

## Line defects in minerals

### Bibliography

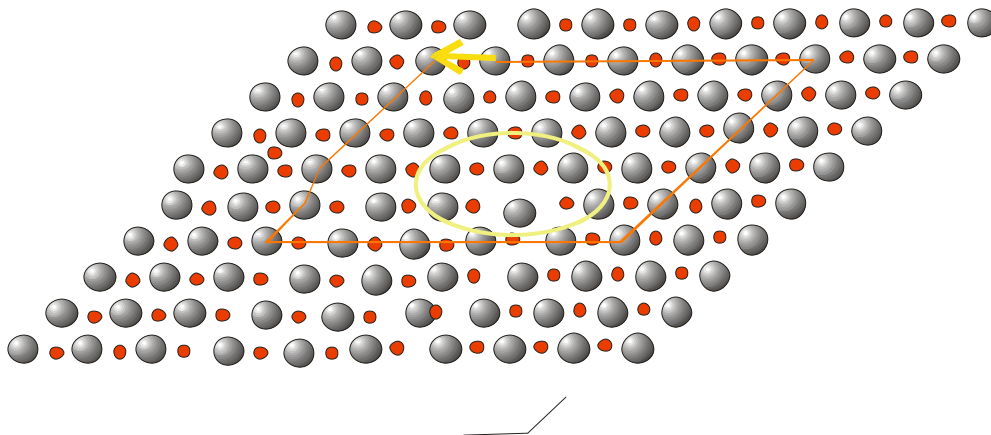
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- Nicolas, J., and J.P. Poirier, *Crystalline plasticity and solid state flow in metamorphic rocks*, 444 pp., Wiley-Interscience, 1976.

### Burgers vectors sf/RH

The Burgers vector,  $\mathbf{b}$ , indicates the displacement suffered by the crystal as the dislocation passes. When the dislocation exits the crystal, the surface expression exhibits a step with a depth  $|\mathbf{b}|$ . Thus the Burgers vector is often called the slip direction. By convention the direction of the Burgers vector is given by completing a circuit of integral steps around the dislocation, keeping the dislocation line length on the right hand side. The closure failure from finish to start defines the Burgers vector.

In the schematic below the dislocation is contained within the yellow ellipse. A circuit of 5 lattice vectors is shown. The yellow arrow shows the magnitude and direction of the closure failure. The region close to the dislocation that is highly disturbed is called the dislocation core (approximated by the ellipse). The exact displacements of the ions in the core region may change as the dislocation moves through the crystal. In general the core region has an associated volume increase and a bonding scheme that is substantially different from that in the defect-free portion of the crystal. Consequently it may be a region of enhanced diffusivity. The core region is probably a few lattice parameters wide; and outside this region, ions are displaced from their equilibrium positions by amounts that can be accommodated by elastic distortions.

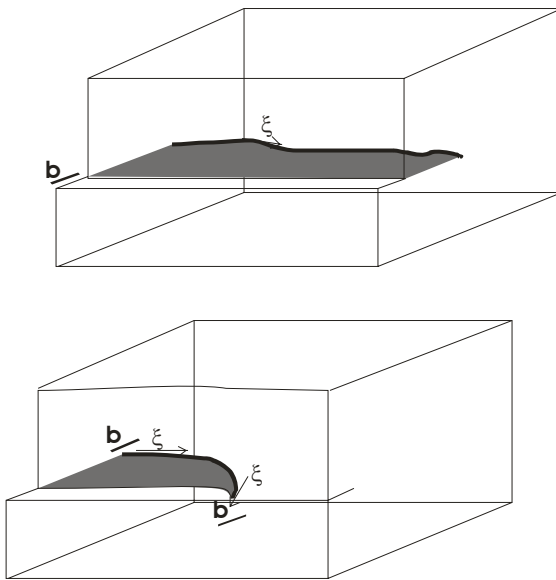
RH/sf



### *Dislocation line vectors*

At any given point, the tangent to the dislocation core region, is defined as the dislocation line vector  $\mathbf{l}$ . The sense of positive direction of  $\mathbf{l}$  is somewhat arbitrary, but once chosen should be consistent along the entire length of the dislocation. In the example above, the line direction is positive **into** the paper. By considering slightly more complicated Burgers circuits, one may prove that the Burger vector must remain unchanged along entire length of the dislocation. Thus, if the dislocation changes its direction in the crystal the relation between the line direction and the Burgers vector changes.

### *Edge and screw*



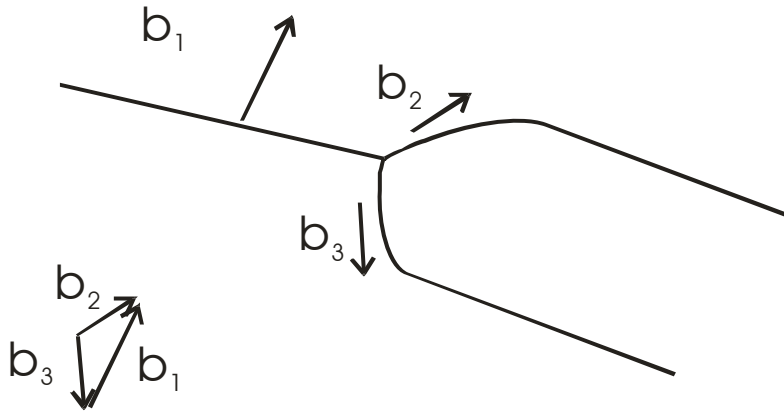
When the line direction and the Burgers vector are perpendicular the dislocation is said to be an **edge** dislocation. When the two are parallel, it is said to be a **screw** dislocation. When the line length and Burgers vector make some other angle the dislocation is said to have **mixed** character.

The dislocation may be curved along its length when viewed at a scale of many lattice dimensions. Clearly, the character of the dislocation may vary from edge to screw along its length.

If the dislocation moves completely through the crystal, one portion of the crystal is displaced relative to the other by one Burgers vector.

### *Dislocation reactions:*

Owing to the fact that the dislocation separates the portion of the crystal that has been distorted from that which has not, it can be proven that a dislocation cannot end in the crystal. It may loop back upon itself, terminate at a grain boundary, surface, or interphase boundary, or react with other dislocations. When the latter occurs, the vector sum of the Burgers vectors must be equal.



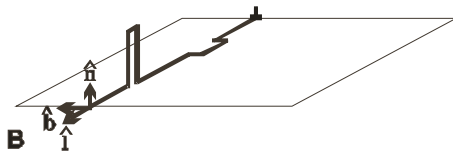
### Slip planes

The slip plane is a plane whose normal is  $\mathbf{n} = \mathbf{b} \times \boldsymbol{\xi}$

A dislocation that is composed of short edge and screw segments is said to be kinked.

When the dislocation departs from its slip plane, it is said to be jogged.

Motion of the dislocation along a given slide plane is called glide and can be accommodated at relatively low temperatures. When the dislocation move perpendicular to the glide plane it is climbing. This motion requires diffusion of ions towards or away from the dislocation and can only be accomplished at higher temperatures or lower strain rates than the glide motion.



Kink in plane  
Jog out of plane



Motion of the dislocation only occurs normal to its line direction. When an edge dislocation moves along its glide plane, no material needs to be removed from the crystal. The motion of the dislocation is said to be conservative

Motion of a screw dislocation never involves diffusion, because there is no unique slip plane ( $\mathbf{b} \parallel \boldsymbol{\xi}$ ). Motion of a screw segment from one lattice plane to another is called cross slip.

*Dislocation slip systems in minerals.*

The combination of a slip plane and a Burgers vector is called a slip system. Dislocation segments in a given slip system can be either edge and screw as long as they have the same Burgers vector. When the crystal is loaded externally to values high enough to cause slip, the dislocation moves, and small atomic adjustments are made in the core structure. The adjustments must be periodic as the dislocation moves from one lattice point to another. The energy necessary to cause the movements is provided by the work done on the system by the external forces. The stress necessary to cause slip, often called *lattice friction*, depends on the detailed crystal geometry, and will, therefore, differ from one slip system to another. Some systems will be easier to activate than others. For elastically isotropic crystals, several rules of thumb can be used to predict the ease of slip:

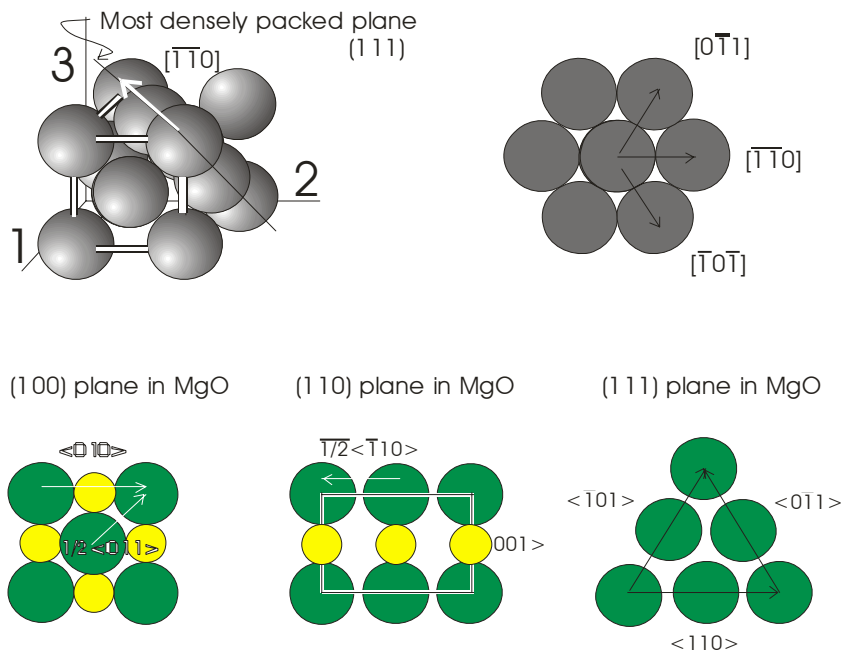
In general, slip planes that are widely spaced and densely packed will be preferred, because widely spaced planes are likely to indicate weaker bonding.

Short Burgers vectors are preferred, because the elastic distortion surrounding the dislocation will be minimized.

In poly ionic materials, those that are elastically anisotropic, (i.e. minerals) or when bonding is dominantly covalent, these rules may be broken.

	System	(Plane) $\langle \mathbf{b} \rangle$	(nm)	remark	
Calcite	$r^-$	$(10\bar{1}4)\langle 20\bar{2}1 \rangle$	0.810	Structural cell	Rhombohedral
	$r^+$	$(10\bar{1}4)\langle \bar{2}021 \rangle$		Shortest vector $\frac{1}{3}\langle 2\bar{1}\bar{1}0 \rangle$	
	$f^-$	$(\bar{1}012)\langle \bar{2}201 \rangle$		Next, $\frac{1}{3}\langle 0\bar{1}11 \rangle$	
	$f^+$	$(\bar{1}012)\langle 2\bar{2}01 \rangle$			
	a	$(\bar{1}2\bar{1}0)\langle \bar{2}021 \rangle$			
	c	$(0001)\langle \bar{1}2\bar{1}0 \rangle$			
Quartz	a on c	$(10\bar{1}0)\langle \bar{1}2\bar{1}0 \rangle$	0.49	Wet quartz, Low T, High $\varepsilon$	Trigonal
	c on a	$(0001)\langle 11\bar{2}0 \rangle$	0.54	Wet quartz	[Kirby and McCormick, 1984] {Linker, 1981 #4307}
	a on m	$(\bar{1}2\bar{1}0)\langle 0001 \rangle$	0.49		{Linker, 1981 #4307}
	c+a on m	$(10\bar{1}0)\langle 1\bar{2}13 \rangle$			
Olivine		$(100)\langle 001 \rangle$		Low T, High str. rt.	Orthorhombic
		$(110)\langle 001 \rangle$		"	
		$(100)\langle 010 \rangle$		{Dubious}	
		$(100)\langle 001 \rangle$		Medium T, str. rt.	
		$(0hk)\langle 100 \rangle$		"	
		$(001)\langle 100 \rangle$		"	
		$(010)\langle 100 \rangle$		High T, low str. + above	

Example 1. Magnesio-wustite, (Mg,Fe)O: FCC,  $Fm\bar{3}m$ ,  $a=0.42-0.43$  nm.  
 {Cordier, 2002 #4304}



The top two figures show an FCC lattice with a monatomic basis. Although (111) is the closest packed plane, (100) and (110) are also relatively closely packed.

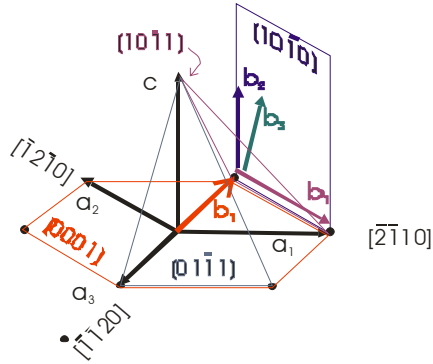
In MgO, two sublattices are present, an anion sub-lattice and a cation sublattice. Electrostatic interactions change the preferred slip plane from (111) to (001) and (110). (See bottom figure). The preferred plane (110) allows the two sublattices to overlap in the core of the dislocation.

In experiments, two slip systems are observed to operate:  $\{110\} \frac{1}{2}\langle\bar{1}10\rangle$  and  $\{001\} \frac{1}{2}\langle\bar{1}10\rangle$ . The Burgers vector has length  $\frac{1}{2}\langle 1\bar{1}0\rangle$  because there are lattice points at  $\langle 000\rangle$  and  $\langle \frac{1}{2} \frac{1}{2} 0\rangle$  in the FCC cell. Slip on  $\{110\}$  planes is much easier and occurs at lower temperatures (for same stress) (or lower stresses for same temperature if T is low).

# Slip Systems in Minerals

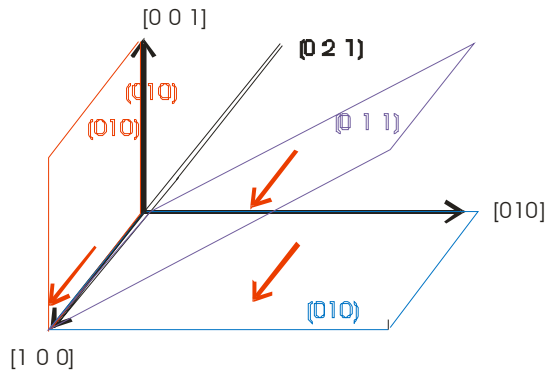
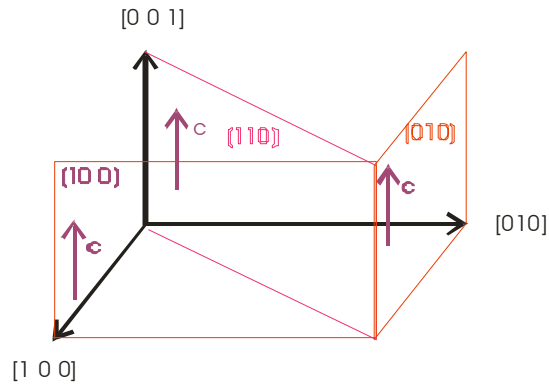
**Quartz**  
 $c = 0.54 \text{ nm}$   
 $a_1 = 0.49 \text{ nm}$

- (0001) basal plane
- (10 $\bar{1}$ 0) m prism
- (01 $\bar{1}$ 1) z rhomb
- (10 $\bar{1}$ 1) r rhomb



**Olivine**

$a = 0.476 \text{ nm}$   
 $b = 1.023 \text{ nm}$   
 $c = 0.599 \text{ nm}$



[Cordier, 2002]

### Example 2: Olivine

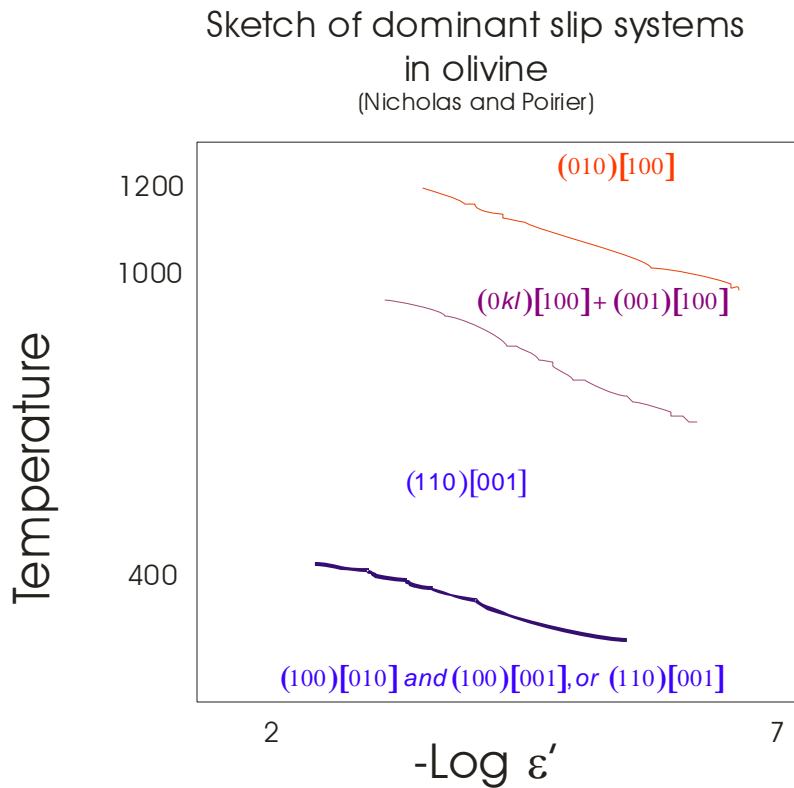
Lattice parameters are  $\mathbf{a} = 4.76 \text{ \AA}$ ;  $\mathbf{b} = 10.21 \text{ \AA}$ ;  $\mathbf{c} = 5.99 \text{ \AA}$ .

Close packed oxygen planes occur along (100).

Next closest packing is along (011), (010), and  $(0\bar{1}1)$ . These are 1<sup>st</sup> order prism planes in the oxygen HCP sublattice.

For all but (010) Si-O bonds must be broken.

[*Nicholas and Poirier, 1976*]{*Cordier, 2002 #4304*}





*Example 3: Quartz*

$(0001)\langle 11\bar{2}0 \rangle$  Basal slip Low T Easiest.

$(10\bar{1}0)\langle 0001 \rangle$  c on 1<sup>st</sup> order prism

$(10\bar{1}0)\langle 11\bar{2}0 \rangle$  a on 1<sup>st</sup> order prism

$(10\bar{1}0)\langle 1\bar{2}13 \rangle$  a+c on 1<sup>st</sup> order prism

$(11\bar{2}0)\langle 0001 \rangle$  c on 2<sup>nd</sup> order prism

