EOS tutorial — PythEOS

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Goals

- Understanding the EOS parameters
- Solving discrepancies using consistent pressure scales

Questions

- PythEOS — Python
- Tutorial scripts — Jupyter notebook / Jupyter lab

Tutorial Materials

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.

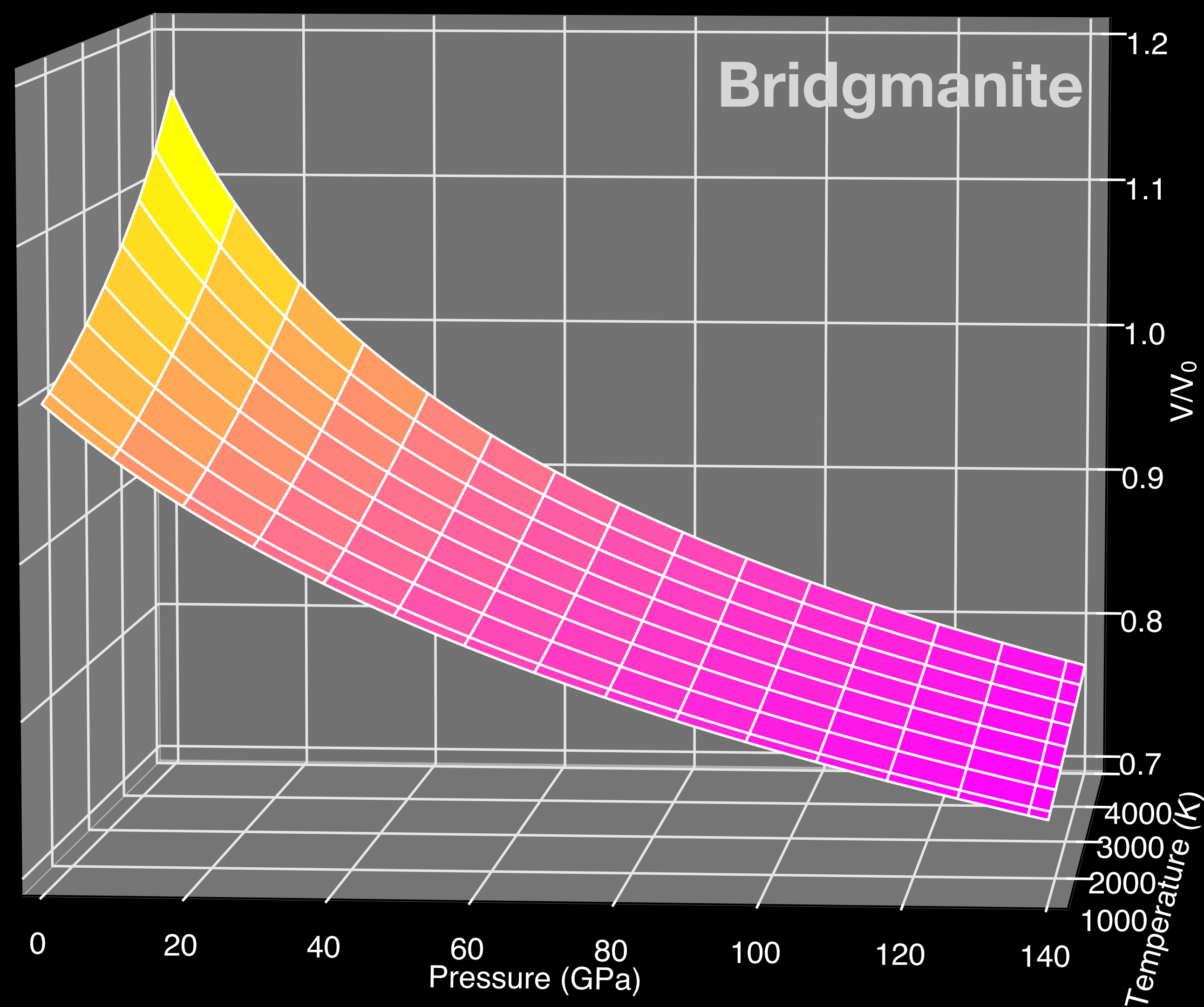
```
git clone https://github.com/SHDShim/CIDER2018-ex.git .
```

P-V-T Equation of State

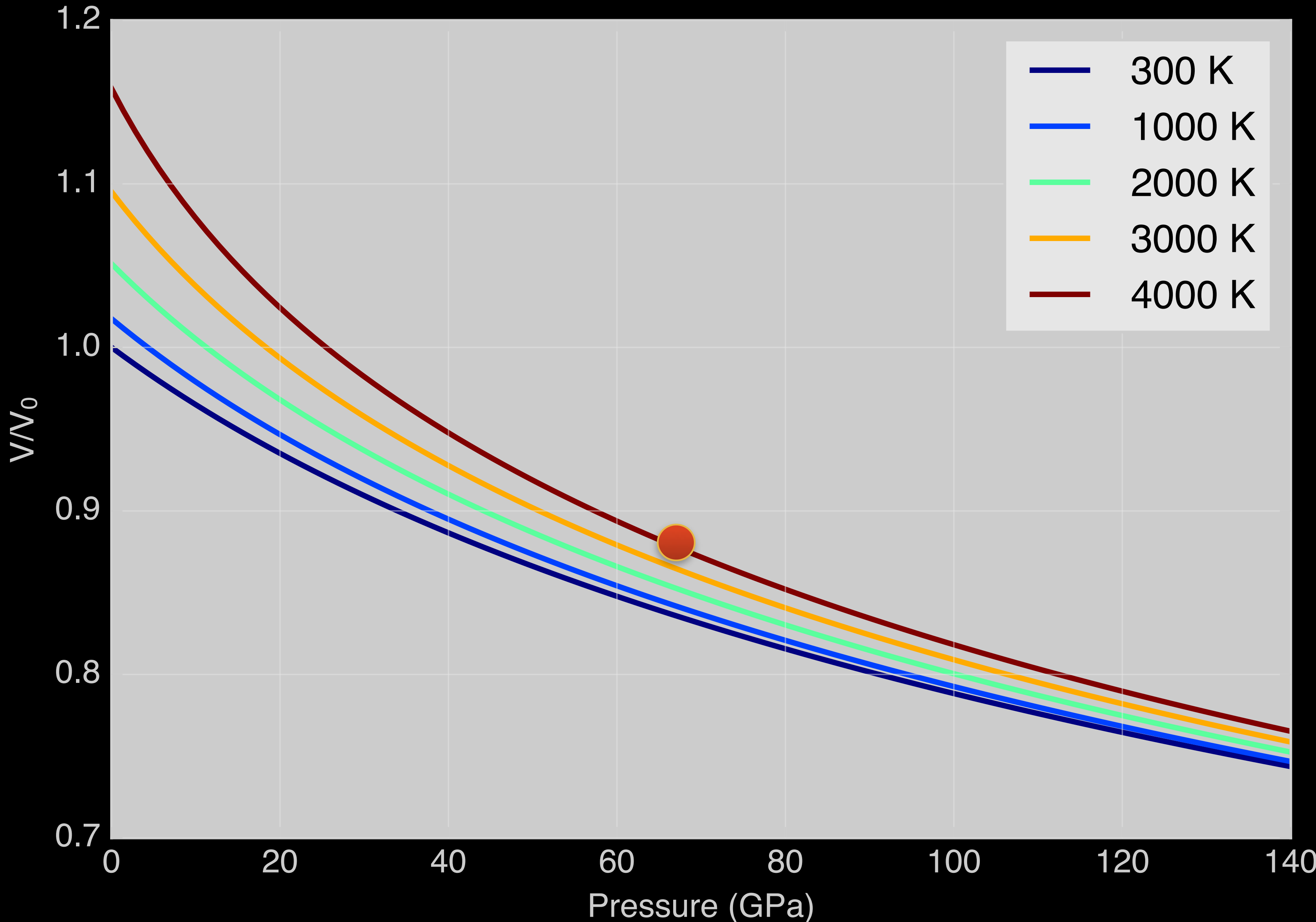
$$F_{total} = F_{st} + F_{vib} + F_{elec}$$

$$P(V,T) = P_{st}(V,T_0) + \Delta P_{th}(V,T)$$

$P-V-T$ EOS


Bridgmanite
1.2
1.1
1.0
0.9
0.8
0.7
V/V0
4000
3000
2000
1000
Temperature (K)
0
20
40
60
80
100
120
140
Pressure (GPa)

$P-V-T$ EOS



300 K
1000 K
2000 K
3000 K
4000 K
1.2
1.1
1.0
0.9
0.8
0.7
V/V0
0
20
40
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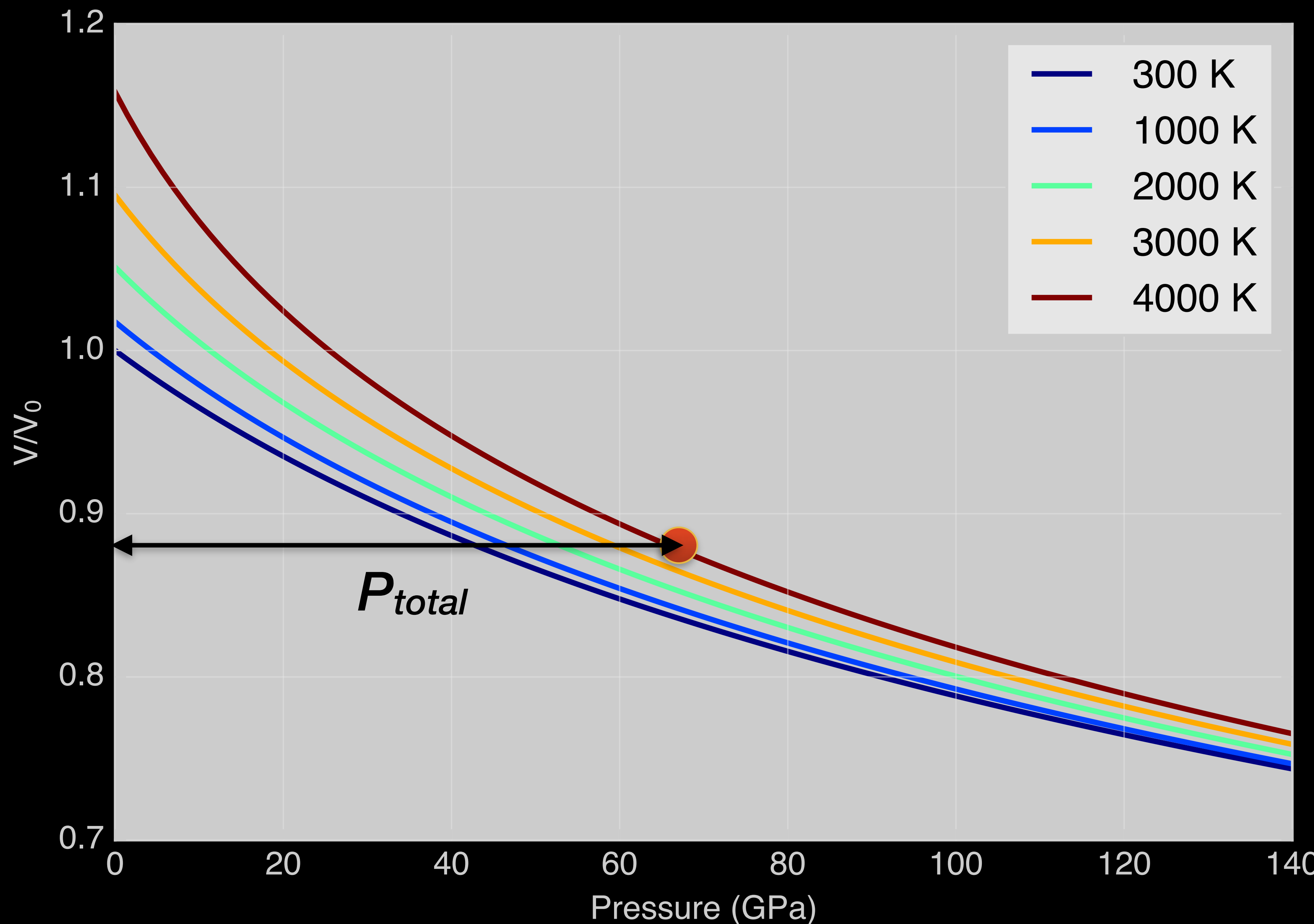
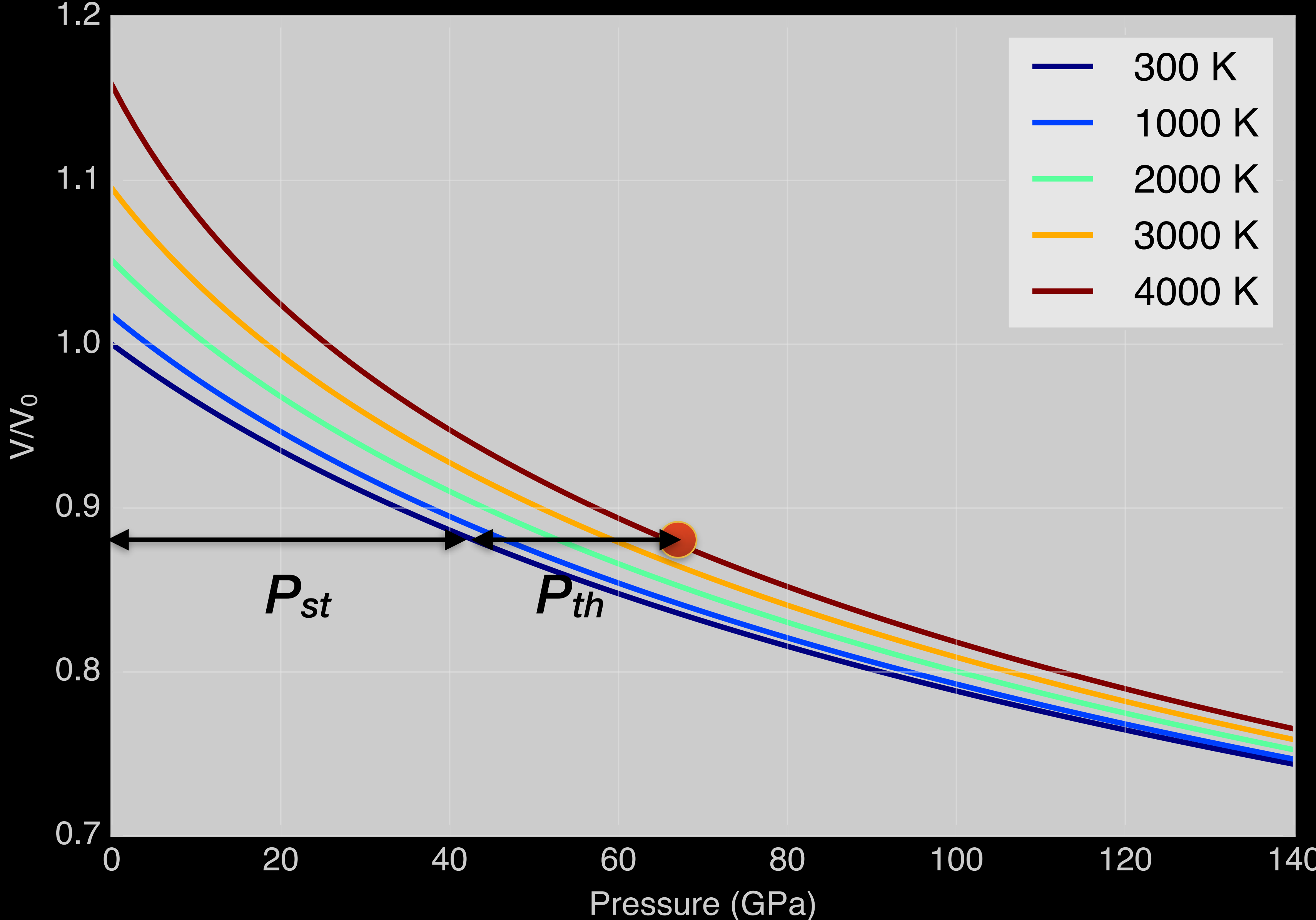
140
Pressure (GPa)

P—V—T EOS



1.2
1.1
1.0
0.9
0.8
0.7
V/V0
0
20
40
60
80
100
120
140
Pressure (GPa)
300 K
1000 K
2000 K
3000 K
4000 K
Ptotal

$P-V-T$ EOS



300 K
1000 K
2000 K
3000 K
4000 K
P_{st}
P_{th}
V/V0
Pressure (GPa)
1.2
1.1
1.0
0.9
0.8
0.7
0
20
40
60
80
100
120
140

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

NATURE | TOOLBOX

Interactive notebooks: Sharing the code

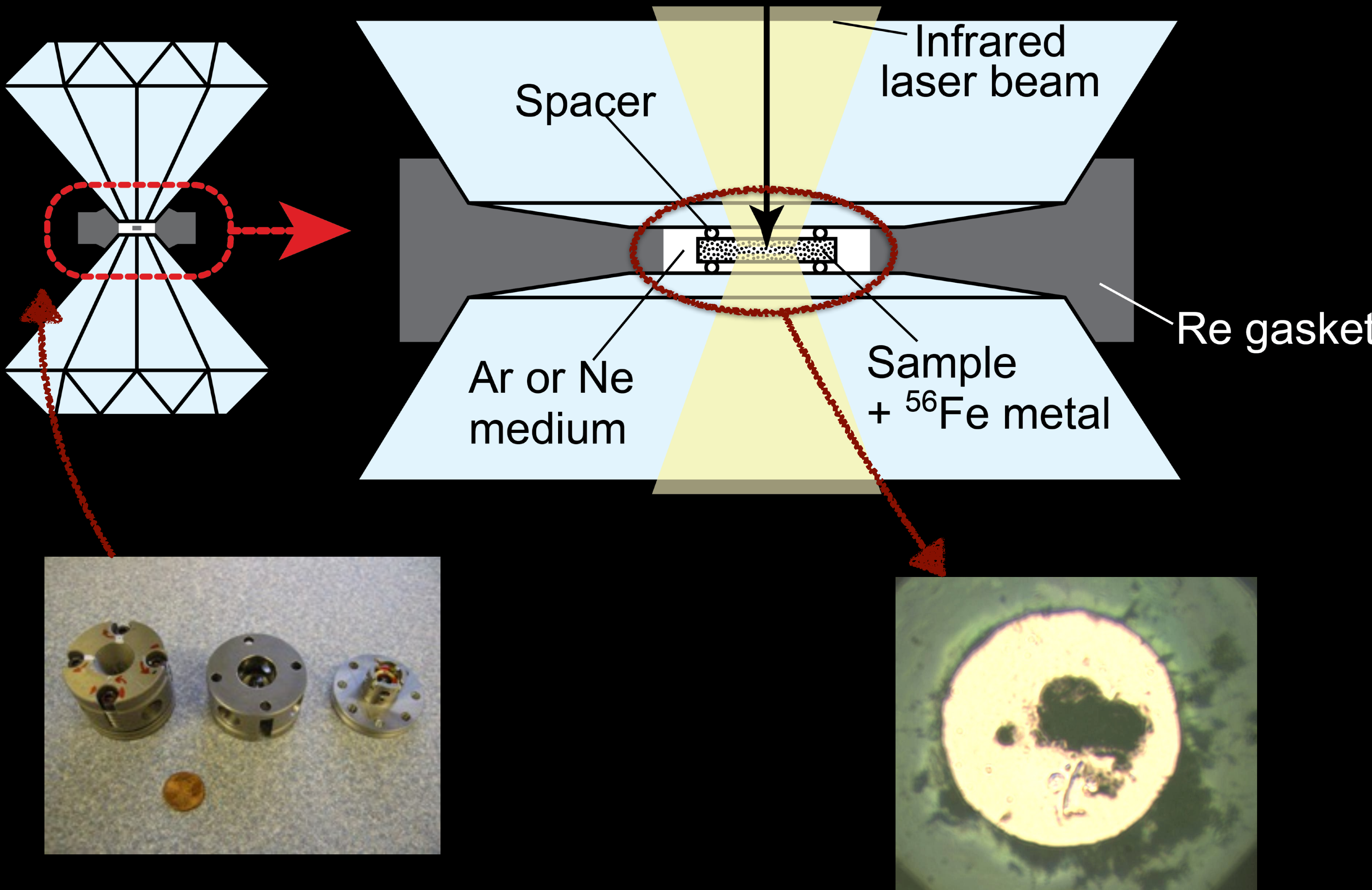
The free IPython notebook makes data analysis easier to record, understand and reproduce.

Helen Shen

05 November 2014

PDF | Rights & Permissions

Experiments



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

- Jamieson (1982), Heinz (1984), Anderson (1989), Shim (2002), Tsuchiya (2003), Dorogokupets (2007, 2015), Ye (2017), …..

- Which one to use?

Table 1
Thermodynamic parameters of gold

Parameter		References
V_0 (Å^3)	67.850 ± 0.004	[27]
K_{0T} (GPa)	167 ± 3	[20–23]
K'_{0T}	5.0 ± 0.2	This study
γ_0	2.97 ± 0.05	[18]
q	1.0 ± 0.1	This study
θ_0 (K)	170	[18]
$3nk$ (J/gK)	0.125	[15]
c_0 (km/s)	3.10 ± 0.02	This study
s	1.525 ± 0.008	This study

Can I reproduce them?

Table 2
Pressure (in GPa) at selected compressions and temperatures using the gold EOS from this study

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

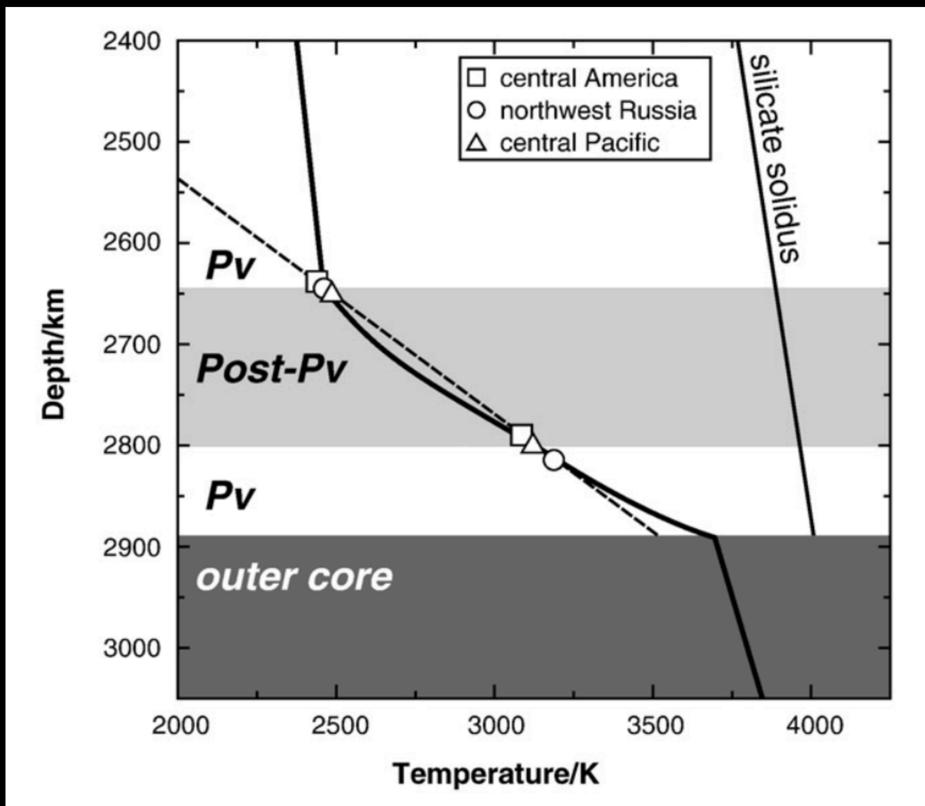
PythEOS

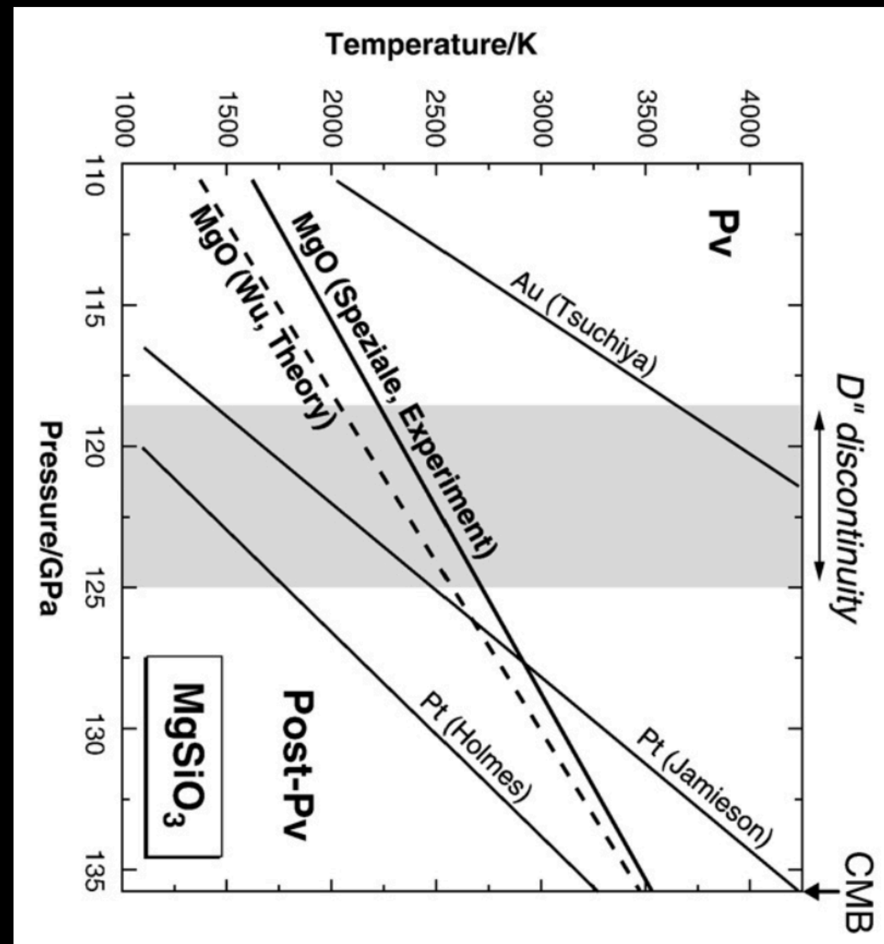
- Accurate calculation of pressure scales
- Conversion of pressures
- Equation of state fit
- Error propagation

Can we resolve the discrepancies among different mineral physics datasets?

d-Mantle_Boundaries.ipynb

Estimating CMB temperature





Tateno 2009

Matching EOSs

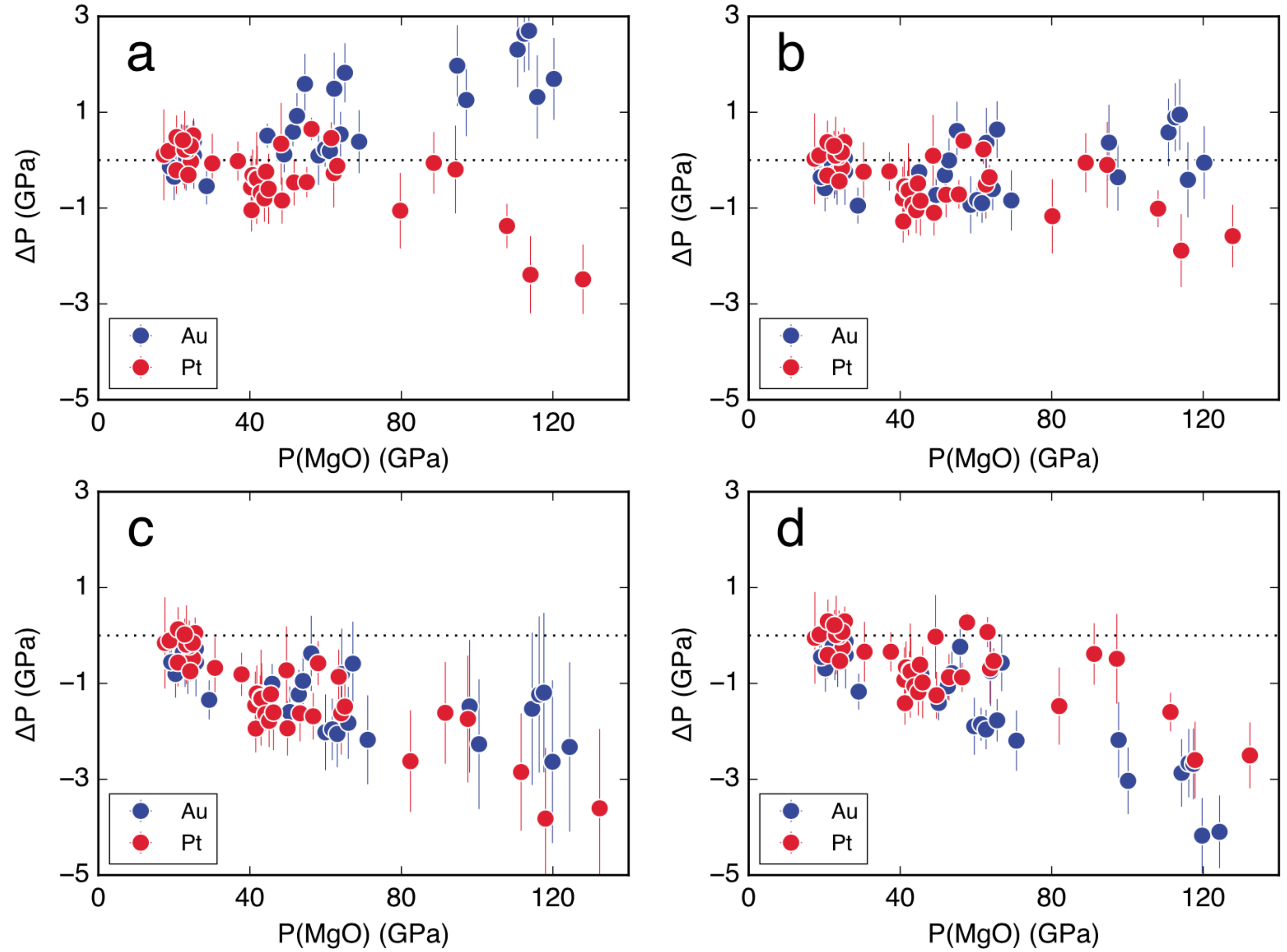


Figure 4. Differences in pressure among the Pt (red), Au (blue), and MgO (dashed lines at 0) scales at 300 K and high pressure. (a) Au-F07, Pt-F07, and MgO-S01; (b) Au-, Pt-, and MgO-D07; (c) Au-Y09, Pt-Y09, and MgO-T09; and (d) Au-, Pt-, and MgO-D15. The error bars are the 1σ uncertainties estimated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

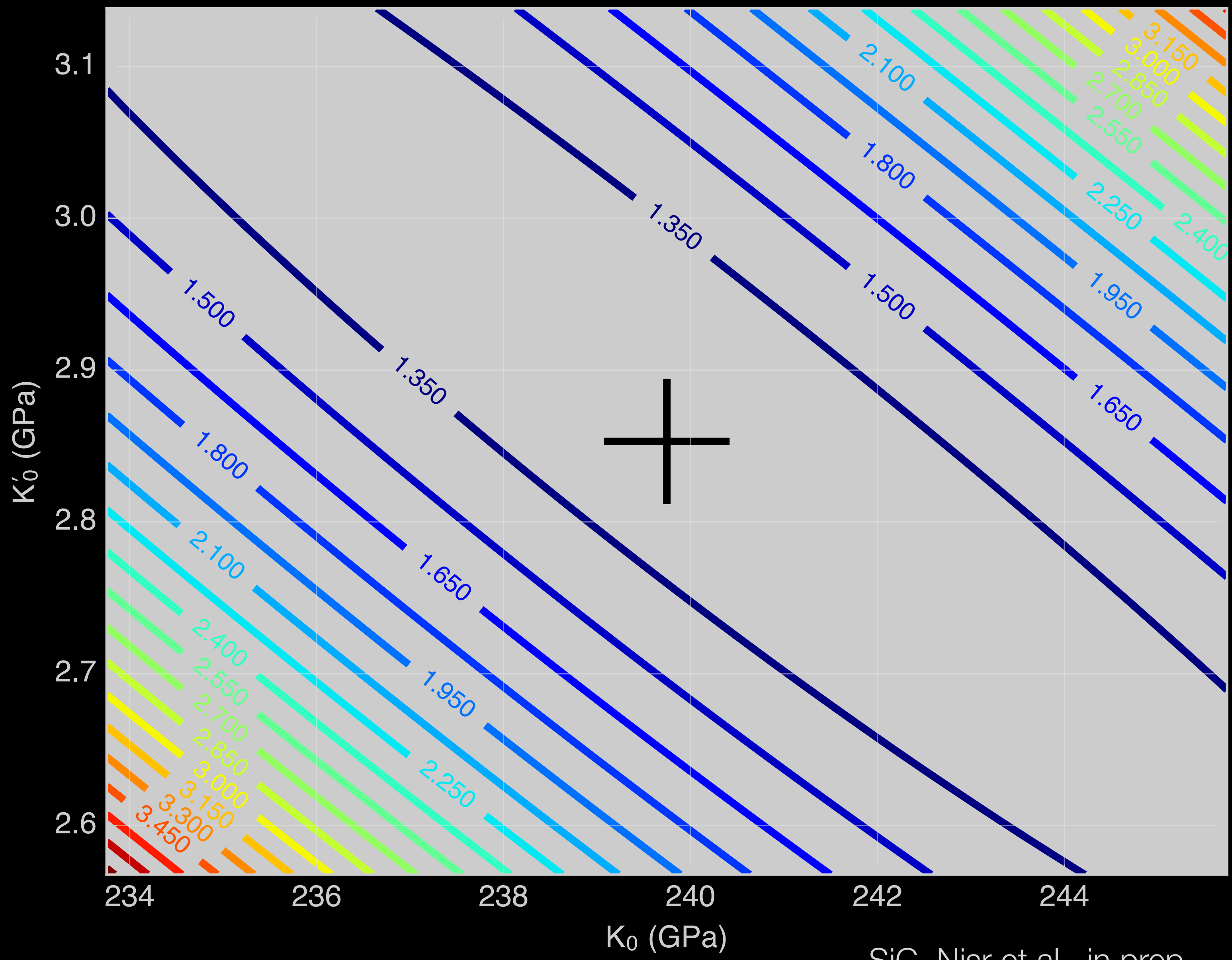
Can use of different pressure scale affect the EOS fitting result?

b-8_pv_eos_fit_multi-scales.ipynb

Parameters to Fit

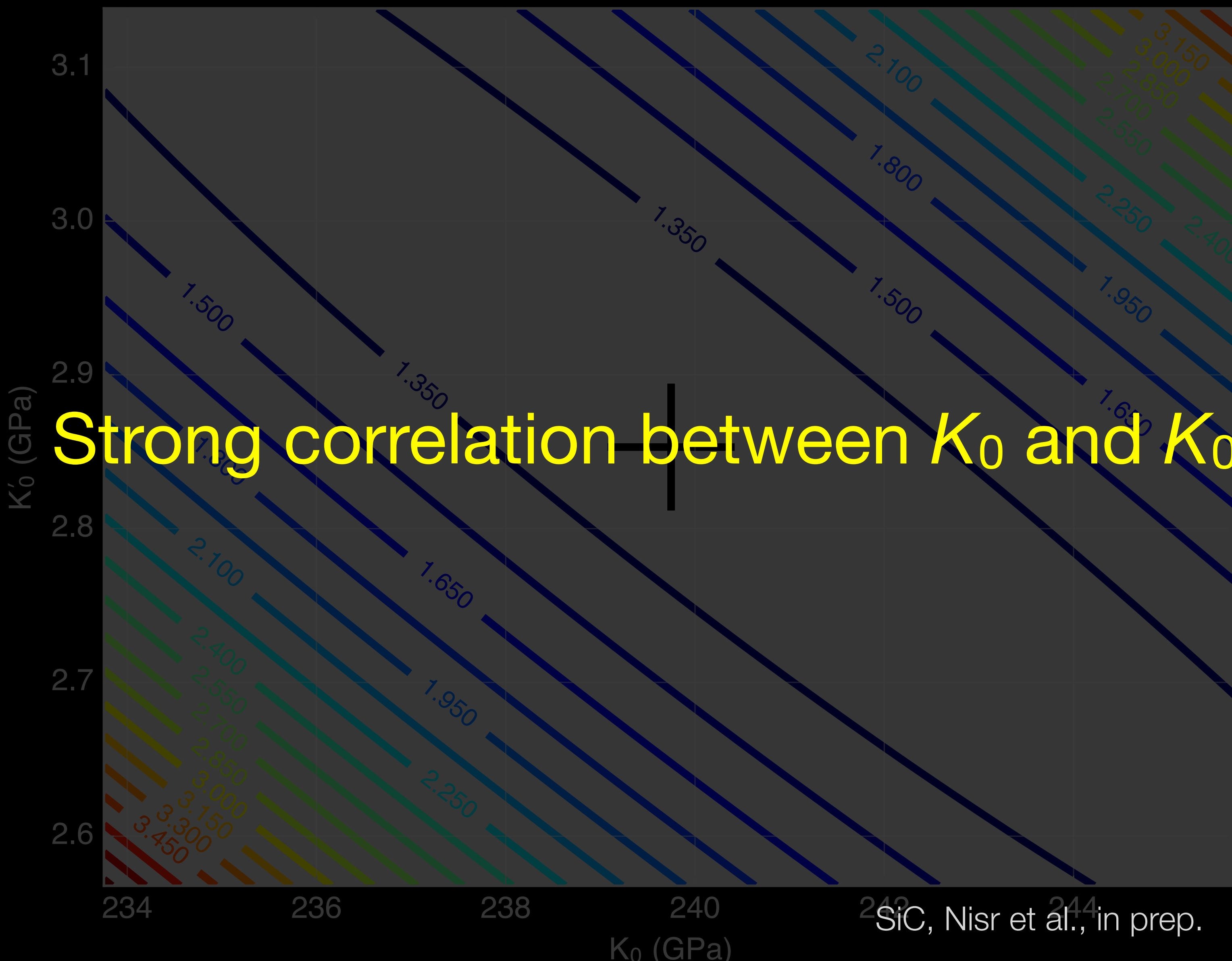
$$V_0, K_0, K'_0$$

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

$$V_0, K_0, K'_0$$

$$\gamma_0, q, \theta_0$$

Caution

Table 1. Model parameters for the equations of state of NaCl-B2, Solid Ne, Au, and Pt

Parameters	NaCl-B2*	Ne*	Au†	Pt‡
V_0, Å^3	41.35	88.967	67.850(4)	60.38(1)
K_{0T}, GPa (Vinet)	26.86(2.90)	1.16(14)	167	277
K'_{0T} (Vinet)	5.25(26)	8.23(31)	6.00(2)	5.08(2)
K_{0T}, GPa (B-M)	30.69(2.90)	1.43(14)	167	277
K'_{0T} (B-M)	4.33(26)	8.02(31)	5.77(2)	4.95(2)
θ_0, K	290	75.1	170	230
γ_0,	1.70	2.05	2.97(3)	2.72(3)
q_0	0.5(3)	0.6(3)	0.6(3)	0.5(5)

Fei et al. (2007)

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γ_0,	1.70	2.05	2.97(3)	2.72(3)
q_0	0.5(3)	0.6(3)	0.6(3)	0.5(5)

Do not mix equations and fitting results

Fei et al. (2007)

How can I reproduce pressure calculations?

a-6_p_scale_test_Speziale_MgO.ipynb