Lecture Notes - Mineralogy - Periclase Structure

- In lab we determined the unit cell for a crystal of synthetic periclase (MgO). Because periclase is cubic, only one lattice parameter (**a**) is needed to completely specify the size and shape of the unit cell. We found that **a** = 0.421 nm (= 4.21 Å). Based on this measurement, the volume (**V**) of the periclase unit cell is 0.074618 nm^3.

- The density of periclase can be determined by a specific gravity measurement using either the Joly or Berman balance. Because periclase is very hygroscopic, the Berman balance with toluene as the fluid is to be recommended. Periclase has a density of 3.56 g/cm^3 (=3.56 x 10^{-21} g/nm^3). One unit cell contains 2.6564 x 10^{-22} gm of periclase. [(0.074618 nm^3/unit cell) x (3.56 x 10^{-21} gm of periclase/nm^3) = (2.6564 x 10^{-22} gm of periclase/unit cell)]

- One gram formula unit (mole) of periclase has a mass (**gfw**) of 40.31 gms and contains **N** (6.023 x 10^{23}) formula units of MgO. Therefore, there are [(6.023 x 10^{23} formula units of MgO)/(40.31 gms) =] 1.494 x 10^{22} formula units of periclase per gram of periclase.

- Using the results of (2) and (3) it is clear that there should be [(1.494 x 10^{22} formula units of periclase/gm of periclase) x (2.6564 x 10^{-22} gm of periclase/unit cell) =] 3.969 formula units of periclase/unit cell. This number **Z** (formula units/unit cell) must be an integer (**Z** = 4) because there cannot be fractions of atoms in the unit cell.

$$\boxed{\mathbf{Z}\left(\frac{\text{formula units}}{\text{unit cell}}\right) = \frac{\mathbf{V\ D\ N}}{\mathbf{M}} \quad \frac{\left(\frac{nm^3}{\text{unit cell}}\right)\left(\frac{gm}{cm^3}\right)\left(\frac{\text{formula units}}{\text{mole}}\right)}{\left(\frac{gm}{\text{mole}}\right)}}$$

- Knowing the value of **Z**, it is possible to determine the exact locations of the Mg and O atoms using the special positions for the periclase space group Fm3m. With the multiplicity of a general position equal to 192, it is clear that Mg and O must be on special positions indeed. From the *International Tables for X-ray Crystallography* (p.338), it is clear that Mg and O **must** occupy special positions *a* and *b* with coordinates 0,0,0 and $^1/_2,^1/_2,^1/_2$, respectively. But which atom is to have 0,0,0 and which is to have $^1/_2,^1/_2,^1/_2$? Careful scrutiny of the structure reveals that there is no difference between the two possibilities; there is only a difference in choice of origin.

- Other crystal structures may be discovered in the same manner as that of periclase. However, for structures with more complexity, data in addition to Z and the crystal's symmetry are required for a complete structure determination.

Periclase MgO

Crystal Data: Cubic. *Point Group:* $4/m\ \overline{3}\ 2/m$. As small octahedra, less commonly cubo-octahedra or dodecahedra, may be clustered; granular, massive.

Physical Properties: *Cleavage:* {001}, perfect; on {111}, good; may exhibit parting on {011}. Hardness = 5.5 D(meas.) = 3.56–3.68 D(calc.) = 3.58 Slightly soluble in H_2O when powdered, to give an alkaline reaction.

Optical Properties: Transparent. *Color:* Colorless, grayish white, yellow, brownish yellow; may be green or black with inclusions; colorless in transmitted light. *Streak:* White. *Luster:* Vitreous.
Optical Class: Isotropic. $n = 1.735$–1.745

Cell Data: *Space Group:* $Fm3m$. a = 4.203–4.212 Z = 4

X-ray Powder Pattern: Synthetic.
2.106 (100), 1.489 (52), 0.9419 (17), 0.8600 (15), 1.216 (12), 2.431 (10), 1.0533 (5)

Chemistry:

	(1)
FeO	5.97
MgO	93.86
Total	99.83

(1) Monte Somma, Italy.

Mineral Group: Periclase group.

Occurrence: A product of the high-temperature metamorphism of magnesian limestones and dolostone.

Association: Forsterite, magnesite (Monte Somma, Italy); brucite, hydromagnesite, ellestadite (Crestmore quarry, California, USA); fluorellestadite, lime, periclase, magnesioferrite, hematite, srebrodolskite, anhydrite (Kopeysk, Russia).

Distribution: On Monte Somma, Campania, Italy. At Predazzo, Tirol, Austria. From Carlingford, Co. Louth, Ireland. At Broadford, Isle of Skye, and Camas Mòr, Isle of Muck, Scotland. From León, Spain. At the Bellerberg volcano, two km north of Mayen, Eifel district, Germany. From Nordmark and Långban, Värmland, Sweden. In mines around Kopeysk, Chelyabinsk coal basin, Southern Ural Mountains, Russia. In the USA, at the Crestmore quarry, Riverside Co., California; from Tombstone, Cochise Co., Arizona; in the Gabbs mine, Gabbs district, Nye Co., Nevada. In Canada, at Oka, Quebec. From ten km west of Cowell, Eyre Peninsula, South Australia.

Name: From the Greek for *to break around*, in allusion to the perfect cubic cleavage.

Type Material: Natural History Museum, Paris, France, 96.1201.

References: (1) Palache, C., H. Berman, and C. Frondel (1944) Dana's system of mineralogy, (7th edition), v. I, 499–500. (2) Deer, W.A., R.A. Howie, and J. Zussman (1962) Rock-forming minerals, v. 5, non-silicates, 1–4. (3) Hazen, R.M. (1976) Effects of temperature and pressure on the cell dimension and X-ray temperature factors of periclase. Amer. Mineral., 61, 266–271. (4) (1953) NBS Circ. 539, 1, 37.

$Fm3m$ O_h^5 No. 225 $F\,4/m\,\bar{3}\,2/m$ $m\,3\,m$ Cubic

Origin at centre ($m3m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions $(0,0,0;\ 0,\tfrac{1}{2},\tfrac{1}{2};\ \tfrac{1}{2},0,\tfrac{1}{2};\ \tfrac{1}{2},\tfrac{1}{2},0)+$	Conditions limiting possible reflections
				General:
192	l	1	$x,y,z;\ z,x,y;\ y,z,x;\ x,z,y;\ y,x,z;\ z,y,x;$ $x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};\ x,\bar{z},\bar{y};\ y,\bar{x},\bar{z};\ z,\bar{y},\bar{x};$ $\bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};\ \bar{x},z,\bar{y};\ \bar{y},x,\bar{z};\ \bar{z},y,\bar{x};$ $\bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x;\ \bar{x},\bar{z},y;\ \bar{y},\bar{x},z;\ \bar{z},\bar{y},x;$ $\bar{x},\bar{y},\bar{z};\ \bar{z},\bar{x},\bar{y};\ \bar{y},\bar{z},\bar{x};\ \bar{x},\bar{z},\bar{y};\ \bar{y},\bar{x},\bar{z};\ \bar{z},\bar{y},\bar{x};$ $\bar{x},y,z;\ \bar{z},x,y;\ \bar{y},z,x;\ \bar{x},z,y;\ \bar{y},x,z;\ \bar{z},y,x;$ $x,\bar{y},z;\ z,\bar{x},y;\ y,\bar{z},x;\ x,\bar{z},y;\ y,\bar{x},z;\ z,\bar{y},x;$ $x,y,\bar{z};\ z,x,\bar{y};\ y,z,\bar{x};\ x,z,\bar{y};\ y,x,\bar{z};\ z,y,\bar{x}.$	hkl: $h+k,k+l,(l+h)=2n$ hhl: $(l+h=2n)$; ↻ $0kl$: $(k,l=2n)$; ↻
				Special: as above, plus
96	k	m	$x,x,z;\ z,x,x;\ x,z,x;\ \bar{x},\bar{x},\bar{z};\ \bar{z},\bar{x},\bar{x};\ \bar{x},\bar{z},\bar{x};$ $x,\bar{x},\bar{z};\ z,\bar{x},\bar{x};\ x,\bar{z},\bar{x};\ \bar{x},x,z;\ \bar{z},x,x;\ \bar{x},z,x;$ $\bar{x},x,\bar{z};\ \bar{z},x,\bar{x};\ \bar{x},z,\bar{x};\ x,\bar{x},z;\ z,\bar{x},x;\ x,\bar{z},x;$ $\bar{x},\bar{x},z;\ \bar{z},\bar{x},x;\ \bar{x},\bar{z},x;\ x,x,\bar{z};\ z,x,\bar{x};\ x,z,\bar{x}.$	no extra conditions
96	j	m	$0,y,z;\ z,0,y;\ y,z,0;\ 0,z,y;\ y,0,z;\ z,y,0;$ $0,\bar{y},\bar{z};\ \bar{z},0,\bar{y};\ \bar{y},\bar{z},0;\ 0,\bar{z},\bar{y};\ \bar{y},0,\bar{z};\ \bar{z},\bar{y},0;$ $0,y,\bar{z};\ \bar{z},0,y;\ y,\bar{z},0;\ 0,\bar{z},y;\ y,0,\bar{z};\ \bar{z},y,0;$ $0,\bar{y},z;\ z,0,\bar{y};\ \bar{y},z,0;\ 0,z,\bar{y};\ \bar{y},0,z;\ z,\bar{y},0.$	
48	i	mm	$\tfrac{1}{2},x,x;\ x,\tfrac{1}{2},x;\ x,x,\tfrac{1}{2};\ \tfrac{1}{2},x,\bar{x};\ \bar{x},\tfrac{1}{2},x;\ x,\bar{x},\tfrac{1}{2};$ $\tfrac{1}{2},\bar{x},\bar{x};\ \bar{x},\tfrac{1}{2},\bar{x};\ \bar{x},\bar{x},\tfrac{1}{2};\ \tfrac{1}{2},\bar{x},x;\ x,\tfrac{1}{2},\bar{x};\ \bar{x},x,\tfrac{1}{2}.$	
48	h	mm	$0,x,x;\ x,0,x;\ x,x,0;\ 0,x,\bar{x};\ \bar{x},0,x;\ x,\bar{x},0;$ $0,\bar{x},\bar{x};\ \bar{x},0,\bar{x};\ \bar{x},\bar{x},0;\ 0,\bar{x},x;\ x,0,\bar{x};\ \bar{x},x,0.$	
48	g	mm	$x,\tfrac{1}{4},\tfrac{1}{4};\ \tfrac{1}{4},x,\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{1}{4},x;\ x,\tfrac{1}{4},\tfrac{3}{4};\ \tfrac{3}{4},x,\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{3}{4},x;$ $\bar{x},\tfrac{1}{4},\tfrac{1}{4};\ \tfrac{1}{4},\bar{x},\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{1}{4},\bar{x};\ \bar{x},\tfrac{1}{4},\tfrac{3}{4};\ \tfrac{3}{4},\bar{x},\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{3}{4},\bar{x}.$	hkl: $h,(k,l)=2n$
32	f	$3m$	$x,x,x;\ x,\bar{x},\bar{x};\ \bar{x},x,\bar{x};\ \bar{x},\bar{x},x;$ $\bar{x},\bar{x},\bar{x};\ \bar{x},x,x;\ x,\bar{x},x;\ x,x,\bar{x}.$	no extra conditions
24	e	$4mm$	$x,0,0;\ 0,x,0;\ 0,0,x;\ \bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x}.$	
24	d	mmm	$0,\tfrac{1}{4},\tfrac{1}{4};\ \tfrac{1}{4},0,\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{1}{4},0;\ 0,\tfrac{1}{4},\tfrac{3}{4};\ \tfrac{3}{4},0,\tfrac{1}{4};\ \tfrac{1}{4},\tfrac{3}{4},0.$	hkl: $h,(k,l)=2n$
8	c	$\bar{4}3m$	$\tfrac{1}{4},\tfrac{1}{4},\tfrac{1}{4};\ \tfrac{3}{4},\tfrac{3}{4},\tfrac{3}{4}.$	
4	b	$m3m$	$\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}.$	no extra conditions
4	a	$m3m$	$0,0,0.$