Geochemistry, Geophysics, Geosystems

Supporting Information for

Disproportionation of iron in almandine-pyrope garnet from 25 to 65 GPa

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Text S1 PerpleX modifications

In order to be able to use PerpleX for predictions of Fe disproportionation as a result of incorporation of an $FeAlO_3$ component in bridgmanite, we had to modify several of the input files needed to run PerpleX. PerpleX is an open-source software available on https://www.perplex.ethz.ch/. We use release version 6.8.9. We added four new phases to the thermodynamic database of Stixrude & Lithgow-Bertelloni (2022): hematite, $FeAlO_3$ (bridgmanite), fcc Fe, and hcp Fe. Parameters for these phases are given in Table S1. For the $FeAlO_3$ Gibbs free energy, we assumed ideal mixing and selected a value to match the results of Liu et al. (2020), which include measurements of the components of bridgmanites of varying composition along the $MgSiO_3$-$FeAlO_3$ join. For hcp and fcc Fe parameters, we fit the PerpleX EOS6 to the data of Dewaele et al. (2006) and Tsujino et al. (2013), respectively. To assign Gibbs Free Energy values for hcp and fcc Fe, we chose values that would match the phase boundary of Komabayashi et al. (2009).

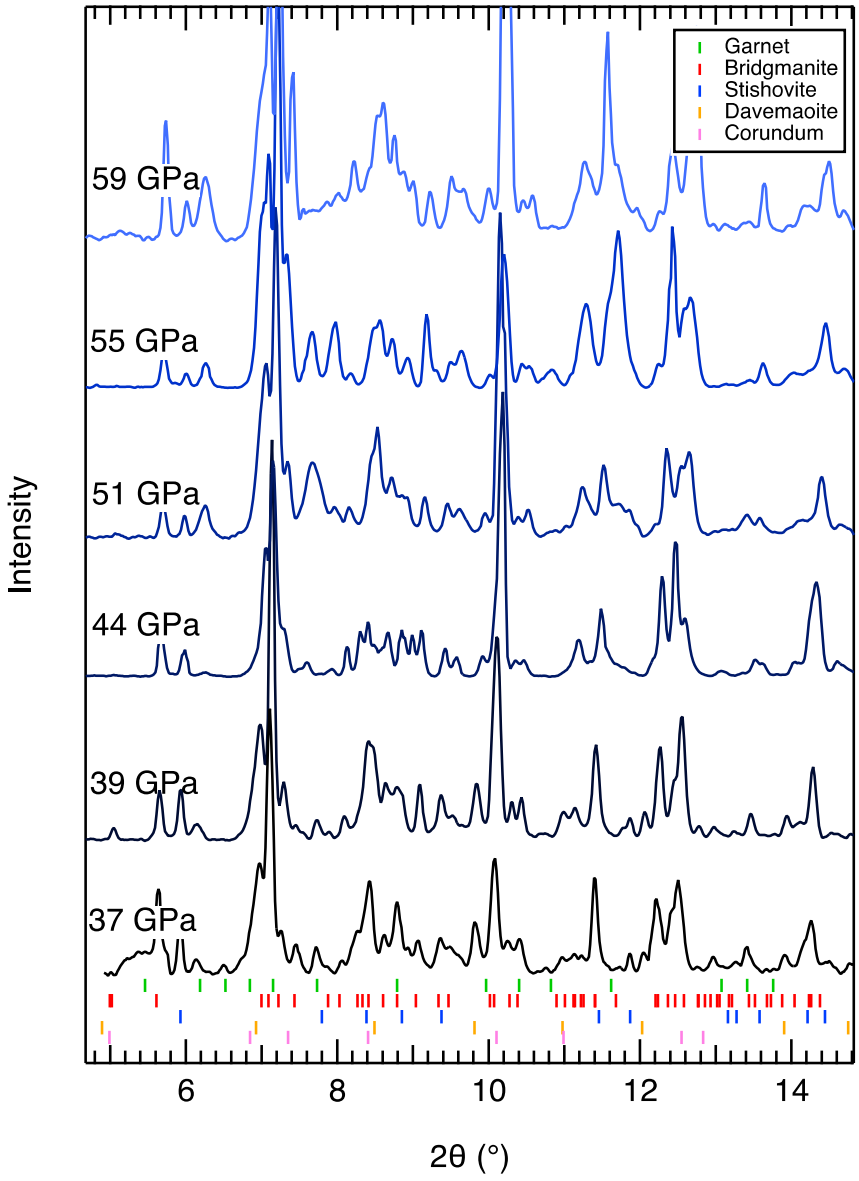

Figure S1. XRD patterns collected at 42 keV on samples with no Ir foils. Pressures given are post-quench based on diamond Raman or stishovite peak.

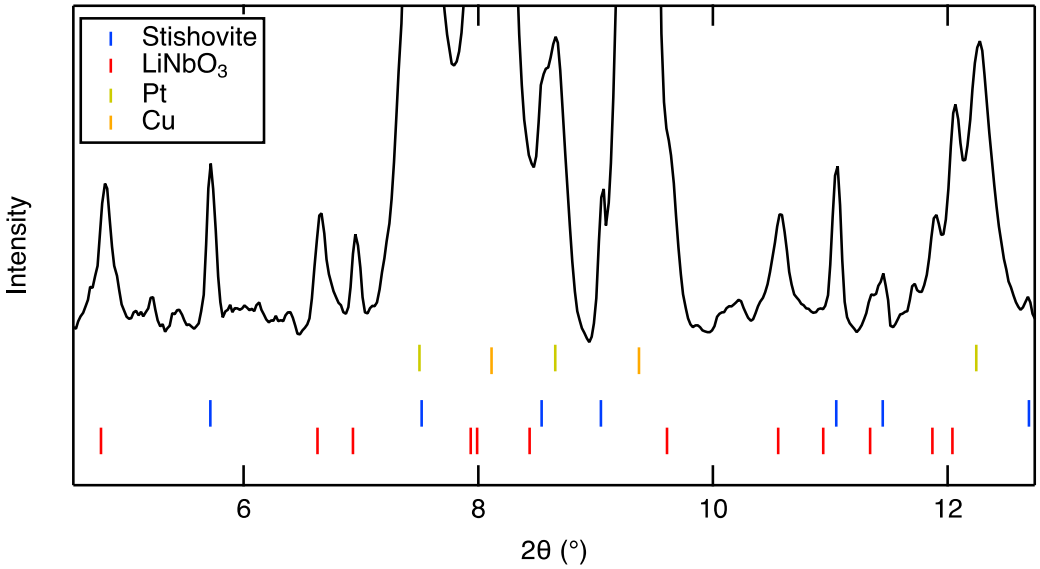

Fig. S2. Example XRD pattern from the K11 thin section XRD map in which the stishovite and $LiNbO_3$ phases are present. X-ray spot size is 2x3 μm.

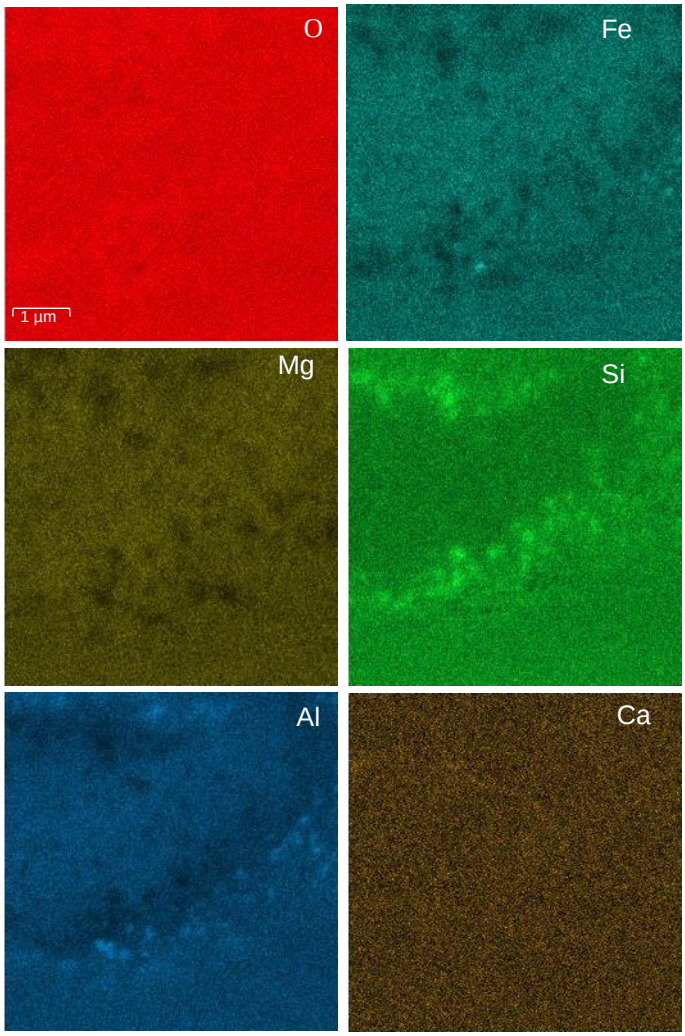

Fig. S3. EDS maps collected at 5 kV on a portion of the laser-heated spot in sample K54 (indicated with dashed box in Fig. 6).

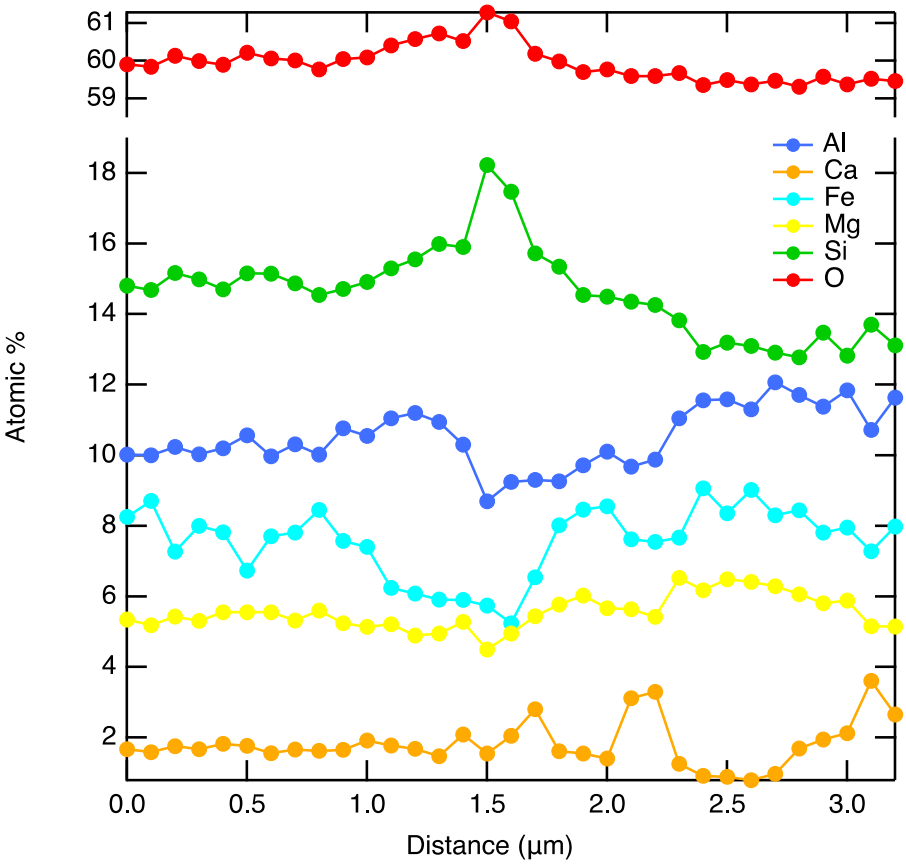

Fig. S4. Line scan collected across the laser-heated spot in K54 at 5 keV. Line corresponds to arrow in Fig. 6 and travels from the center to the edge of the laser heated spot.

Element	Atomic %
Mg	5.03
Al	9.87
Si	15
Ca	1.85
Mn	0.28
Fe	7.97
O	59.98

Table S1. WDS measurements on the natural almandine-pyrope garnet.

Parameter	PerpleX variable	hematite	$FeAlO_3$ bridgmanite	fcc Fe[6]	hcp Fe[7]
EoS		6	6	6	6
F_0 [J/mol]	G0	-743740.7[1]	-1180000	0	-150
-# atoms pfu	S0	-5	-5	-1	-1
$-V_0$ [J/bar]	V0	-3.027[1]	-2.768[3]	-6.859	-6.710
K_0 [bar]	c1	1996000[1]	2070000[3]	1685000	1650000
K’	c2	4.0[1]	3.73[3]	4.724	4.97
T_D [K]	c3	551.6762[2]	858.26509[4]	340	417
g_0	c4	1.8970[2]	1.54222[4]	2.650	2.431114
q_0	c5	1	0.84088[4]	1	1

1. Holland & Powell (2002)
2. Holland & Powell (2011)
3. Myhill (2018)
4. Stixrude & Lithgow-Bertelloni (2021) (same as values for Al bdm endmember)
5. Tsujino et al. (2013)
6. Dewaele et al. (2006)

Table S2. Parameters used for modified thermodynamic database in PerpleX modeling in this work.