12.109 Lecture Notes
September 8, 2005

Rock Forming Minerals I
Structure and composition of: OLIVINE, SPINEL, GARNET

OLIVINE
Major constituent mineral of the earth's upper mantle, found in peridotite (rock composed of >50% olivine mineral)
$(Mg,Fe)_2SiO_4$
That is, solid solution of forsterite Mg_2SiO_4 and fayalite Fe_2SiO_4

Solid solution – continuous variation in chemical composition & physical properties

Polymorphism – same chemical composition, different crystal structure

Polymorphs of olivine at high pressure are wadsleyite and ringwoodite. The transition to wadsleyite occurs at ~310 km depth, and to ringwoodite at ~410 km depth. Ringwoodite has the spinel structure.

Coordination number – the number of anions surrounding the cation
See work by Linus Pauling, 1932
"Pauling's rules" for crystal structures, assumes ionic bonding
Ionic structure understood using electrostatic rules of attraction and repulsion
Cations and anions surround each other to neutralize charge – can rationalize crystal structure with coordination number

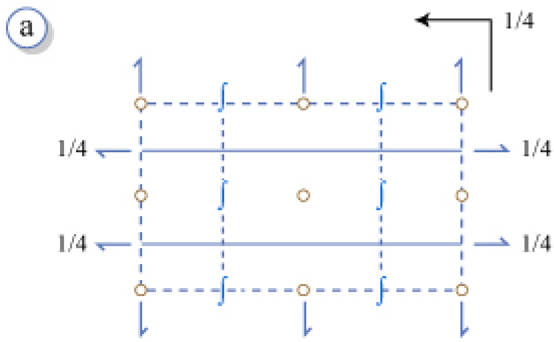
<u>Structure of olivine</u>
Two types of coordination in olivine – octahedral (6 anions around 1 cation)
tetrahedral (4 anions around 1 cation)
coordination polyhedron – shape that you get when you connect the centers of the anions that surround the cation

Pauling radius ratio rule – $\frac{r_{cation}}{r_{anion}}$ correlated with coordination #

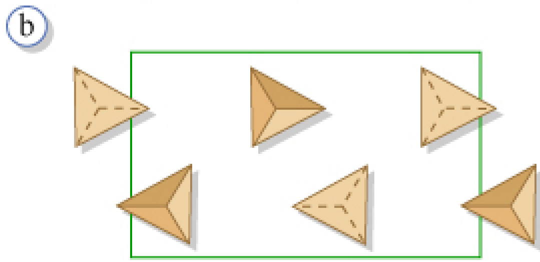
coordination	Average ratio	
(4) tetrahedral	.225	
(6) octahedral	.414	
(8) cubic	.732	
(12) dodecahedral	1	(spherical packing)

Ex. forsterite Mg_2SiO_4
Si^{4+} in tetrahedral site, Mg^{2+} in octahedral site, O atoms anions
Forms octahedral chains/strips
Strips impart directionality → PHYSICAL PROPERTIES consistent with symmetry
Strips bound together by isolated tetrahedral strips

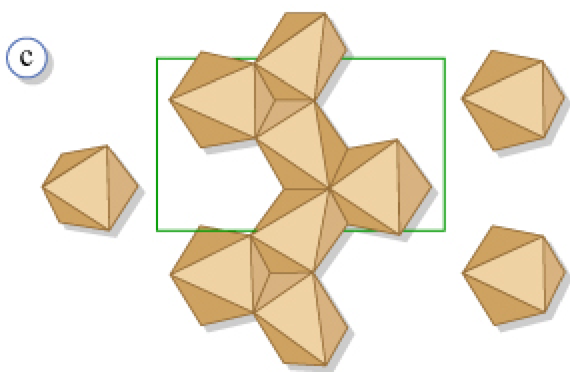
STRUCTURE OF OLIVINE



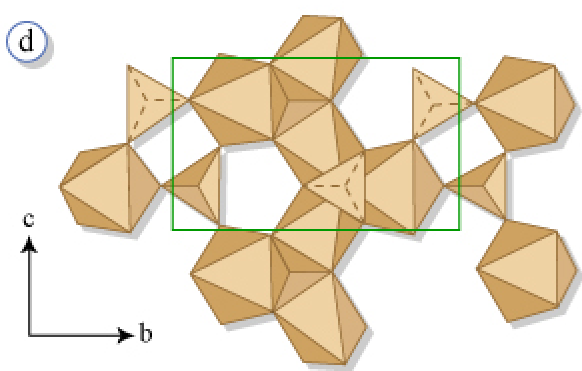
The space group Pbnm projected down the direction. The dotted lines are not glide planes, but only outline the unit cell.



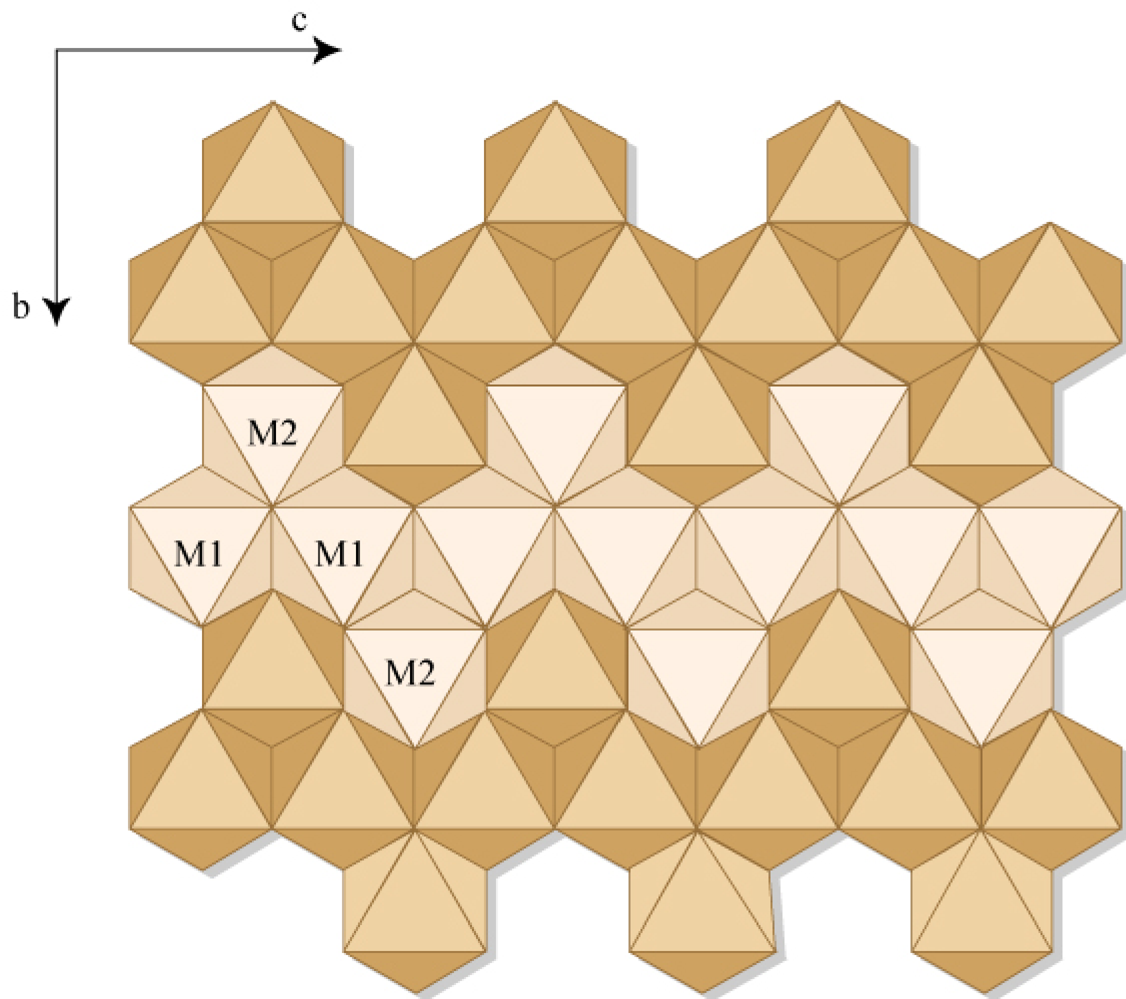
The positions of tetrahedra at the same scale as the space-group projection.



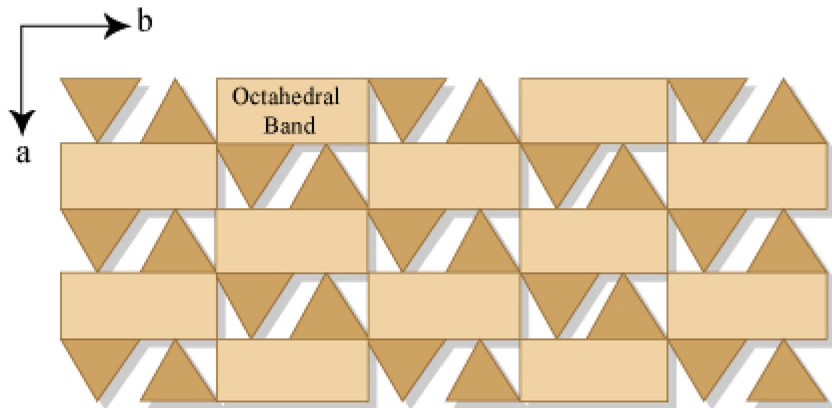
The octahedra band in the same orientation. The smaller octahedra that form the "backbone" of the chain contain M1 sites, while the larger ones that alternate on either side of the chain contain M sites. The octahedra shown contain cations at height x = 0.5. Identical chains fill the void on either side of the central chain shown at heights x = 0 and 1.



The tetrahedra of (b) superimposed on the octahedral chains of (c). The two outer pairs of tetrahedra are in the same layer as the octahedra (the "x = 0.5 layer"), while the two tetrahedra above the octahedral chain are in the "x = 0 layer" and the link that octahedral chain to one directly above in the "x = 0.5 layer" of the next unit cell above.

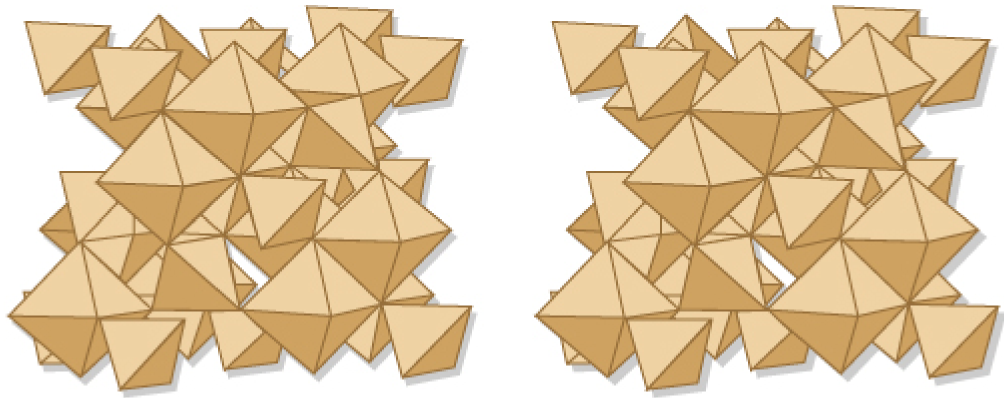


The octahedral chains in olivine, drawn as if the mineral were ideally close packed. Identities of M1 and M2 are indicated. The darker octahedral chains are at height x = 0 and the lighter chain is at height x = 0.5 along the a direction.



A schematic view of the olivine structure projected down the c direction. Rectangles represent the edge-sharing octahedral chain and triangles the independent tetrahedra that share edges and corners with octahedra.

SPINEL
$MgAl_2O_4$
Cubic close packed oxygen structure
|A rotate upper layer by 120º, place on lower layer
|B
|C
Mg tetrahedral, Al octahedral
High symmetry → 3 crystallographically distinct sites: tetrahedral site, octahedral site, anion site
Notated $Mg^{IV}Al_2^{VI}O_4$ (does not follow radius ratio rule)
Structure solved by W.L. Bragg

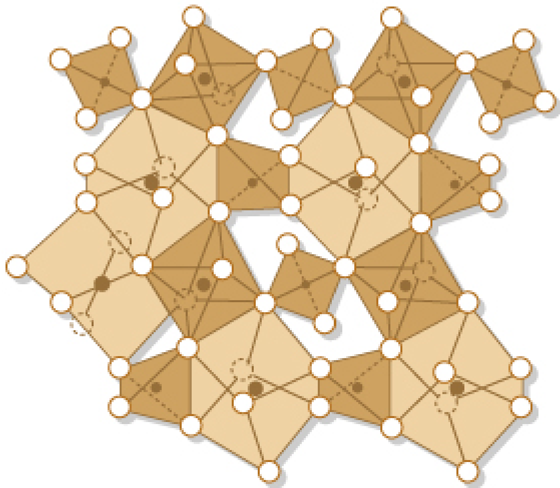


Stereoscopic view of the spinel structure.

Inverse spinels include magnetite and ulvospinel
Ulvospinel $Fe^{IV}(Ti, Fe)_2{}^{VI}O_4$

GARNET (cubic/isometric symmetry)
Common mineral in peridotite and crustal metamorphic rocs
Shows a lot of solid solution chemical variation

A Portion of the Garnet Structure Showing the High Proportion of Shared Polyhedral Edges



1. Yttrogarnet	$Y_3Al_2Al_3O_{12}$
2. Yamatoite	$Mn_3V_2Si_3O_{12}$
3. Goldmanite	$Ca_3V_2Si_3O_{12}$
4. Kimzeyite	$Ca_3Zr_2Al_2SiO_{12}$
5. Ferric-kimzeyite	$Ca_3Zr_2Fe_2SiO_{12}$
6. Uvarovite	$Ca_3Cr_2Si_3O_{12}$
7. Andradite	$Ca_3Fe_2Si_3O_{12}$
8. Pyrope	$Mg_3Al_2Si_3O_{12}$
9. Spessartine	$Mn_3Al_2Si_3O_{12}$
10. Hydrogrossular	$Ca_3Al_2H_{12}O_{12}$
11. Grossular	$Ca_3Al_2Si_3O_{12}$
12. Almandine	$Fe_3Al_2Si_3O_{12}$
13. Schorlomite	$Ca_3Ti_2Fe_2TiO_{12}$
14. Hydrogrossular	$Ca_3Al_2H_{12}O_{12}$
15. Hydroandradite	$Ca_3Fe_2H_{12}O_{12}$
16. Repeat from step number 8	
17. Knorringite (= hanléite)	$Mg_3Cr_2Si_3O_{12}$
18. Repeat from step number 9	
19. Khoharite	$Mg_3Fe_2Si_3O_{12}$
20. Skiagite	$Fe_3Fe_2Si_3O_{12}$
21. Calderite	$Mn_3Fe_2Si_3O_{12}$
22. Blythite	$Mn_3Mn_2Si_3O_{12}$

Pyralspite group
Ugrandite group
Yttrogarnet – "YAG" lasers
At high pressures, pyroxene becomes majorite, a garnet structure