

# Dislocations dans les minéraux: une affaire de cœur

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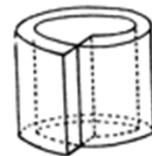
*Institut Universitaire de France*



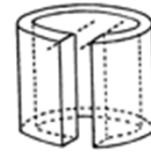
# Volterra's distortions



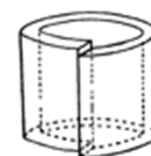
Vito Volterra (1860-1940)  
Italian mathematician and physicist



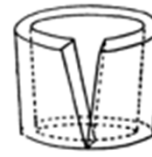
Distorsion d'Ordre 1



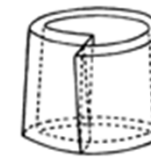
Distorsion d'Ordre 2



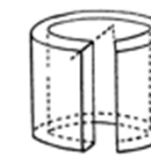
Distorsion d'Ordre 3



Distorsion d'Ordre 4



Distorsion d'Ordre 5



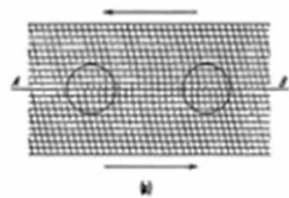
Distorsion d'Ordre 6

Vito Volterra, Sur l'équilibre des corps élastiques  
multiplement connexes, 1907

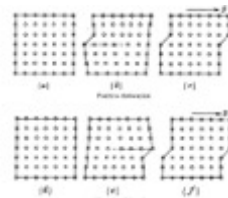
# The concept of dislocations



Egon Orowan



Sir Geoffrey Ingram Taylor

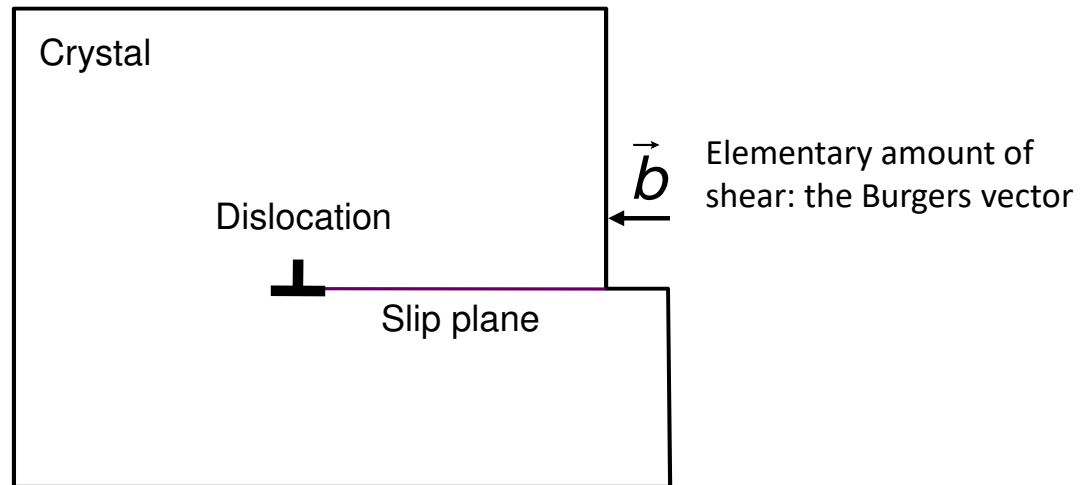


Michael Polanyi



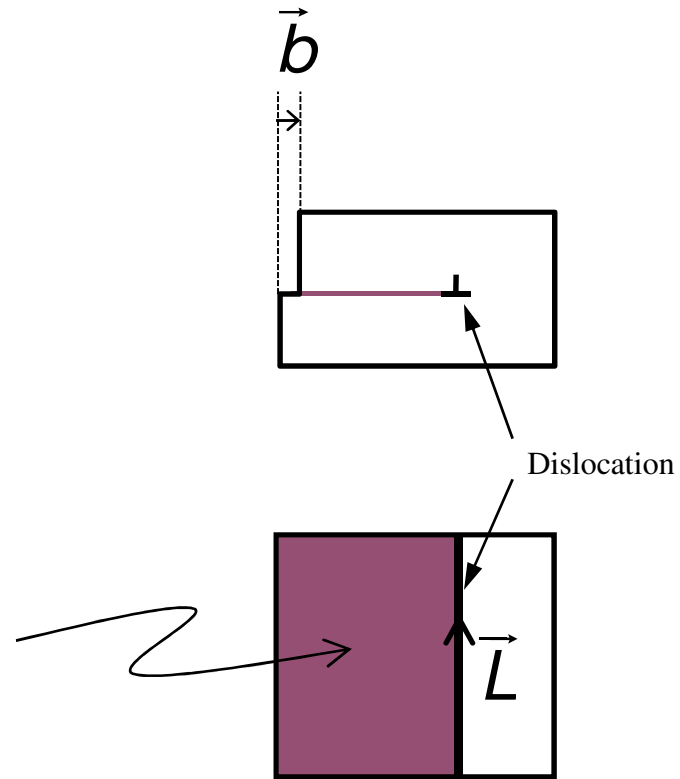
1934

# Shearing crystals

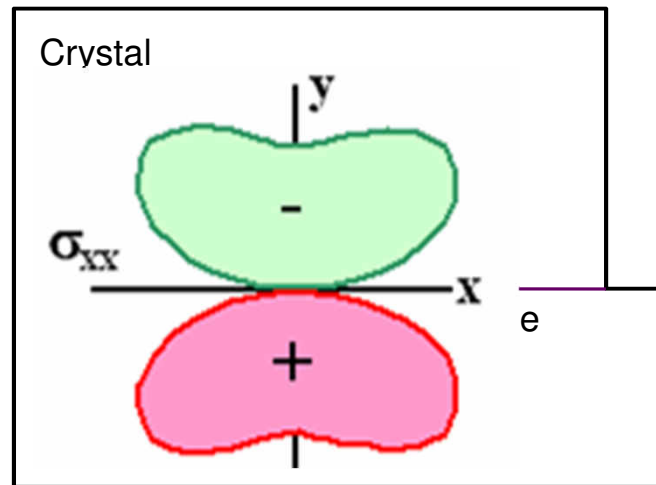


# Dislocations: important parameters

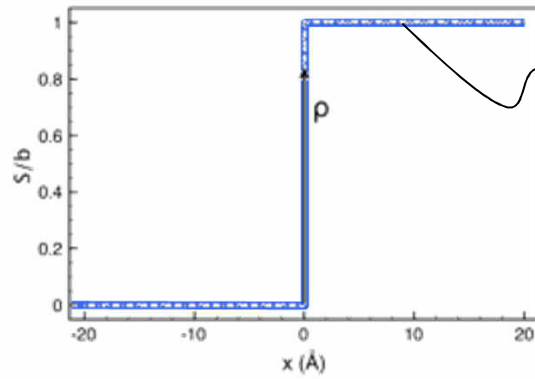
- Elementary amount of shear: the Burgers vector
- Dislocation line orientation (local)
- Slip plane: contains  $L$  and  $b$



# Dislocations: the far field



Volterra dislocation



Shear profile

# Dislocations: the far field

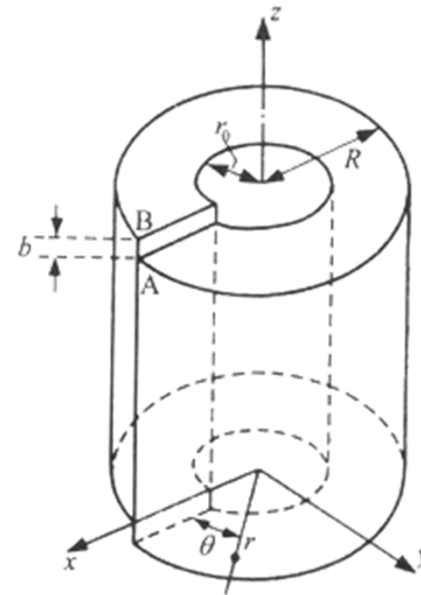
Elasticity theory

- *Screw dislocation*

$$\bar{R} = \frac{\bar{b}}{2\pi} \theta$$

Strain: 
$$\bar{\varepsilon} = \frac{b}{4\pi r} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

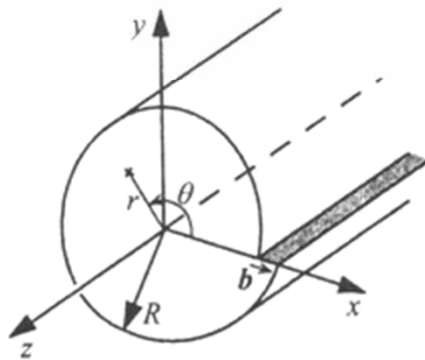
Stress: 
$$\bar{\sigma} = \frac{\mu b}{2\pi r} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$



# Dislocations: the far field

- Elasticity theory
  - *Edge dislocation*

$$R_r = \frac{b}{2\pi} \left[ -\frac{(1-2\nu)}{(2(1-\nu))} \sin\theta \ln r + \frac{\sin\theta}{4(1-\nu)} + \theta \cos\theta \right]$$
$$R_\theta = \frac{b}{2\pi} \left[ -\frac{(1-2\nu)}{(2(1-\nu))} \cos\theta \ln r + \frac{\cos\theta}{4(1-\nu)} - \theta \sin\theta \right]$$

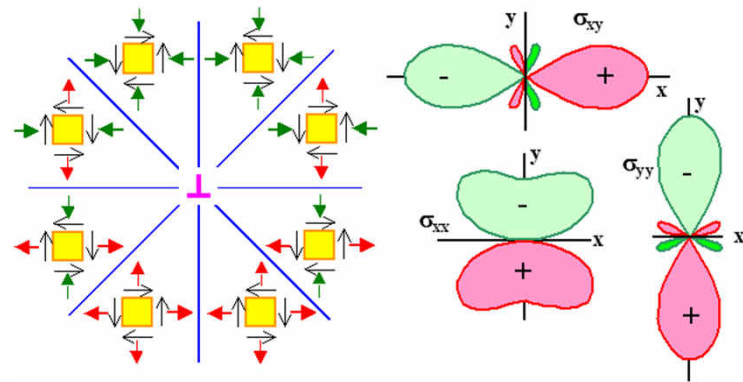
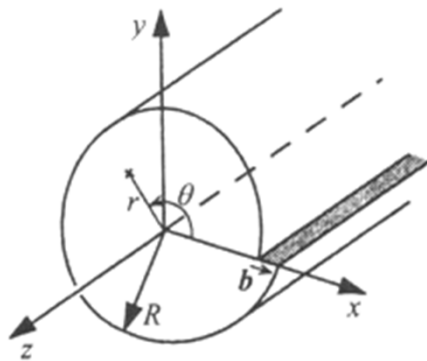




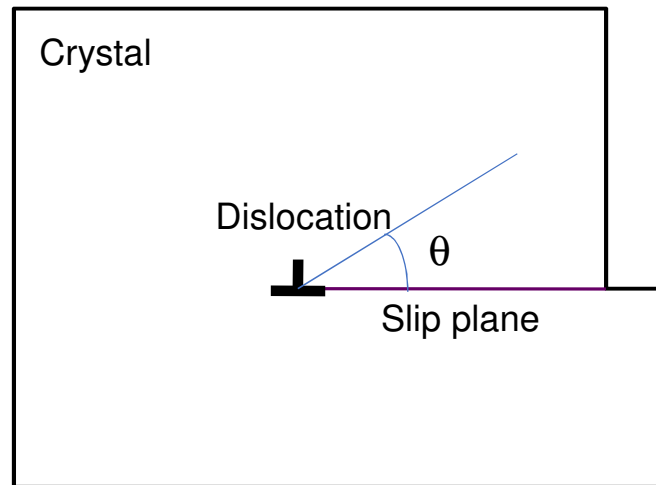
# Dislocations: the far field

- Elasticity theory
  - *Edge dislocation*

$$\bar{\sigma} = \frac{\mu b}{2\pi(1-\nu)} \begin{pmatrix} -\frac{y(3x^2 + y^2)}{(x^2 + y^2)^2} & \frac{x(x^2 - y^2)}{(x^2 + y^2)^2} & 0 \\ \frac{x(x^2 - y^2)}{(x^2 + y^2)^2} & \frac{y(x^2 - y^2)}{(x^2 + y^2)^2} & 0 \\ 0 & 0 & \frac{-2\nu y}{x^2 + y^2} \end{pmatrix}$$

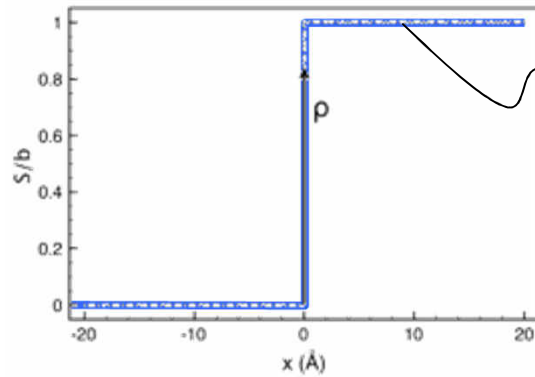


# Volterra dislocations: the far field



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

Volterra dislocation

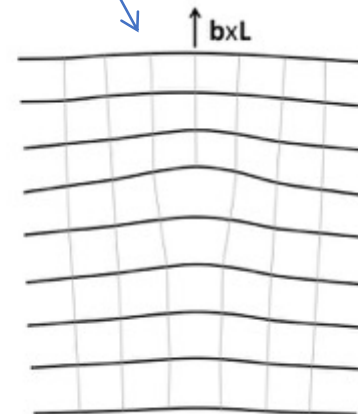
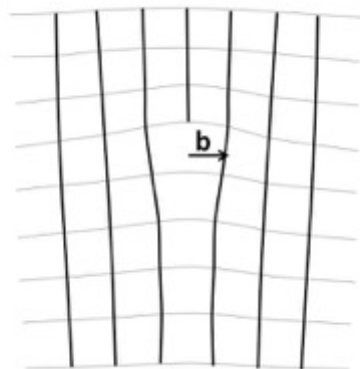


Shear profile

# Dislocations: the displacement field

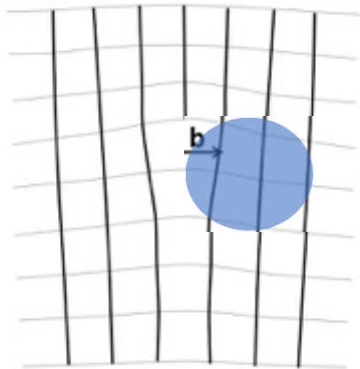
- *Mixed dislocation (general case)*

$$\bar{R} = \frac{1}{2\pi} \left[ \bar{b}\theta + \bar{b}_e \frac{\sin 2\theta}{4(1-\nu)} + (\bar{b} \times \bar{L}) \cdot \left( \frac{(1-2\nu)}{2(1-\nu)} \ln r + \frac{\cos 2\theta}{4(1-\nu)} \right) \right]$$

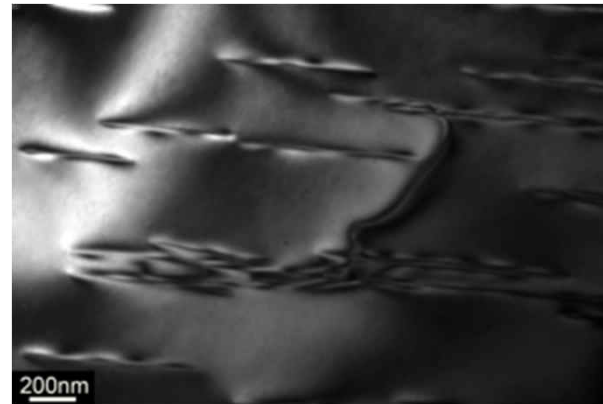


# Dislocations: observations

- Transmission electron microscopy

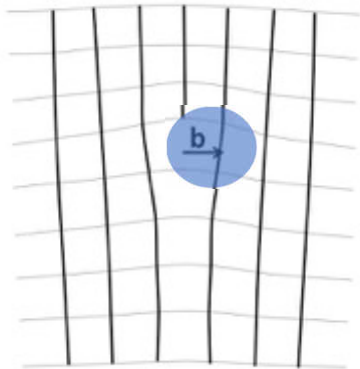


Dark Field

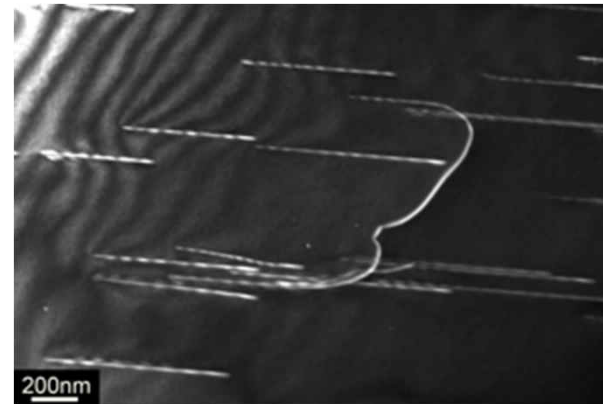


# Dislocations: observations

- Transmission electron microscopy

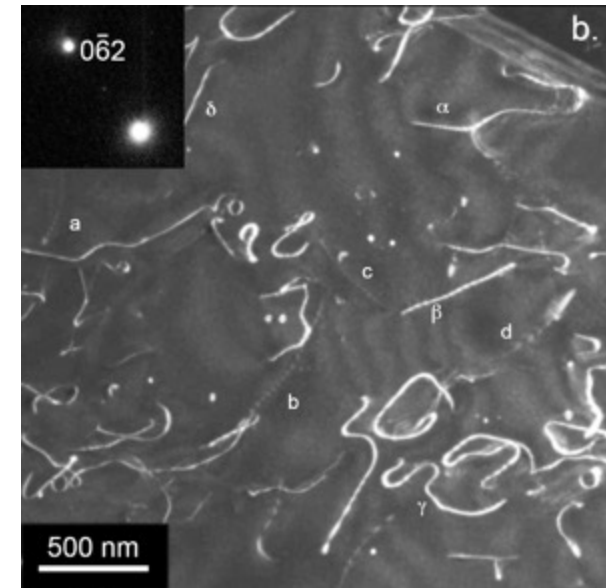
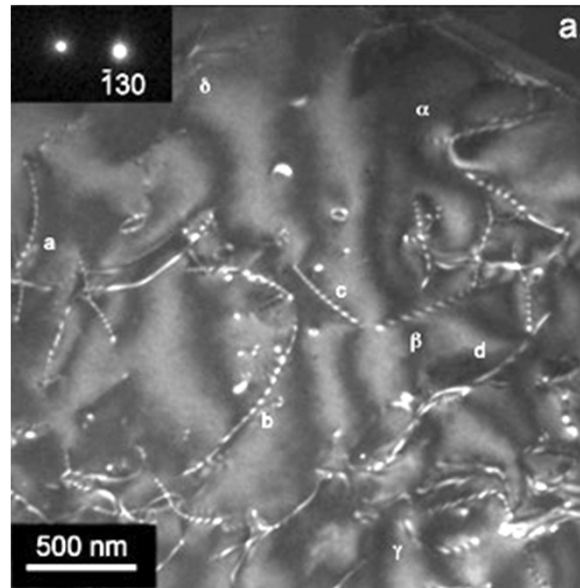
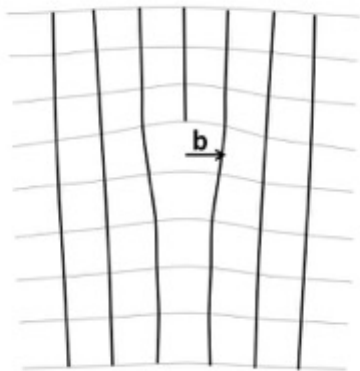


Weak-Beam Dark Field



# Dislocations: observations

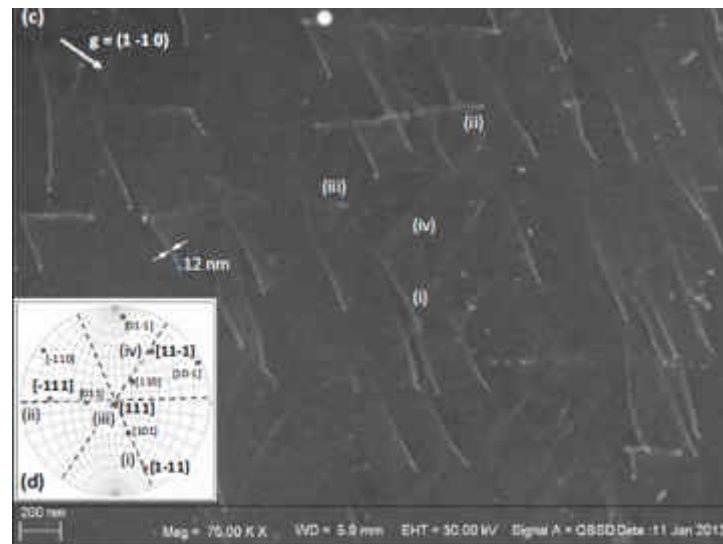
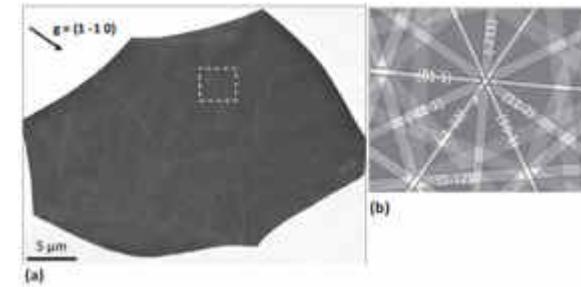
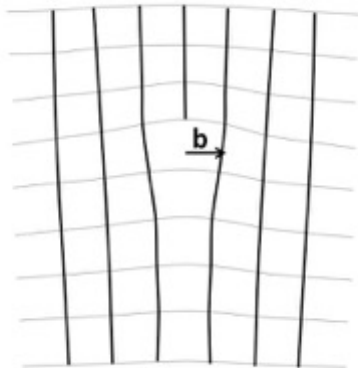
- Transmission electron microscopy



Olivine deformed at 900°C – Sample courtesy S. Demouchy

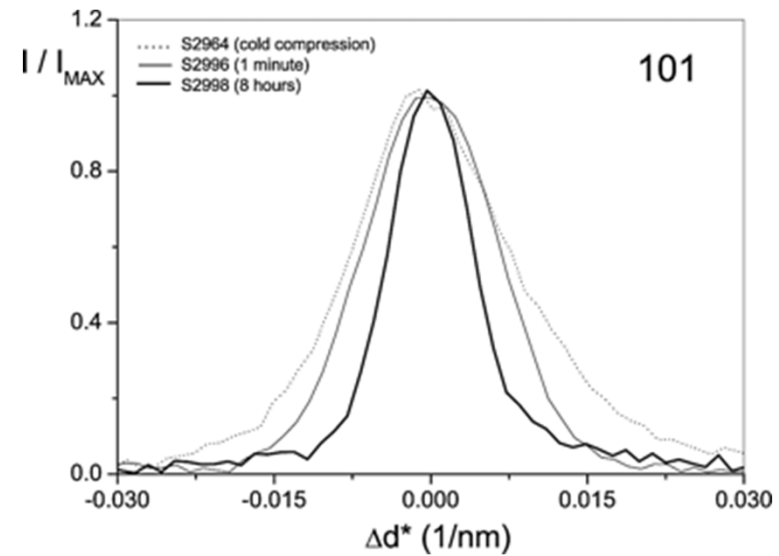
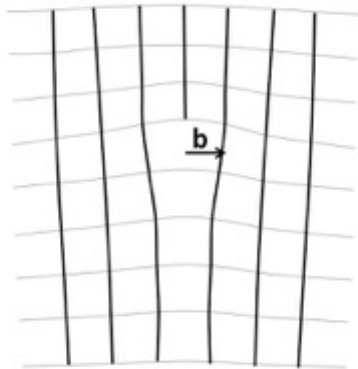
# Dislocations: observations

- Electron Channelling Contrast Imaging (ECCI) in the SEM



# Dislocations: observations

- X-ray diffraction peak broadening analysis (strain anisotropy)

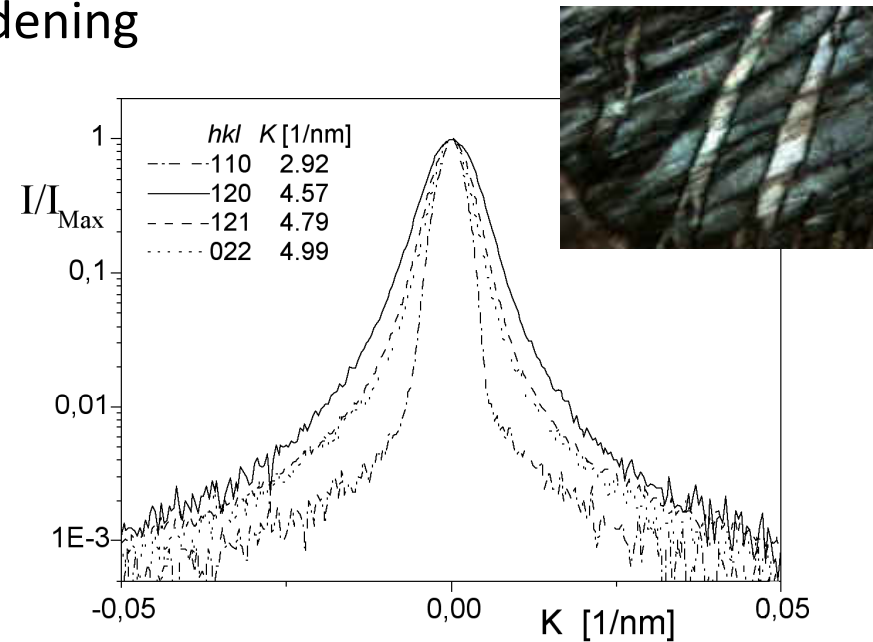
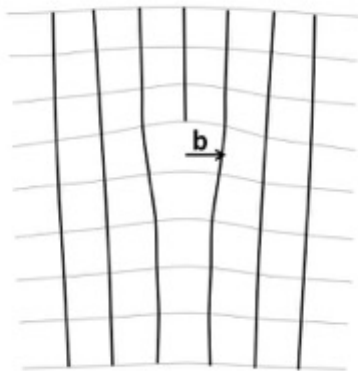


Shear deformation of forsterite – Couvy et al. (2004) Eur. J. Mineral.



# Dislocations: observations

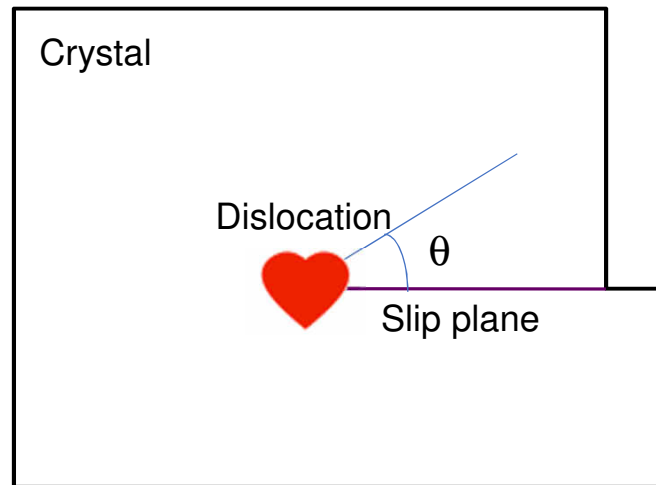
- X-ray diffraction peak broadening analysis (strain anisotropy)



Cordier, Ungár, Zsoldos & Tichy (2004) Nature 428, 837-840

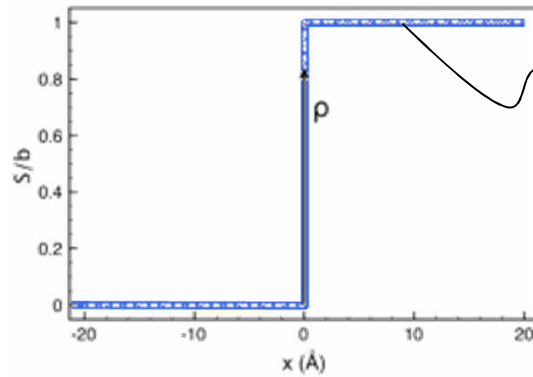
# Volterra dislocations: the core

$$E_{el} = \frac{\mu b^2}{4\pi K} \ln \left( \frac{R}{r_0} \right)$$



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

Volterra dislocation



Shear profile



THE SIZE OF A DISLOCATION

By R. PEIERLS, The University, Birmingham

ABSTRACT. Calculations are made of the size of a dislocation and of the critical shear stress for its motion.

It is generally supposed that the plastic deformation of crystals proceeds by means of the propagation of dislocations along the slip planes. Since a dislocation consists of a displacement of a great many atoms, it is obviously impossible to obtain a rigorous solution of the equilibrium conditions for all these atoms. Dr Orowan has shown me how to obtain an idealized model, which leads to equations that can be solved, of the forces in a dislocation, and in this note I shall report on the results.

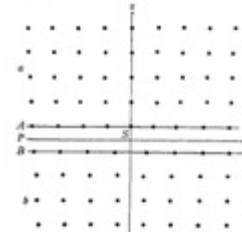
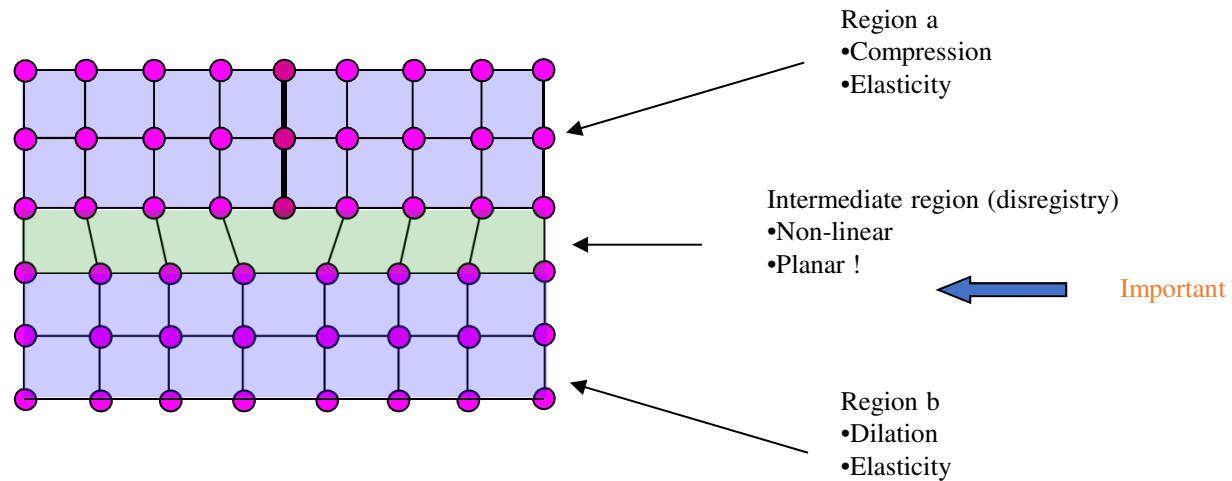


Figure 1.

The type of dislocation which I have investigated is sketched in figure 1. The slip plane  $P(x=0)$  divides the crystal into an upper part  $a$  and a lower part  $b$ . These are symmetrical about the vertical plane  $S(x=0)$ . The central plane  $S$  lies in a net plane in the upper half-crystal  $a$ , and half way between two net planes in  $b$ . The  $y$  axis is at right angles to the plane of the figure (i.e. the line in which the plane  $S$  meets the slip plane  $P$ ) is called the dislocation line. In the neighbourhood of this line the atoms of  $a$  are moved inwards and those of  $b$  are moved apart, so that at great distances from the dislocation line the two planes  $A$  and  $B$  which are immediately above and below the slip plane are again in correct alignment,  $A$  containing, however, one row of atoms more than  $B$ .

The atoms in the plane  $A$  are then subject to two forces: (i) The interaction

# Modeling dislocations using the Peierls-Nabarro model



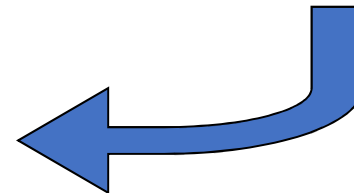
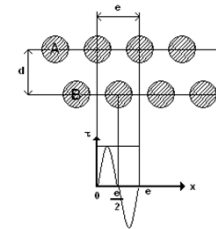
# Modeling dislocations using the Peierls-Nabarro model

$$\frac{K}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x-x'} \left[ \frac{dS(x')}{dx'} \right] dx' = \frac{K}{2\pi} \int_{-\infty}^{+\infty} \frac{\rho(x')}{x-x'} dx' = F(S(x))$$



Sinusoidal  
(assumed !)

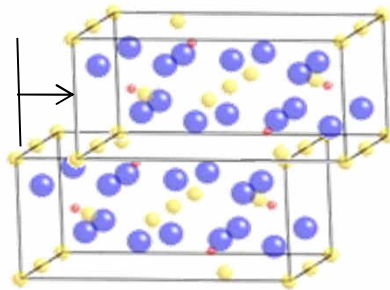
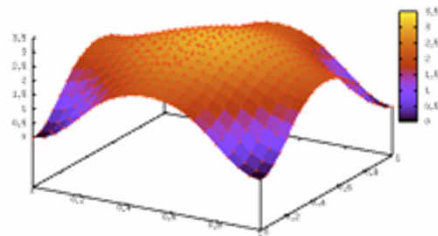
$$F(S(x)) = \tau^{\max} \sin\left(\frac{2\pi S(x)}{b}\right)$$



$$\sigma_p = \frac{Kb}{a'} \exp\left(-\frac{2\pi\xi}{a'}\right)$$

# Modeling dislocations using the Peierls-Nabarro model

$$\frac{K}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x-x'} \left[ \frac{dS(x')}{dx'} \right] dx' = \frac{K}{2\pi} \int_{-\infty}^{+\infty} \frac{\rho(x')}{x-x'} dx' = F(S(x))$$

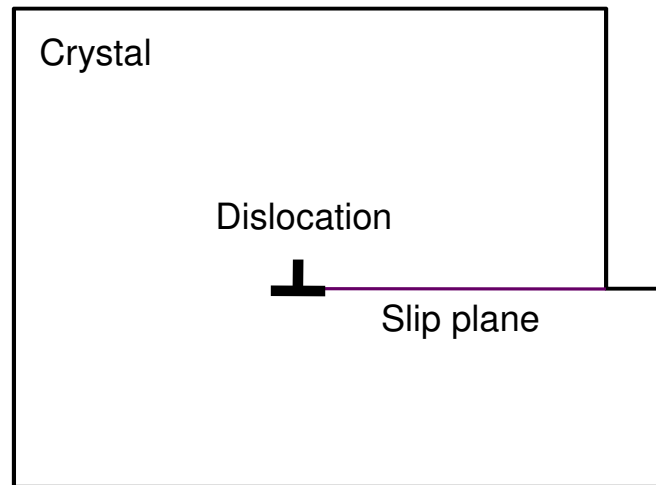


Generalised Stacking Faults (GSF)

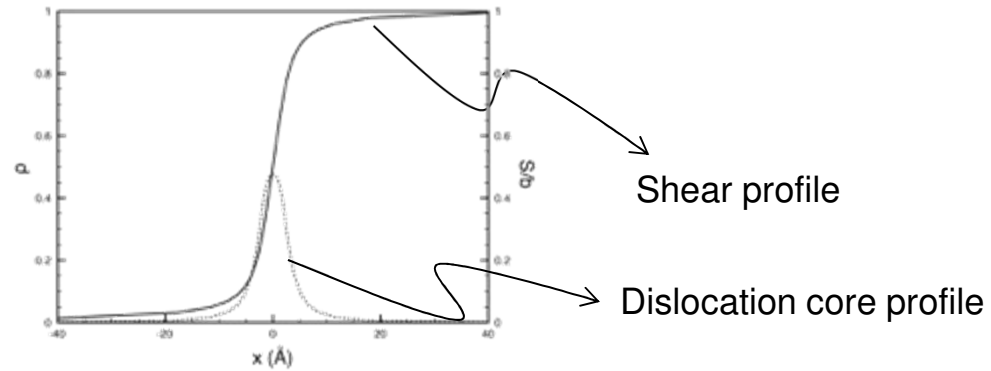
Can be calculated *ab initio*

$$F(S) = -\frac{\partial \gamma}{\partial S}$$

# Modeling dislocations using the Peierls-Nabarro model

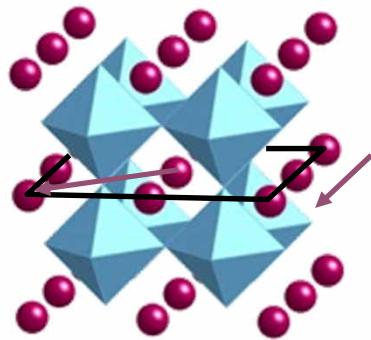


Peierls dislocation

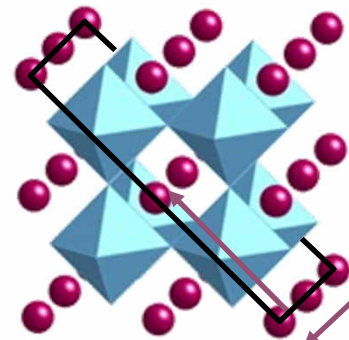


# Testing the Peierls-Nabarro model: SrTiO<sub>3</sub>

$\langle 100 \rangle \{010\}$   $a = 3.905 \text{ \AA}$



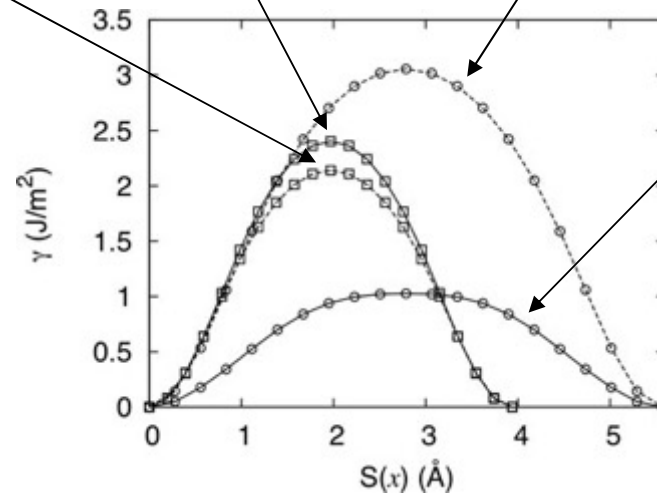
$a = 5.52 \text{ \AA}$   $\langle 110 \rangle \{1\bar{1}0\}$





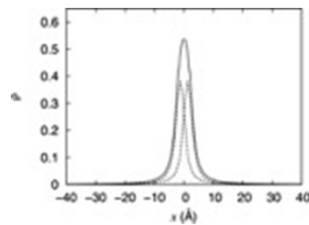
# SrTiO<sub>3</sub>: generalized stacking faults

$\langle 100 \rangle \{010\}$      $\langle 100 \rangle \{011\}$      $\langle 110 \rangle \{001\}$      $\langle 110 \rangle \{1\bar{1}0\}$

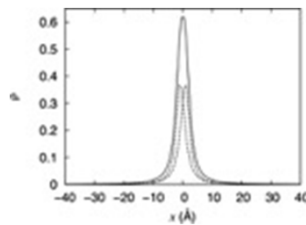


# SrTiO<sub>3</sub>: generalized stacking faults

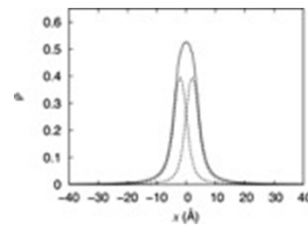
$\langle 100 \rangle \{ 010 \}$



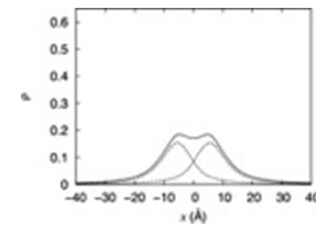
$\langle 100 \rangle \{ 011 \}$

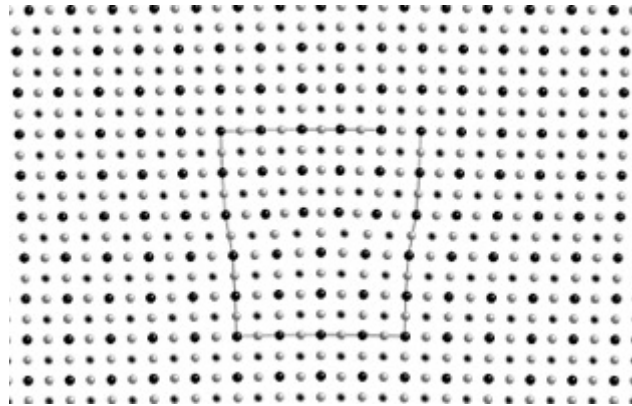


$\langle 110 \rangle \{ 001 \}$

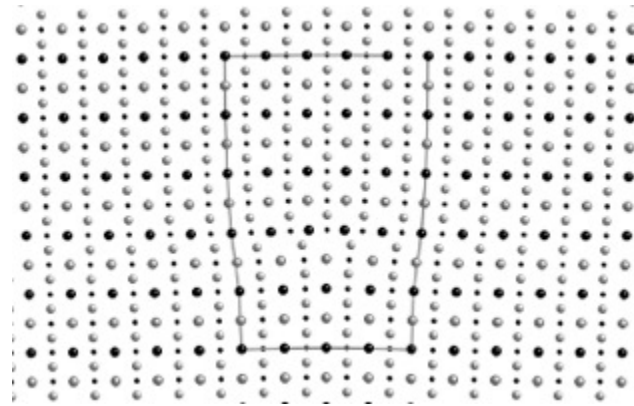


$\langle 110 \rangle \{ 1\bar{1}0 \}$

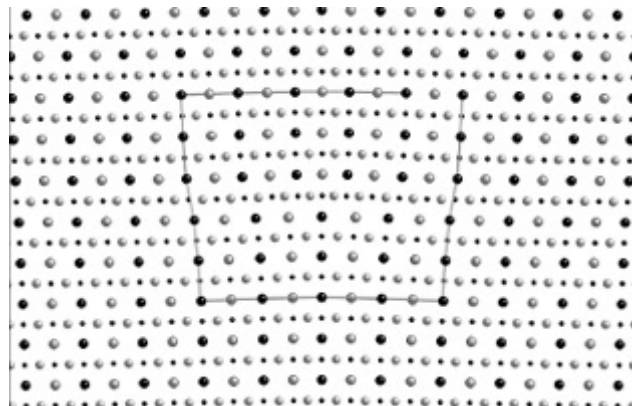




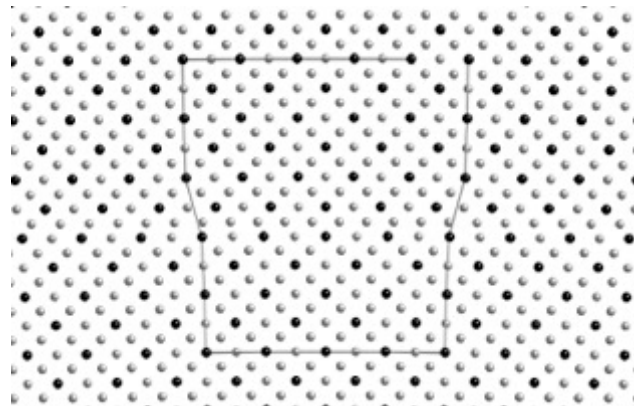
$\langle 100 \rangle \{010\}$



$\langle 100 \rangle \{011\}$



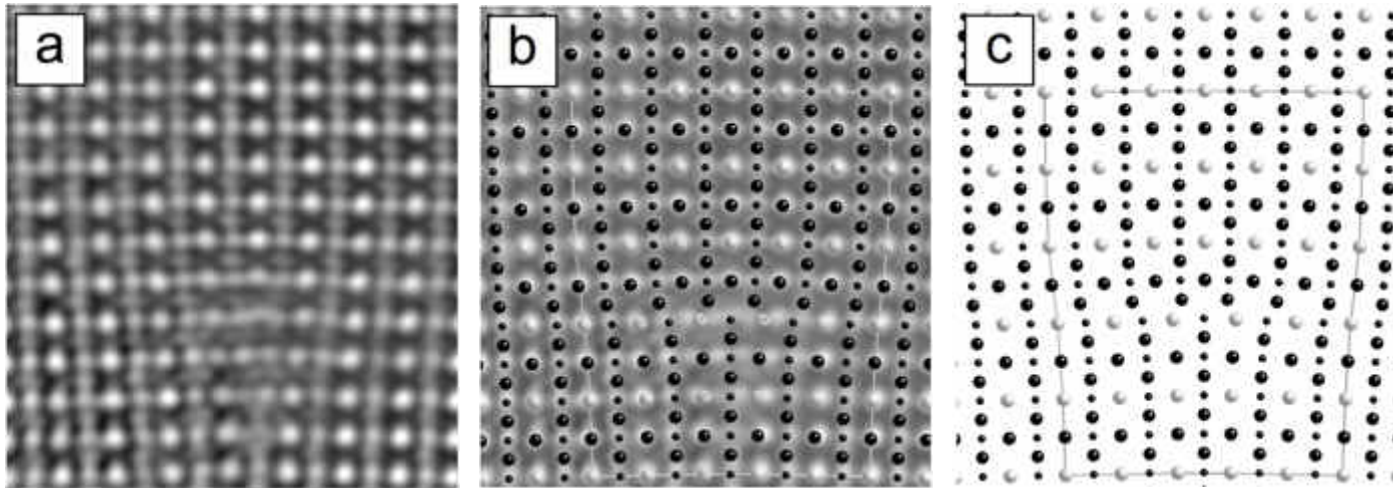
$\langle 110 \rangle \{001\}$



$\langle 110 \rangle \{1\bar{1}0\}$

# Testing the Peierls-Nabarro model: $\text{SrTiO}_3$

Comparison with HRTEM images



Atomic scale model  
Peierls-Nabarro  
Courtesy Ferré et al. (2008)

# The Peierls-Nabarro model: lattice friction

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Analytical model: Joos & Duesberry (1997)

Dimensionless parameter:  $\Gamma = \zeta/d'$

Two cases:

- Narrow cores  $\Gamma \ll 1$  
$$\sigma_p(\Gamma \ll 1) = \frac{3\sqrt{3}}{8} \tau_{\max} \frac{d'}{\pi\zeta}$$

- Wide cores  $\Gamma \gg 1$  
$$\sigma_p(\Gamma \gg 1) = \frac{Kb}{d'} \exp\left(\frac{-2\pi\zeta}{d'}\right).$$

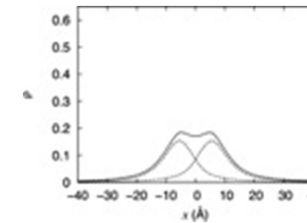
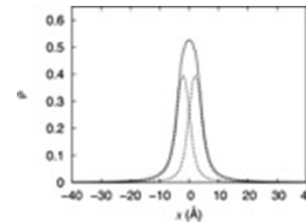
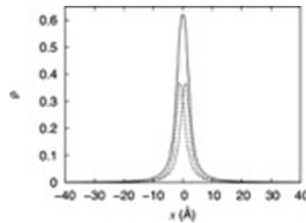
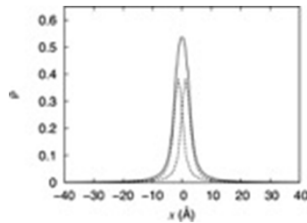
# SrTiO<sub>3</sub>: lattice friction

$\langle 100 \rangle \{ 010 \}$

$\langle 100 \rangle \{ 011 \}$

$\langle 110 \rangle \{ 001 \}$

$\langle 110 \rangle \{ 1\bar{1}0 \}$



Edge (GPa)

0.6

0.6

1.2

0.004

Screw (GPa)

0.7

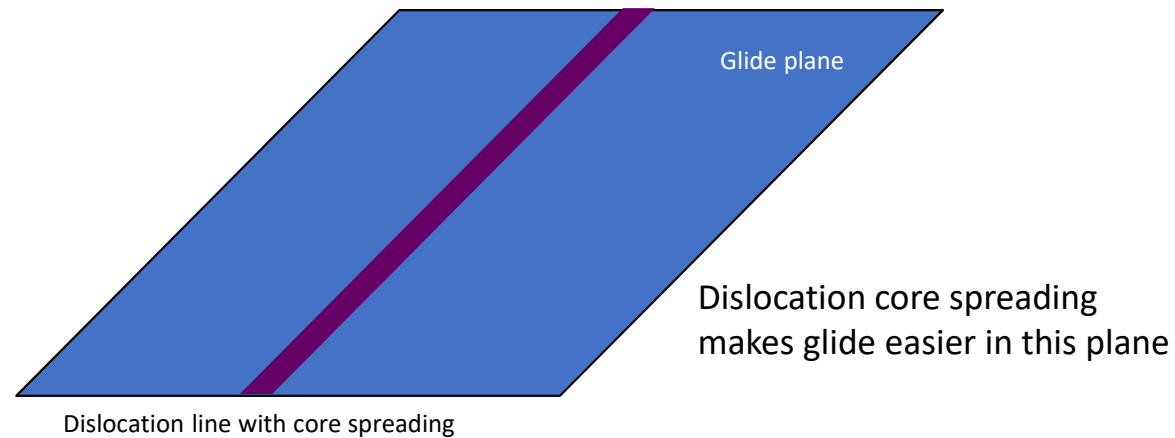
9.9

0.9

0.006

# When the core structure determines the glide plane

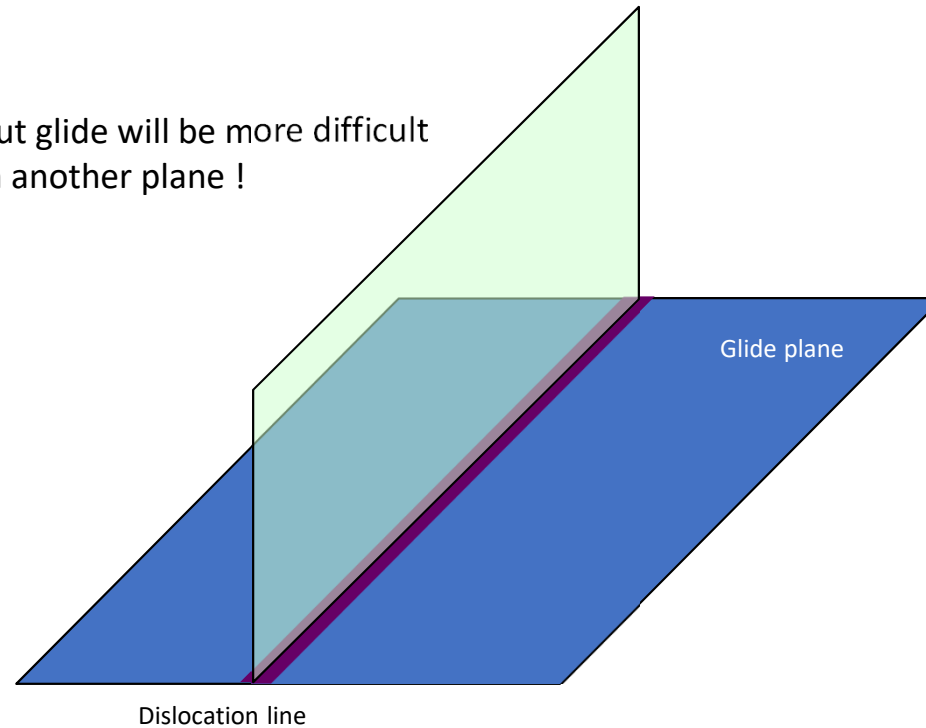
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# When the core structure determines the glide plane

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But glide will be more difficult in another plane !



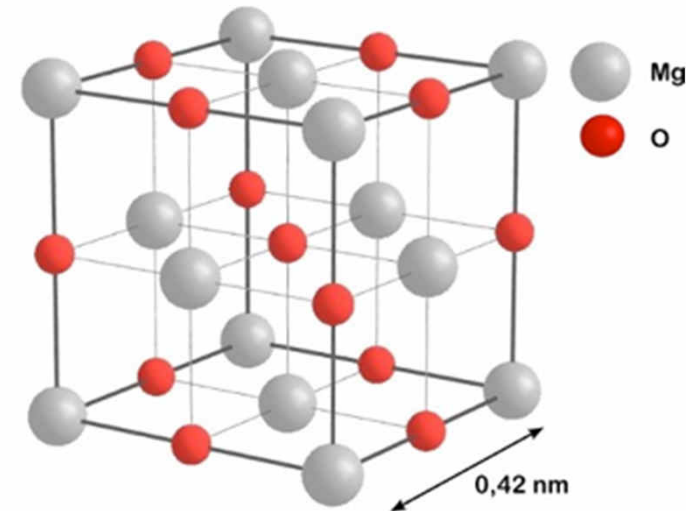


# “Predicting” slip systems in MgO

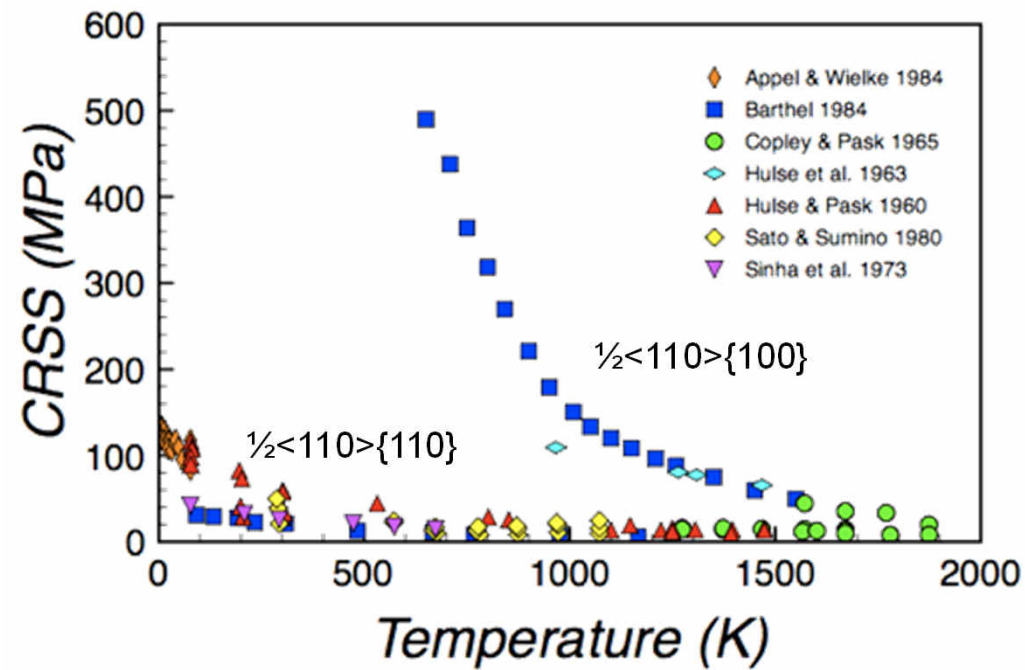
B1 cubic crystal structure (space group  $Fm\bar{3}m$ )

Rock-salt (NaCl) structure.

Lattice parameter is about 4.21 Å

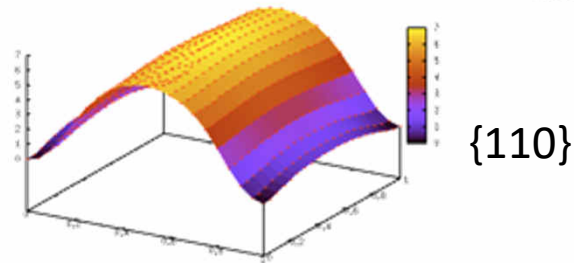
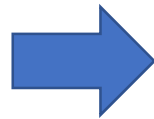
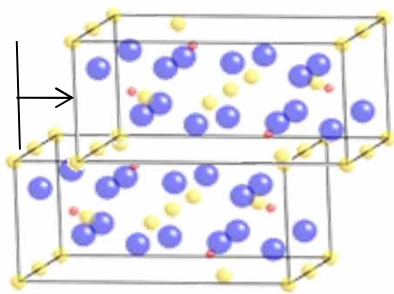


# “Predicting” slip systems in MgO

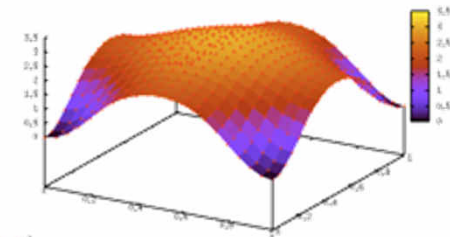


# “Predicting” slip systems in MgO with the Peierls-Nabarro model

$$\frac{K}{2\pi} \int_{-\infty}^{+\infty} \frac{1}{x-x'} \left[ \frac{dS(x')}{dx'} \right] dx' = \frac{K}{2\pi} \int_{-\infty}^{+\infty} \frac{\rho(x')}{x-x'} dx' = F(S(x))$$



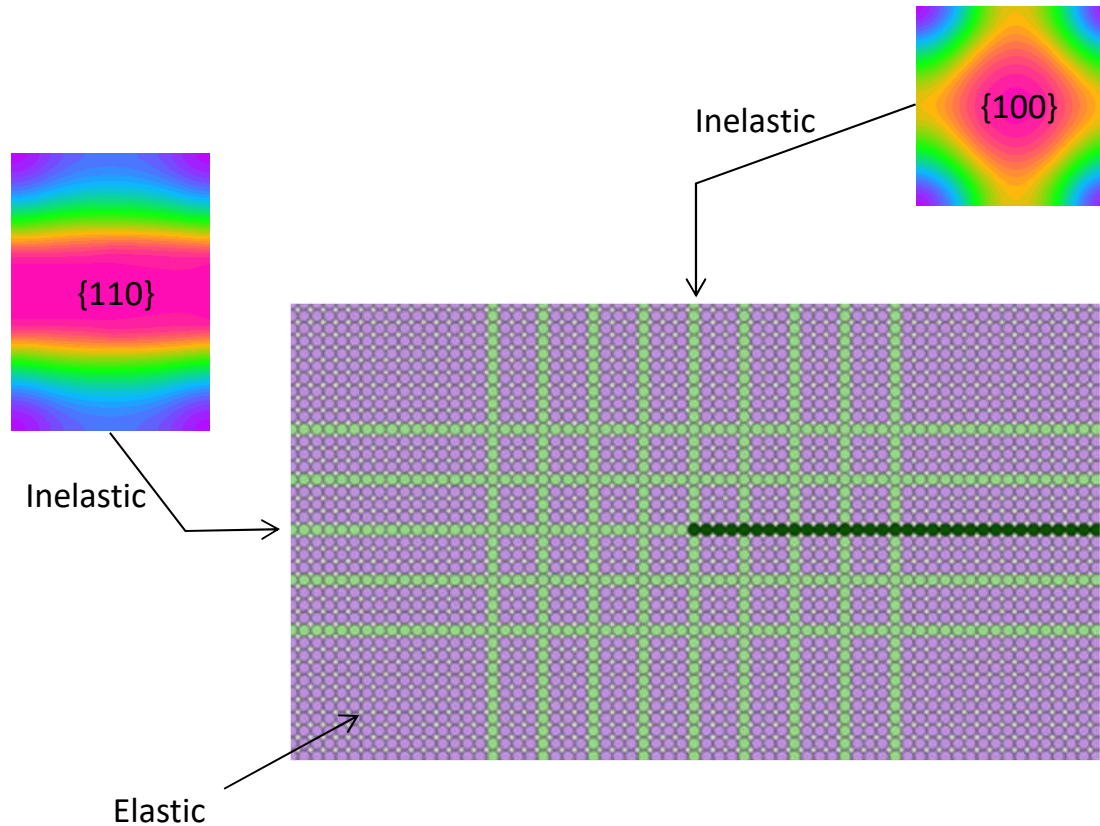
{110}



{100}

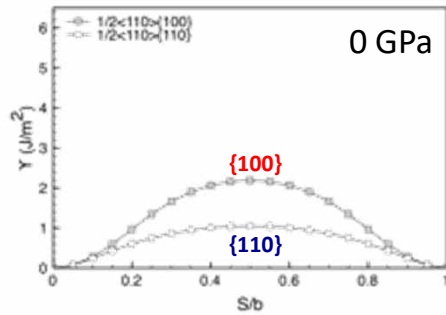


# “Predicting” slip systems in MgO with the Peierls-Nabarro Galerkin model



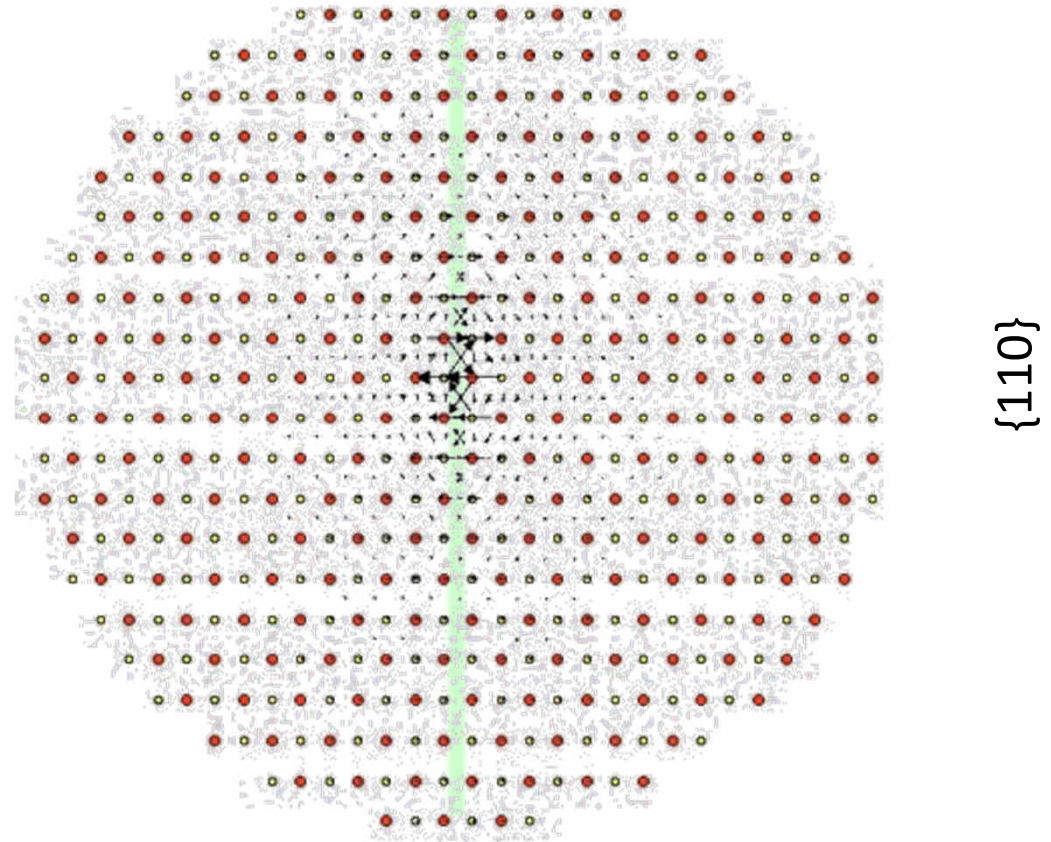
C. Denoual (CEA-DAM)

# “Predicting” slip systems in MgO with the Peierls-Nabarro Galerkin model

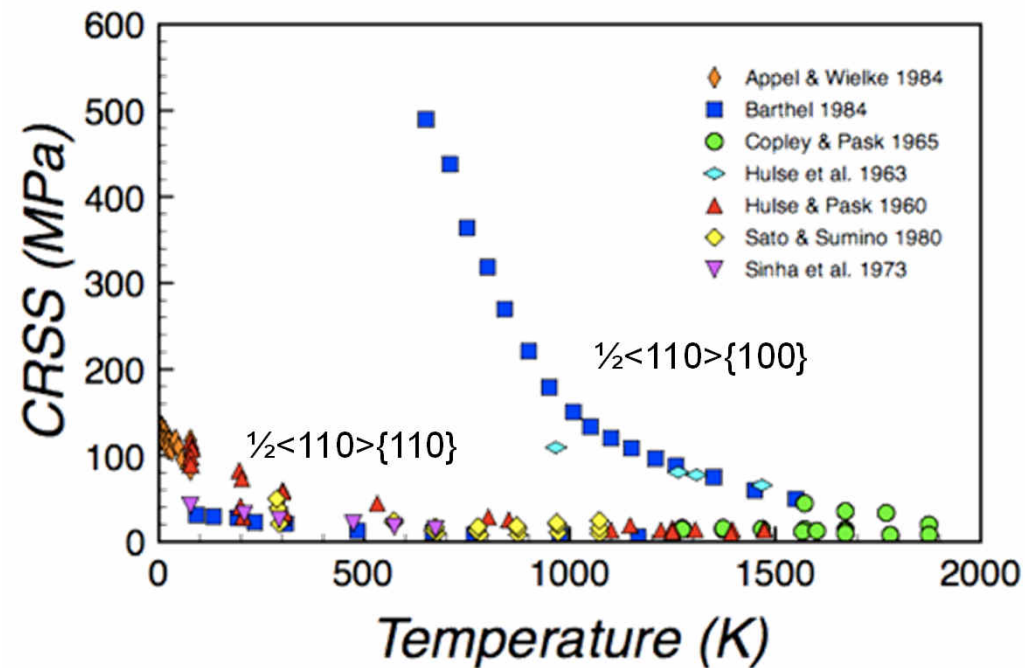


0 GPa

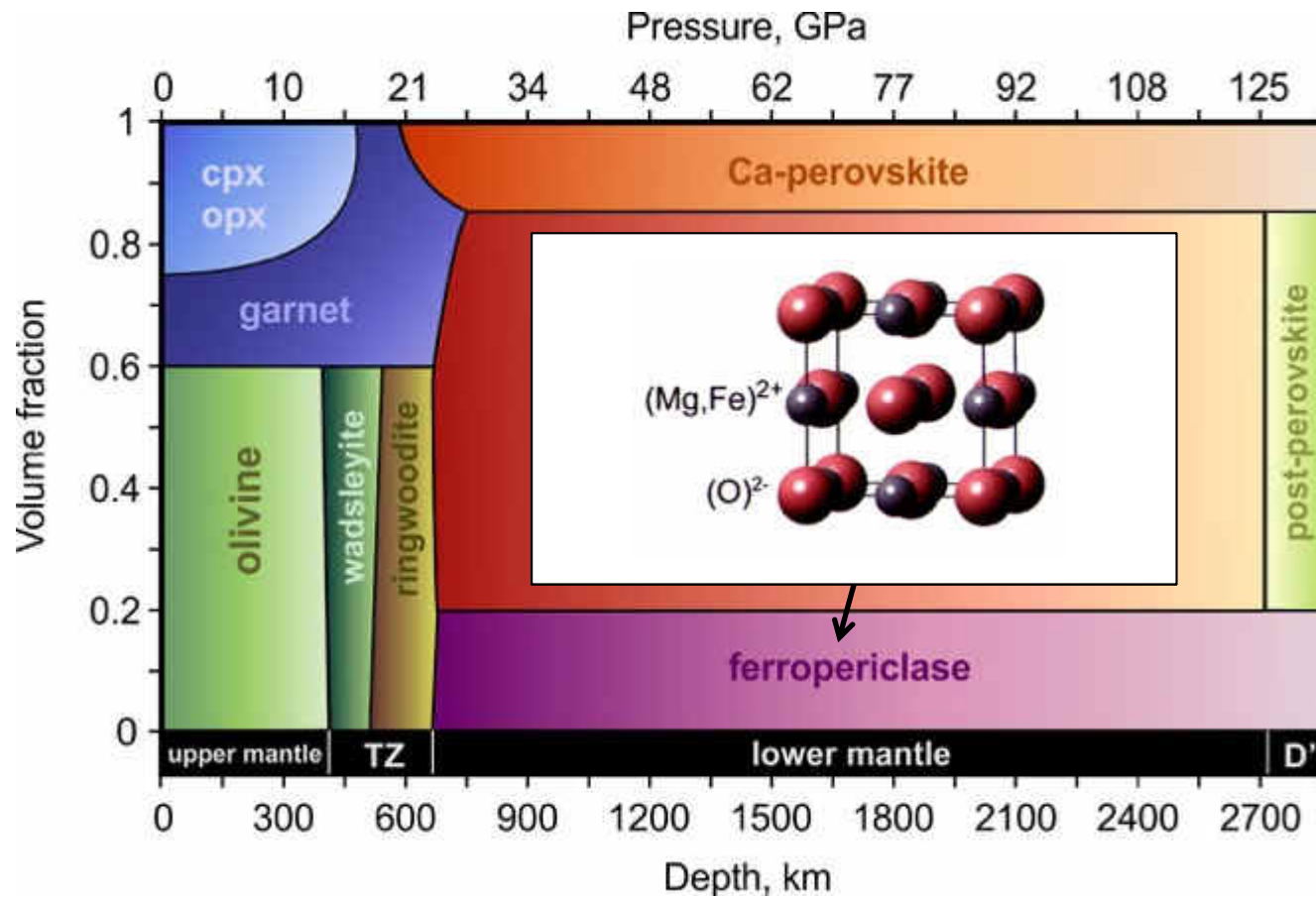
Glide in {110}



# “Predicting” slip systems in MgO with the Peierls-Nabarro Galerkin model



# (Mg,Fe)O in the mantle



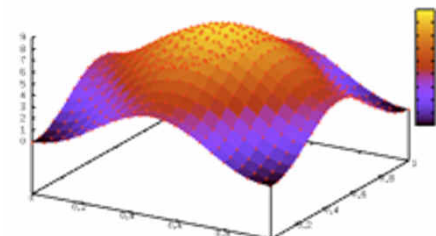
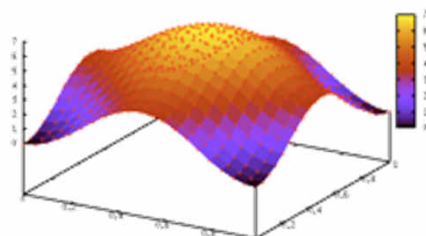
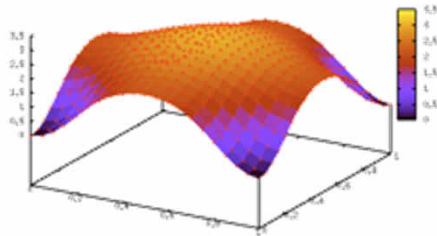


# Predicting slip systems in MgO with the Peierls-Nabarro Galerkin model

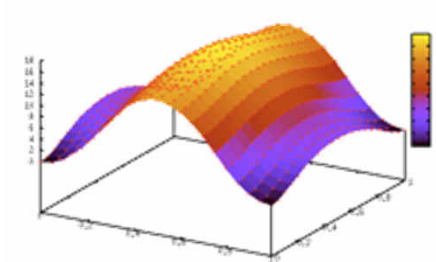
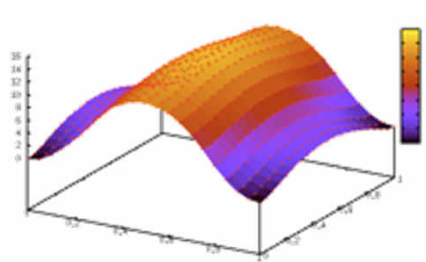
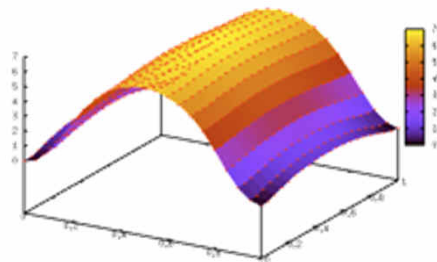
0 GPa

60 GPa

100 GPa



{100}

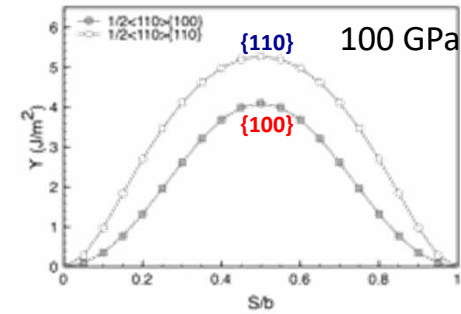
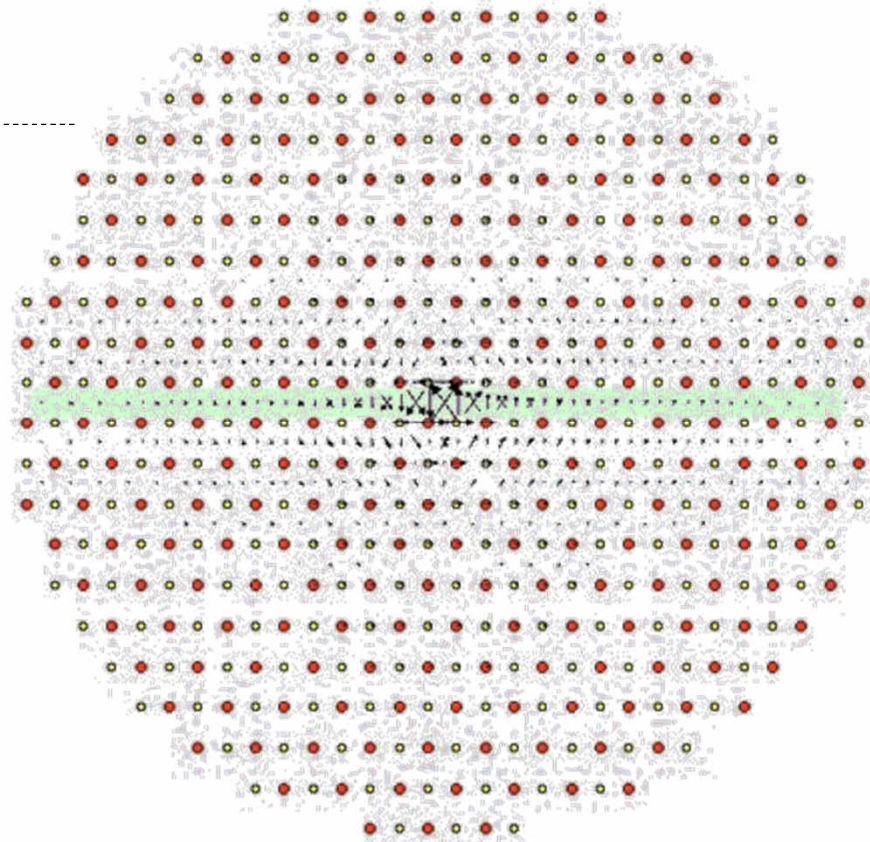


{110}



# Predicting slip systems in MgO with the Peierls-Nabarro Galerkin model

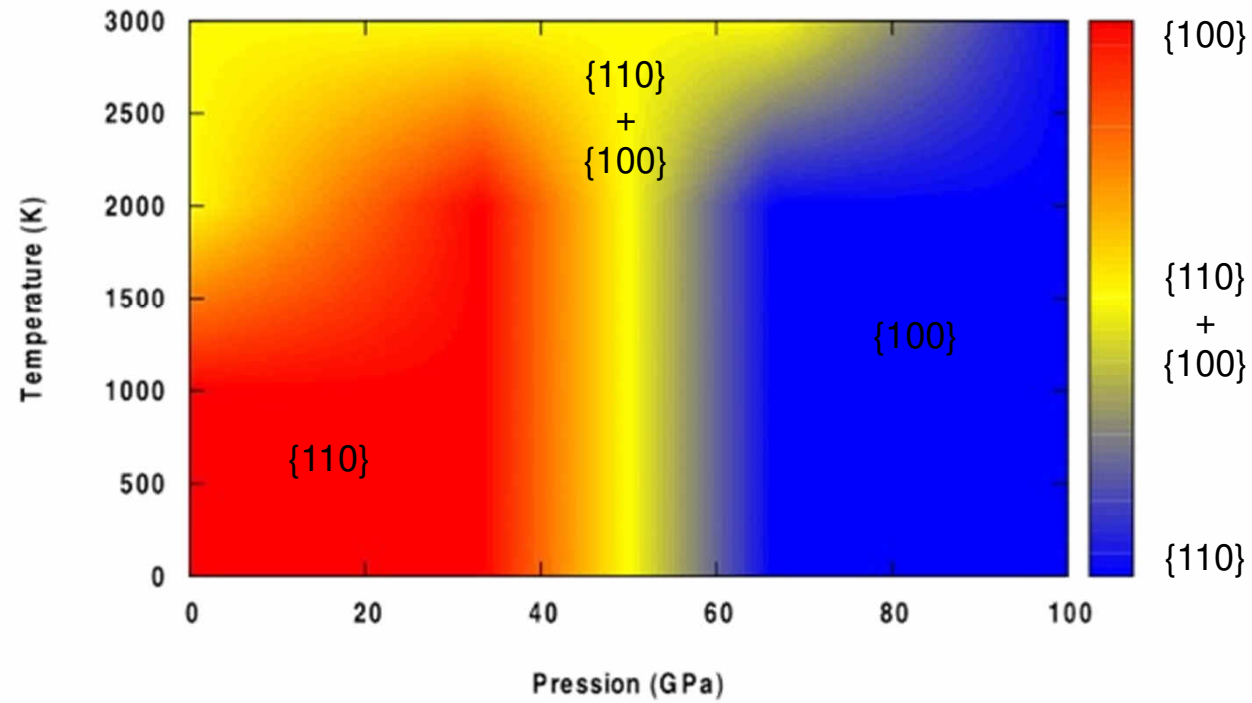
{100}



100 GPa

Glide in {100}

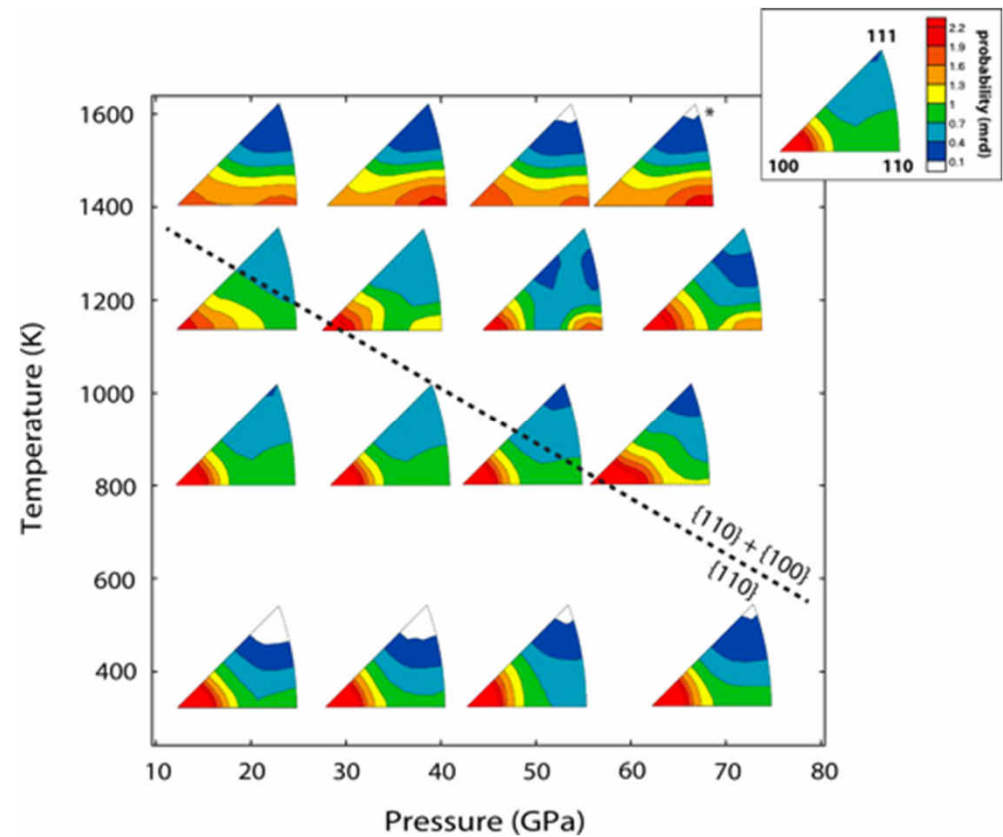
# Predicting slip systems in MgO with the Peierls-Nabarro Galerkin model



$$\dot{\epsilon} = 10^{-4} \text{ s}^{-1}; \rho = 10^{12} \text{ m}^{-2}$$

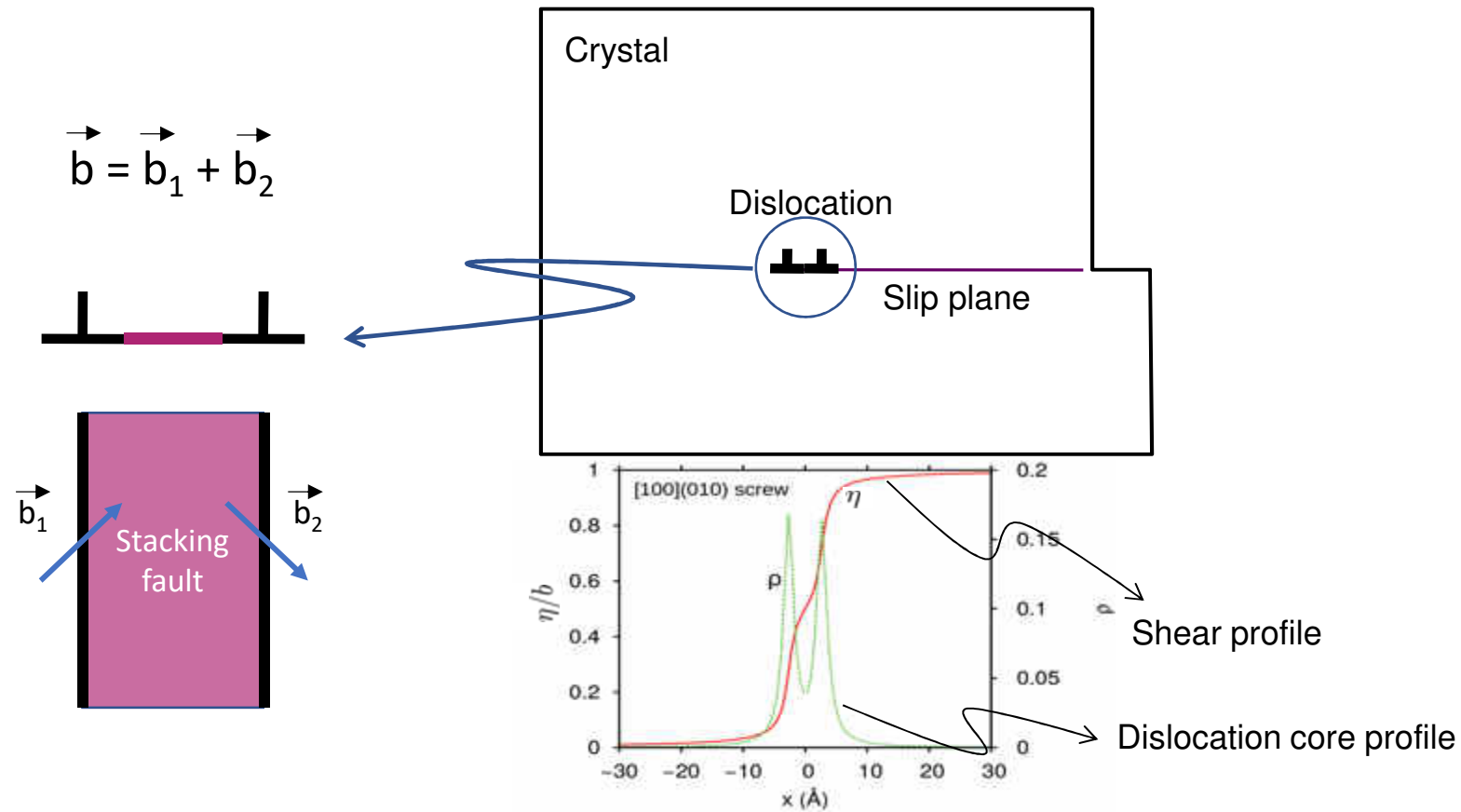
# Experimental evidence

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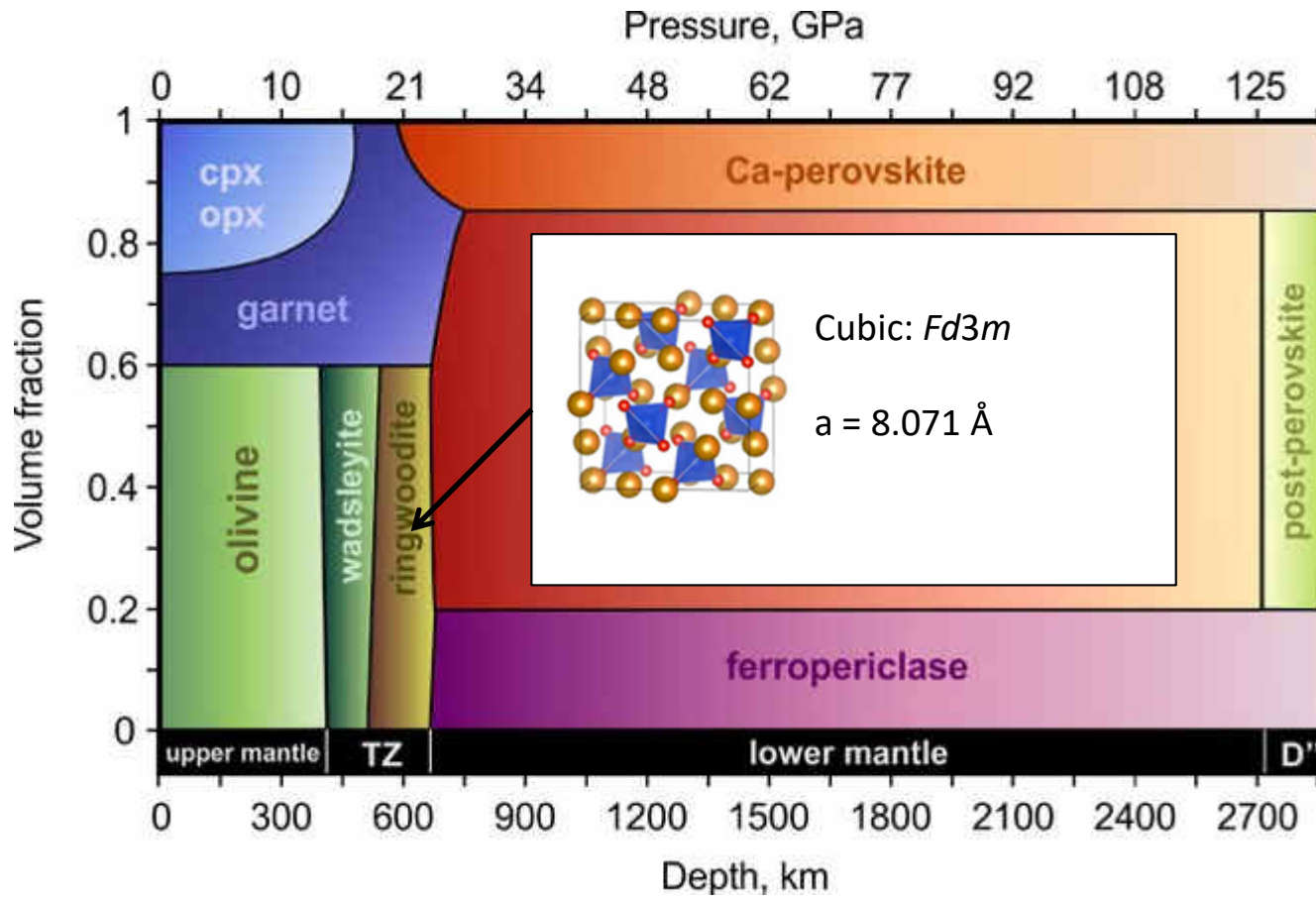
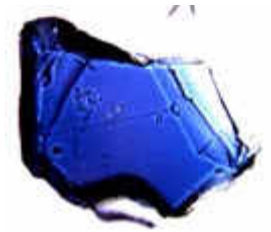


*J. Immoor et al. / Earth and Planetary Science  
Letters 489 (2018) 251–257*

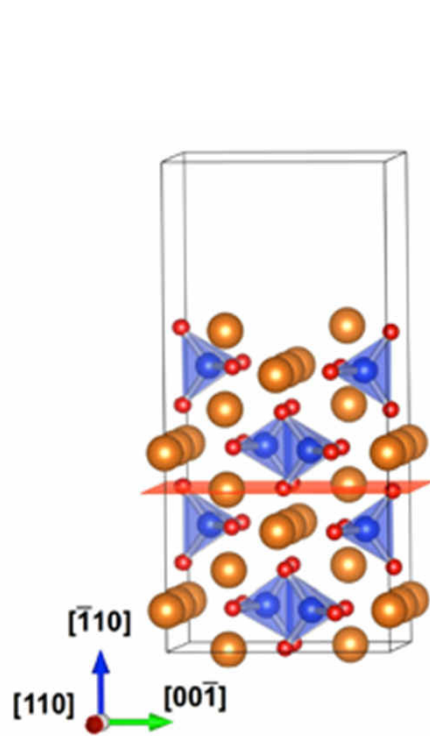
# Beyond core spreading: dissociation



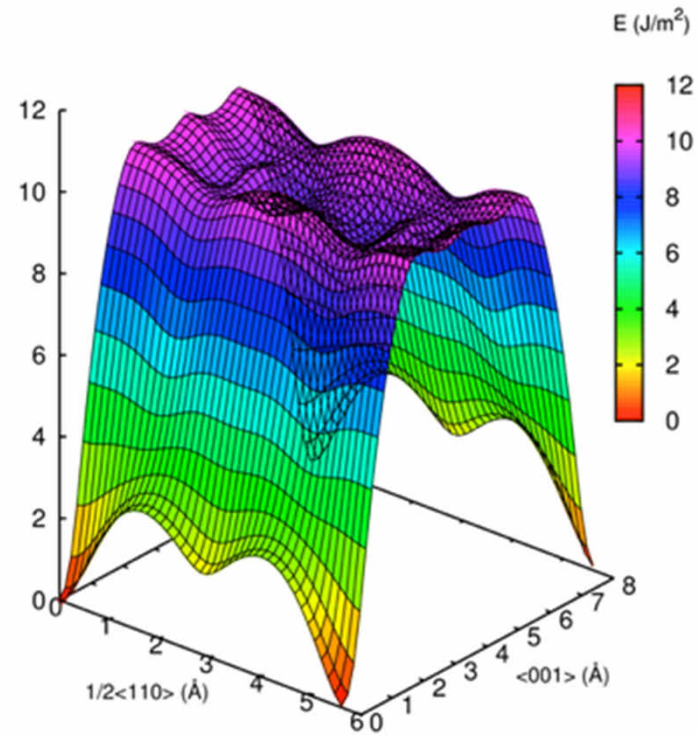
# Ringwoodite ( $\text{Mg}_2\text{SiO}_4$ )



# Ringwoodite: generalized stacking faults



Ringwoodite (20 GPa)  
(110) plane

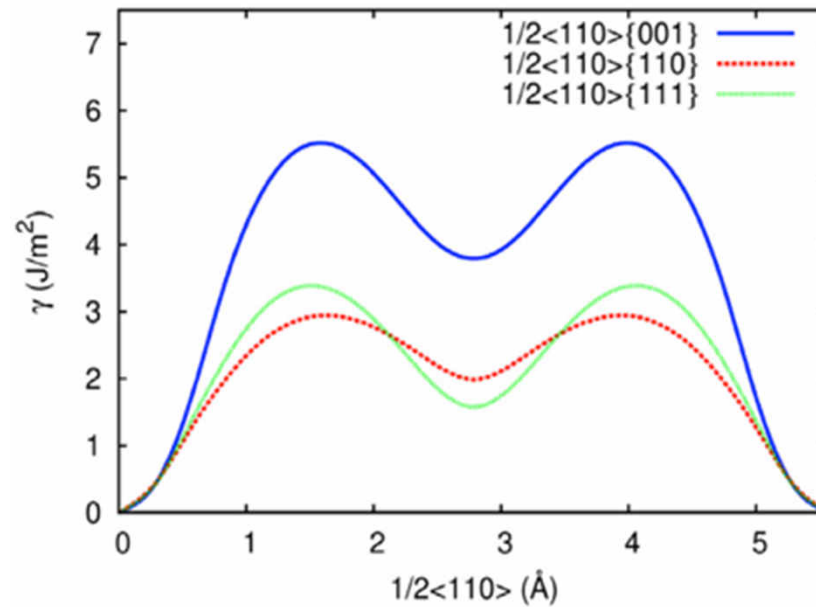


Easy shear path along the  $1/2\langle 110 \rangle$  direction

Defines the **Burgers vector**

# Ringwoodite: generalized stacking faults

Ringwoodite (20 GPa)

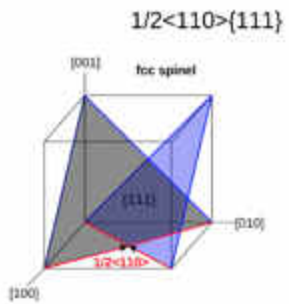
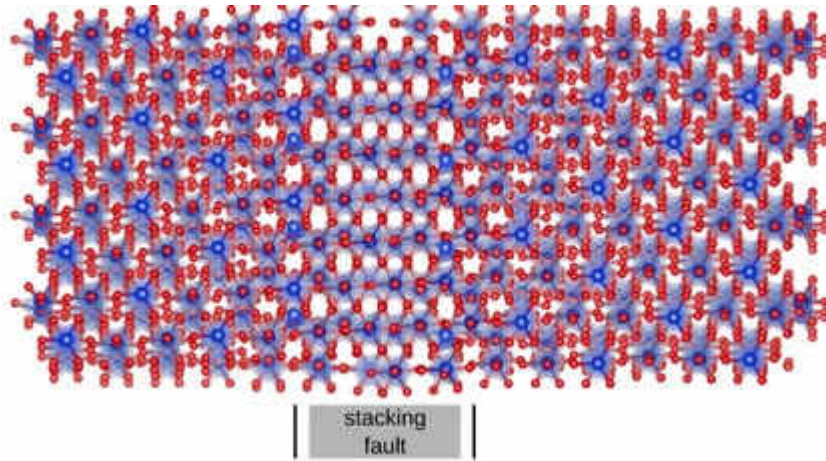


Easy shear path along the  $1/2[-110]$  direction

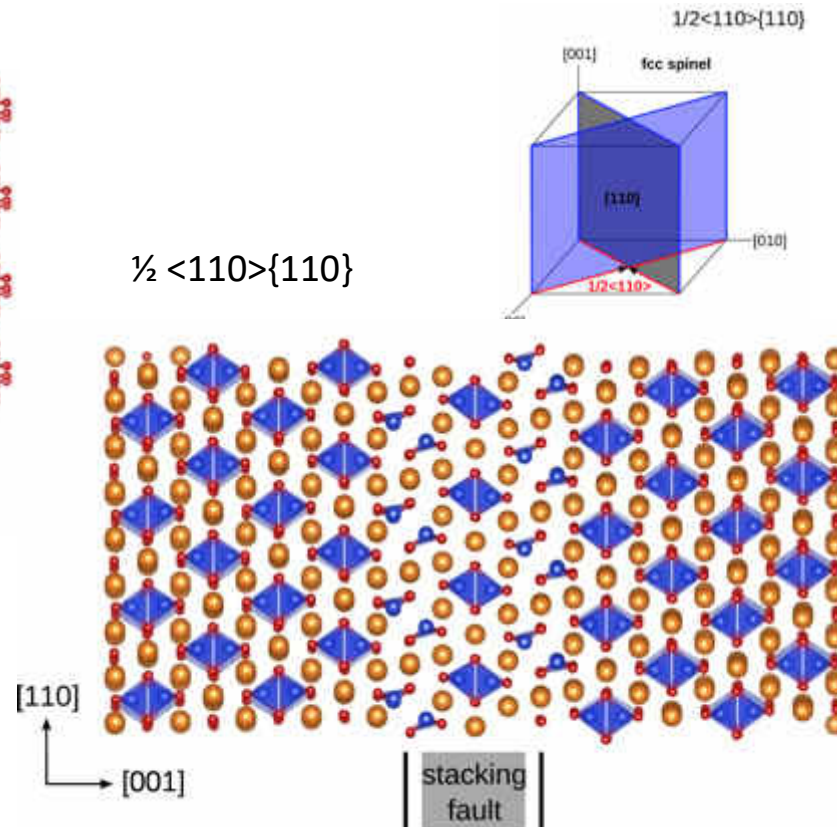


# Ringwoodite: dissociated dislocations

$\frac{1}{2} \langle 110 \rangle \{111\}$

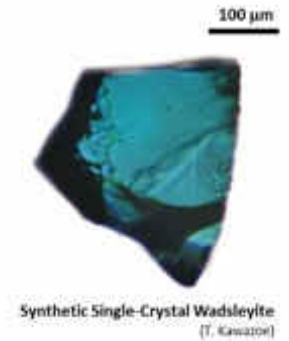
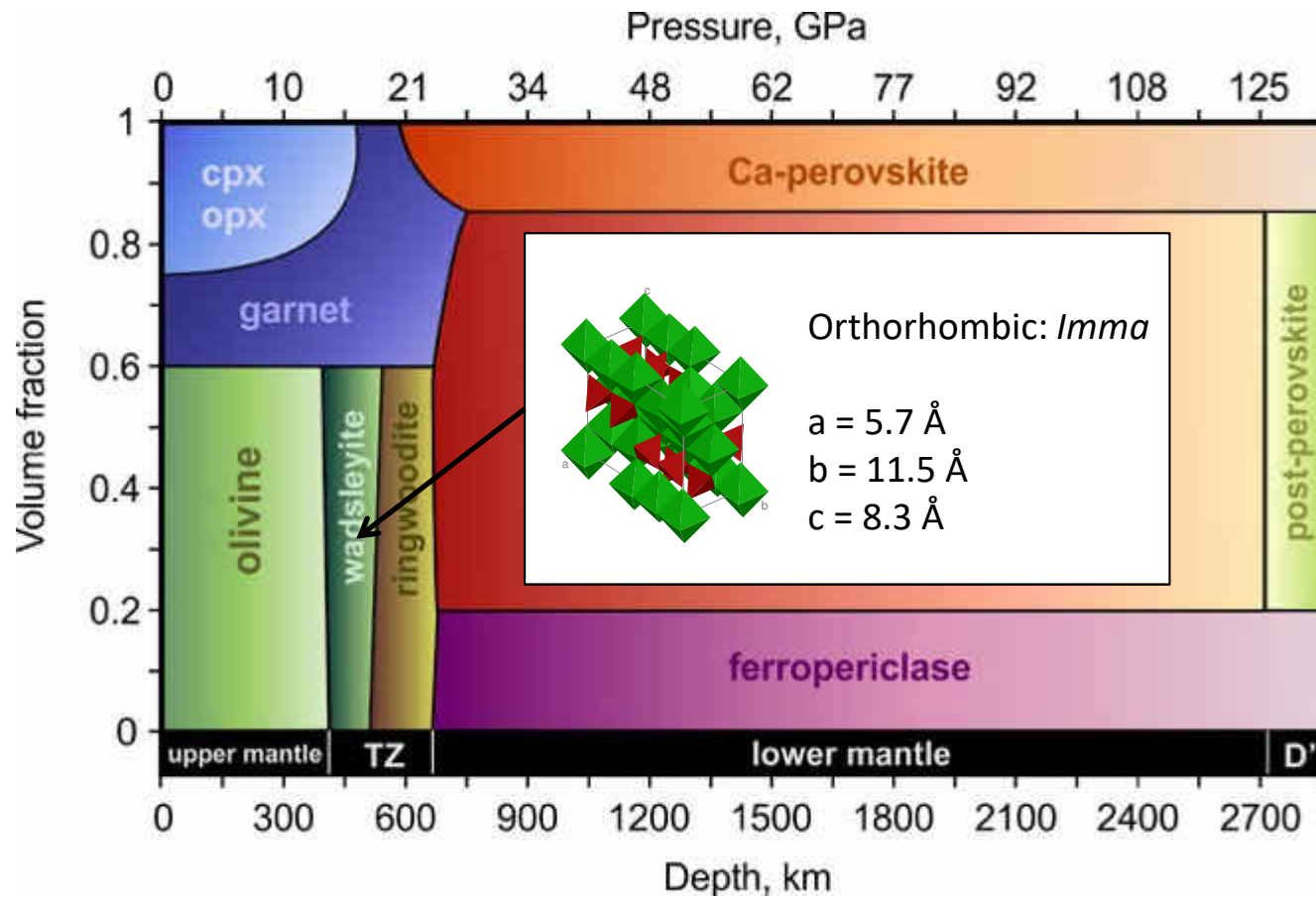


$\frac{1}{2} \langle 110 \rangle \{110\}$



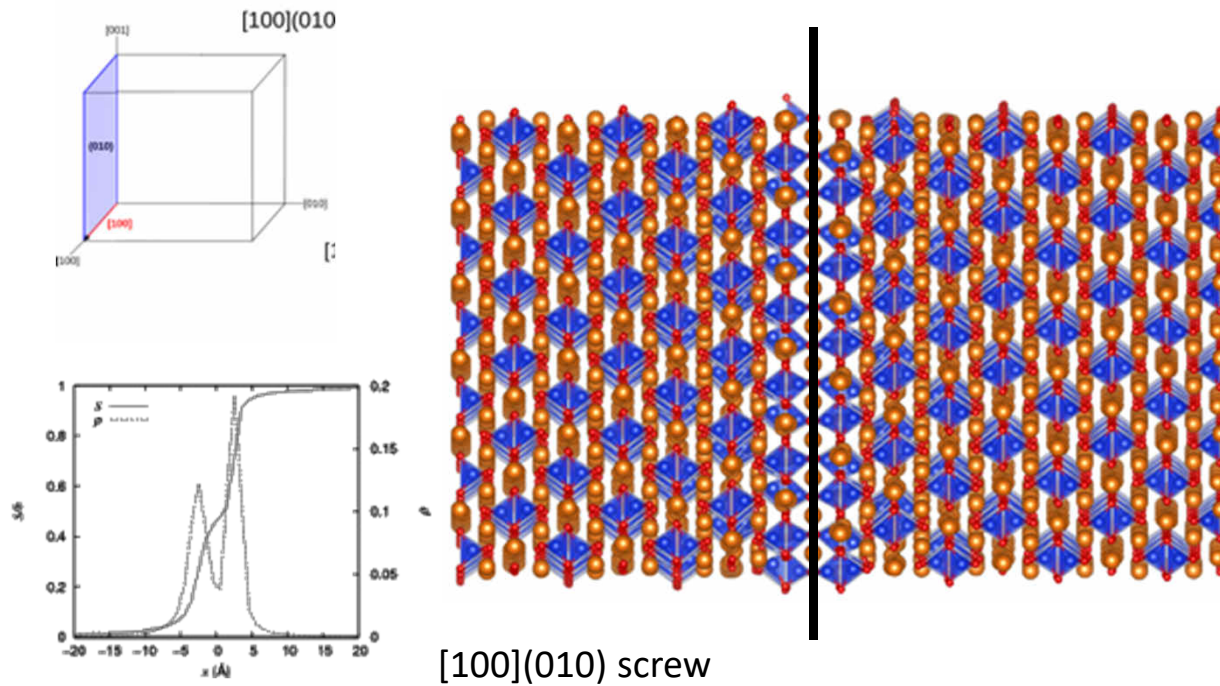


# Wadsleyite ( $\text{Mg}_2\text{SiO}_4$ )



# Wadsleyite ( $\text{Mg}_2\text{SiO}_4$ )

[100] glide: the shortest lattice repeat (5.5 Å)



E. Thurel PhD thesis

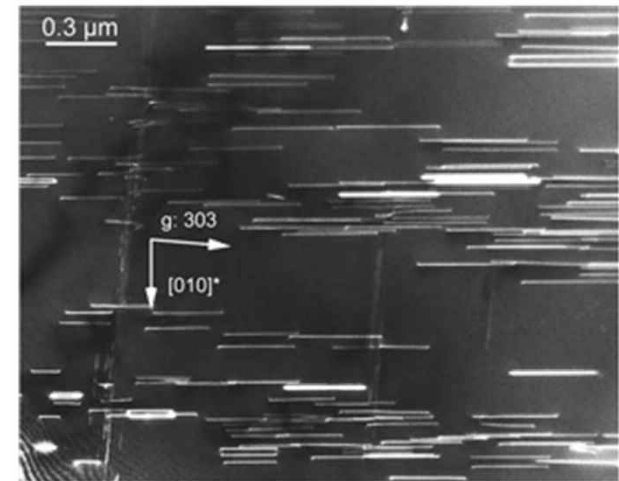


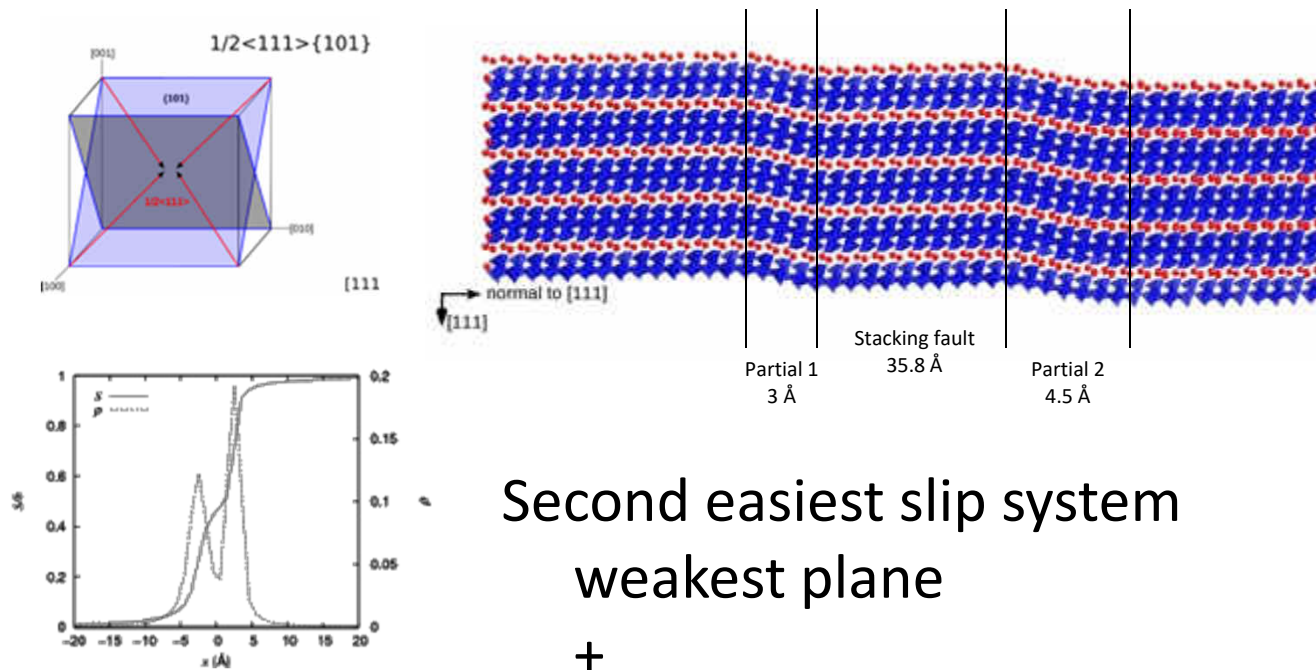
Fig. 13 [100] dislocations gliding in (010). Some [010] dislocations gliding in (101) can be seen through their residual contrast. Weak-beam dark field  $g: 303$

Easiest slip system

# Wadsleyite ( $\text{Mg}_2\text{SiO}_4$ )

E. Thurel PhD thesis

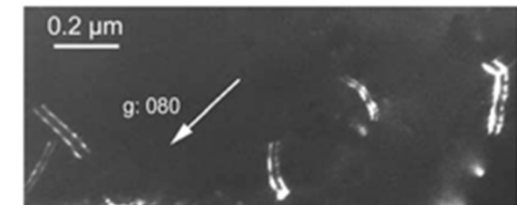
$\frac{1}{2}\langle 111 \rangle \{101\}$  (7.5 Å)



$\frac{1}{2} [111](101)$

Second easiest slip system  
 weakest plane  
 +  
 Wide dissociation (5-8 b)

Wadsleyite deformed at 18 GPa - 1600°C



Dissociated  $\frac{1}{2}\langle 111 \rangle$  dislocations gliding in  $\{101\}$

# Wadsleyite (Mg<sub>2</sub>SiO<sub>4</sub>)

19

[010] dislocations: the largest lattice repeat (11.5 Å)

## DISLOCATION CORES IN CRYSTALS WITH LARGE UNIT CELLS

F.R.N. Nabarro  
Department of Physics, University of the Witwatersrand,  
Johannesburg, South Africa.

Résumé - Une maille cristalline peut être grande dans 0, 1, 2 ou 3 directions, et peut être définie comme petite, allongée, raccourci ou grande. Les propriétés mécaniques, et en particulier, la structure de coeur des dislocations dépendent des forces aussi bien que de la longueur des liaisons dans les trois directions principales. Si nous ne distinguons que les catégories courte/longue et forte/faible, nous trouvons 20 catégories cristallines plastiques. Des exemples de quelques-unes de ces catégories sont discutées et la largeur et les contraintes de Peierls de quelques-unes de leurs dislocations sont considérées. Les défauts d'empilement et les dislocations partielles compliquent l'analyse. L'influence des liaisons courte/longue et forte/faible sur la stabilité des dislocations creuses et sur les tubes de corrosion est examinée, et certains problèmes concernant les dislocations de croissance et les tubes de corrosion sont mentionnés.

Abstract - A crystal cell may be large in 0, 1, 2 or 3 directions, so that it may be described as small, prolate, oblate or large. The mechanical properties, and in particular the dislocation structure, depend on the strengths as well as the lengths of the bonds in the three principal directions. If we distinguish only the classes short/long and strong/weak, we find 20 plastic crystal classes. Examples of some of these classes are discussed, and the widths and Peierls stresses of some of their dislocations are considered. Stacking faults and partial dislocations complicate the analysis. The influence of short/long and strong/weak bonds on the stability of hollow dislocations and etch tubes is examined, and some problems concerning growth dislocations and etch tubes are mentioned.

Acta Cryst. (1951). 4, 497

## Capillary Equilibria of Dislocated Crystals

By F. C. FRANK  
H. H. Wills Physical Laboratory, University of Bristol, England

(Received 2 November 1950)

It is shown that a dislocation whose Burgers vector exceeds a critical value, of the order of magnitude 10 Å, is only in equilibrium with an empty tube at its core. This is not the case in metals or other simple crystalline solids, but is likely to be the case in protein crystals, which therefore, unfortunately, do not provide good models of simple crystalline substances in respect of dislocations. The same causes generally give rise to a dimple or crater where a dislocation meets a free surface, and the shape of this crater is calculated. Though shallow in form, it is infinitely deep except at a habit face of a crystal, where it is of finite depth and may be totally absent.

### 1. The equilibrium of open-cored dislocations

It will be shown that for a dislocation of large Burgers vector\* there exists a state of equilibrium in which the core of the dislocation is an empty tube. We shall find, however, that this is not the case for the elementary dislocations of a typical metal or simple ionic crystal; but it may be so for substances with large unit cells, of the order of 10 Å, or more, e.g. some silicates. It will assuredly be the case in protein crystals.

For simplicity we consider the case of a screw dislocation in a material with isotropic elastic constants. Strain-energy densities are of similar magnitude at similar distances from dislocations of other orientation and in materials of naturally occurring degrees of anisotropy in their elastic behaviour. Let there be an empty cylinder of radius  $r$ , the dislocation line lying in the cylinder. Then the shear strain at the surface of the cylinder is  $b/2\pi r$ , where  $b$  is the modulus of the Burgers vector. There is consequently a strain-energy density here of  $\mu b^2/8\pi^2 r^2$ , where  $\mu$  is the rigidity modulus.

Suppose that a shell of material of thickness  $dr$  evaporates from this cylinder and deposits elsewhere, on a surface of the material whose radius of curvature is negligibly large. The interior cylindrical surface is thus enlarged. If  $\gamma$  is the specific surface free energy of the

substance, the total increase in free energy per unit length of cylinder is

$$dF = 2\pi\gamma dr - (\mu b^2/8\pi^2 r^2) 2\pi r dr. \quad (1)$$

There is an equilibrium when  $dF/dr$  is zero, i.e. when

$$r = \mu b^2/8\pi^2 \gamma. \quad (2)$$

Now, empirically the rigidities and surface energies of substances tend to vary in a parallel manner so that  $\gamma/\mu$  is very roughly a constant length (cf. Table 1), a typical value being say  $\frac{1}{2}$  Å. In consequence  $r$  is less than 1 Å, unless  $b$  exceeds 4–5 Å. The implied assumption of linear elasticity is then invalid. If  $b$  were as large as 100 Å, as would be appropriate in protein crystals, this objection would disappear, and we may conclude that the typical dislocation in such a crystal would, in equilibrium, have a hollow core of the order of 1000 Å in diameter. This brings the unfortunate conclusion that these crystals, the ones in which we can most easily see the constituent parts, do not furnish satisfactory analogues of simpler crystals with regard to dislocations.

Let us now make an approximate allowance for the non-linear elastic behaviour. We shall assume that stress is related to strain by Hooke's law up to a strain of 0.1 and thereafter is constant (as in Figs. 1 (ii) and 2 (ii)). The strain-energy density is

$$\begin{aligned} \mu b^2/8\pi^2 r^2 & \quad (r \geq 5b/\pi); \\ \mu b^2/20\pi r - \mu/200 & \quad (r < 5b/\pi). \end{aligned} \quad (3)$$

\* The Burgers vector is the name we give to what Burgers (1939) called the 'strength' of a dislocation. This vector is parallel to the dislocation line in a 'screw' and normal to it in an 'edge' dislocation, these being only particular cases of the general situation. A simple account of the geometry and elastic fields of dislocations is given by Cottrell (1949).

Table 1. Approximate rigidities and surface energies of solids

Substance	Rigidity modulus $\mu$ ( $10^{11}$ erg cm. <sup>-2</sup> )	Surface energy $\gamma$ (erg cm. <sup>-2</sup> )	$\gamma/\mu$ ( $10^{-8}$ cm.)	Reference
Copper	4.4	1400	0.32	Udin <i>et al.</i> (1949)
Sodium chloride	1.5	155	0.10	Rose (1936), Shuttleworth (1949)
Argon	0.106	42	0.40	Mackenzie & Mott (1950), Shuttleworth (1949)
Mica	8.0	4500 (in vacuum) 400 (in air)	0.56 0.05	Obreimoff (1930) Orowan (1933)

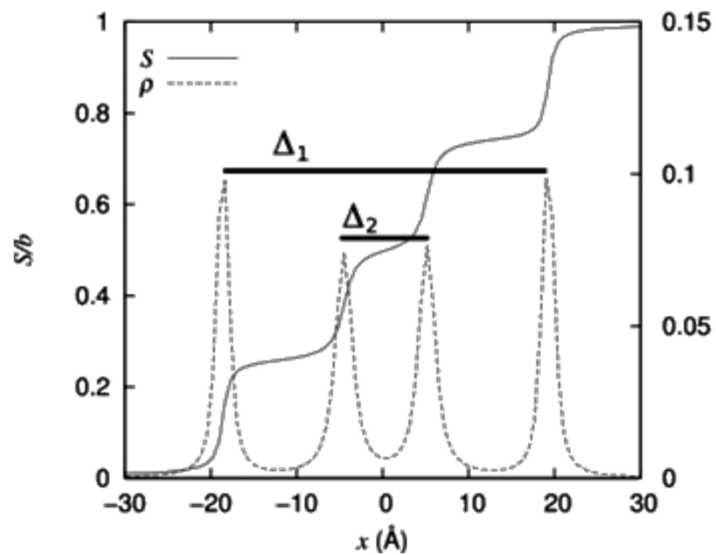
A C 4

32

# Wadsleyite ( $\text{Mg}_2\text{SiO}_4$ )

[010] dislocations: the largest lattice repeat (11.5 Å)

Peierls model of the edge [010](100) dislocation



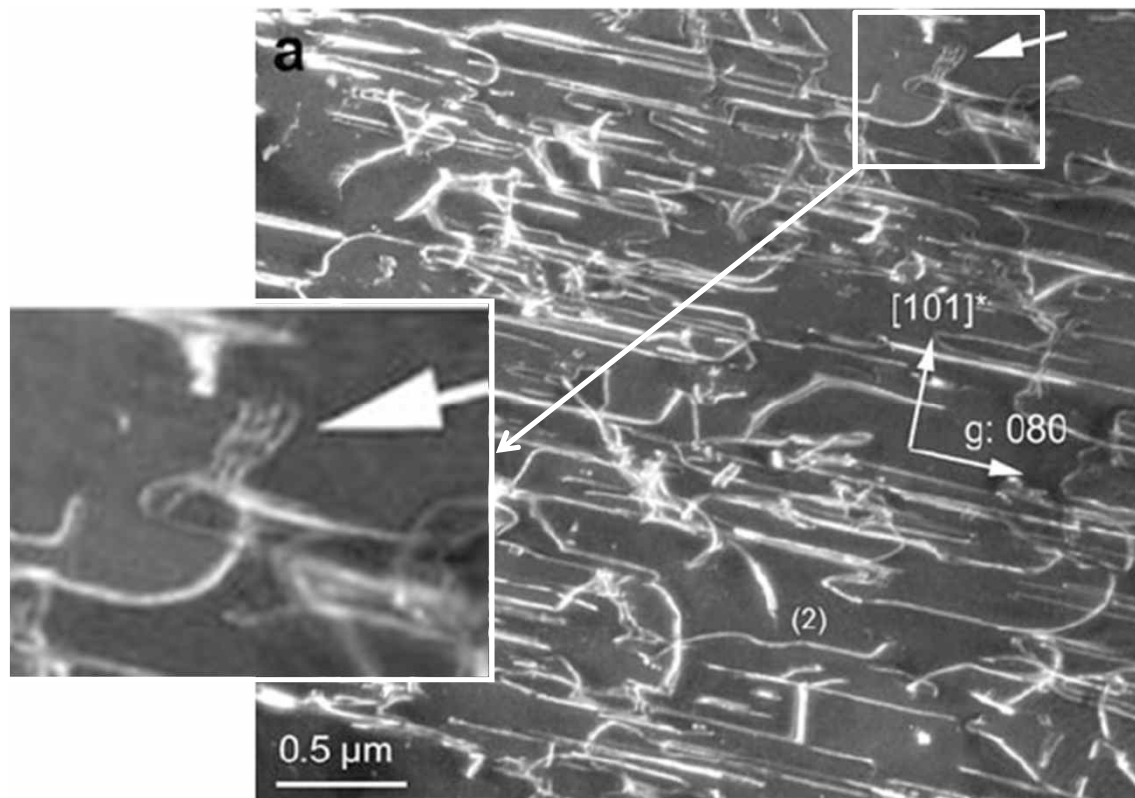
$$[010] \rightarrow \frac{1}{4}[010] + \frac{1}{4}[010] + \frac{1}{4}[010] + \frac{1}{4}[010]$$



# Wadsleyite ( $\text{Mg}_2\text{SiO}_4$ )

[010] dislocations: the largest lattice repeat (11.5 Å)

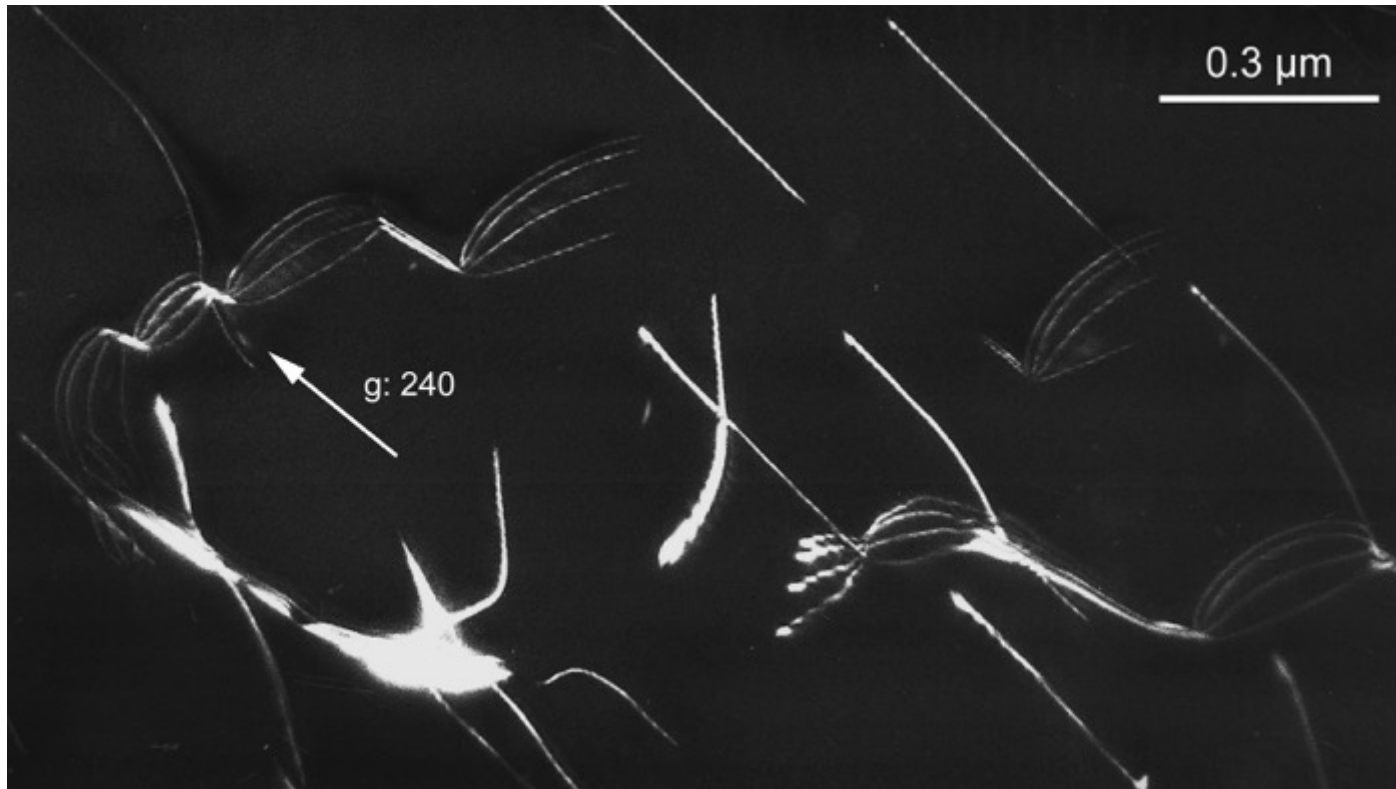
Wadsleyite deformed at 17 GPa - 1500°C



# Wadsleyite ( $\text{Mg}_2\text{SiO}_4$ )

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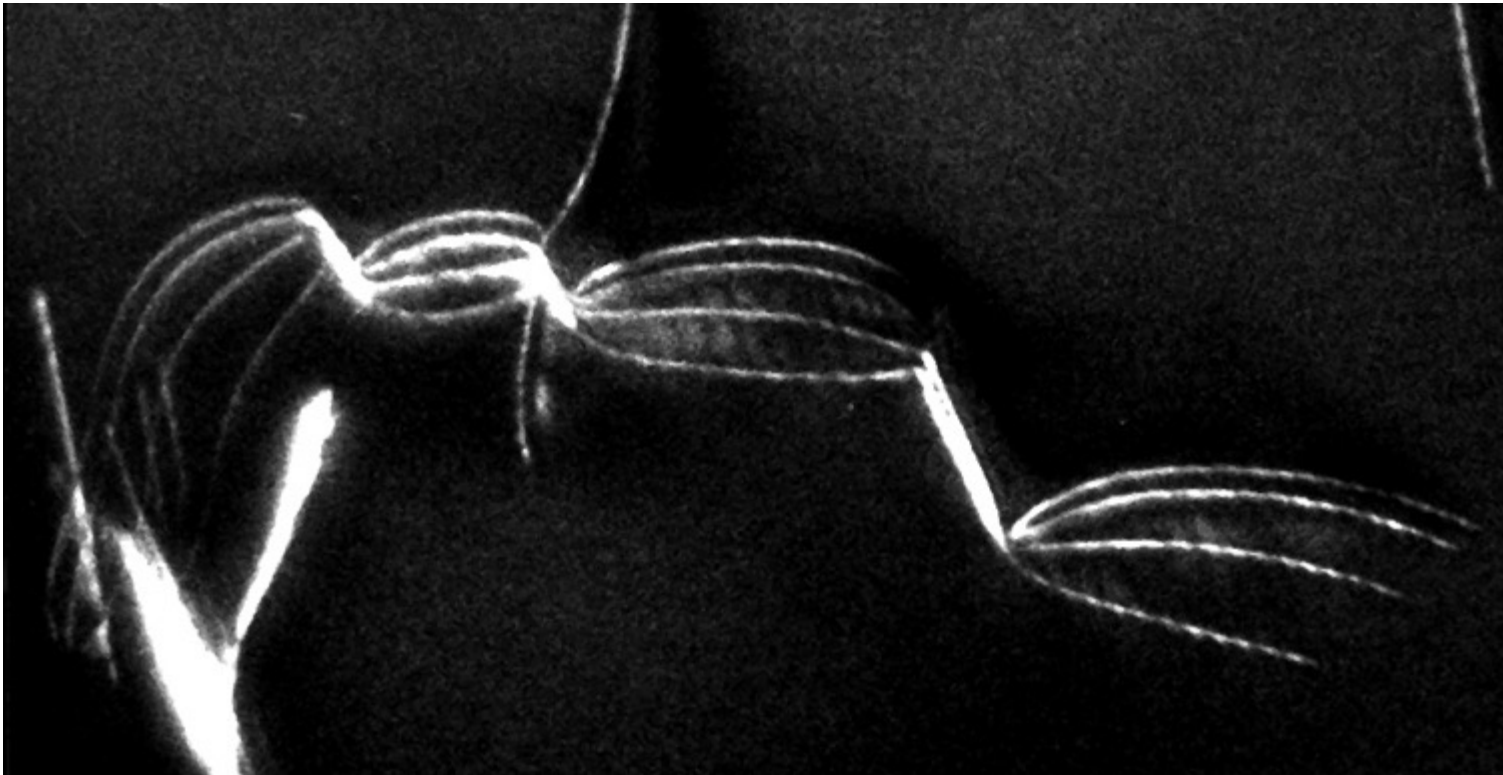
[010] dislocations: the largest lattice repeat (11.5 Å)



# Wadsleyite ( $\text{Mg}_2\text{SiO}_4$ )

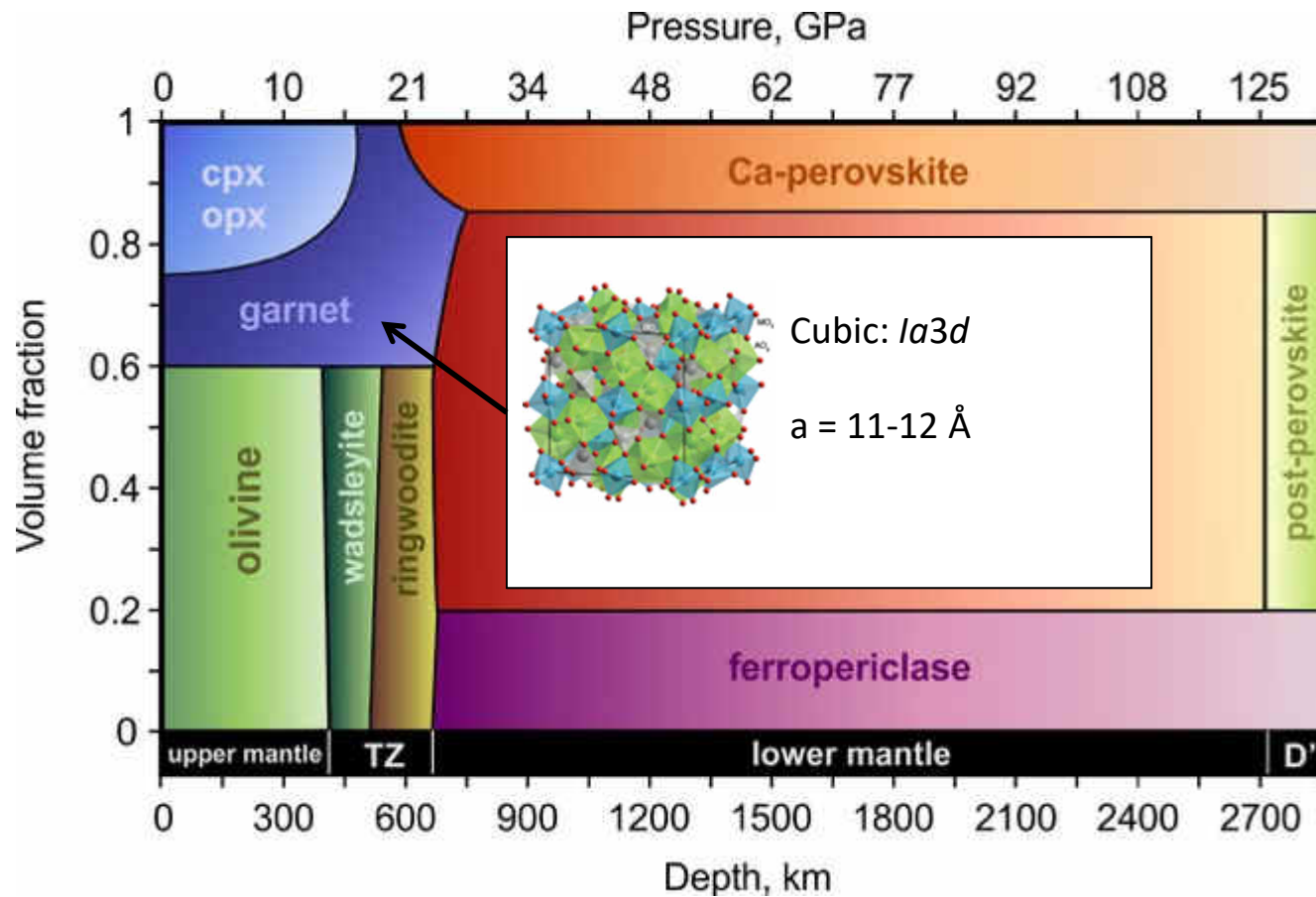
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[010] dislocations: the largest lattice repeat (11.5 Å)





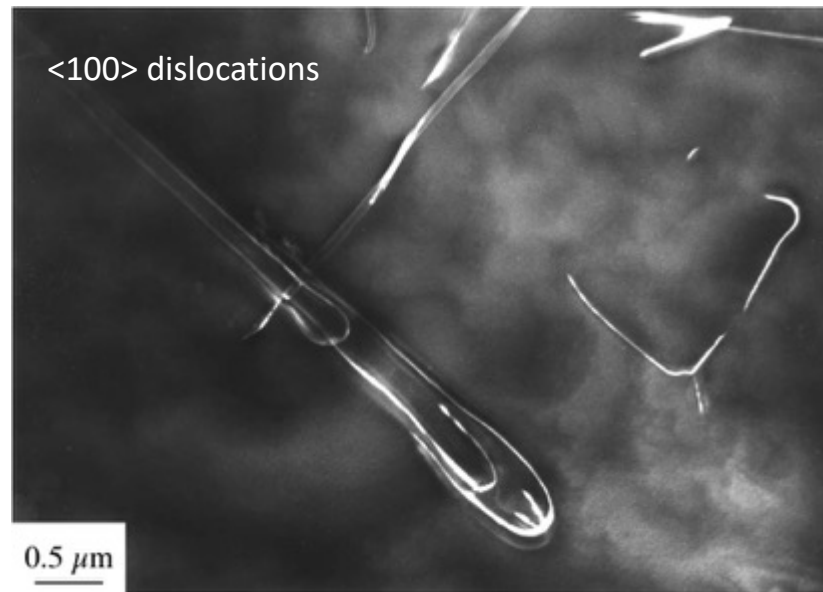
# Garnets $X_3Y_2Z_3O_{12}$



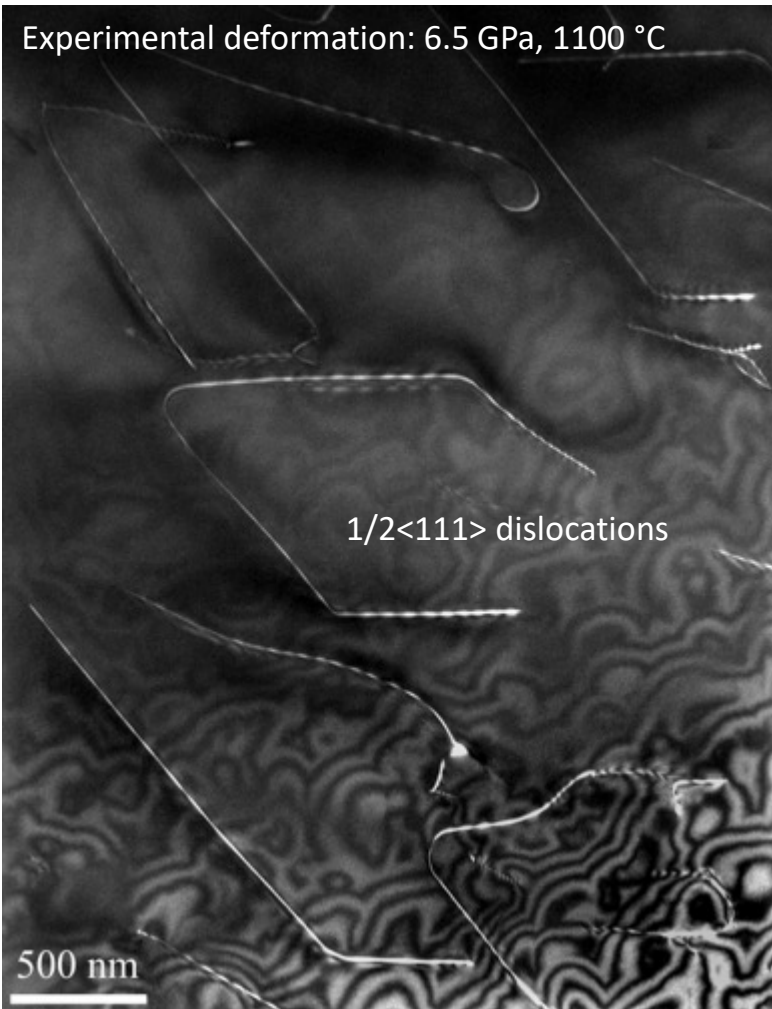
# Garnets

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Experimental deformation: 6.5 GPa, 900 °C

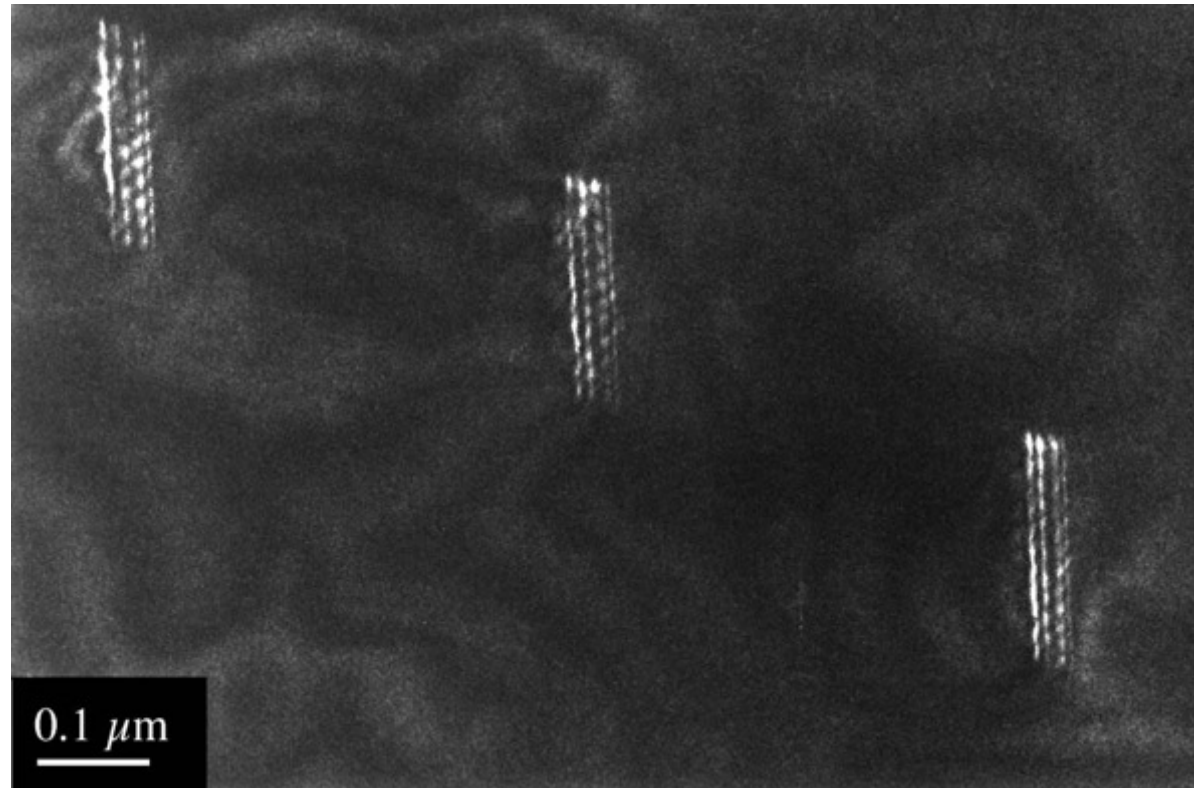


V. Voegelé et al. Physics of the Earth and Planetary Interiors  
108 (1998) 305–318



# Garnets

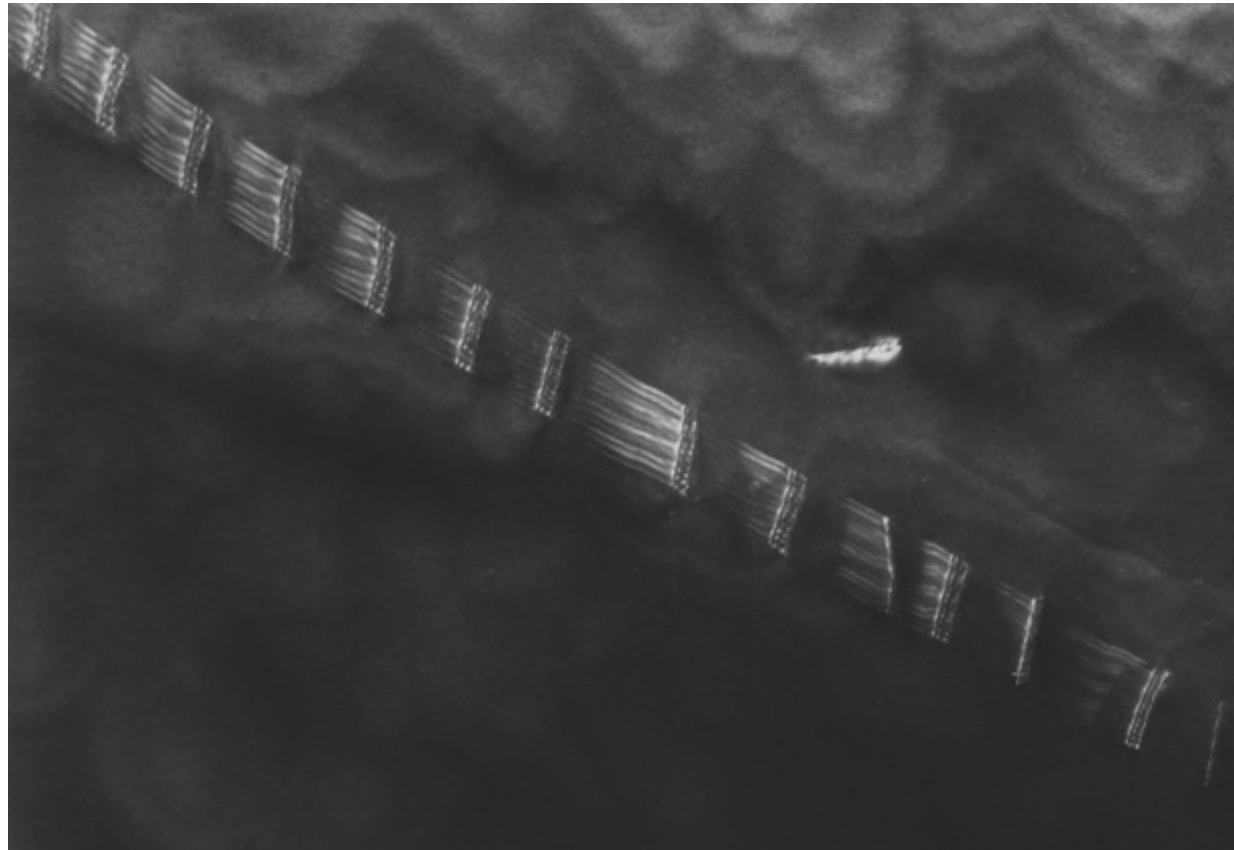
Eclogites from the Alps



V. Voegelé et al. *Physics of the Earth and Planetary Interiors* 108 (1998) 319–338

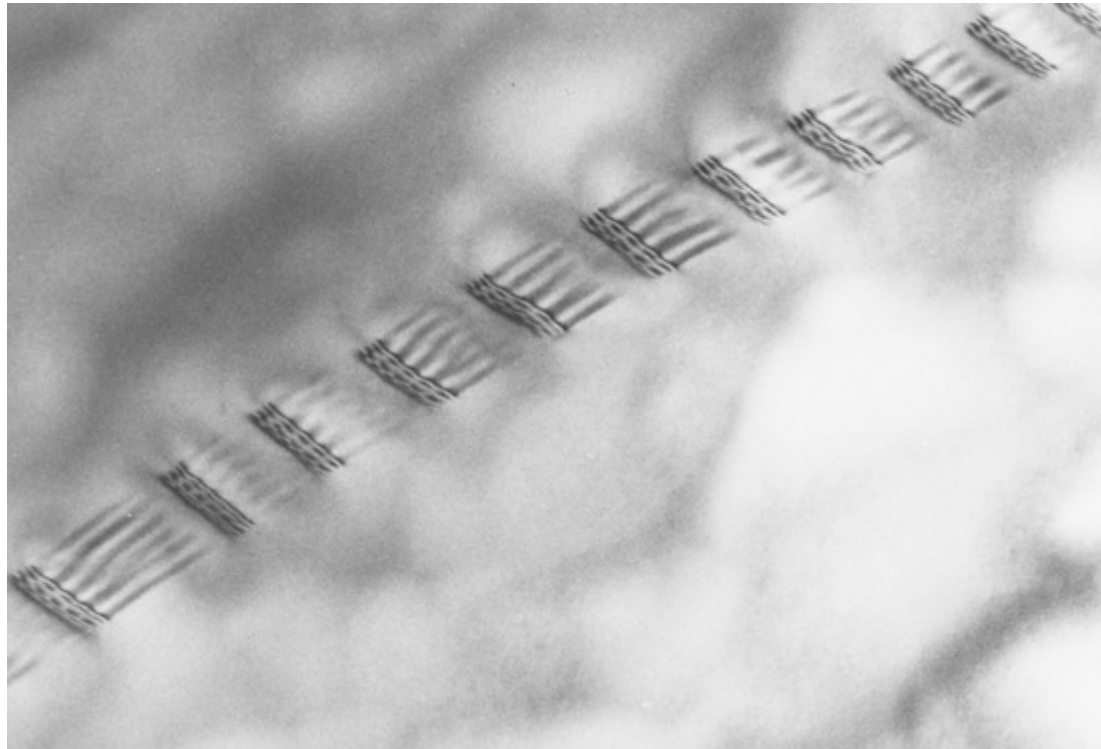
# Garnets

Eclogites from the Alps



# Garnets

Eclogites from the Alps

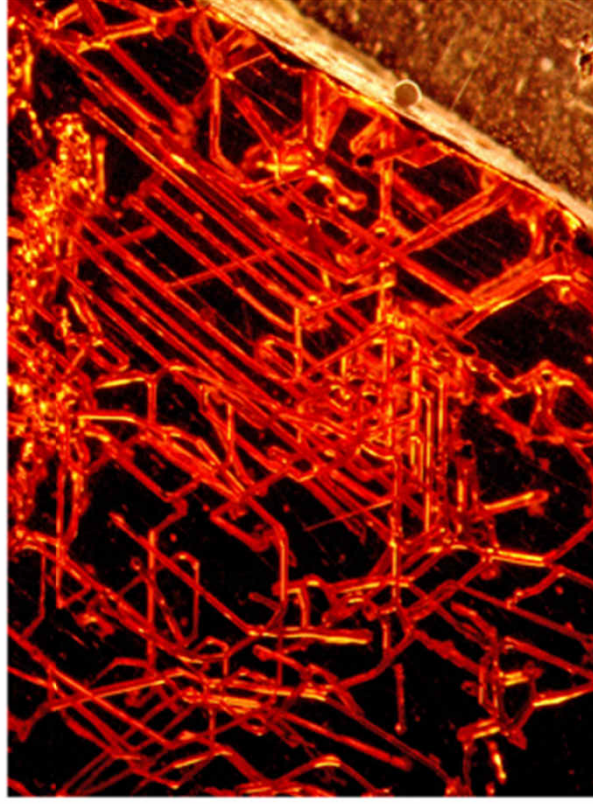


V. Voegelé et al. *Physics of the Earth and Planetary Interiors* 108 (1998) 319–338

The New York Times

## Something Digs Intricate Tunnels in Garnets. Is It Alive?

The deep red gems have long been found marred with internal markings. Researchers propose a new explanation involving fungal microorganisms who have found a nice place to live.











Letter

On the formation of arrays of micro-tunnels in pyrope and almandine garnets

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<sup>2</sup>Department of Materials Science and Engineering, Case Western Reserve University, Cleveland, Ohio 44106, U.S.A.

<sup>3</sup>Departments of Mechanical Engineering, Materials Science and Engineering, Earth and Planetary Sciences, Johns Hopkins University, Baltimore, Maryland 21210, U.S.A.

Abstract

A recent paper devoted to unusual fine-scale tubular tunnels found in pyrope and almandine garnets suggested that the 5 to 100  $\mu\text{m}$  diameter tunnels were produced by an endolithic organism that is able to chemically dissolve and penetrate the mineral, perhaps in search of nutrients. The hypothesized microbial boring of the garnets was based on the finding of endolithic remains in the tunnels, but boring alone does not adequately explain the linear, highly aligned or occasionally branched tunnels that have been imaged. We have prepared this short Letter, in the spirit of Occam's Razor, to highlight the very probable role that dislocations play in the creation of such tunnels by preferential etching of a dislocation-rich deformation microstructure. The geometrical features of the tunnels possess all the characteristics of classical dislocation substructures that have been observed in natural and synthetic garnets.

**Keywords:** Garnets, dislocations, etching, tunnels

Introduction

The intricate and beautiful X-ray computed tomographic images recently published by Ivarsson et al. (2018) contain clear evidence of highly aligned parallel tunnels that originate at the mineral surface and extend into the interior, see, for example, Figure 1. These tunnels form highly regular miniature palisades in some regions; in others, they exist as more chaotic branched networks with kinks and junctions with uniquely prescribed angles. The networks of curvilinear, branching, and anastomosing (interconnected) tunnels were interpreted as evidence that these tunnels are independent of crystallography, thus providing an indirect foundation for the authors' hypothesis of biological tunneling (Ivarsson et al. 2018). Unfortunately, this interpretation completely misses the striking geometric similarities between the tunnels in these tomographic images and published observations and understanding of dislocation microstructures in both natural and synthetic garnets [see, for example, Rabier (1995, 1979); Rabier et al. (1976a, 1981); Garem et al. (1982); Rabier and Garem (1984); Allen et al. (1987); Karato et al. (1995); Blumenthal and Phillips (1996); Voegelé et al. (1998a, 1998b)].

As is well known, dislocations are prominent in virtually all crystalline materials. Dislocation generation, multiplication, and motion are widely recognized as a common deformation response of crystalline materials to externally applied shear stresses and have been extensively observed and characterized in metals and alloys, minerals, ceramics, and semiconductors. The absence of dislocations in the pyrope and almandine garnets under discussion, if true, would be remarkable.

Here, we briefly review and discuss dislocations in garnets, tunnel formation due to abiogenic etching of dislocations in minerals, and the similarities between the geometry of dislocation substructures

and the intricate tunnels and networks observed in these pyrope and almandine garnets (Ivarsson et al. 2018).

Dislocations in garnets

The relationship between dislocations and plasticity in garnets is well established. Synthetic garnets of technological interest such as  $\text{Y}_3\text{Al}_5\text{O}_{12}$  (YAG, yttrium aluminum garnet),  $\text{Y}_2\text{Fe}_5\text{O}_{12}$  (YIG, yttrium iron garnet), and  $\text{Gd}_3\text{Ga}_5\text{O}_{12}$  (GGG, gadolinium gallium garnet) were first studied by Rabier and colleagues (Rabier et al. 1976a; Rabier 1979) and have exceptional plastic properties compared to other oxide crystals (Garem et al. 1982; Rabier and Garem 1984; Blumenthal and Phillips 1996). Likewise, the resistance to plastic deformation in natural garnets is significantly greater than that of most other minerals of the Earth's mantle (Karato et al. 1995; Voegelé et al. 1998a). This is related to the very large Burgers vectors of dislocations in garnets and to a "corrugated" oxygen sublattice, which promotes very high atomic-level friction stresses on moving dislocations.

The description of the garnet structure in terms of coordination polyhedra, so common in the mineralogical literature, has proven to be very useful in understanding dislocation properties in synthetic garnets (Rabier et al. 1976b). The garnet structure can be regarded as a body-centered cubic (bcc) lattice with a very large unit cell. The edge of the bcc unit cell is of order 1.2 nm, whereas most common minerals have considerably smaller unit cells. Thus, the magnitude of the smallest perfect unit Burgers vector,  $\mathbf{b} = \frac{1}{2}\langle 111 \rangle$ , is about 1.0 nm. This results in a very large strain energy, proportional to  $G\mathbf{b}^2$  per unit length of dislocation ( $G$  is the elastic shear modulus). The strain energy of a dislocation can be lowered by spreading of its core and by dissociation of the parent dislocation into partial dislocations that bound a planar stacking fault. The dissociated configuration is glissile as long as it remains on the glide plane, but it becomes sessile when reconfigured off of the glide plane (Garem et al. 1982; Blumenthal and Phillips 1996).

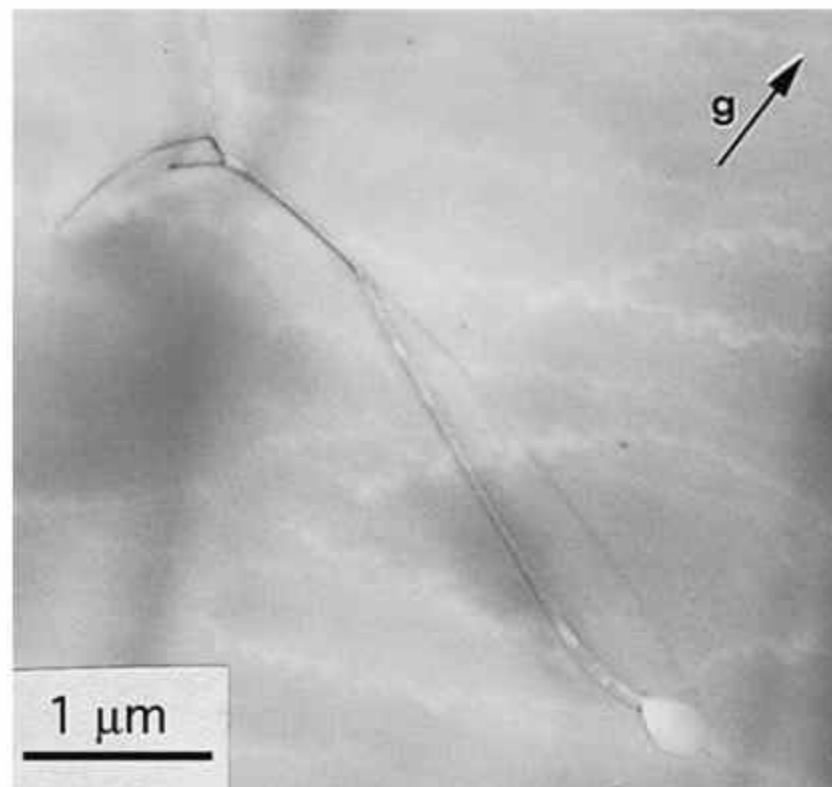


Fig. 17. Eclogite from Yakutia pipe. Hollow core. Bright field.  $g$ : 400.

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Letter

On the formation of arrays of micro-tunnels in pyrope and almandine garnets

Jacques Rabier<sup>1</sup>, Arthur H. Heuer<sup>2</sup>, and Kevin J. Henker<sup>3,\*</sup>

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<sup>2</sup>Department of Materials Science and Engineering, Case Western Reserve University, Cleveland, Ohio 44106, U.S.A.

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Abstract

A recent paper devoted to unusual fine-scale tubular tunnels found in pyrope and almandine garnets suggested that the 5 to 100 μm diameter tunnels were produced by an endolithic organism that is able to chemically dissolve and penetrate the mineral, perhaps in search of nutrients. The hypothesized microbial boring of the garnets was based on the finding of endolithic remains in the tunnels, but boring alone does not adequately explain the linear, highly aligned or occasionally branched tunnels that have been imaged. We have prepared this short Letter, in the spirit of Occam's Razor, to highlight the very probable role that dislocations play in the creation of such tunnels by preferential etching of a dislocation-rich deformation microstructure. The geometrical features of the tunnels possess all the characteristics of classical dislocation substructures that have been observed in natural and synthetic garnets.

**Keywords:** Garnets, dislocations, etching, tunnels

Introduction

The intricate and beautiful X-ray computed tomographic images recently published by Ivarsson et al. (2018) contain clear evidence of highly aligned parallel tunnels that originate at the mineral surface and extend into the interior, see, for example, Figure 1. These tunnels form highly regular miniature palisades in some regions; in others, they exist as more chaotic branched networks with kinks and junctions with uniquely prescribed angles. The networks of curvilinear, branching, and anastomosing (interconnected) tunnels were interpreted as evidence that these tunnels are independent of crystallography, thus providing an indirect foundation for the authors' hypothesis of biological tunneling (Ivarsson et al. 2018). Unfortunately, this interpretation completely misses the striking geometric similarities between the tunnels in these tomographic images and published observations and understanding of dislocation microstructures in both natural and synthetic garnets [see, for example, Rabier (1995, 1979); Rabier et al. (1976a, 1981); Garem et al. (1982); Rabier and Garem (1984); Allen et al. (1987); Karato et al. (1995); Blumenthal and Phillips (1996); Voegelé et al. (1998a, 1998b)].

As is well known, dislocations are prominent in virtually all crystalline materials. Dislocation generation, multiplication, and motion are widely recognized as a common deformation response of crystalline materials to externally applied shear stresses and have been extensively observed and characterized in metals and alloys, minerals, ceramics, and semiconductors. The absence of dislocations in the pyrope and almandine garnets under discussion, if true, would be remarkable.

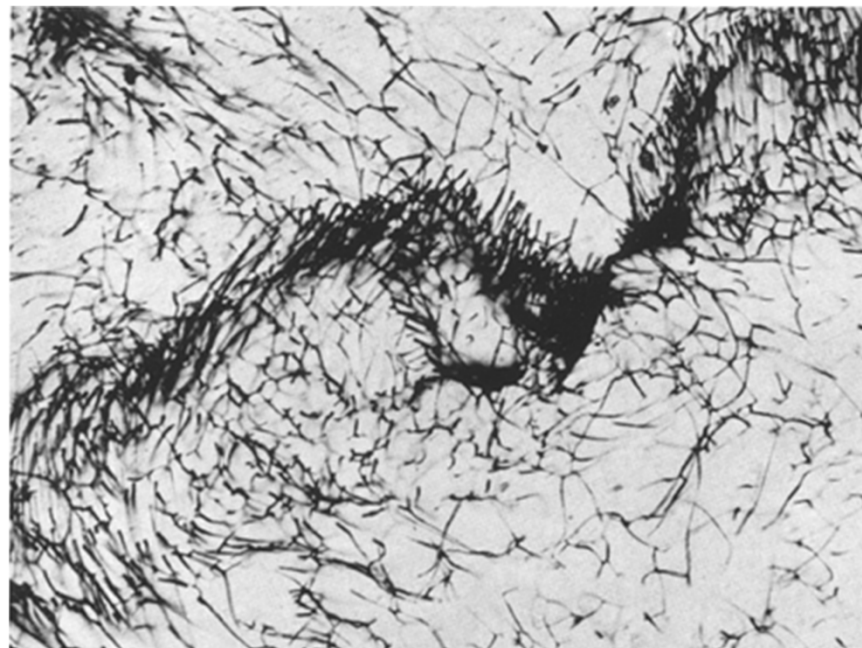
Here, we briefly review and discuss dislocations in garnets, tunnel formation due to abiogenic etching of dislocations in minerals, and the similarities between the geometry of dislocation substructures

and the intricate tunnels and networks observed in these pyrope and almandine garnets (Ivarsson et al. 2018).

Dislocations in garnets

The relationship between dislocations and plasticity in garnets is well established. Synthetic garnets of technological interest such as Y<sub>3</sub>Al<sub>5</sub>O<sub>12</sub> (YAG, yttrium aluminum garnet), Y<sub>2</sub>Fe<sub>17</sub>O<sub>19</sub> (YIG, yttrium iron garnet), and Gd<sub>3</sub>Ga<sub>5</sub>O<sub>12</sub> (GGG, gadolinium gallium garnet) were first studied by Rabier and colleagues (Rabier et al. 1976a; Rabier 1979) and have exceptional plastic properties compared to other oxide crystals (Garem et al. 1982; Rabier and Garem 1984; Blumenthal and Phillips 1996). Likewise, the resistance to plastic deformation in natural garnets is significantly greater than that of most other minerals of the Earth's mantle (Karato et al. 1995; Voegelé et al. 1998a). This is related to the very large Burgers vectors of dislocations in garnets and to a "corrugated" oxygen sublattice, which promotes very high atomic-level friction stresses on moving dislocations.

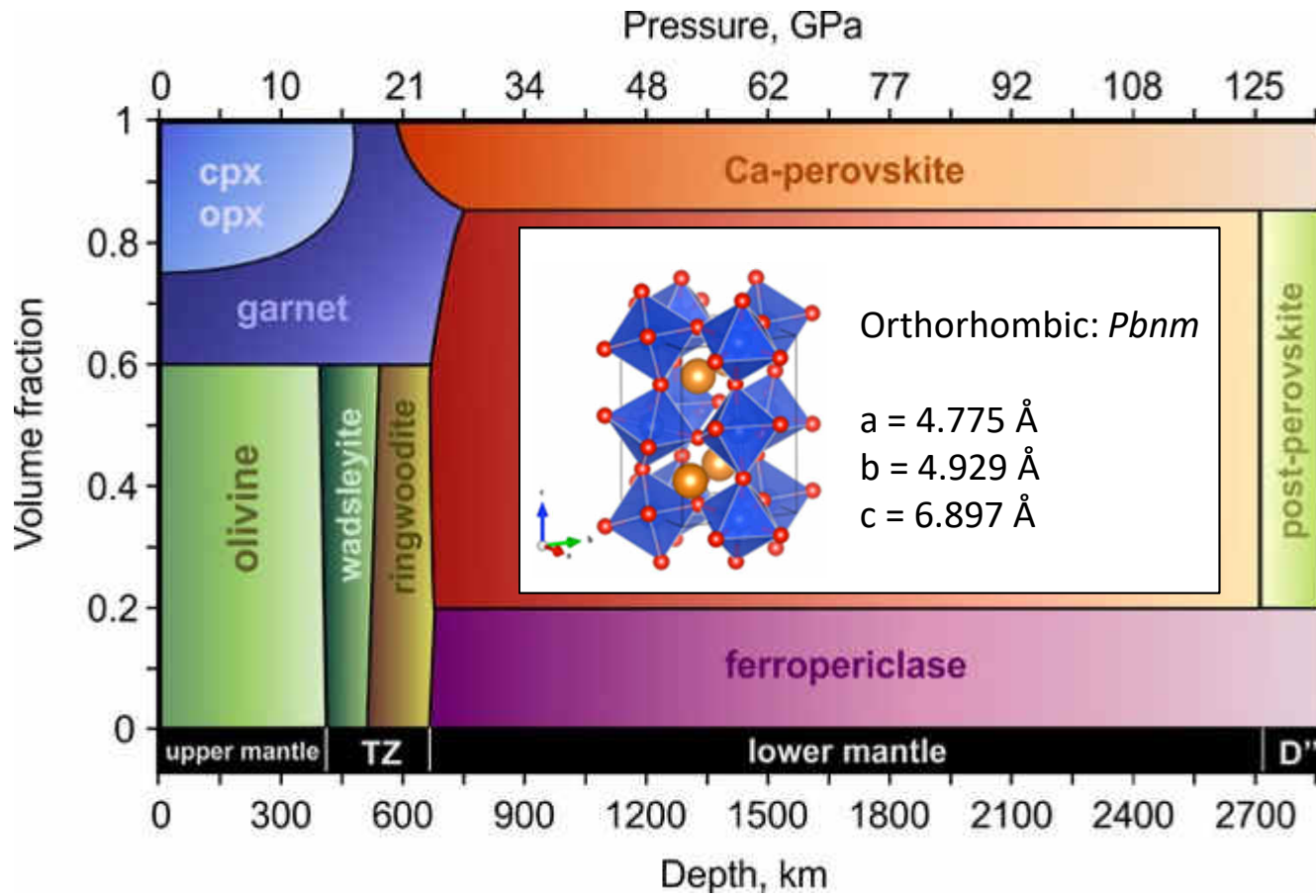
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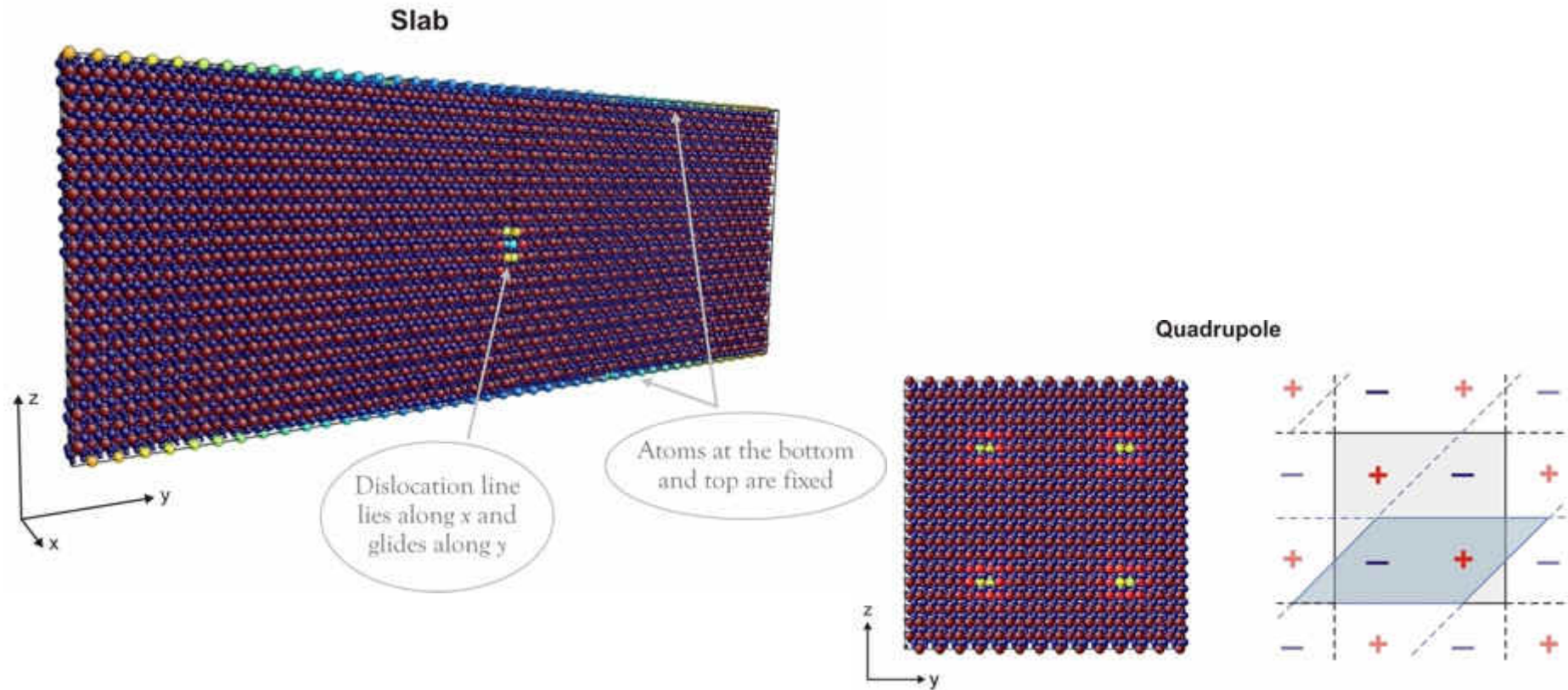
Carstens (1969) Contr. Mineral. and Petrol. 24, 368-353

\* E-mail: henker@jhu.edu, Orcid 0000-0002-5008-2222

# Bridgmanite ( $\text{MgSiO}_3$ )

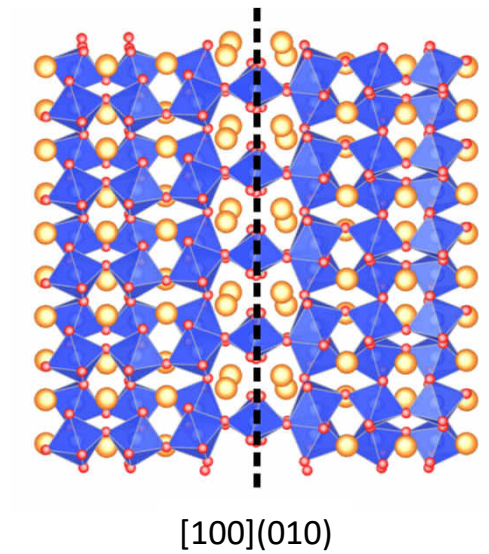


# Modelling dislocations at the atomic scale

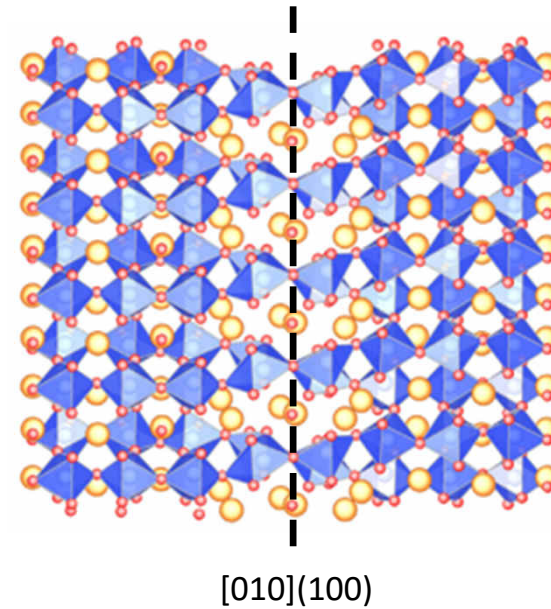


# Modeling dislocations in bridgmanite at 30 GPa

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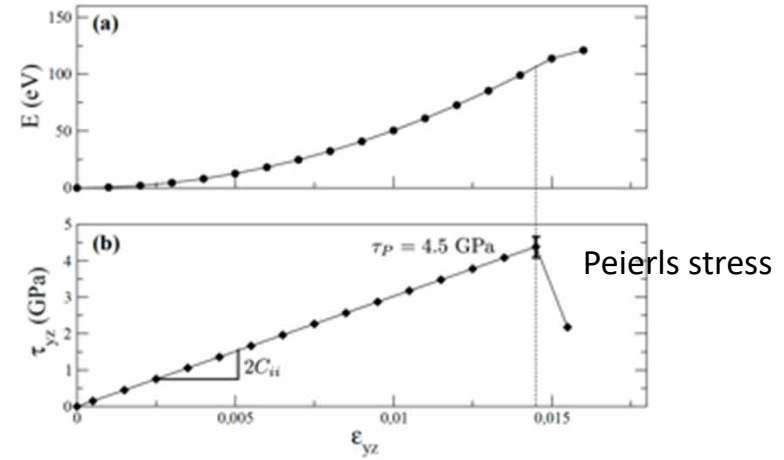
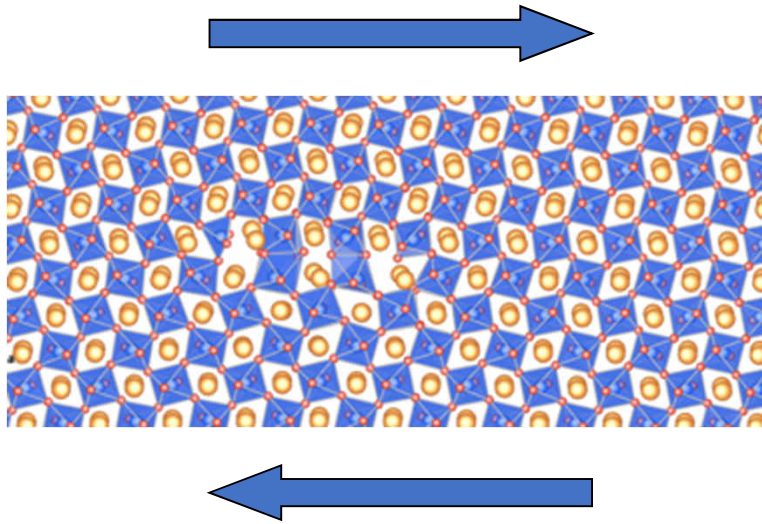
Screw dislocations



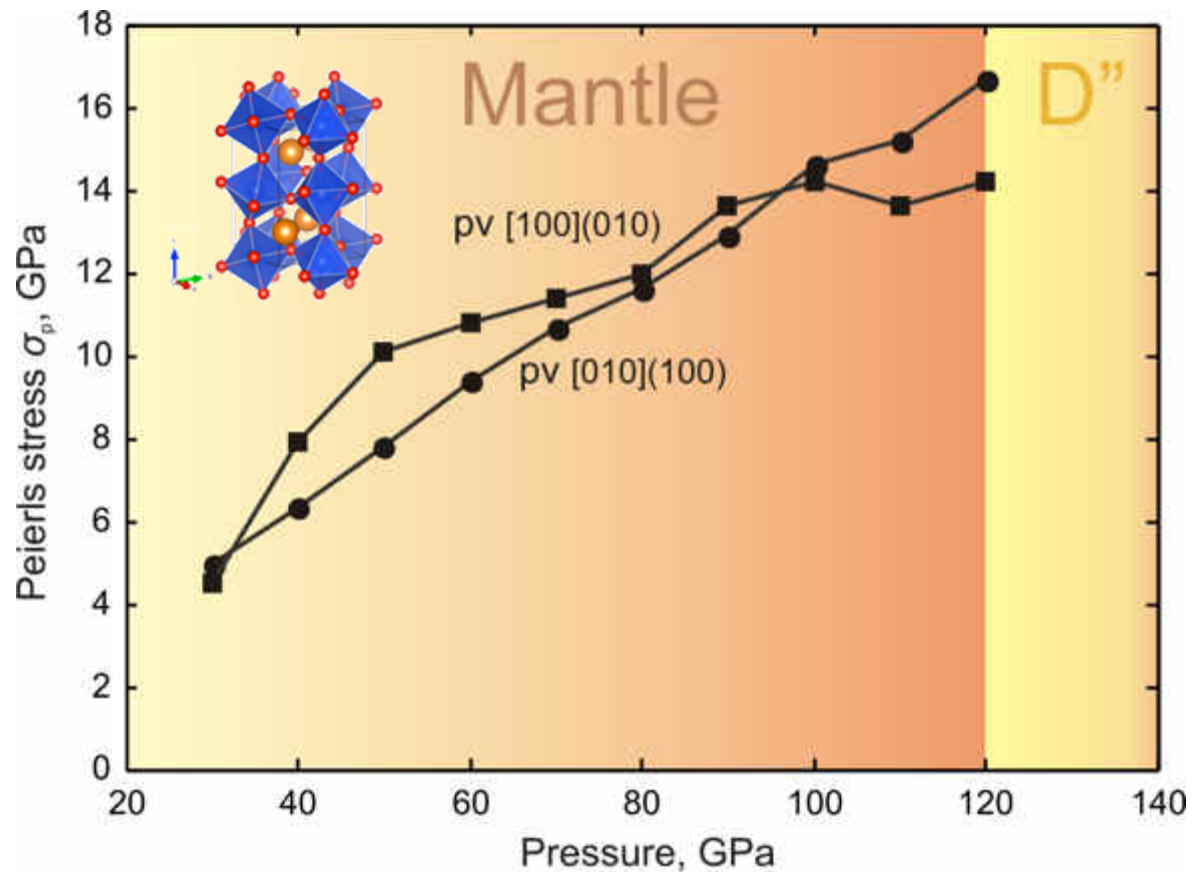
Hirel et al. (2014)



# Modeling lattice friction



# Lattice friction in bridgmanite: influence of P



Hirel et al. Acta Mat 2014

# Experiments under lower mantle conditions

## GEOPHYSICS

### Shear deformation of bridgmanite and magnesiowüstite aggregates at lower mantle conditions

Jennifer Girard, George Amulele,\* Robert Farla,†  
Anwar Mohiuddin, Shun-ichiro Karato‡

Rheological properties of the lower mantle have strong influence on the dynamics and evolution of Earth. By using the improved methods of quantitative deformation experiments at high pressures and temperatures, we deformed a mixture of bridgmanite and magnesiowüstite under the shallow lower mantle conditions. We conducted experiments up to about 100% strain at a strain rate of about  $3 \times 10^{-5} \text{ second}^{-1}$ . We found that bridgmanite is substantially stronger than magnesiowüstite and that magnesiowüstite largely accommodates the strain. Our results suggest that strain weakening and resultant shear localization likely occur in the lower mantle. This would explain the preservation of long-lived geochemical reservoirs and the lack of seismic anisotropy in the majority of the lower mantle except the boundary layers.

The large, rocky lower mantle is mostly composed of (Mg,Fe)SiO<sub>3</sub> bridgmanite (~70%) and (Mg,Fe)O magnesiowüstite (~20%) (and a few percent of calcium perovskite CaSiO<sub>3</sub>) (1). Many of Earth's geochemical and geophysical questions depend strongly on the rheological properties of materials in this region. For instance, geochemical observations suggest that the lower mantle hosts a large amount of incompatible elements working as a reservoir of these elements (2, 3). The degree of preservation of these reservoirs is controlled by the nature of mixing or stirring of materials (4, 5), which strongly depends on the rheological properties of materials in this region. However, very little is currently known about the rheological properties of materials in the lower mantle because of the difficulties in quantitative experimental studies of deformation under the conditions of the lower mantle.

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\*Present address: Department of Earth and Planetary Sciences, Macquarie University, Sydney, NSW, Australia. †Present address: Bayerisches Geoinstitut, Universität Bayreuth, Bayreuth, Germany.  
‡Corresponding author. E-mail: shun-ichiro.karato@yale.edu

The main difficulties include the controlled generation of stress (or strain rate) and reliable measurements of stress and strain under the high-pressure and -temperature conditions [e.g., (6)]. Consequently, previous studies on plastic deformation of lower mantle minerals were either performed at high pressures and low temperatures (7–10), at high pressures and high temperatures, without stress-strain rate control (11), or on analog materials at low pressures (12–14). Applying low-temperature experiments to Earth's interior is difficult because rheological properties are highly sensitive to temperature. Also the mechanisms by which deformation occurs are sensitive to temperature and strain rate, creating extrapolation issues for both low-temperature and poorly controlled strain-rate (stress) measurements [e.g., (15)]. Furthermore, microstructural evolution often leads to strain-dependent rheological behavior, which is particularly important for a sample containing two materials with a large strength contrast (16). The lower mantle approximates a two-phase mixture (bridgmanite and magnesiowüstite) with presumably a large strength contrast [e.g., (13, 17, 18)], and therefore large strain (>30%) experiments are essential to

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Girard et al. (2016) Science

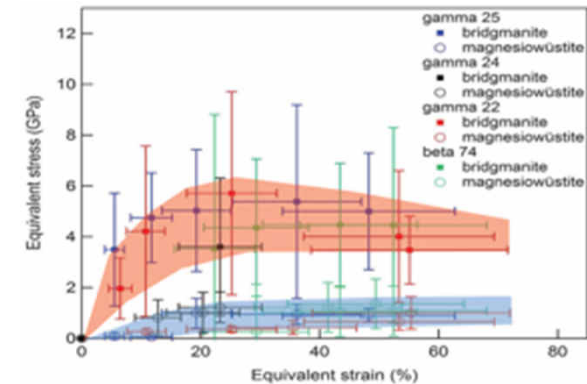
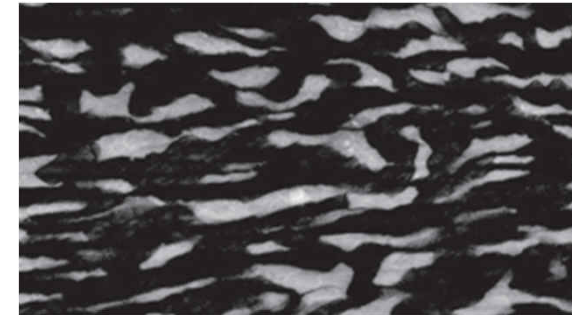
27 GPa  
2130 K



Rotational Drickamer apparatus

Yamazaki & Karato (2001)

SEM on deformed sample



Synchrotron: rheological data

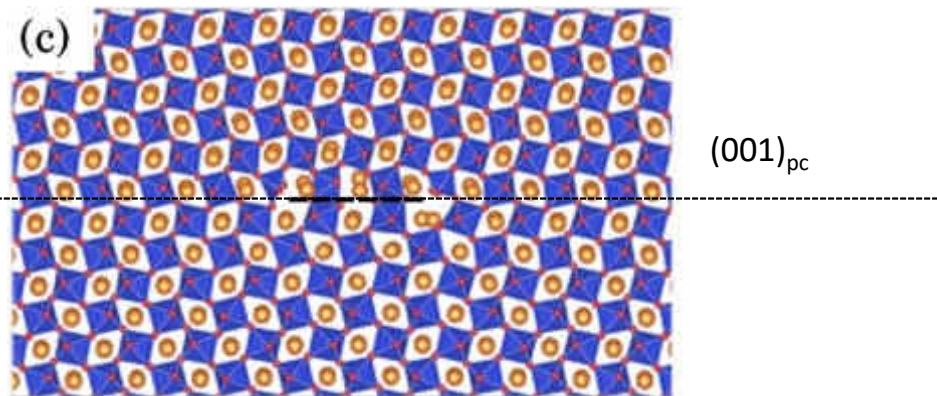


# Dislocations in perovskites

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Edge dislocations

$\text{MgSiO}_3$   $[110]_{\text{pc}}$



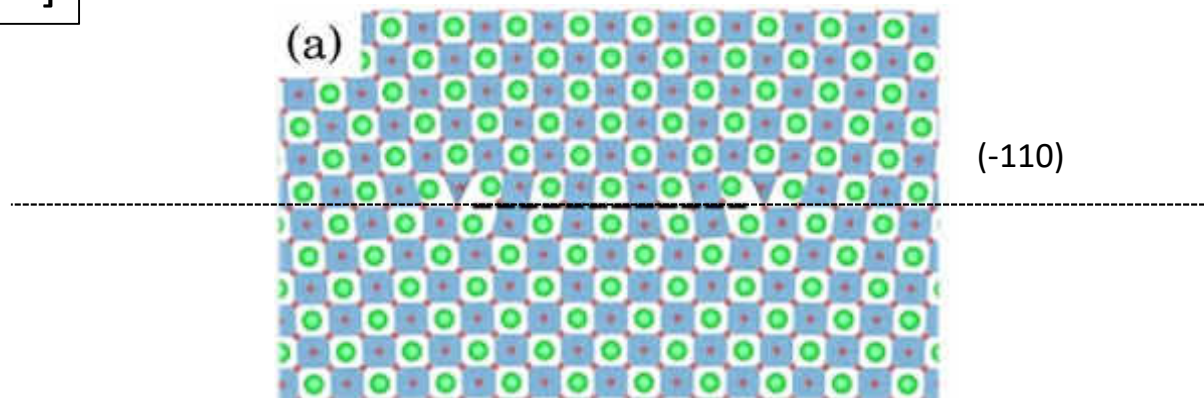
Hirel et al. Scripta Mat (2016)

# Dislocations in perovskites

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Edge dislocations

SrTiO<sub>3</sub> [110]

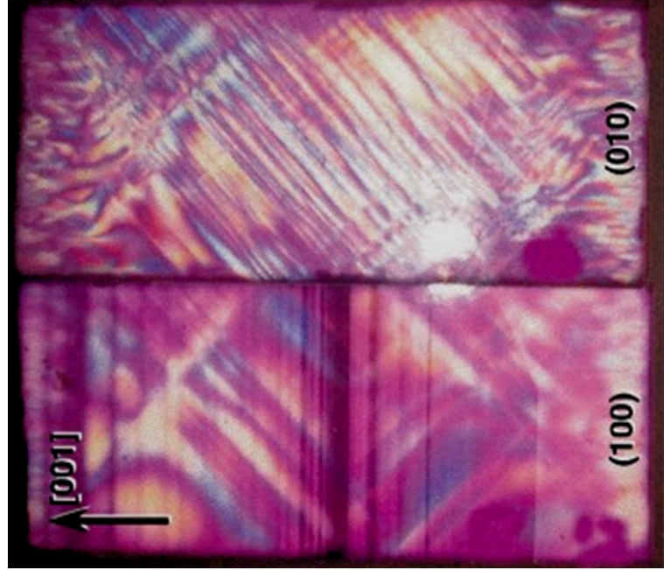
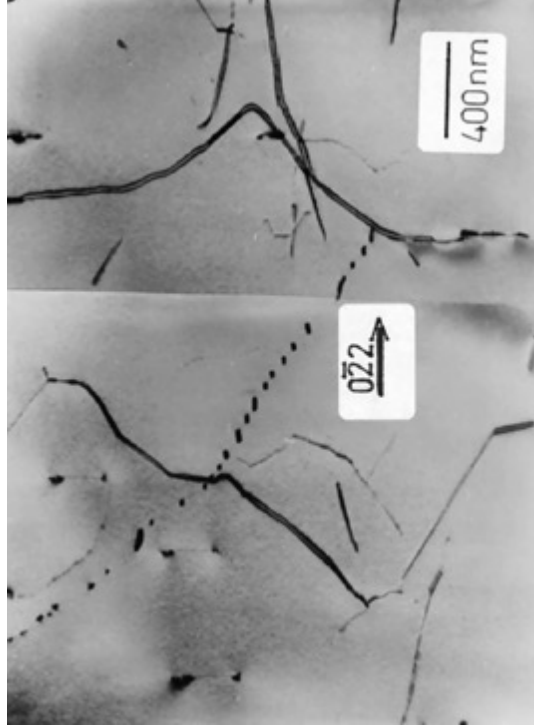


Hirel et al. Scripta Mat (2016)

## Surprising Results of a Study on the Plasticity in Strontium Titanate

Dieter Brunner, Shahram Taeri-Baghadrani, Wilfried Sigle, and Manfred Rühle\*

Max-Planck-Institut für Metallforschung, D-70174 Stuttgart, Germany

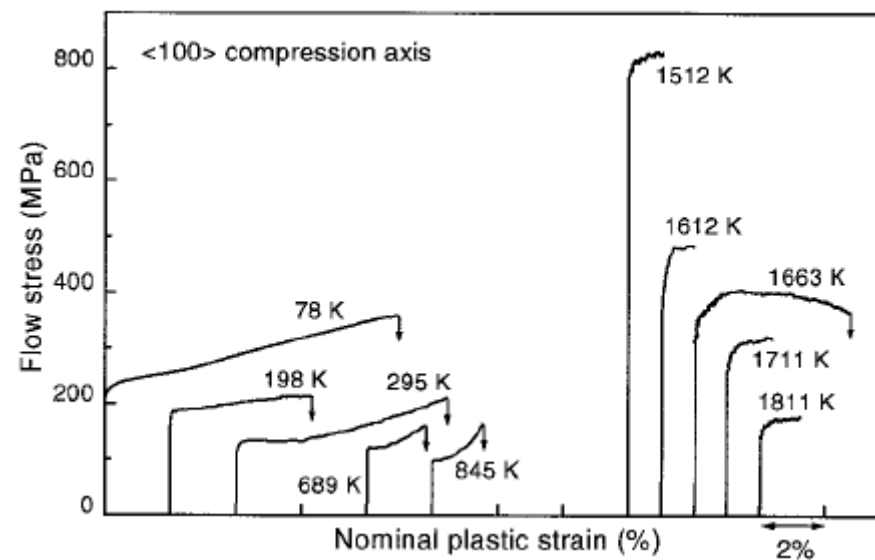


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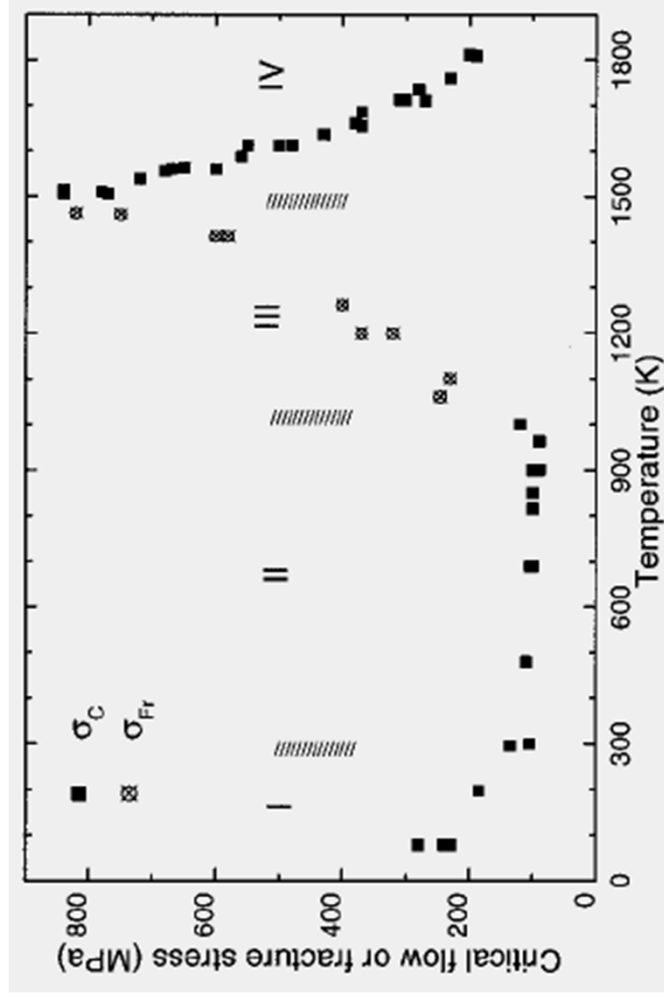
$\text{SrTiO}_3$   $\langle 110 \rangle$  slip



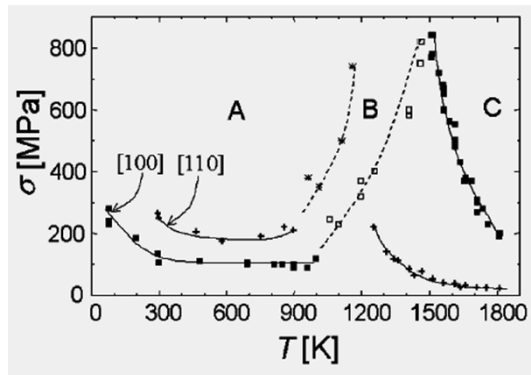
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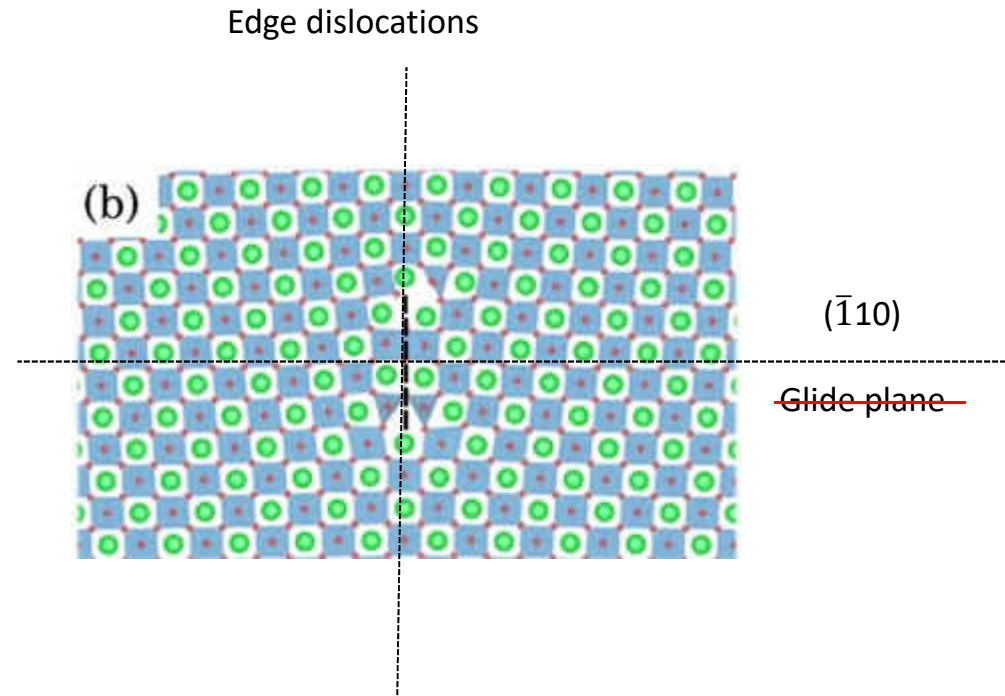
Max-Planck-Institut für Metallforschung, D-70174 Stuttgart, Germany



# SrTiO<sub>3</sub> high temperature: climb dissociation



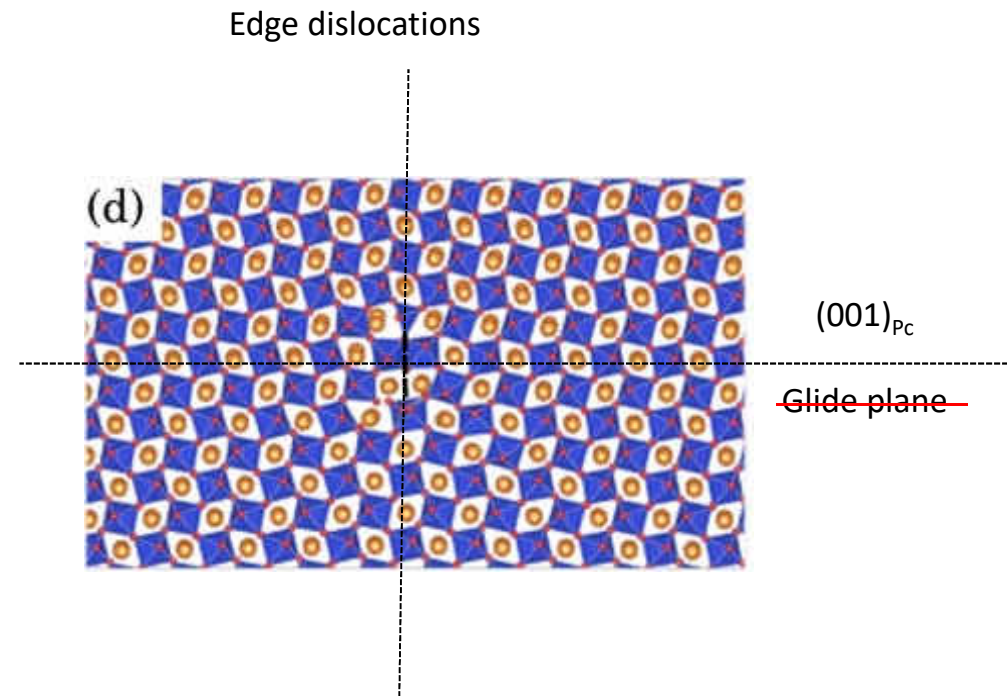
Brunner et al. (2001)  
Gumbsch et al. (2001)



Hirel et al. Scripta Mat (2016)

# MgSiO<sub>3</sub> high temperature: climb dissociation

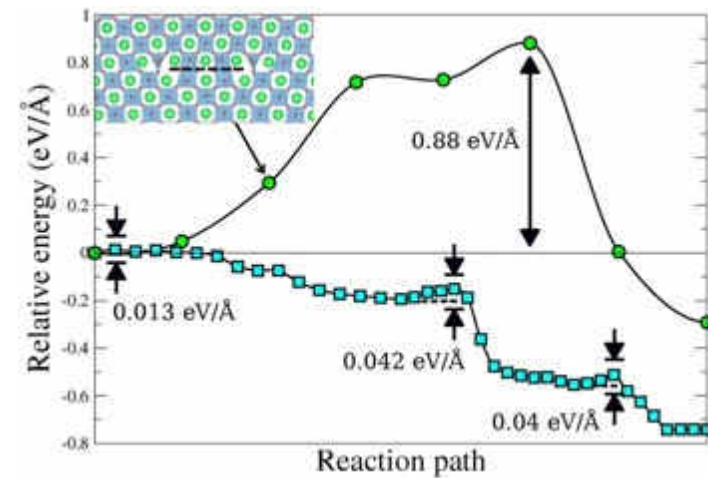
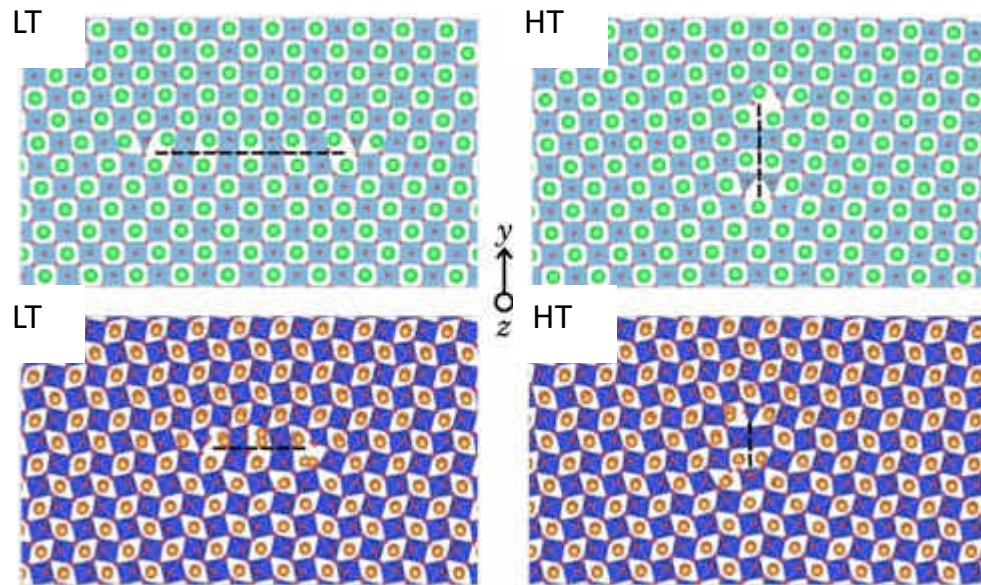
MgSiO<sub>3</sub> [110]<sub>pc</sub>



Hirel et al. Scripta Mat (2016)



# Climb dissociation in perovskite

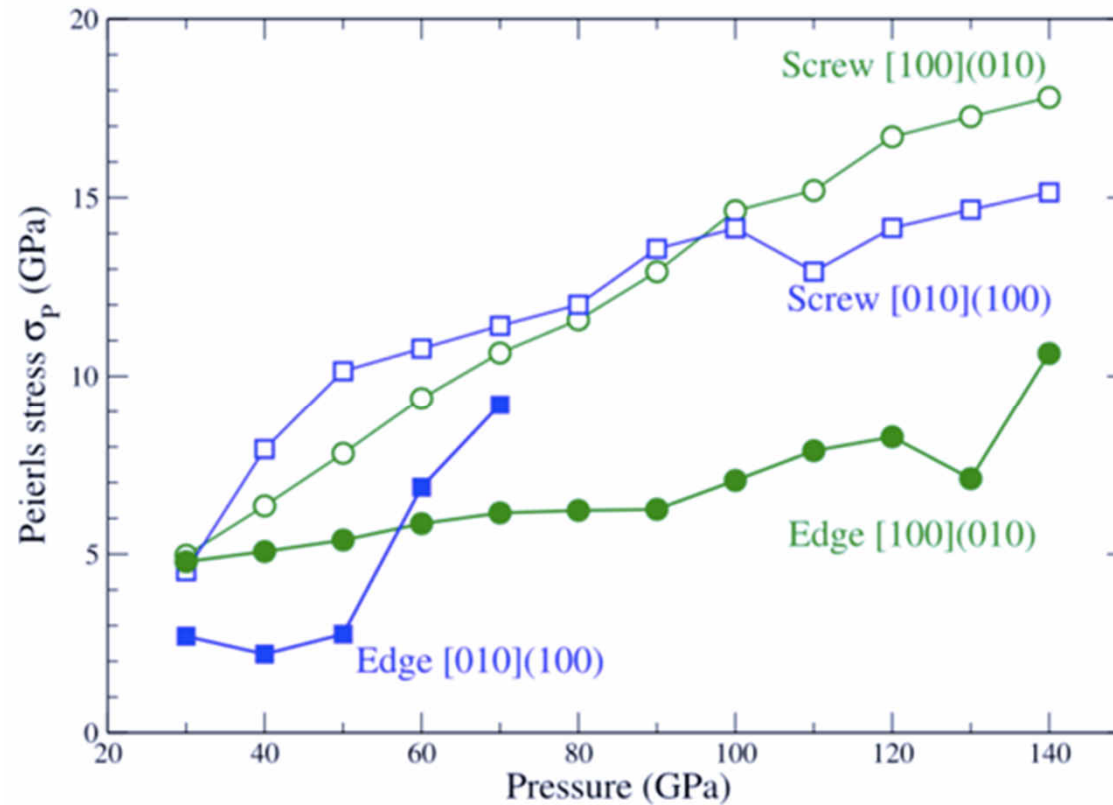


Hirel et al. (2016)



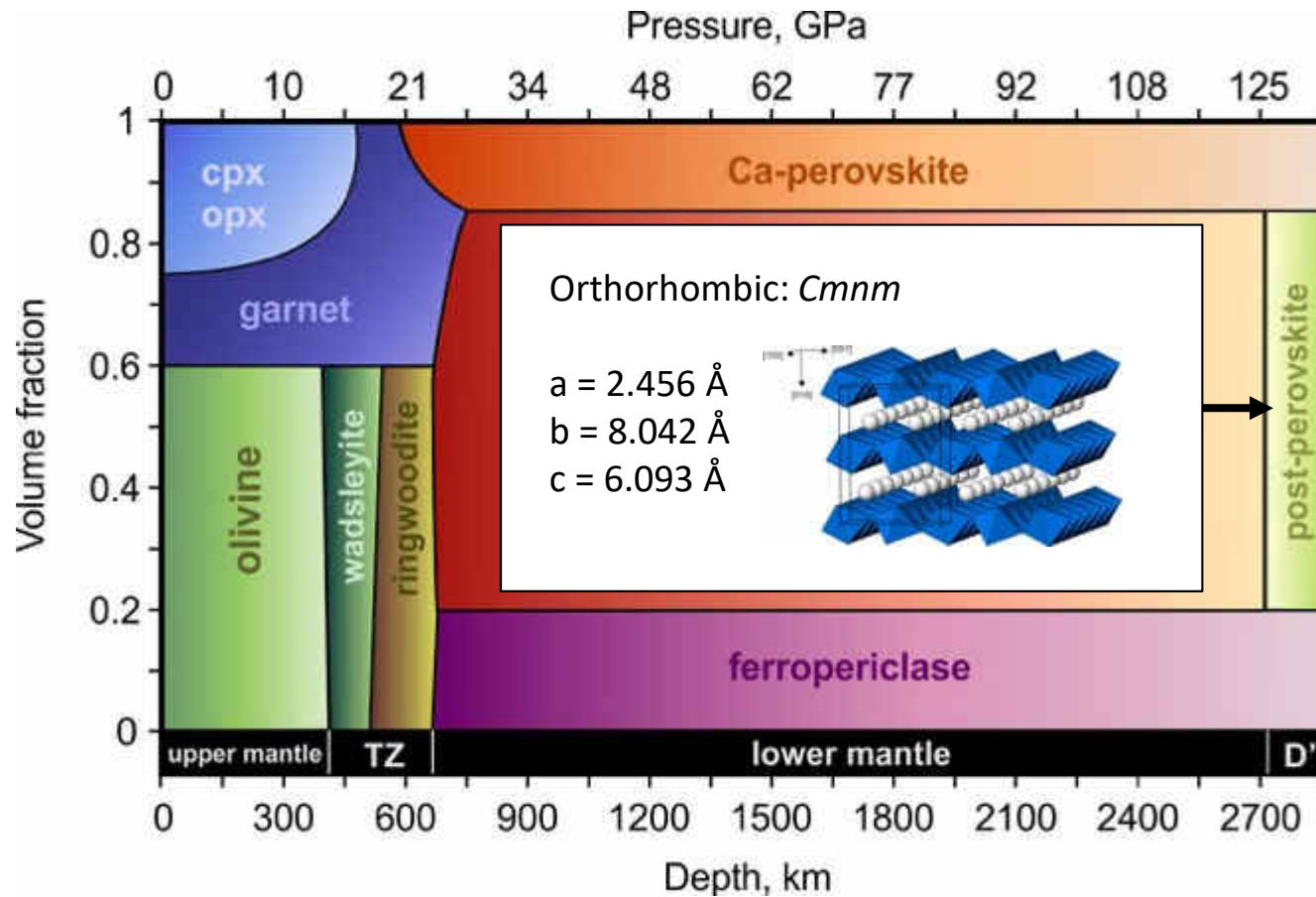
# Lattice friction in MgSiO<sub>3</sub> bridgmanite

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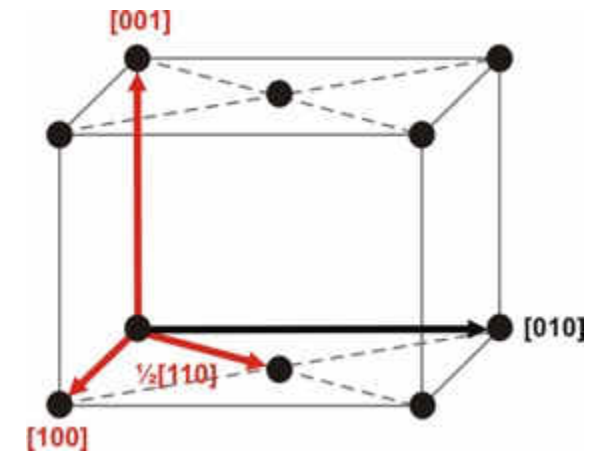
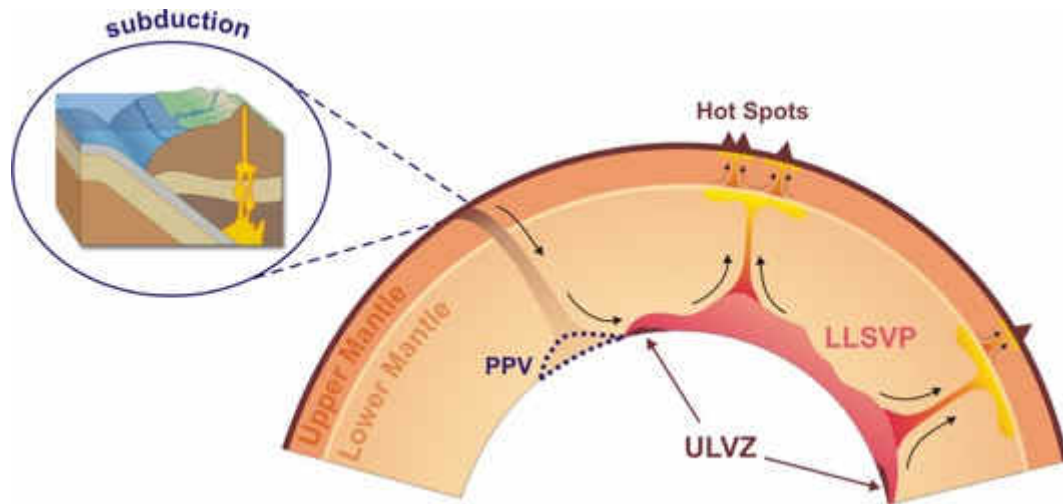


Hirel et al. Acta Mat 2014

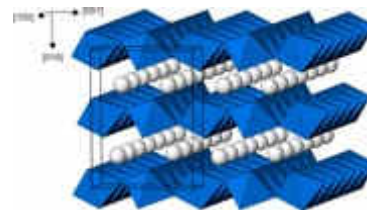
# Post-perovskite ( $\text{MgSiO}_3$ )



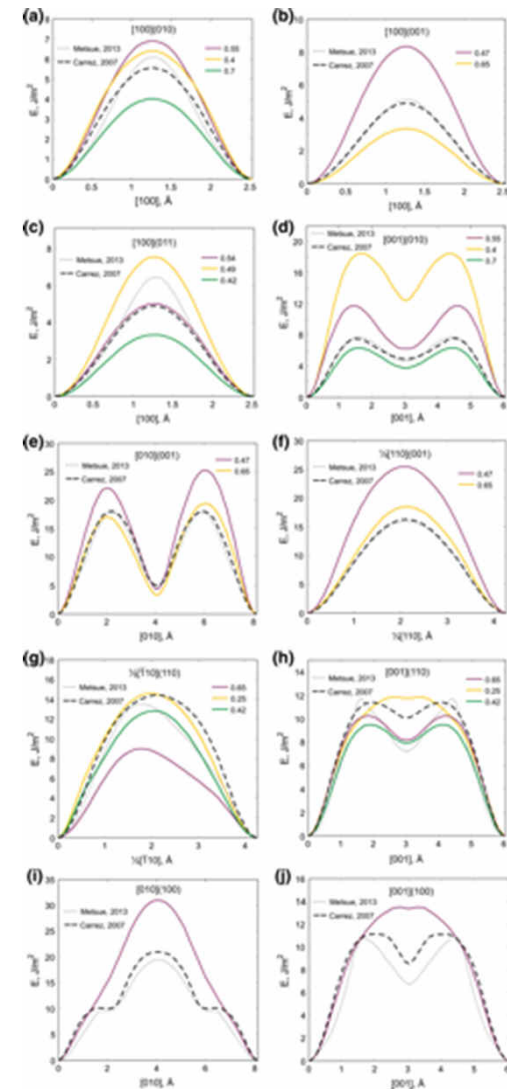
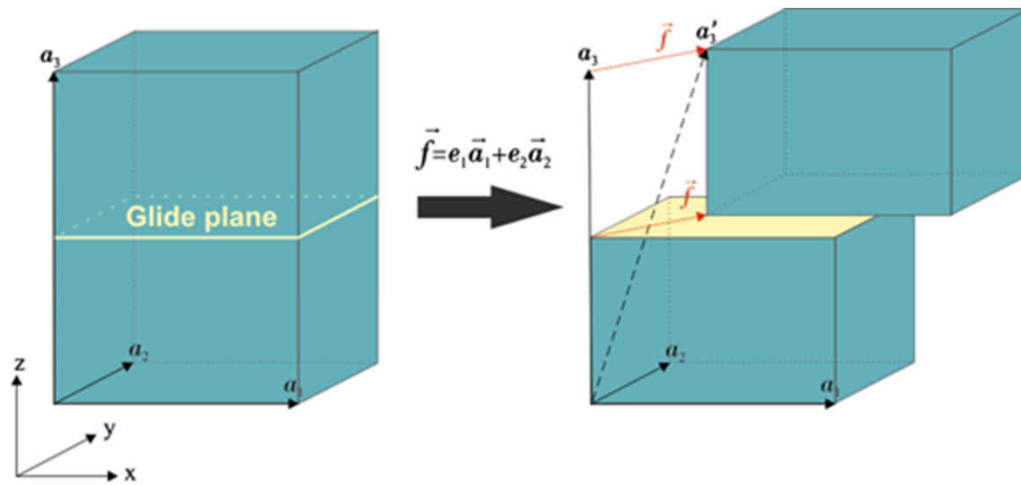
# Post-perovskite ( $\text{MgSiO}_3$ )



Possible Burgers vectors



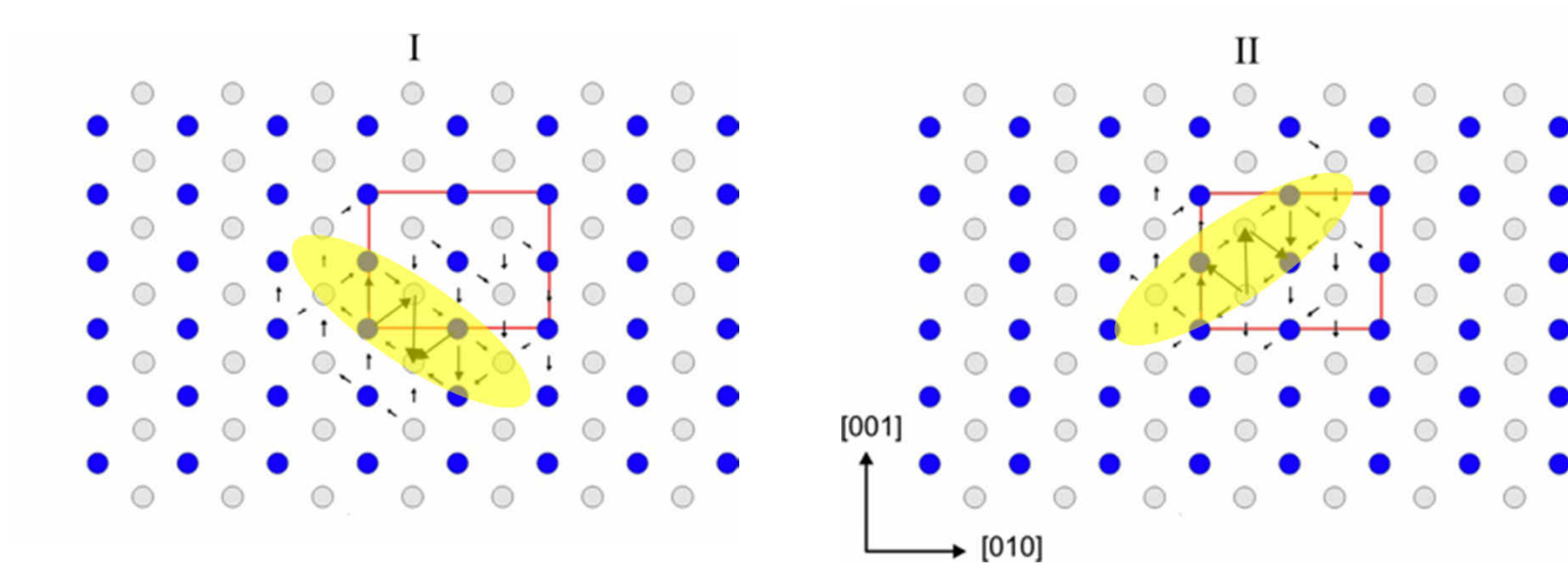
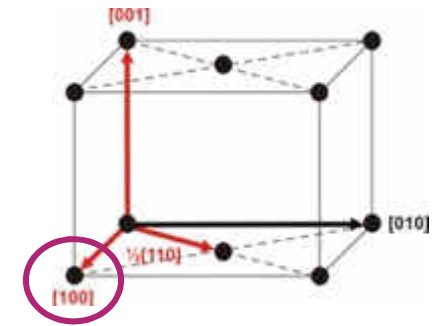
# Post-perovskite ( $\text{MgSiO}_3$ )



# Post-perovskite ( $\text{MgSiO}_3$ )

[100] glide: the shortest lattice repeat (2.456 Å)

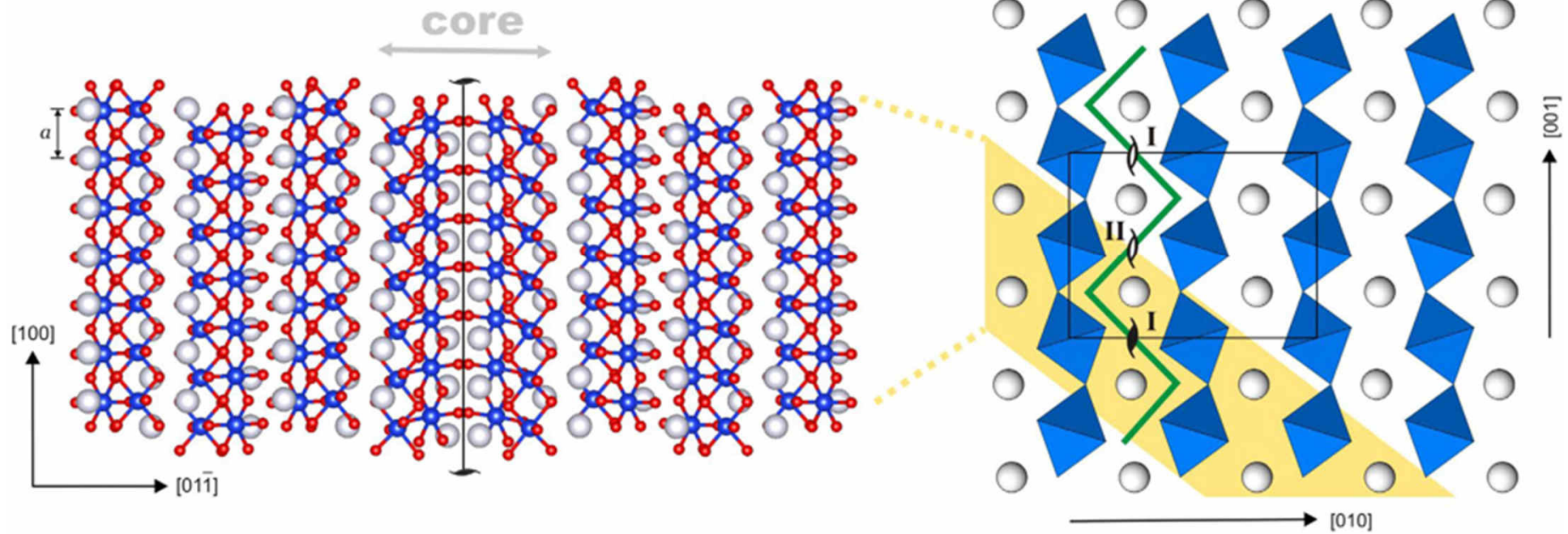
Screw dislocation



# Post-perovskite ( $\text{MgSiO}_3$ )

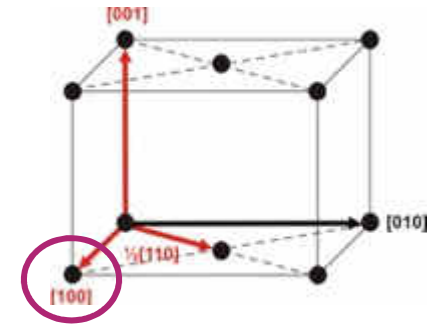
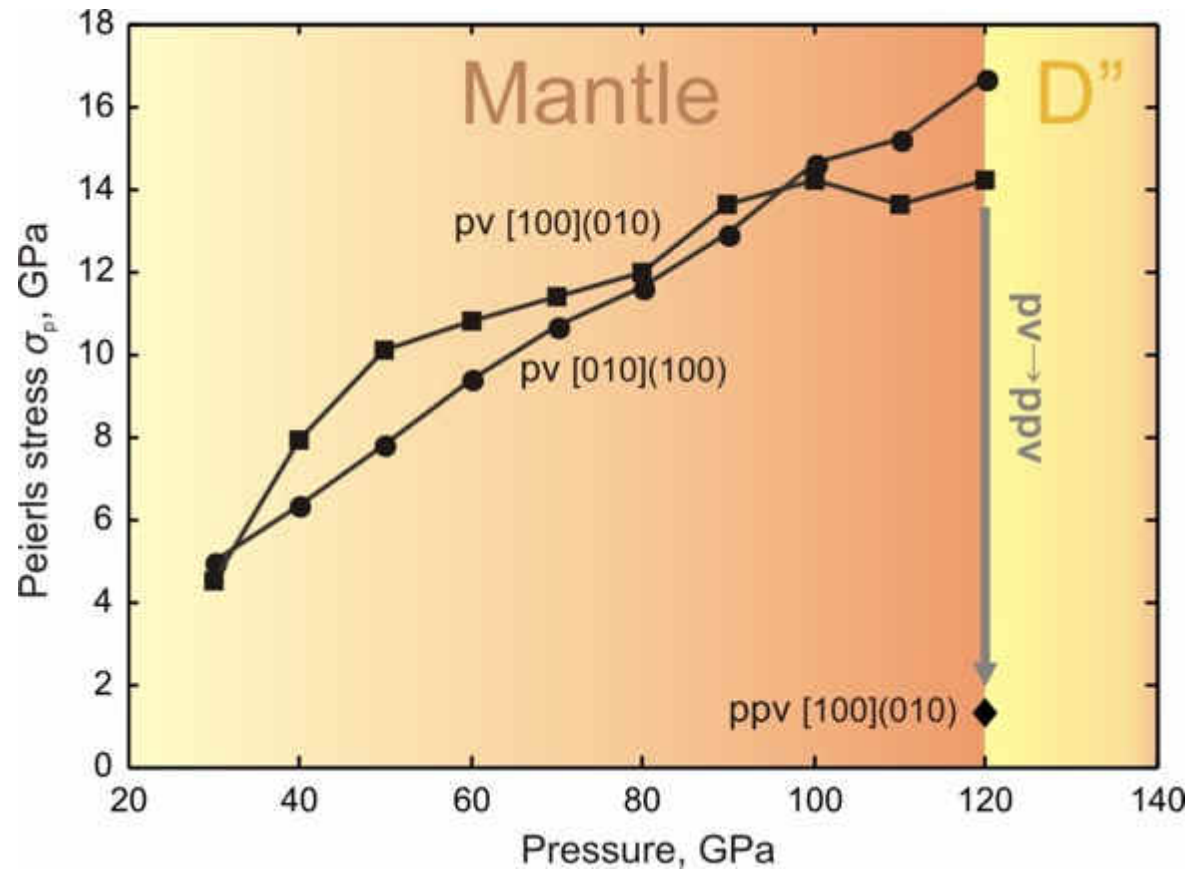
[100] glide: the shortest lattice repeat (2.456 Å)

Screw dislocation





# Post-perovskite ( $\text{MgSiO}_3$ )

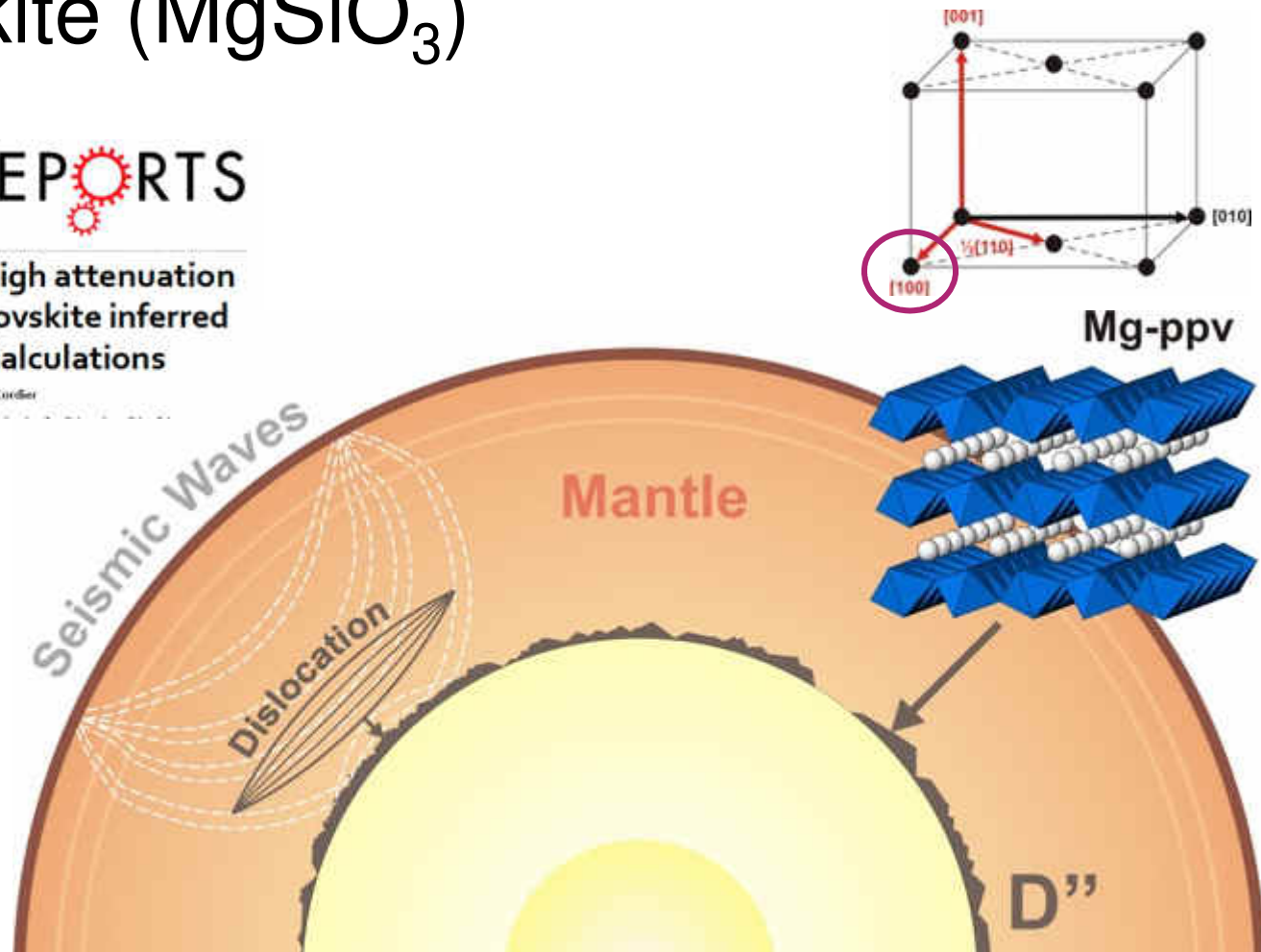


# Post-perovskite ( $\text{MgSiO}_3$ )

SCIENTIFIC REPORTS

OPEN Low viscosity and high attenuation in  $\text{MgSiO}_3$  post-perovskite inferred from atomic-scale calculations

Received: 26 July 2016  
Accepted: 13 September 2016  
Alexandra M. Goryainova, Philippe Carrez & Patrick Cordier

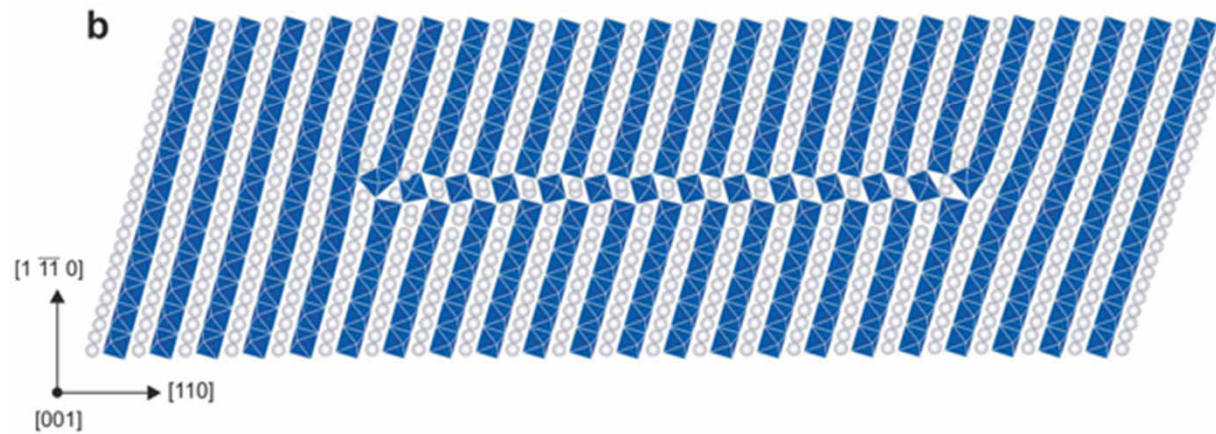
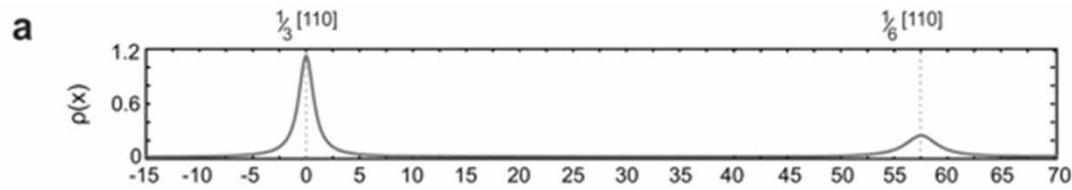
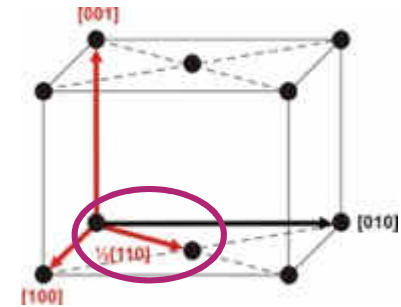




# Post-perovskite ( $\text{MgSiO}_3$ )

$\frac{1}{2} [110]$  glide: the 2<sup>nd</sup> shortest lattice repeat (4.2 Å)

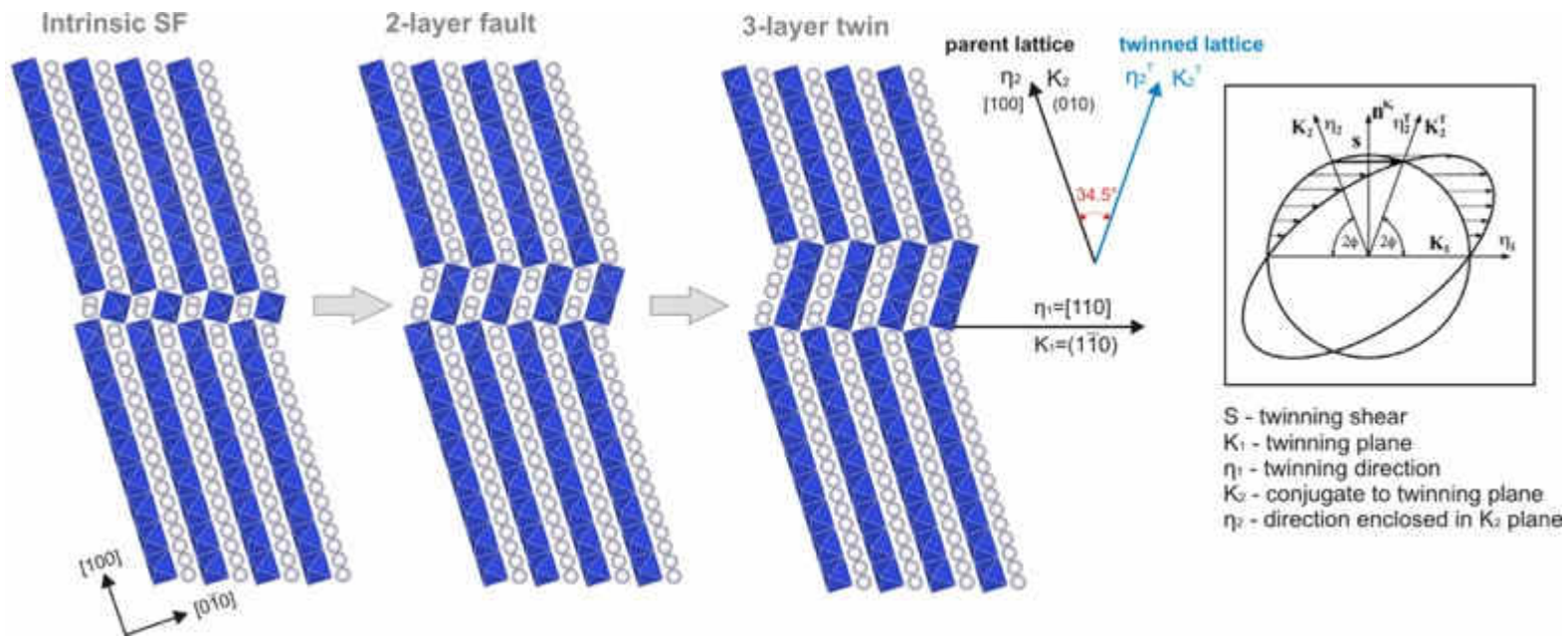
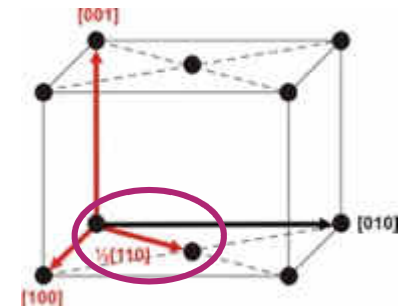
$\frac{1}{2} [110](1\bar{1}0)$  edge dislocation



# Post-perovskite ( $\text{MgSiO}_3$ )

$\frac{1}{2} [110]$  glide: the 2<sup>nd</sup> shortest lattice repeat (4.2 Å)

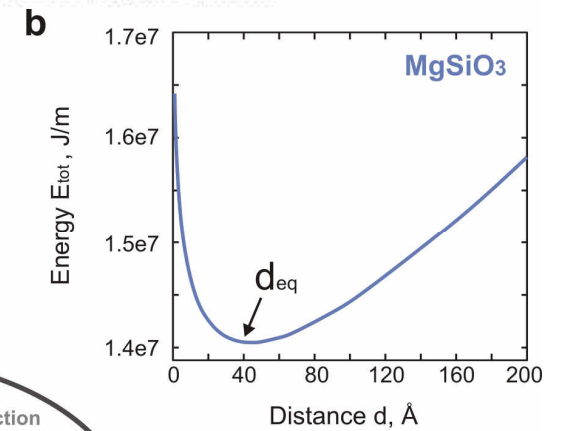
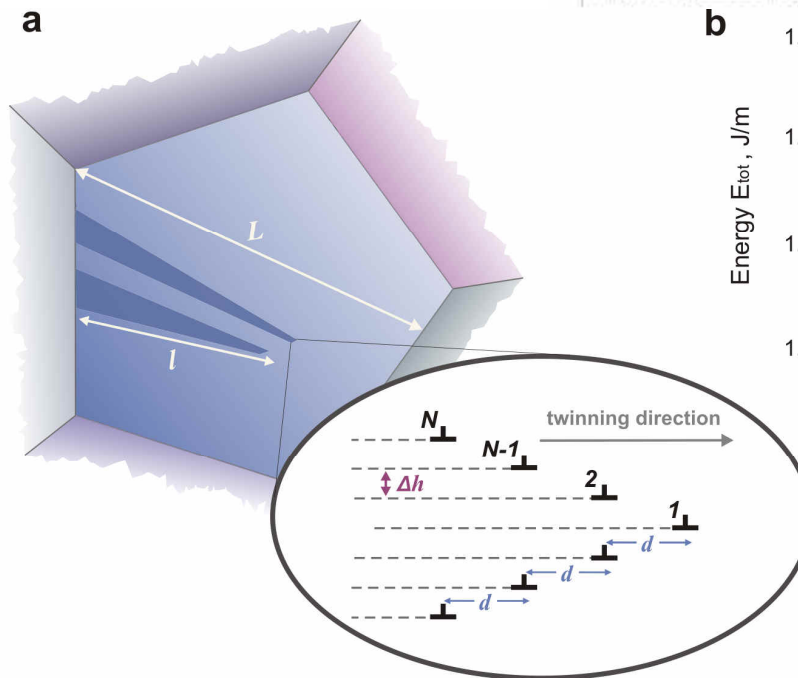
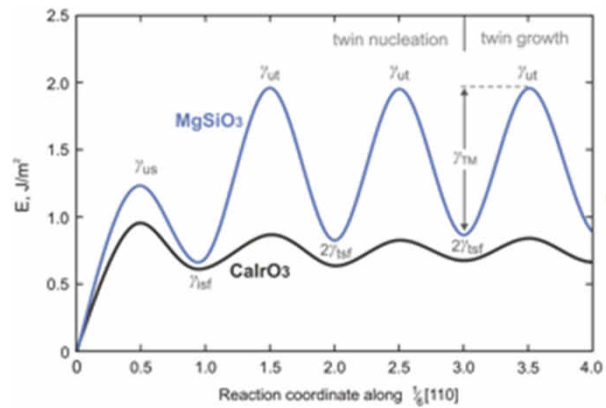
$\frac{1}{6} [110](1\bar{1}0)$  edge dislocation



# Post-perovskite ( $\text{MgSiO}_3$ )

OPEN Prediction of Mechanical Twinning in Magnesium Silicate Post-Perovskite

Philippe Carrez, Alexandra M. Goryaeva & Patrick Cordier



# Notes and thoughts

- Dislocations are two-fold
  - Far-field: elasticity
  - Near field: atomic configurations
- The dislocation cores control the mobility
- In materials with complex crystal chemistry (and sometimes low symmetries) dislocation cores can exhibit various configurations
- Great progress have been made on the modeling side
- Observations are needed



# THANK YOU

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