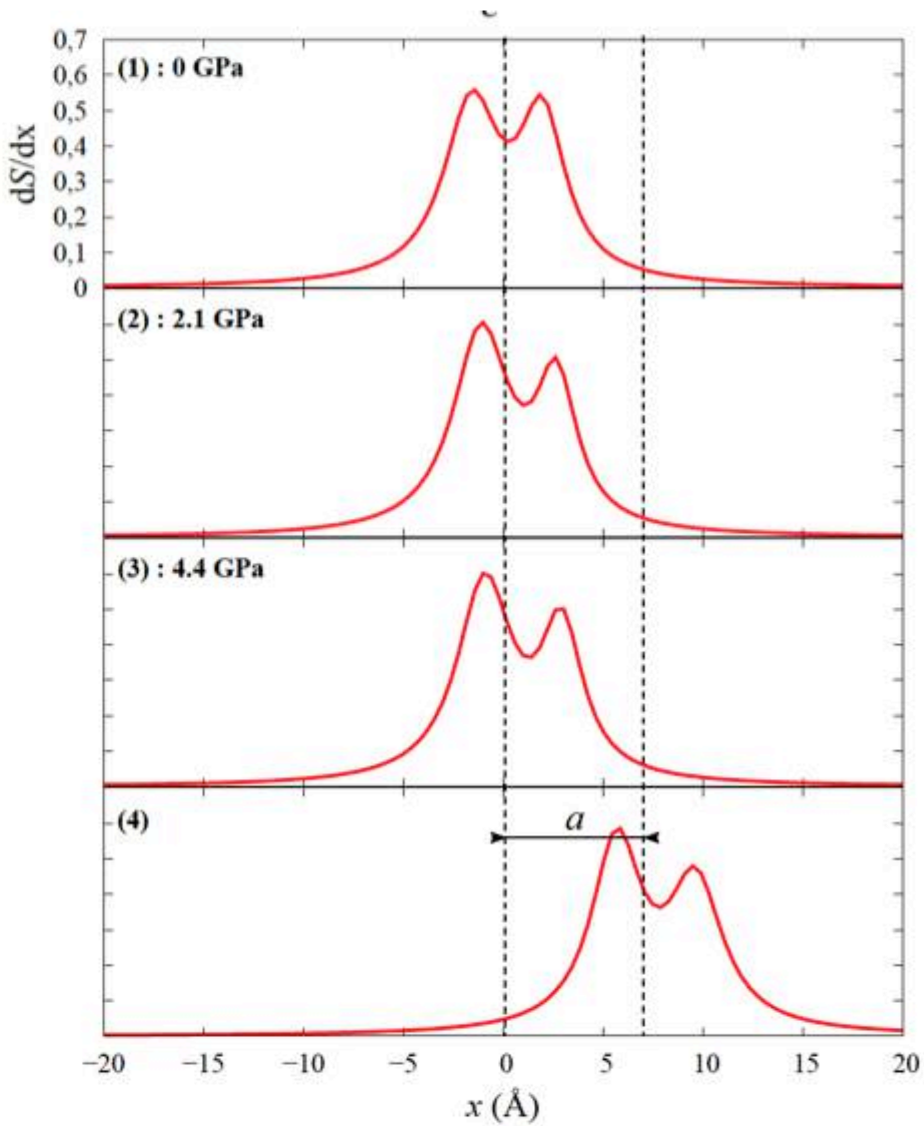


[001] dislocation in $MgSiO_3$ Pv

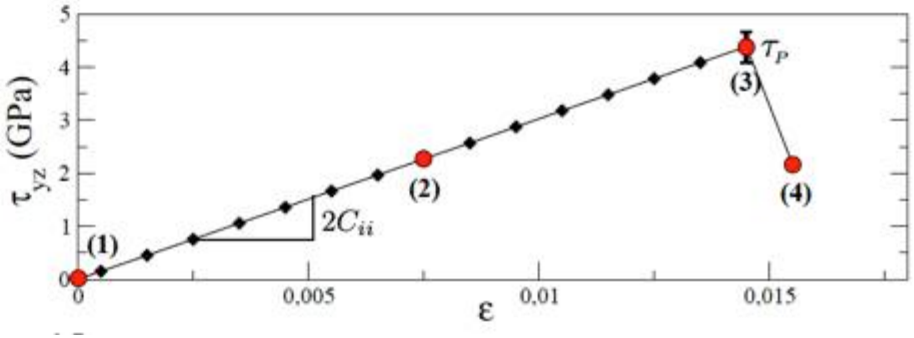
Peierls potential computed using NEB
Example of screw [010](100) dislocation



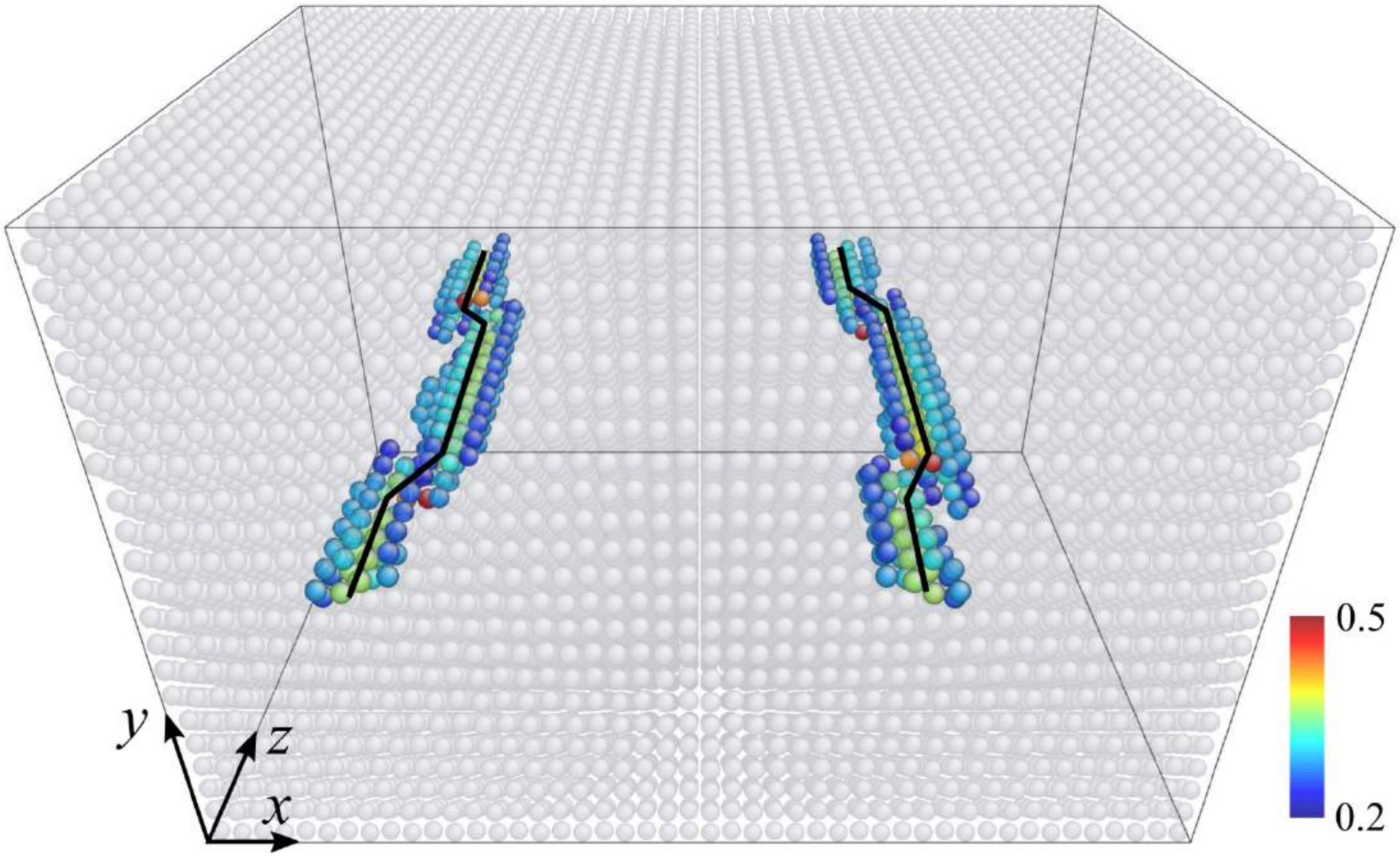
Dislocation core structure and Peierls stress



[100](010) in bridgmanite at 30 GPa



Kink pair nucleation energy computed within periodic cell

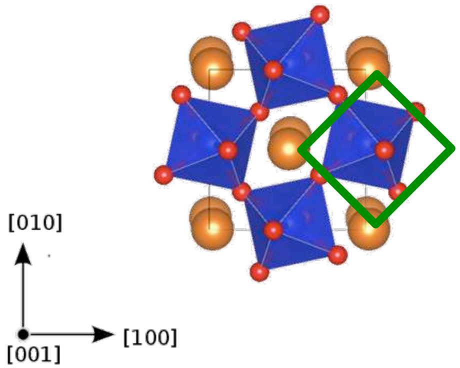


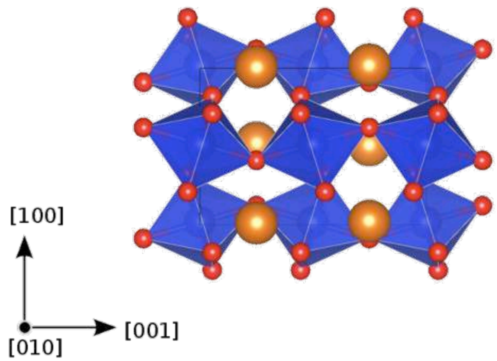
Dipole configuration of kinked dislocation => kink energy Hk = 9.5 eV (P=30 GPa)

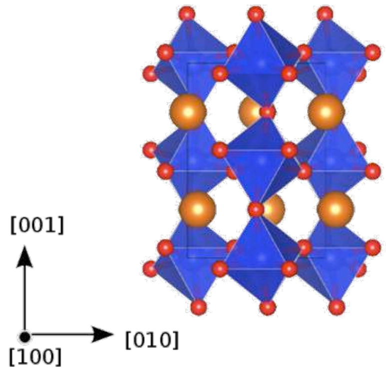
$$H_k = \frac{\mu b^3}{2}\sqrt{\tau_P/\mu}$$

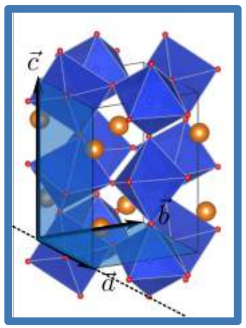
Kraych et al. (PRB 2016)

Two slip systems : [100](010) and [010](100)

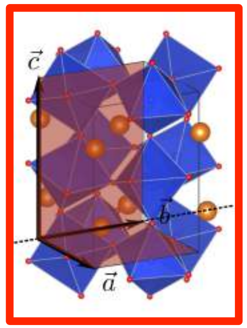








[100]

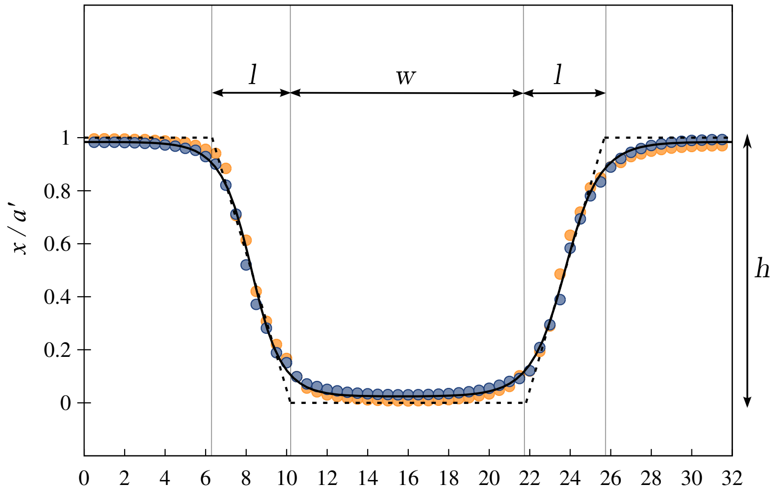


[010]

Two slip systems consistent with classical <110>{110} slip system observed in perfect cubic perovskite (ex. $SrTiO_3$, known to be ductile)

ΔH^* function of stress

Kink-pairs configuration: Trapezoidal shape described using *l*, *w* and *h*



$$
\begin{aligned}
2H_k &= \Delta H_k^*(\tau = 0) \\
&= \frac{\mu b^2}{2\pi}\left[\frac{l^2 + a'^2/(1-\upsilon)}{\sqrt{l^2+a'^2}} \ln\left(\frac{\sqrt{l^2+a'^2}}{e\rho}\right)\right. \\
&\quad \left. - l\ \ln(l/e\rho) + l\ \ln\left(\frac{2l}{l+\sqrt{l^2+a'^2}}\right) + l - \sqrt{l^2+a'^2}\right] \\
&\quad + 2\frac{\sqrt{l^2+a'^2}}{a}\int_0^{a'} V_P(x)dx.
\end{aligned}
$$

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KINK PAIR NUCLEATION AND CRITICAL SHEAR STRESS

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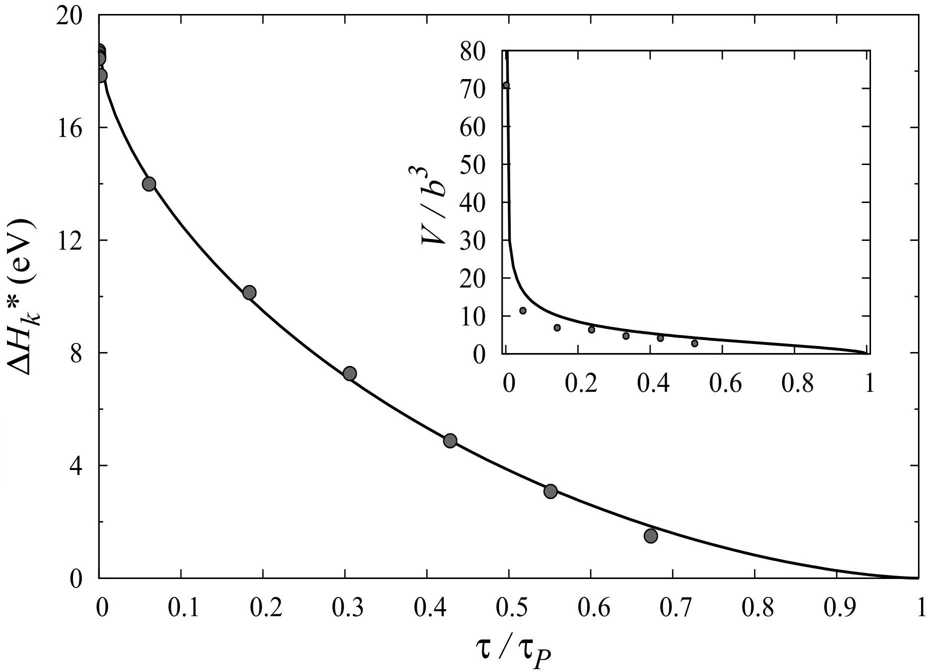
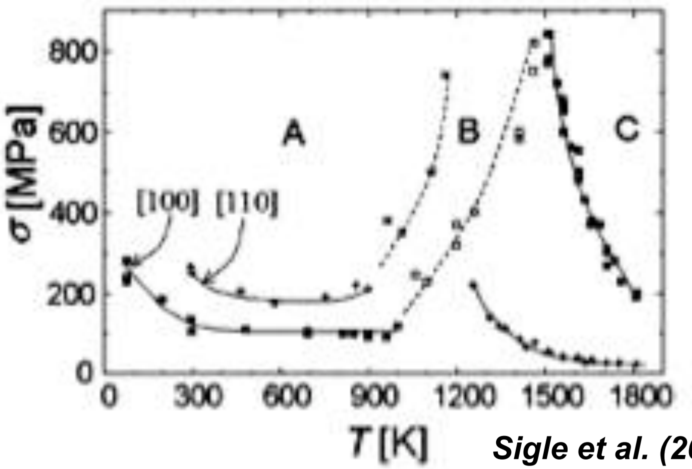
$$\Delta H_k = \Delta E_{elas} + \Delta W_P - W_\tau$$

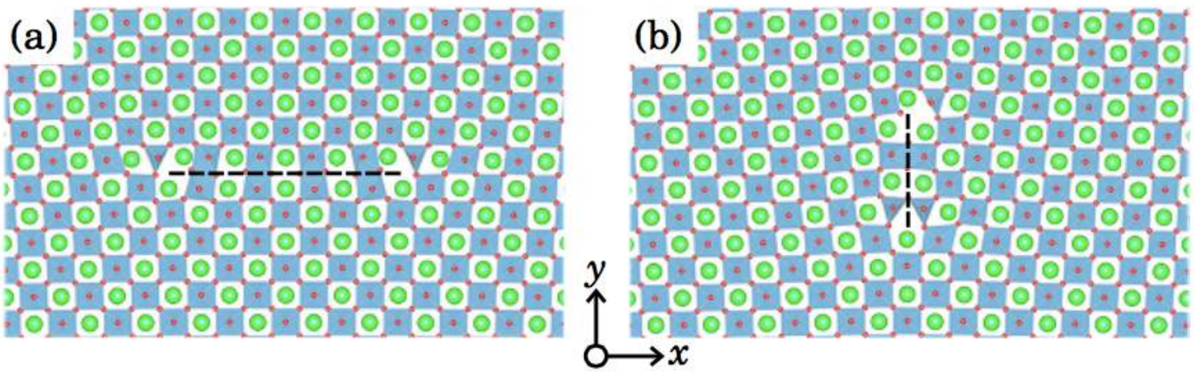


Kraych et al. (PRB 2016)

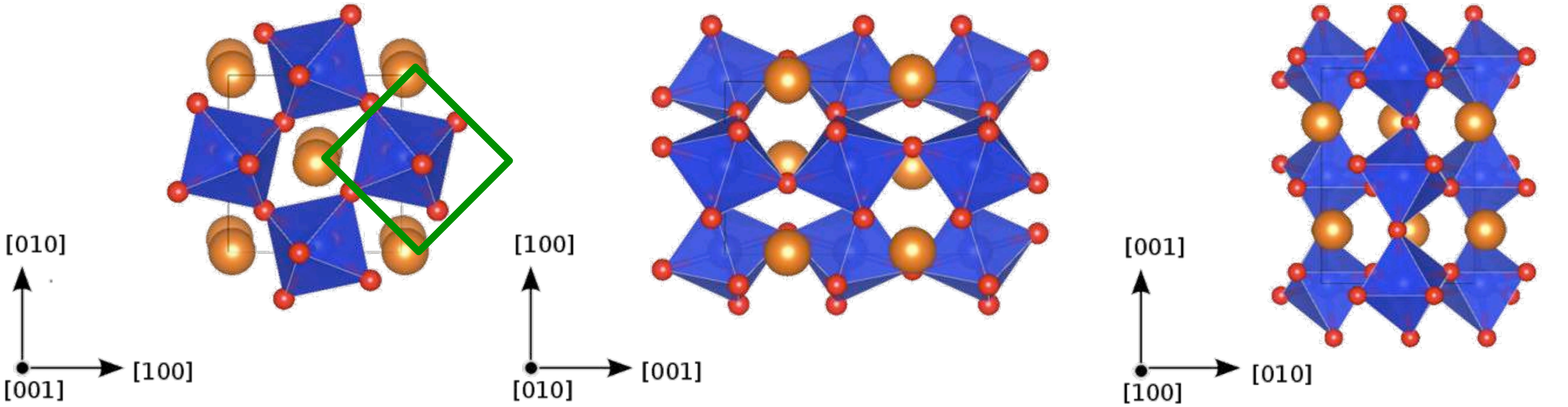
$SrTiO_3$ cubic perovskite mechanical properties



Sigle et al. (2006)

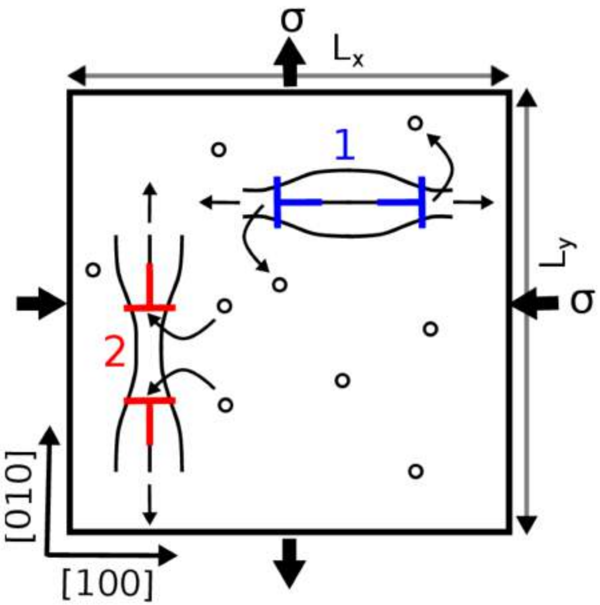


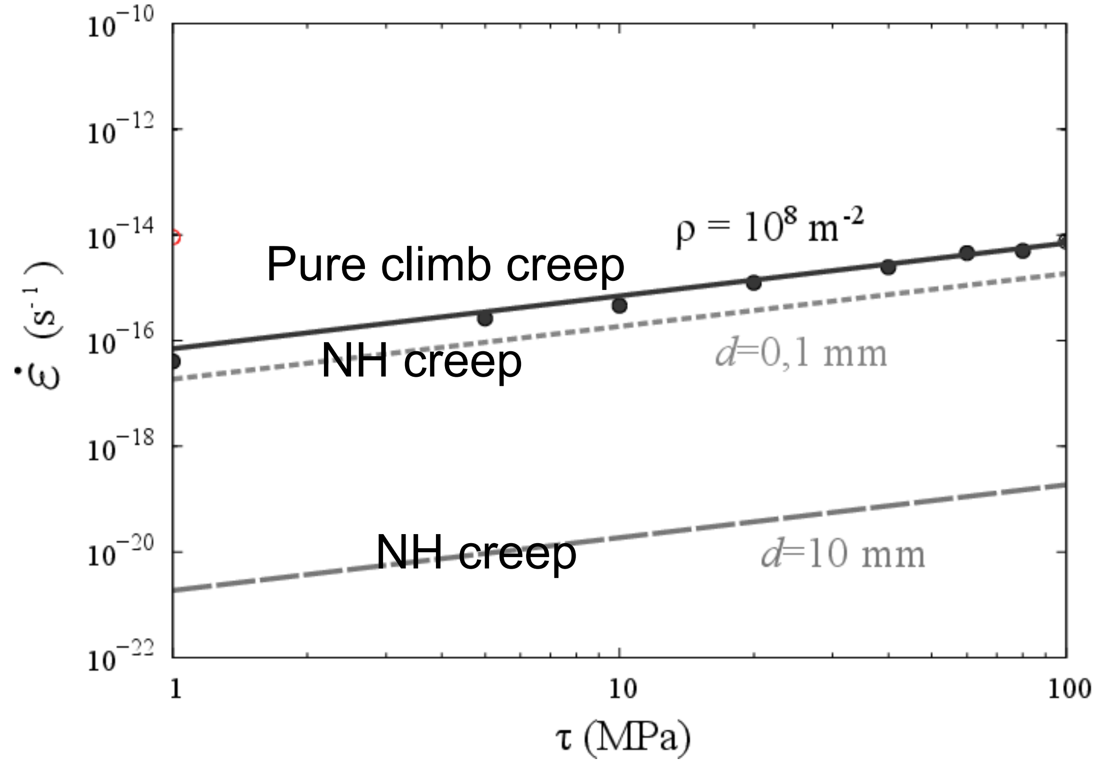
Hirel et al. (under review Scripta Mat.)



Cubic		Orthorhombic
$\langle 100\rangle_c\{010\}_c$	$[100]_c(010)_c$	$[110]_o(\bar{1}10)_o$
	$[010]_c(001)_c$	$[\bar{1}10]_o(001)_o$
	$[001]_c(010)_c$	$[001]_o(\bar{1}10)_o$
$\langle 100\rangle_c\{011\}_c$	$[001]_c(110)_c$	$[001]_o(010)_o$
	$[001]_c(1\bar{1}0)_c$	$[001]_o(100)_o$
$\langle 110\rangle_c\{001\}_c$	$[110]_c(001)_c$	$[010]_o(001)_o$
	$[1\bar{1}0]_c(001)_c$	$[100]_o(001)_o$
$\langle 110\rangle_c\{1\bar{1}0\}_c$	$[1\bar{1}0]_c(110)_c$	$[100]_o(010)_o$
	$[110]_c(1\bar{1}0)_c$	$[010]_o(100)_o$

2.5 DD simulations of pure climb creep



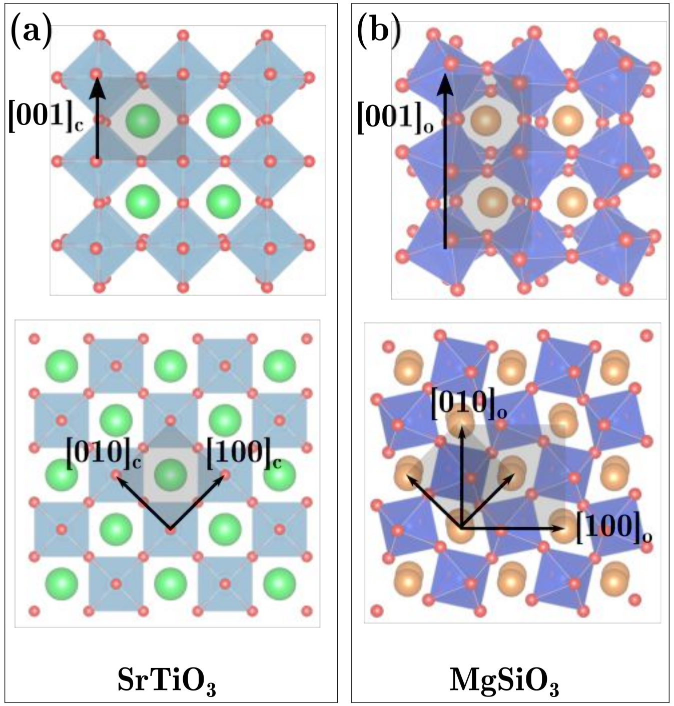


d > 0,1 mm → Pure climb creep > NH creep

$$\dot{\epsilon} = \alpha \frac{D_{sd}\,\sigma\,\Omega}{d^2 k_b T}$$

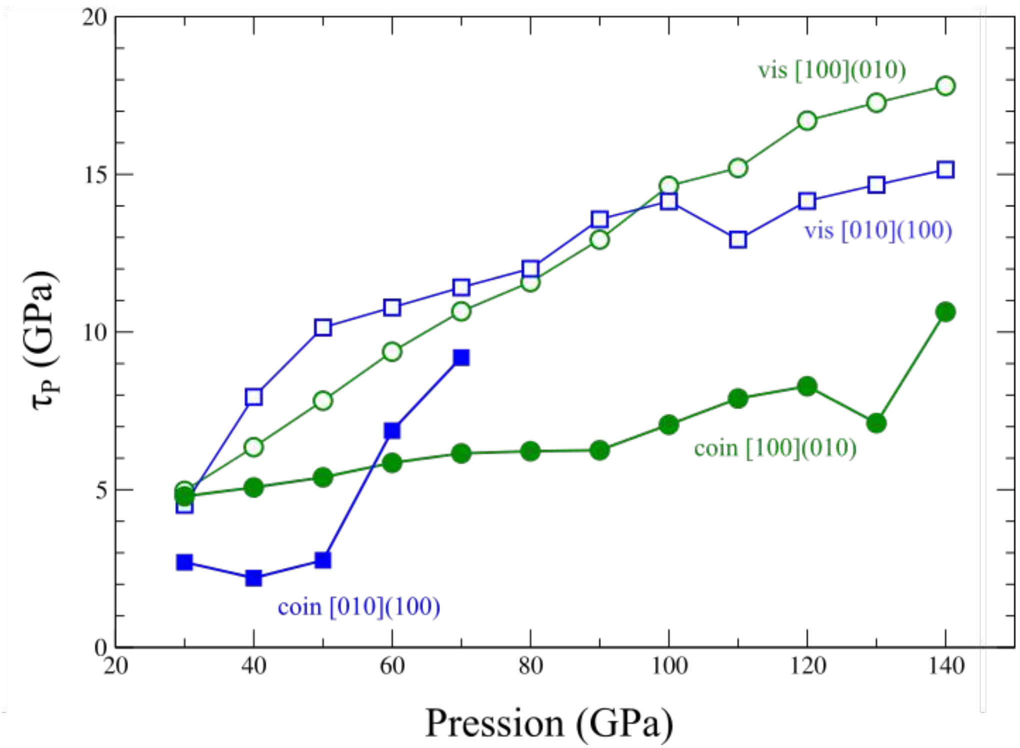
Poirier, Creep of crystals (198

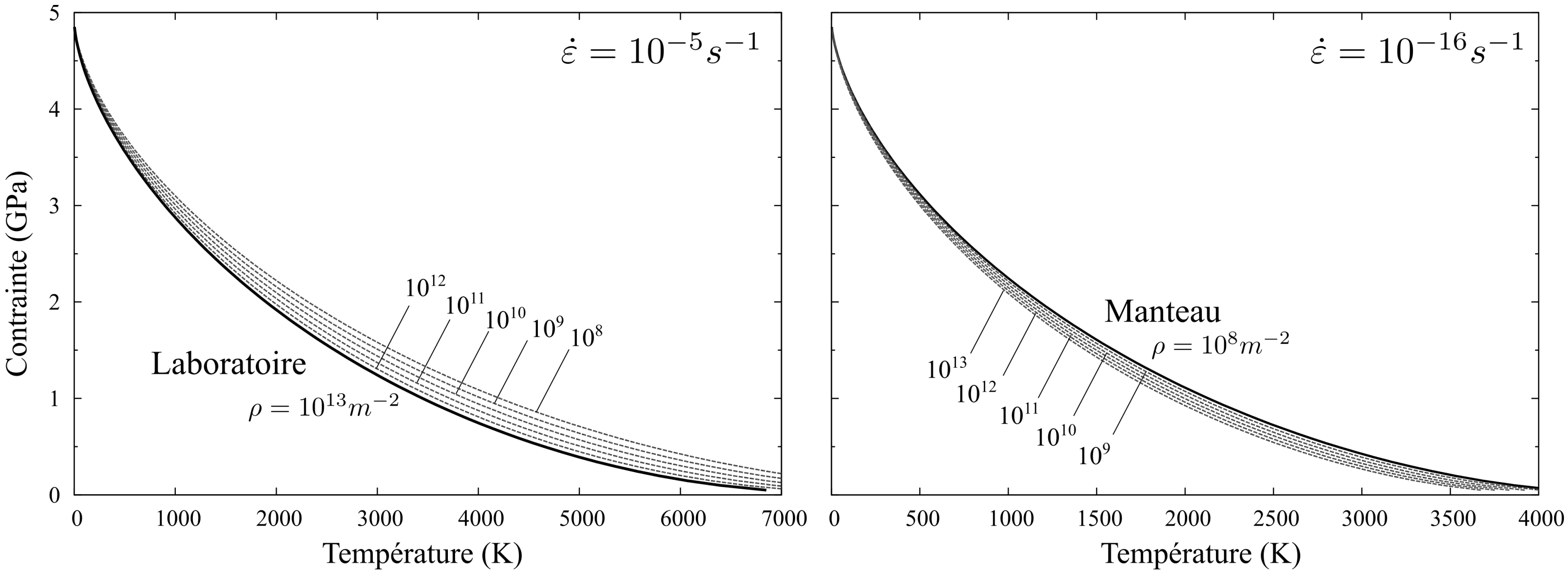
Slip systems ; orthorhombic -> cubic



$[100]_{ortho}$; $[010]_{ortho} \rightarrow <110>_{cubic}$

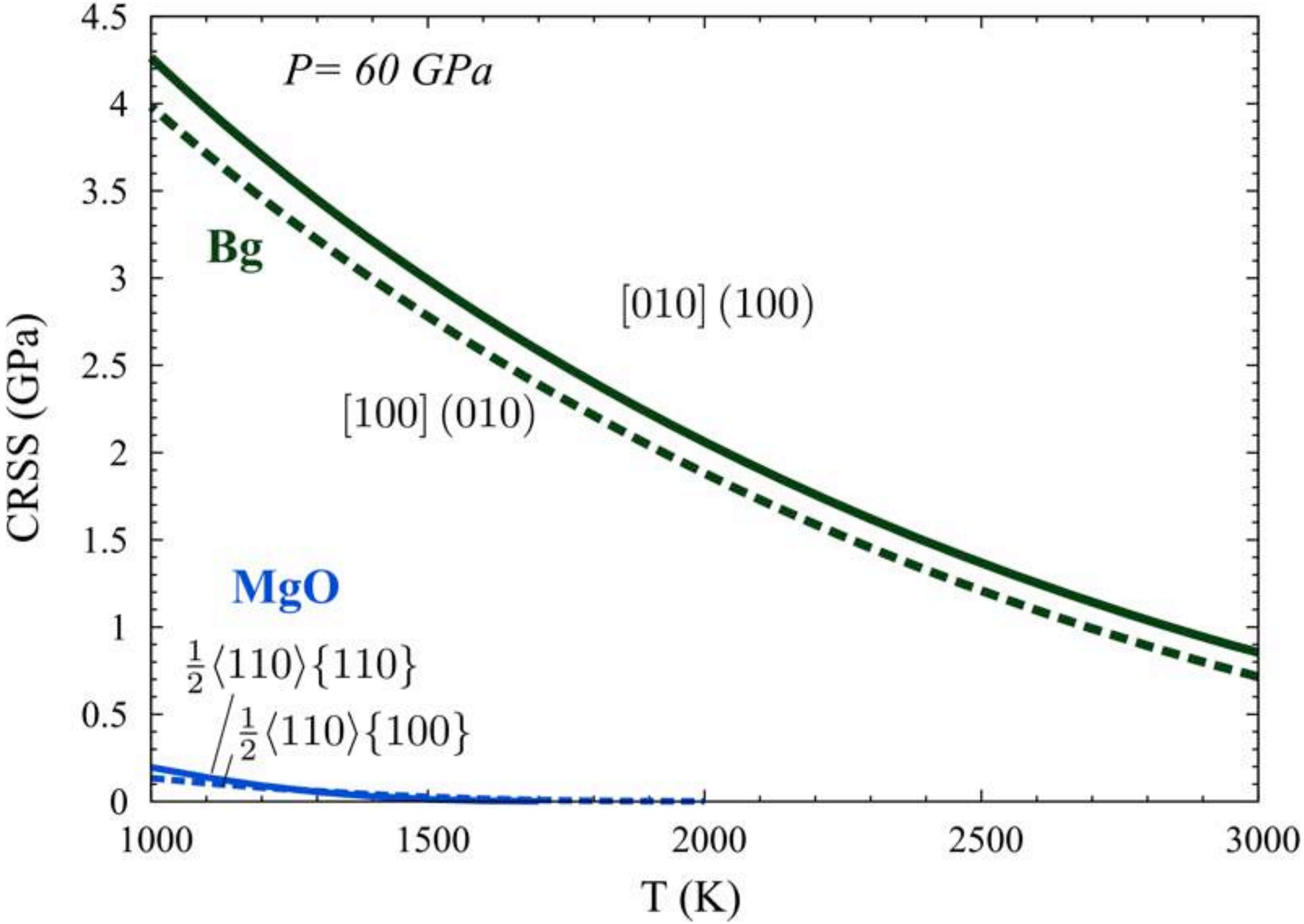
$[001]_{ortho}$; $[110]_{ortho} \rightarrow <100>_{cubic}$





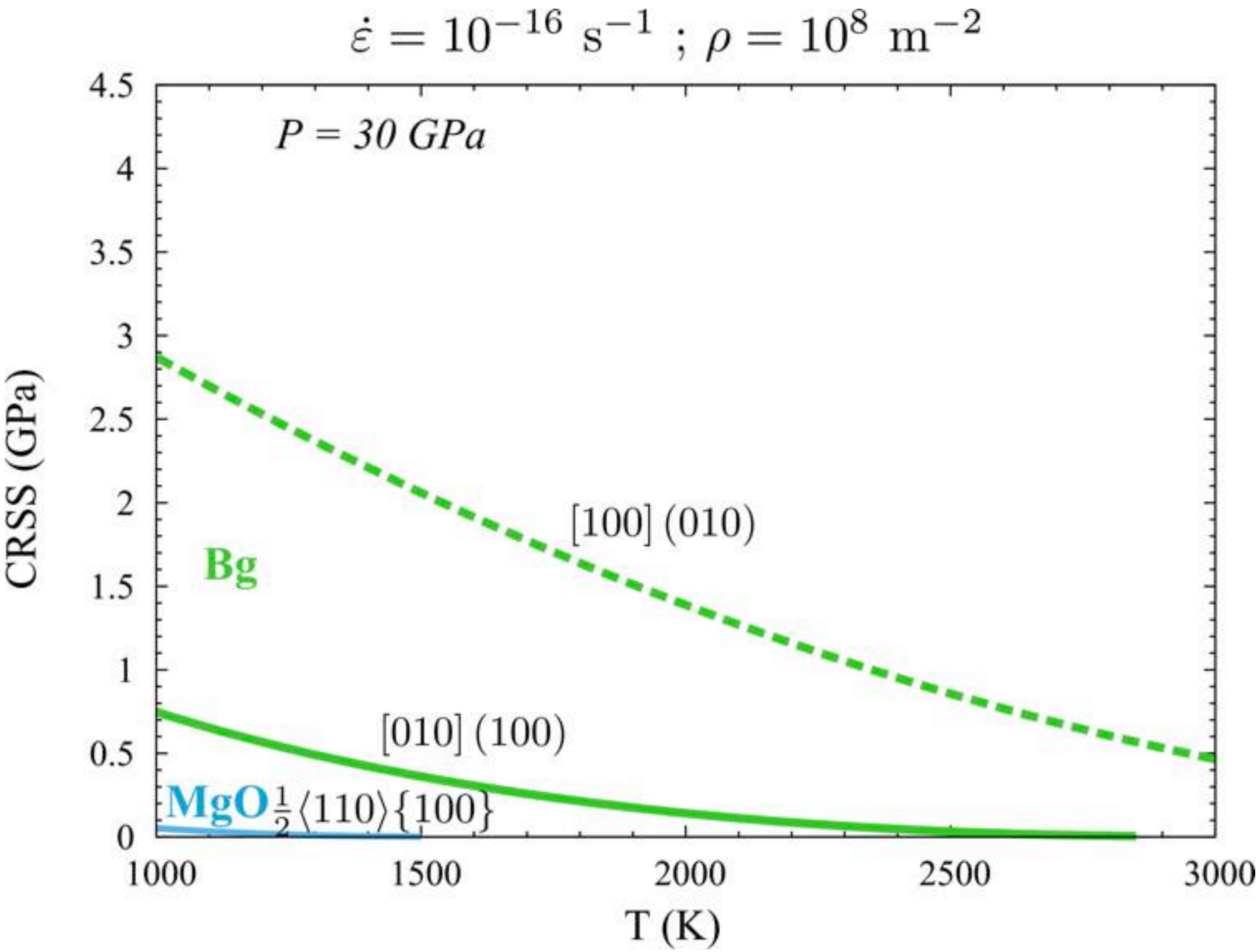
$$\dot{\gamma} = \rho b v_s$$

$MgSiO_3$ perovskite (60 GPa)



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

$MgSiO_3$ perovskite (30 GPa)



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