Document S2 (Pseudosection modeling)

Supplementary material for:

Various antiphase domains in garnet-hosted omphacite in low temperature eclogite: A FIB–TEM study on heterogeneous ordering processes

Ryo Fukushima[1], Tatsuki Tsujimori[1,2], Nobuyoshi Miyajima[3]

[1] Graduate School of Science, Tohoku University, Sendai 980-8578, Japan
[2] Center for Northeast Asian Studies, Tohoku University, Sendai 980-8576, Japan
[3] Bayerisches Geoinstitut, Universität Bayreuth, 95440 Bayreuth, Germany

Corresponding author: Ryo Fukushima
E-mail address: ryo.fukushima.p7@dc.tohoku.ac.jp
Address: Graduate School of Science, Tohoku University, 41 Kawauchi, Aoba, Sendai 980-8578, Japan
Phone/Fax: +81-22-795-6236

Journal: American Mineralogist

Pseudosection modeling

In order to confirm omphacite can be formed simultaneously with growth of the garnet (core: $prp_5alm_{67}sps_3grs_{24}$, rim: $prp_8alm_{61}sps_2grs_{30}$), we simulated it with pseudosection modeling by considering a prograde metamorphic path and fractional crystallization of the garnet. For simplicity, we neglected thermal overstepping of garnet nucleation. We used the software Theriak-Domino (de Capitani and Brown 1987; de Capitani and Petrakakis 2010) and thermodynamic data of Holland and Powell (1998). Mixing models are shown in Table S2. The whole rock composition of Syros eclogite was obtained by calculating an average of some eclogite compositions in Laurent et al. (2018) (Table S3). We chose a water-saturated MnNCKFMASHO + Ti + CO_2 system. An activity of CO_2 was fixed to 0.03 (Schumacher et al. 2008).

First of all, assuming that the garnet grew earliest in the eclogite, we started with estimating the *P*–*T* condition under which the garnet core was thermodynamically stable. We found that the *P*–*T* condition under which the garnet core had nucleated was at (~500°C, 2.0 GPa). Then an imaginary *P*–*T* path from (~500°C, 2.0 GPa) to (~530°C, 2.2 GPa) was set to define the garnet-fractionated bulk composition. Finally, we obtained the final condition at (~550°C, 2.5 GPa). It should be noted that the final condition is calculated without CO_2 so that we can obtain a reasonable value of pressure there. The estimated *P*–*T* path is similar to the *P*–*T* paths of Trotet et al. (2001) and Laurent et al. (2018).

We then calculated changes in amount of pyroxene and its end-members as garnet grew (Figs. S2 and S3). Our estimation shows that the amount of pyroxene approximately increases and the hedenbergite concentration decreases during the rim growth.

Table S2. Mixing models used in the pseudosection modeling.

Phase	Model
Garnet: [Mg, Fe, Ca, Mn]$_3$Al$_2$Si$_3$O$_8$ (End-members: pyrope, almandine, grossular and spessartine)	Dale et al. (2000) except for spessartine: $W_{py\text{–}gr}$ = 33 kJ, $W_{py\text{–}alm}$ = 2.5 kJ The spessartine end-member is considered as ideal one.
Na-pyroxene: [Ca, Na][Mg, Fe, Al]Si$_2$O$_6$ (End-members: diopside, hedenbergite, jadeite and omphacite)	Holland and Powell (1996) except that aegrine is ignored.
Epidote: Ca$_2$Al$_2$[Al, Fe^{3+}]Si$_3$O$_{12}$(OH) (End-members: clinozoisite and epidote)	Ideal
Chlorite: [Mg, Fe, Mn]$_4$[Mg, Fe, Al, Mn]$_2$[Si, Al]$_2$Si$_2$O$_{10}$(OH)$_8$ (End-members: Al-free chlorite, clinochlore, daphnite, amesite and Mn-chlorite)	Holland et al. (1998)
White mica: [K, Na][Mg, Fe, Al][Al][Si, Al]$_2$Si$_2$O$_{10}$(OH)$_2$ (End-members: muscovite, celadonite, Fe-celadonite and paragonite)	Keller et al. (2005)
Carbonate: [Ca, Mg]CO$_3$ (End-members: calcite, dolomite and magnesite)	Holland and Powell (2003)
Amphibole: [Na, Ca]$_2$[Mg, Fe, Al]$_2$[Mg, Fe]$_3$Si$_8$O$_{22}$(OH)$_2$ (End-members: glaucophane, ferroglaucophane, tschermakite, Fe-tschermakite, tremolite, ferroactinolite)	Modified after White et al. (2003) and Wei et al. (2003): $W_{gl\text{–}tr}$ = 77 kJ, $W_{gl\text{–}fact}$ = 83 kJ, $W_{ts\text{–}tr}$ = 20 kJ, $W_{ts\text{–}fact}$ = –38 kJ, $W_{tr\text{–}fact}$ = 10 kJ, $W_{fgl\text{–}fact}$ = 77 kJ, $W_{fgl\text{–}tr}$ = 83 kJ, $W_{fts\text{–}fact}$ = 20 kJ, $W_{fts\text{–}tr}$ = –38 kJ
Feldspar: [K, Na][AlSi$_3$O$_8$]–Ca[Al$_2$Si$_2$O$_8$] (End-members: sanidine, $C\bar{1}$ anorthite and high-albite)	Holland and Powell (2003)
Ilmenite: [Fe, Mg, Mn]TiO$_3$ (End-members: ilmenite, geikielite and pyrophanite)	Ideal

Single end-member minerals: quartz, lawsonite, and titanite

Table S3. Whole rock chemical compositions of the eclogite used for the pseudosection modeling (normalized wt%). For growth of the rim of the garnet, we used a garnet-fractionated bulk-rock composition.

	Nucleation	Rim growth
SiO_2	52.59	56.22
TiO_2	1.38	1.71
Al_2O_3	14.67	13.13
FeO^T	10.39	5.45
MnO	0.18	0.00
MgO	5.89	7.07
CaO	8.73	8.78
Na_2O	4.66	5.77
K_2O	1.51	1.87
total	100.00	100.00

FeO^T= total Fe as FeO
The whole rock composition for the eclogite from Syros is the average of whole rock compositions of SY1401, SY1460 and SY1418 in Laurent et al. (2018).

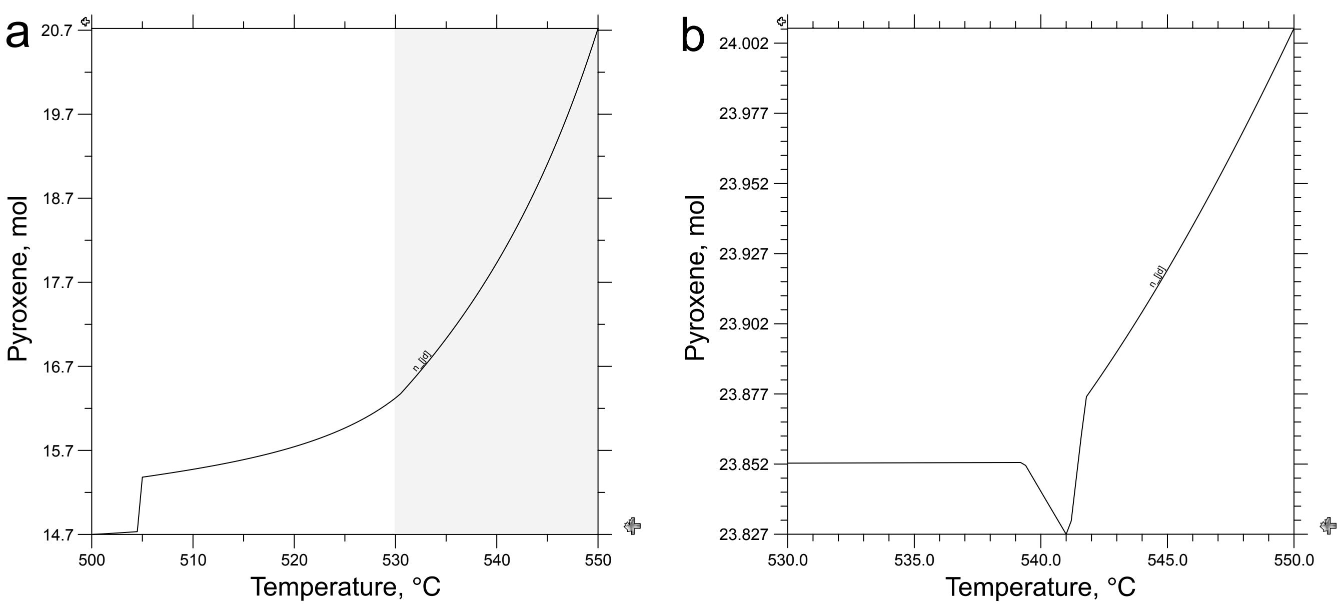

Figure S2. Results of estimation of the amount of pyroxene: **a** during the growth of the garnet core (500–530°C, without fill); **b** during the growth of the garnet rim.

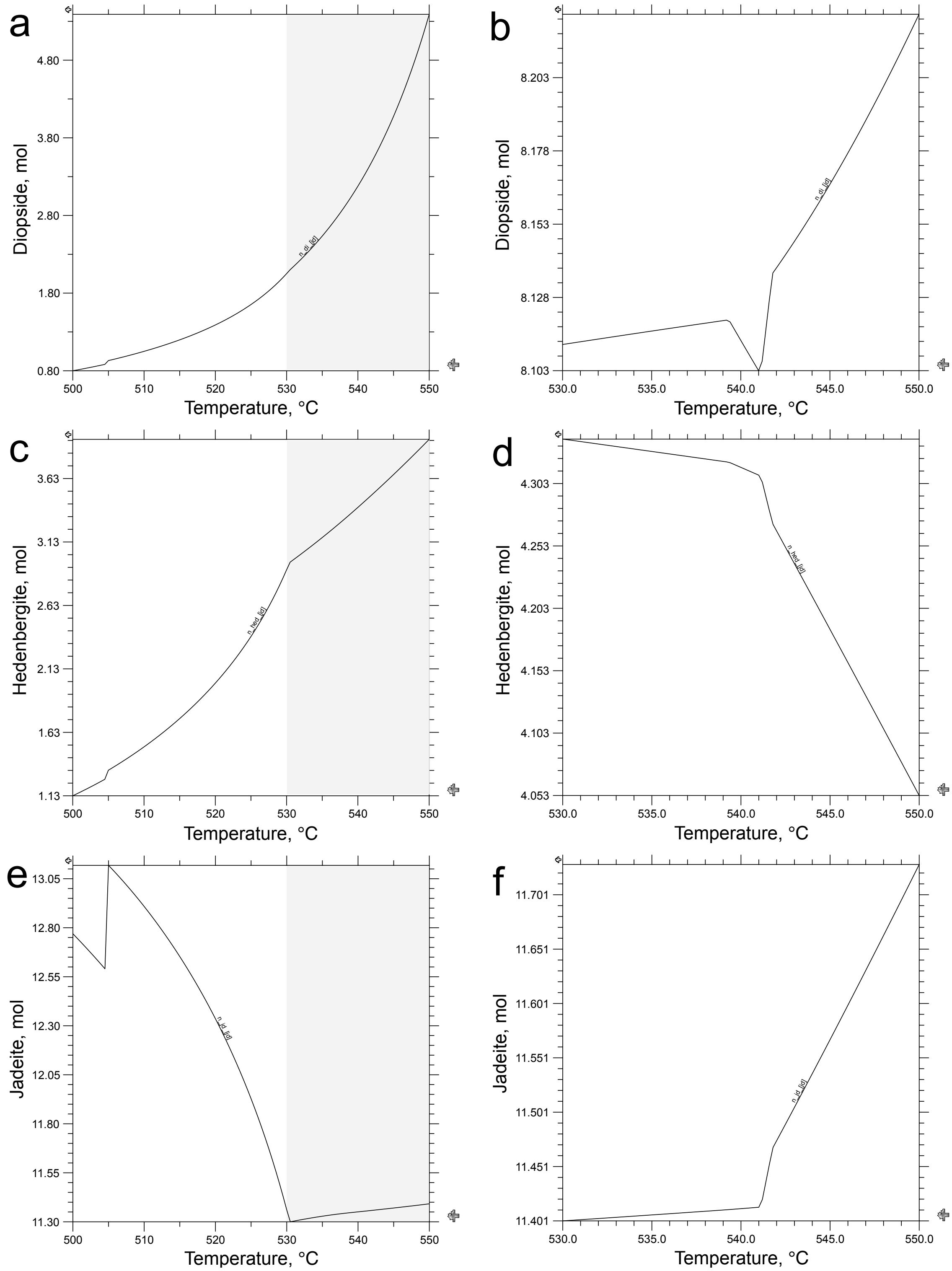

Figure S3. Results of estimation of the amount of pyroxene end-members: **a**, **b** diopside; **c**, **d** hedenbergite; **e**, **f** jadeite. The left-side figures show the results during the growth of the garnet core (500–530℃, without fill), while the right-side figures show that during the growth of the garnet rim.

References

Dale, J., Holland, T., and Powell, R. (2000) Hornblende ± garnet ± plagioclase thermobarometry: a natural assemblage calibration of the thermodynamics of hornblende. Contributions to Mineralogy and Petrology, 140, 353–362.

de Capitani, C., and Brown, T.H. (1987) The computation of chemical equilibrium in complex systems containing non-ideal solutions. Geochimica et Cosmochimica Acta, 51, 2639–2652.

de Capitani, C., and Petrakakis, K. (2010) The computation of equilibrium assemblage diagrams with Theriak/Domino software. American Mineralogist, 95, 1006–1016.

Holland, T., and Powell, R. (1996) Thermodynamics of order-disorder in minerals: II. Symmetric formalism applied to solid solutions. American Mineralogist, 81, 1425–1437.

Holland, T., and Powell, R. (1998) An internally consistent thermodynamic data set for phases of petrological interest. Journal of Metamorphic Geology, 16, 309–343.

Holland, T., and Powell, R. (2003) Activity–composition relations for phases in petrological calculations: an asymmetric multicomponent formulation. Contributions to Mineralogy and Petrology, 145, 492–501.

Holland, T., Baker, J., and Powell, R. (1998) Mixing properties and activity-composition relationships of chlorites in the system MgO-FeO-Al_2O_3-SiO_2-H_2O. European Journal of Mineralogy, 10, 395–406.

Keller, L.M., de Capitani, C., and Abart, R. (2005) A quaternary solution model for white micas based on natural coexisting phengite–paragonite pairs. Journal of Petrology, 46, 2129–2144.

Laurent, V., Lanari, P., Naïr, I., Augier, R., Lahfid, A., and Jolivet, L. (2018) Exhumation of eclogite and blueschist (Cyclades, Greece): Pressure–temperature evolution determined by thermobarometry and garnet equilibrium modeling. Journal of Metamorphic Geology, 36, 769–798.

Schumacher, J.C., Brady, J.B., Cheney, J.T., and Tonnsen, R.R. (2008) Glaucophane-bearing marbles on Syros, Greece. Journal of Petrology, 49, 1667–1686.

Trotet, F., Vidal, O., and Jolivet, L. (2001) Exhumation of Syros and Sifnos metamorphic rocks (Cyclades, Greece). New constraints on the PT paths. European Journal of Mineralogy, 13, 901–920.

Wei, C.J., Powell, R., and Zhang, L.F. (2003) Eclogites from the south Tianshan, NW China: petrological characteristic and calculated mineral equilibria in the Na_2O–CaO–FeO–MgO–Al_2O_3–SiO_2–H_2O system. Journal of Metamorphic Geology, 21, 163–179.

White, R.W., Powell, R., and Phillips, G.N. (2003) A mineral equilibria study of the hydrothermal alteration in mafic greenschist facies rocks at Kalgoorlie, Western Australia. Journal of Metamorphic Geology, 21, 455–468.