CIDER 2006 Summer Program

Mineral Physics Component

Min Phys 1  Thermodynamics (Lars)
Min Phys 2  Mantle Mineralogy (Lars)
Tutorial 1  Constructing Earth Models (Lars)
Tutorial 2  Melts (Marc)
Min Phys 3  Equation of state and Lattice Dynamics (Tom)
Min Phys 4  Phase Equilibria (Marc)
Min Phys 5  Elasticity (Tom)
Tutorial 3  Equation of state data analysis (Tom)
Min Phys 6  Fluids and Melts (Marc)

Mantle Phases

Wadsleyite (wa); Ringwoodite (ri); akimotoite (ak); Mg-perovskite (mgpv); Ca-perovskite (capv); Ferropericlase (fp)
1. Some simple principles of phase equilibria

2. Some experimental and practical considerations

3. Topical aspects of phase equilibria in and near the transition zone

(But beware: simple thermodynamics can be inconvenient with some EOS)

\[
P = \frac{3}{2} K \left[ \left( \frac{V_0}{V} \right)^{7/3} - \left( \frac{V_0}{V} \right)^{5/3} \right] \left[ 1 - \frac{3}{4} (4 - K') \left( \frac{V_0}{V} \right)^{2/3} - 1 \right]
\]

\[
V(P, T) = V(1, T) \left( 1 + \frac{K' P}{K T} \right)^{1/K'}
\]

S = \int \frac{C}{T} dT - \int \frac{P V_0 dP}{T}

V = V(T, P)

Murnaghan EOS
\[ 0 = \Delta G = \Delta H^0 + \int_{T^0}^{T} \Delta C_p \, dT - T \left[ \Delta S^0 + \int_{T^0}^{T} \frac{\Delta C_p}{T} \, dT \right] + \int_{P^0}^{P} \Delta V \, dP \]

\[ \Delta G = -RT \ln \frac{X_{Mg}^{ol} a_{Mg}^{ol}}{a_{Mg}^{wd} X_{Mg}^{wd}} = -RT \ln \frac{X_{Mg}^{ol} \gamma_{Mg}^{ol}}{X_{Mg}^{wd} \gamma_{Mg}^{wd}} \]

\[ \Delta G = -RT \ln K_D - \frac{RT}{X_{Mg}^{wd}} \ln \frac{X_{Mg}^{ol} \gamma_{Mg}^{ol}}{X_{Mg}^{wd} \gamma_{Mg}^{wd}} \]

\[ RT \ln \gamma_{Mg}^{wd} = W_{FeMg}^{wd} X_{Mg}^{wd} \]

\[ RT \ln \gamma_{Fe}^{wd} = W_{FeMg}^{wd} X_{Mg}^{wd} \]
\[
G'_\text{Anorthite} = G_{\text{Liquid}} + RT \ln \frac{X_{\text{CaFeSi}_3O_8}}{Y_{\text{CaFeSi}_3O_8}}
\]
DIA Press

Why use simple or analogue materials in phase equilibria experiments? (a partial list):

1. To isolate, detect, and characterize the effects of minor phases or components.
2. To reduce problems in experimental design.
3. To obtain results at more tractable temperatures, pressures, etc.
4. To obtain more favorable kinetics.
5. To magnify compositional effects.
6. To reduce the thermodynamic variance of the system.
Fig. 4. Phase relations in pyrolite at 1600 °C determined on the basis of the results of in situ X-ray diffraction experiments. Dashed

Nishiyama et al. 2004 -MgO (Matsui) Pressure Scale

Litasov et al. (2004) Au (Tsuchiya, 2003) pressure scale
Phase Relations of Subducted Crust

Ono et al. (2001)

Mantle Phases

Temperature (K)

Wadsleyite (wa); Ringwoodite (r); akimotoite (ak); Mg-perovskite (mgpv); Ca-perovskite (capv); Ferropericlase (fp)

Atomic Fraction

Depth (km)
Frost, 2003

Frost (2003) 12.5 GPa, 1400 °C
Schmidt and Poli (1998)
Dense Hydrous Magnesian Silicates (DHMS)

<table>
<thead>
<tr>
<th>Minerals</th>
<th>Formula</th>
<th>$\text{H}_2\text{O}$ (wt.%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorite</td>
<td>$\text{Mg}_5\text{Al}_2\text{Si}<em>3\text{O}</em>{10} (\text{OH})_8$</td>
<td>13</td>
</tr>
<tr>
<td>Serpentine</td>
<td>$\text{Mg}_3\text{Si}_2\text{O}_5 (\text{OH})_4$</td>
<td>4.28</td>
</tr>
<tr>
<td>Chondrodite</td>
<td>$\text{Mg}_5\text{Si}_2\text{O}_8 (\text{OH})_2$</td>
<td>5.30</td>
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<tr>
<td>Clinohumite</td>
<td>$\text{Mg}_9\text{Si}<em>4\text{O}</em>{16} (\text{OH})_2$</td>
<td>3</td>
</tr>
<tr>
<td>10 Å Phase</td>
<td>$\text{Mg}_3\text{Si}<em>4\text{O}</em>{14} \text{H}_6$</td>
<td>13</td>
</tr>
<tr>
<td>Phase A</td>
<td>$\text{Mg}_7\text{Si}_2\text{O}_8 (\text{OH})_6$</td>
<td>12</td>
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<tr>
<td>Phase E</td>
<td>$\text{Mg}_2.3\text{Si}_1.25\text{H}_2\text{O}_6$</td>
<td>11.40</td>
</tr>
<tr>
<td>Superhydrous phase B/phase C$^a$</td>
<td>$\text{Mg}_8\text{Si}<em>3\text{O}</em>{14} (\text{OH})_4$</td>
<td>5.80</td>
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<td>Phase D(G)$^a$</td>
<td>$\delta_6$</td>
<td>14.5–18</td>
</tr>
</tbody>
</table>

*Figure 1.* Crystal structure of phase D projected along c. Shaded and unshaded octahedra represent SiO$_4$ and MgO$_6$ octahedra, respectively. Large spheres represent Mg and small ones H.
H$_2$O should thicken 410 km discontinuity

Bercovici and Karato, 2003

Wood, 1995