EOS tutorial — PythEOS

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Acknowledgement: NSF-CSED, NSF-FESD, NSF-EAR, NASA-NExSS, Keck
Goals

• Understanding the EOS parameters

• Solving discrepancies using consistent pressure scales
Questions

• PythEOS — Python

• Tutorial scripts — Jupyter notebook / Jupyter lab
1. Anaconda distribution of python 3.6 is already installed in your VirtualMachine.

2. Start the VirtualMachine.

3. Login as “mineralphysics”.

4. Right click in an empty area of the desktop and “create new … > folder”. Then make a folder, “EOS_ex”.

5. Right click the newly created folder and choose “open in new terminal”

6. Type the following command in the terminal.

   ```
   git clone https://github.com/SHDShim/CIDER2018-ex.git
   ```
P-V-T Equation of State

\[ F_{\text{total}} = F_{\text{st}} + F_{\text{vib}} + F_{\text{elec}} \]

\[ P(V, T) = P_{\text{st}}(V, T_0) + \Delta P_{\text{th}}(V, T) \]
$P-V-T$ EOS

Bridgmanite
$P-V-T$ EOS
$P-V-T$ EOS

![Graph showing the relationship between pressure ($P$) and volume ($V$) at different temperatures ($T$). The graph includes lines for temperatures of 300 K, 1000 K, 2000 K, 3000 K, and 4000 K. The $P_{total}$ label indicates the total pressure as a function of pressure (GPa).]
$P-V-T$ EOS

![Graph showing $P-V$ relations with different temperatures.

- $P_{st}$
- $P_{th}$

Pressure (GPa) vs. \( V/V_0 \) for temperatures 300 K, 1000 K, 2000 K, 3000 K, and 4000 K.]
Parameters

\[ P_{st} = f(V \mid V_0, K_0, K'_0) \]

\[ \Delta P_{th} = f(V, T \mid \gamma_0, q, \theta_0) \]
Understanding the EOS parameters

0-eos.ipynb
Running Jupyter Lab

$ cd ~

$ source activate root

$ jupyter lab
Jupyter Lab

- Code cell
- Markdown cell
- Code, table, figures, animations, equations, bibliography, ..., all together in one document.
- Reproducibility and transparency
Shortcut Keys to Remember

• Shift + Enter

• Option + Enter

• Command + Enter

• Esc + m

• Esc + y
Interactive notebooks: Sharing the code

The free IPython notebook makes data analysis easier to record, understand and reproduce.

Helen Shen

05 November 2014
Experiments

- Infrared laser beam
- Re gasket
- Sample + $^{56}$Fe metal
- Ar or Ne medium
- Spacer
P-V-T Equation of State

\[ P(V, T) = P_{st}(V, T_0) + \Delta P_{th}(V, T) \]
Popular Pressure Scales

- MgO, Pt, Au, NaCl, KCl, Ne, Ar …
- Ruby, Diamond, …

- Are they all consistent with each other?
- Which one is accurate?
Gold


- Which one to use?
Can I reproduce them?

### Table 1

Thermodynamic parameters of gold

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_0$ (Å³)</td>
<td>67.850 ± 0.004</td>
<td>[27]</td>
</tr>
<tr>
<td>$K_{OT}$ (GPa)</td>
<td>167 ± 3</td>
<td>[20-23]</td>
</tr>
<tr>
<td>$K'_{OT}$</td>
<td>5.0 ± 0.2</td>
<td>This study</td>
</tr>
<tr>
<td>$\gamma_0$</td>
<td>2.97 ± 0.05</td>
<td>[18]</td>
</tr>
<tr>
<td>$q$</td>
<td>1.0 ± 0.1</td>
<td>This study</td>
</tr>
<tr>
<td>$\theta_0$</td>
<td>170</td>
<td>[18]</td>
</tr>
<tr>
<td>$\beta n$ (J/gK)</td>
<td>0.125</td>
<td>[15]</td>
</tr>
<tr>
<td>$c_0$ (km/s)</td>
<td>3.10 ± 0.02</td>
<td>This study</td>
</tr>
<tr>
<td>$s$</td>
<td>1.525 ± 0.008</td>
<td>This study</td>
</tr>
</tbody>
</table>

### Table 2

Pressure (in GPa) at selected compressions and temperatures using the gold EOS from this study

<table>
<thead>
<tr>
<th>$1 - V/V_0$</th>
<th>300 K</th>
<th>500 K</th>
<th>1000 K</th>
<th>1500 K</th>
<th>2000 K</th>
<th>2500 K</th>
<th>3000 K</th>
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</thead>
<tbody>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>1.42</td>
<td>4.99</td>
<td>8.56</td>
<td>12.14</td>
<td>15.72</td>
<td>19.30</td>
</tr>
<tr>
<td>0.02</td>
<td>3.55</td>
<td>4.97</td>
<td>8.53</td>
<td>12.11</td>
<td>15.69</td>
<td>19.26</td>
<td>22.84</td>
</tr>
<tr>
<td>0.04</td>
<td>7.55</td>
<td>8.96</td>
<td>12.53</td>
<td>16.11</td>
<td>19.68</td>
<td>23.26</td>
<td>26.84</td>
</tr>
<tr>
<td>0.06</td>
<td>12.06</td>
<td>13.48</td>
<td>17.04</td>
<td>20.62</td>
<td>24.19</td>
<td>27.77</td>
<td>31.35</td>
</tr>
<tr>
<td>0.08</td>
<td>17.16</td>
<td>18.57</td>
<td>22.13</td>
<td>25.71</td>
<td>29.28</td>
<td>32.86</td>
<td>36.44</td>
</tr>
<tr>
<td>0.10</td>
<td>22.91</td>
<td>24.32</td>
<td>27.88</td>
<td>31.45</td>
<td>35.03</td>
<td>38.61</td>
<td>42.19</td>
</tr>
<tr>
<td>0.12</td>
<td>29.42</td>
<td>30.82</td>
<td>34.38</td>
<td>37.95</td>
<td>41.53</td>
<td>45.10</td>
<td>48.68</td>
</tr>
<tr>
<td>0.14</td>
<td>36.77</td>
<td>38.17</td>
<td>41.73</td>
<td>45.30</td>
<td>48.88</td>
<td>52.45</td>
<td>56.03</td>
</tr>
<tr>
<td>0.16</td>
<td>45.11</td>
<td>46.50</td>
<td>50.06</td>
<td>53.63</td>
<td>57.20</td>
<td>60.78</td>
<td>64.35</td>
</tr>
<tr>
<td>0.18</td>
<td>54.56</td>
<td>55.95</td>
<td>59.50</td>
<td>63.07</td>
<td>66.64</td>
<td>70.22</td>
<td>73.80</td>
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<tr>
<td>0.20</td>
<td>65.29</td>
<td>66.68</td>
<td>70.22</td>
<td>73.79</td>
<td>77.37</td>
<td>80.94</td>
<td>84.52</td>
</tr>
<tr>
<td>0.22</td>
<td>77.50</td>
<td>78.89</td>
<td>82.43</td>
<td>85.99</td>
<td>89.57</td>
<td>93.14</td>
<td>96.72</td>
</tr>
<tr>
<td>0.24</td>
<td>91.42</td>
<td>92.80</td>
<td>96.33</td>
<td>99.90</td>
<td>103.47</td>
<td>107.05</td>
<td>110.62</td>
</tr>
<tr>
<td>0.26</td>
<td>107.32</td>
<td>108.69</td>
<td>112.22</td>
<td>115.78</td>
<td>119.35</td>
<td>122.93</td>
<td>126.50</td>
</tr>
<tr>
<td>0.28</td>
<td>125.51</td>
<td>126.87</td>
<td>130.40</td>
<td>133.96</td>
<td>137.53</td>
<td>141.10</td>
<td>144.68</td>
</tr>
<tr>
<td>0.30</td>
<td>146.38</td>
<td>147.73</td>
<td>151.25</td>
<td>154.81</td>
<td>158.38</td>
<td>161.95</td>
<td>165.53</td>
</tr>
<tr>
<td>0.32</td>
<td>170.38</td>
<td>171.73</td>
<td>175.24</td>
<td>178.79</td>
<td>182.36</td>
<td>185.93</td>
<td>189.51</td>
</tr>
<tr>
<td>0.34</td>
<td>198.07</td>
<td>199.40</td>
<td>202.90</td>
<td>206.46</td>
<td>210.02</td>
<td>213.59</td>
<td>217.17</td>
</tr>
</tbody>
</table>
PythEOS

- Accurate calculation of pressure scales
- Conversion of pressures
- Equation of state fit
- Error propagation
Can we resolve the discrepancies among different mineral physics datasets?

d-Mantle_Boundaries.ipynb
Estimating CMB temperature

Tateno 2009
Matching EOSs

Figure 4. Differences in pressure among the Pt (red), Au (blue), and MgO (dashed lines at 0) scales at 300 K and high pressure. (a) Au-F07, Pt-F07, and MgO-S01; (b) Au-, Pt-, and MgO-D07; (c) Au-Y09, Pt-Y09, and MgO-T09; and (d) Au-, Pt-, and MgO-D15. The error bars are the 1σ uncertainties estimated from the uncertainties in the measured unit cell volume and the uncertainties of the thermoelastic properties provided in the original papers.

Ye et al. 2017 JGR
Other Uncertainty Sources

• Stress conditions
• Temperature conditions
• Extreme thermal contribution — electronic contribution in metal pressure standards
Can use of different pressure scale affect the EOS fitting result?

b-8_pv_eos_fit_multi-scales.ipynb
Parameters to Fit

\[ V_0, K_0, K'_0 \]
Example: Isotherm Fitting

SiC, Nisr et al., in prep.
Example: Isotherm Fitting

Strong correlation between $K_0$ and $K_0'$. SiC, Nisr et al., in prep.
Can use of different pressure scale affect the EOS fitting result?

c-10_pvt-eos_fit.ipynb
Parameters to Fit

\[ V_0, K_0, K'_0 \]
\[ \gamma_0, q, \theta_0 \]
Table 1. Model parameters for the equations of state of NaCl-B2, Solid Ne, Au, and Pt

<table>
<thead>
<tr>
<th>Parameters</th>
<th>NaCl-B2*</th>
<th>Ne*</th>
<th>Au†</th>
<th>Pt‡</th>
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<tr>
<td>$V_0$, Å³</td>
<td>41.35</td>
<td>88.967</td>
<td>67.850(4)</td>
<td>60.38(1)</td>
</tr>
<tr>
<td>$K_0$, GPa (Vinet)</td>
<td>26.86(2.90)</td>
<td>1.16(14)</td>
<td>167</td>
<td>277</td>
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<td>$K_0$ (Vinet)</td>
<td>5.25(26)</td>
<td>8.23(31)</td>
<td>6.00(2)</td>
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<td>$K_0$, GPa (B-M)</td>
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</tr>
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<td>290</td>
<td>75.1</td>
<td>170</td>
<td>230</td>
</tr>
<tr>
<td>$\gamma_0$</td>
<td>1.70</td>
<td>2.05</td>
<td>2.97(3)</td>
<td>2.72(3)</td>
</tr>
<tr>
<td>$q_0$</td>
<td>0.5(3)</td>
<td>0.6(3)</td>
<td>0.6(3)</td>
<td>0.5(5)</td>
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Fei et al. (2007)
## Caution

Do not mix equations and fitting results

---

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<td>$\eta_0$</td>
<td>0.5(3)</td>
<td>0.6(3)</td>
<td>0.6(3)</td>
<td>0.5(5)</td>
</tr>
</tbody>
</table>

Fei et al. (2007)
How can I reproduce pressure calculations?

a-6_p_scale_test_Speziale_MgO.ipynb