

Geothermometry and Fe³⁺ Partitioning within an Olivine Metagabbro and a Fayalite Granite in the Adirondack Mountains, NY

Mary Beth Cheversia

Department of Geology, The College of Wooster, Wooster, OH 44691
Faculty sponsor: Lori Bettison-Varga, The College of Wooster

Rebecca Stamski

Department of Geology, Amherst College, Amherst, MA 01002
Faculty sponsor: Peter Crowley, Amherst College

INTRODUCTION

This study focused on the compositions of minerals within an olivine metagabbro and a fayalite granite from the Adirondack Mountains of northern New York State. Synchrotron microscale X-ray absorption near edge structure (SmX, or XANES) spectroscopy (Delaney *et al.*, 1996) was used to analyze Fe³⁺/ΣFe within the Fe-bearing silicates present in our samples. Because this type of research is in its infancy, the results provide new insight into the partitioning of Fe²⁺ and Fe³⁺ between minerals, and may be used to explain this area's metamorphic history. We compared temperatures calculated by methods that assume all iron is Fe²⁺ to temperature calculations that take into account Fe³⁺/ΣFe determined by the SmX analyses. Finally, we examined how Fe³⁺ is partitioned between minerals both within our samples and within samples from the Adirondack region. The results demonstrate the importance of incorporating Fe³⁺/ΣFe data into geothermometry.

GEOLOGIC SETTING AND SAMPLE SELECTION

Three major orogenic events ca. 1350-1000 Ma have been recognized within the Adirondacks, the latest of which, the Ottowan Orogeny (ca. 1090 Ma), had the most influence on the geologic record. This most recent stage involved continental collision resulting in granulite facies metamorphism (Bohlen *et al.*, 1992; McLelland *et al.*, 1996; Olson, 1992). The Ottowan event produced a bull's eye pattern of isotherms in which temperature decreases from >775°C in the Adirondack Highlands to <625°C in the Adirondack Lowlands (Figure 1). Samples of olivine metagabbro and fayalite granite were collected from areas near the 750°C and 675°C isotherms, respectively.

Sample AK97-27 was collected on the Blue Ridge Highway from a road cut exposing well-foliated, dark colored, medium- to coarse-grained olivine metagabbro. The mineral assemblage of this metagabbro includes spinel-clouded plagioclase, hornblende, orthopyroxene, garnet, biotite, and various oxides and sulfides; our sample contained no olivine. The metagabbro, dated at 1143.6±7 Ma using U-Pb Zircon technique (McLelland and Chiarenzelli, 1989), is contemporaneous with the anorthosite massifs. Due to the spacial and chronological proximity of the anorthosite to the metagabbro, the latter is understood to be parental to the former (Frederick *et al.*, 1994).

Sample AK97-19 is a dark grey-green fayalite granite collected from a low road cut near the town of Wanakena. The mineral assemblage includes mesoperthite, quartz, hedenbergite, fayalite, hornblende, albite, ilmenite, magnetite, and zircon. The albite occurs as rims around the mesoperthite and may represent metamorphic recrystallization (Tucker and McKinney, 1997). Unlike almost all intrusive rocks in the Adirondacks, the fayalite granite appears to be virtually undeformed and unmetamorphosed and is not foliated. It cross-cuts metamorphic fabric in the country rock. These observations suggest it was late syn- or post-tectonic. The granite has been dated at approximately 1045 Ma; this time may represent the conclusion of regional high grade metamorphism (McLelland *et al.*, 1996).

EXPERIMENTAL METHODS

One-inch round thin sections were made from sample AK97-19 and AK97-27. Each thin section was examined petrographically and selected mineral grains were analyzed using a scanning electron microscope with an energy dispersive spectrometer (SEM/EDS) at Amherst College. From this technique we obtained major element chemistry of Fe-bearing minerals. Fe³⁺/ΣFe of selected mineral grains was determined by the SmX method using the intense X-ray beam supplied by the National Synchrotron Light Source (NSLS) located at the Brookhaven National Laboratory (BNL). The SmX technique is described in Delaney *et al.*, (1996) and Crowley *et al.*, (this volume). Upon our return to Amherst, we employed geothermometers based on several different mineral pairs to derive temperatures for AK97-19 and AK97-27. In all possible cases, we compared the temperatures obtained using

We spent 6 days at the National Synchrotron Light Source (NSLS) at the Brookhaven National Lab (BNL) using beamline X26a to do the SmX analyses. While at Brookhaven, someone was at the beamline 24 hours/day. At 7 AM & 7 PM the synchrotron beam was "dumped" and electrons were reinjected and accelerated to recreate the synchrotron beam. Before and after beam injection the magnetite, hematite and fayalite standards had to be repeatedly analyzed. We tended to work in 6 hour shifts, with each group responsible for analyzing the standards at either the start or end of their run. For the last 6 days of the project, we returned to Amherst and integrated the SmX results with our earlier microprobe analyses.

Halle Morrison and Zoë Brown helped with some of the ground-truthing of the SmX method. They looked at garnet with a wide range of Fe^{3+}/Fe^{2+} . The SmX results were compared with those determined by Mössbauer spectroscopy and estimated by garnet stoichiometry and garnet molar volume. Their results clearly showed that there were problems with using the Bajt et al. (1994) method with garnet and suggested revisions.

Dan Harrington and Anna Monders examined Fe^{3+} partitioning and geothermometry from a metanorthosite from presumed highest temperature part of the Adirondack highlands. Their geothermometry yields temperatures similar to those of Spear & Markussen (1997). Their results suggest a relatively small Fe^{3+}/Fe^{2+} partitioning at these high temperatures.

Mary Beth Cheversia and Becky Stamski examined Fe^{3+} partitioning and geothermometry from an olivine metagabbro and a fayalite granite from presumed lower temperature parts of the Adirondack highlands. Their geothermometry indicates a protracted thermal history that starts at temperatures greater than those suggested by the Bohlen et al. (1985) isograd pattern.

Heidi Guetschow and Ethan Gutmann examined Fe^{3+} partitioning and geothermometry in the Popple Hill gneiss formation, from the amphibolite facies Adirondack lowlands. Their geothermometry yielded lower temperatures than were found in the highlands. Furthermore, their results suggest a relatively larger Fe^{3+}/Fe^{2+} partitioning than was found at higher temperatures in the highlands.

Rachel Graham and Sue Young Jin studied the Fe^{3+} partitioning and geothermometry in the Carthage-Colton Mylonite Zone. They compared the compositions of mineral grains within a shear zone to those outside the shear zone.

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only SEM/EDS data (i.e., with no Fe³⁺ data) to the temperatures that were adjusted by our SmX Fe³⁺ results in order to determine the effect of Fe³⁺/ΣFe on our calculated temperatures.

RESULTS AND DISCUSSION

Major element compositions of minerals used to calculate temperatures are given in Table 2 and Table 3. Table 1 displays the temperatures, calculated using four different methods, each of which makes distinct assumptions about the Fe³⁺ contents of the minerals used in our geothermometry.

Calculated temperatures for the olivine metagabbro were relatively consistent and realistic. Our first approach, **(T(I))**, Table 1) assumed that all iron was Fe²⁺ and yielded temperatures ranging from 670°C - 852°C. When we utilized our SmX Fe³⁺ data for all minerals except garnet, for which we assumed Fe³⁺ = 0, **(T(II))**, Table 1) our temperatures dropped slightly to 580°C - 745°C. In our third approach, **(T(III))**, Table 1) all minerals were adjusted by SmX Fe³⁺ data and the resulting temperatures were similar to those of **(T(I))**, ranging from 680°C - 846°C. Finally, because this project's garnet SmX analyses may be questionable, we determined temperatures for AK97-27 using a fourth method in which we utilized SmX data for all minerals except garnet. Thus, we calculated the Fe³⁺ of garnet based upon cation stoichiometry, in which Fe³⁺ = 2-Al, and derived temperatures that ranged from 605°C - 755°C **(T(IV))**, Table 1). We believe this may be the most reliable method. Hence, the olivine metagabbro seems to have equilibrated at or below the 750°C isotherm of Bohlen *et al.* (1992).

The temperature of the fayalite granite, AK97-19, was determined using two thermometers. The first thermometer, created by Holland and Blundy (1992), utilized a hornblende-plagioclase pair for which we had no available SmX data and gave a temperature of 848°C. In addition, we calculated temperatures by way of the two-feldspar thermometer of Haselton *et al.* (1983), using mesoperthite and metamorphic albite. From this latter thermometer, we obtained temperatures less than 500°C using data from a distinct albite lamellae (AK9719-20) and a distinct K-feldspar lamellae (AK9719-21) from within the same mesoperthite grain. We also calculated a temperature of 408°C for a pair that included a metamorphic albite (AK9719-15) and a distinct K-feldspar lamellae (AK9719-17). Finally, we reintegrated the bulk composition of the mesoperthite using the compositions of the lamellae and the estimated volumetric contribution of albite and K-feldspar lamellae. Thermometry calculations using this value and that of a metamorphic albite (AK9719-19), yielded a temperature of 660°C (see Table 3 for SEM/EDS analyses of these points). The feldspar analyses probably indicate exsolution temperatures that are lower than the results from the hornblende-plagioclase thermometer. Our data suggest a wide range of temperatures for the fayalite granite, which are broadly coincident with predictions of Bohlen *et al.* (1992).

Fe³⁺ does not greatly influence the predicted temperatures of the olivine metagabbro, as evidenced by the similarities between the results of **(T(I))** and **(T(III))**. This is consistent with the lack of Fe³⁺ partitioning between Fe-bearing minerals found in this sample. Fe³⁺/ΣFe is in the range of 0.13 to 0.16 in all the Fe-bearing phases that we examined. However, Fe³⁺ in the fayalite granite showed some preference for clinopyroxene over fayalite: the clinopyroxene has an Fe³⁺/ΣFe of 0.09 to 0.20 while the fayalite has an Fe³⁺/ΣFe of 0.05. Due to a lack of sufficient SmX data, we are uncertain of the influence of temperature upon this partitioning in AK97-19. On a regional scale, rocks from the Adirondack Lowlands (Guttman and Guetschow, this volume), which have lower temperatures (<650°C), are more oxidized than our moderate to high temperature rocks and the high temperature anorthosite of the Adirondack Highlands (Harrington and Monders, this volume).

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Table 1: Geothermometry data (at 7 kbars) for AK97-27

<u>Mineral Pair & Sample Number*</u>	<u>T(I)</u>	<u>T(II)</u>	<u>T(III)</u>	<u>T(IV)</u>
¹ garnet 41 / biotite 35	852°C	745°C	845°C	755°C
² garnet 41 / hornblende 44	670°C	620°C	680°C	630°C
³ garnet 41 / orthopyroxene 24	705°C	580°C	710°C	605°C
⁴ hornblende 22 / plagioclase 23	835°C	n.a.	846°C	n.a.
⁴ hornblende 43 / plagioclase 36	796°C	n.a.	788°C	n.a.
⁴ hornblende 44 / plagioclase 36	798°C	n.a.	775°C	n.a.

* T(I) = All Fe as Fe²⁺, T(II) = Fe³⁺ by SmX, except garnet where Fe³⁺ = 0, T(III) = Fe³⁺ by SmX, T(IV) = Fe³⁺ by SmX, except garnet where Fe³⁺ = 2-Al.

Thermometers taken from: ¹Ferry and Spear (1978); ²Graham and Powell (1984); ³Lee and Ganguly, (1988); ⁴Holland and Blundy (1992).

Figure 1: Adirondack sample location map, including isotherms from Bohlen (1985).

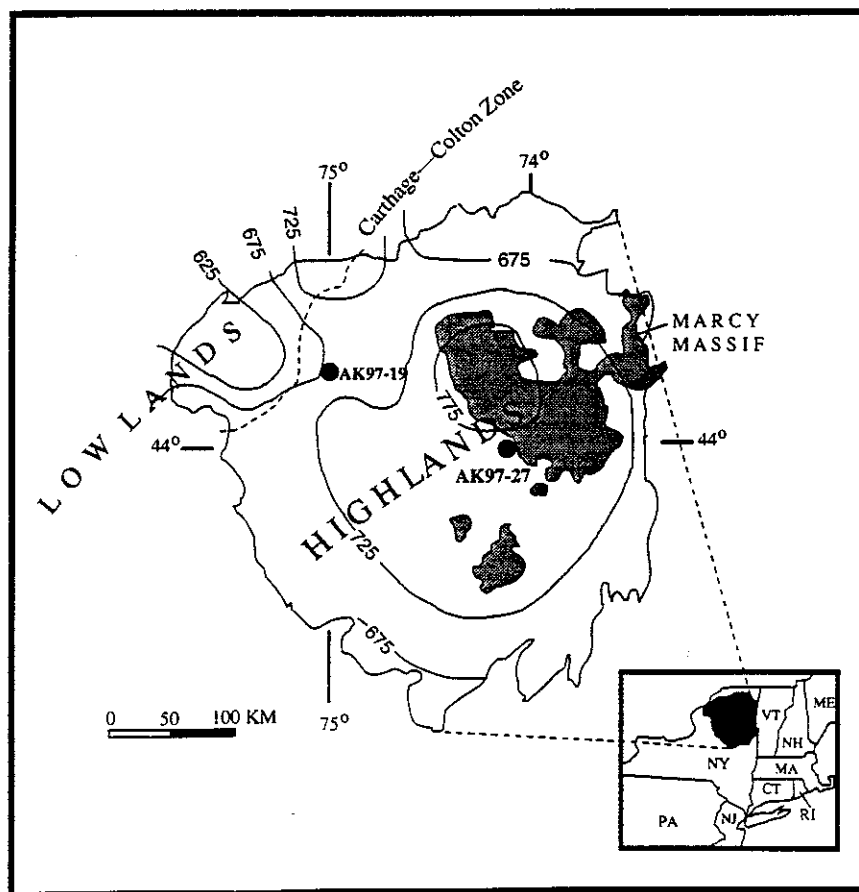


Table 2: SEM/EDS compositional data with Fe³⁺/ΣFe determined by SmX

AK97: Mineral	19-2 fayalite	19-7 cpx	19-28 cpx	19-29 cpx	27-22* hnbnd	27-24 opx	27-35 biotit	27-41 garnet	27-43 hnbnd	27-44 hnbnd
Wt % oxide										
SiO ₂	28.79	47.09	49.31	49.40	40.41	50.87	36.09	38.65	40.52	41.55
Al ₂ O ₃	0.03	0.57	0.89	0.80	13.30	2.12	14.18	21.49	13.49	13.55
TiO ₂	0.00	0.03	0.22	0.18	3.27	0.03	4.66	0.02	3.36	3.11
MgO	0.44	0.94	1.03	1.16	9.81	19.60	12.42	6.47	9.59	10.56
FeO	64.50	25.83	24.43	23.30	12.82	21.42	14.68	23.95	12.93	13.07
Fe ₂ O ₃	3.77	2.67	4.98	6.48	2.42	3.88	2.66	3.98	2.74	2.17
MnO	1.50	0.46	0.58	0.52	0.09	0.27	0.03	1.02	0.06	0.07
CaO	0.00	19.07	19.13	19.39	10.95	0.30	0.04	4.88	10.91	10.77
Na ₂ O	0.44	0.89	1.19	0.62	2.73	0.10	0.00	0.06	2.33	2.50
K ₂ O	0.03	0.00	0.04	0.00	1.07	0.02	9.77	0.06	1.12	1.10
BaO	0.00	0.14	0.00	0.00	0.00	0.06	0.23	0.00	0.00	0.00
Cl	0.07	0.04	0.00	0.01	0.22	0.00	0.18	0.00	0.18	0.18
total	99.58	97.74	101.80	101.85	97.09	98.67	94.94	100.56	97.23	98.62
Stoichiometry	O=4	O=6	O=6	O=6	O=23	O=6	O=22	O=12	O=23	O=23
Si	0.974	1.976	1.967	1.964	6.105	1.935	5.522	2.978	6.110	6.150
Al	0.001	0.028	0.041	0.037	2.367	0.095	2.556	1.952	2.399	2.365
Ti	0.000	0.001	0.007	0.005	0.372	0.001	0.536	0.001	0.380	0.346
Mg	0.023	0.059	0.061	0.069	2.210	1.112	2.832	0.744	2.156	2.331
Fe ²⁺	1.803	0.876	0.766	0.716	1.519	0.643	1.768	1.463	1.520	1.528
Fe ³⁺	0.095	0.081	0.141	0.179	0.258	0.105	0.288	0.219	0.289	0.228
Mn	0.042	0.017	0.020	0.018	0.012	0.009	0.004	0.066	0.008	0.008
Ca	0.000	0.858	0.818	0.825	1.773	0.012	0.007	0.402	1.762	1.708
Na	0.029	0.072	0.092	0.048	0.799	0.007	0.000	0.008	0.680	0.716
K	0.001	0.000	0.002	0.000	0.206	0.001	1.908	0.006	0.216	0.208
Ba	0.000	0.002	0.000	0.000	0.000	0.001	0.014	0.000	0.000	0.000
Cl	0.006	0.004	0.000	0.001	0.073	0.000	0.060	0.000	0.059	0.057
total	2.973	3.974	3.915	3.862	15.693	3.920	15.495	7.839	15.580	15.643
Fe ³⁺ /ΣFe	0.05	0.09	0.16	0.20	0.15	0.14	0.14	0.13	0.16	0.13

Table 3: SEM/EDS compositional data for points with no available SmX data

AK97: Mineral	19-15 albite	19-17 k-spar	19-18 hnbnd	19-19 albite	19-20 albite	19-21 k-spar	27-23 plag	27-36 plag
Wt % oxide								
SiO ₂	64.94	66.74	39.31	68.10	66.55	63.89	57.72	57.93
Al ₂ O ₃	19.25	18.34	7.99	20.42	18.72	17.57	25.83	25.42
TiO ₂	0.00	0.00	2.24	0.05	0.00	0.00	0.03	0.06
MgO	0.00	0.00	0.96	0.00	0.00	0.00	0.00	0.00
FeO	0.27	0.37	33.61	0.32	0.17	0.11	0.01	0.03
MnO	0.03	0.00	0.36	0.00	0.04	0.00	0.00	0.00
CaO	1.21	0.06	9.89	1.07	0.48	0.00	8.07	7.92
Na ₂ O	10.80	1.06	1.76	11.59	11.02	0.62	6.76	7.24
K ₂ O	0.09	15.46	1.70	0.06	0.08	14.92	0.14	0.17
BaO	0.00	0.24	0.00	0.01	0.00	0.04	0.03	0.04
Cl	0.00	0.00	0.51	0.00	0.03	0.00	0.00	0.00
total	96.61	102.26	98.31	101.62	97.10	97.14	98.59	98.79
Stoichiometry	O=8	O=8	O=23	O=8	O=8	O=8	O=8	O=8
Si	2.956	3.014	6.507	2.948	3.006	3.028	2.620	2.631
Al	1.033	0.976	1.558	1.042	0.997	0.981	1.382	1.361
Ti	0.000	0.000	0.278	0.002	0.000	0.000	0.001	0.002
Mg	0.000	0.000	0.237	0.000	0.000	0.000	0.000	0.000
Fe	0.010	0.014	4.652	0.011	0.007	0.004	0.000	0.001
Mn	0.001	0.000	0.050	0.000	0.002	0.000	0.000	0.000
Ca	0.059	0.003	1.753	0.049	0.023	0.000	0.392	0.385
Na	0.953	0.092	0.566	0.973	0.966	0.057	0.595	0.638
K	0.005	0.890	0.358	0.003	0.005	0.902	0.008	0.010
Ba	0.000	0.004	0.000	0.000	0.000	0.001	0.001	0.001
Cl	0.000	0.000	0.186	0.000	0.003	0.000	0.000	0.000
total	5.017	4.993	16.145	5.028	5.009	4.973	4.999	5.029

* Percent Fe³⁺ for hornblende AK9727-22 was estimated from average of percent Fe³⁺ in AK9727-43 and AK9727-44

Interrelationships Between Molar Volume and Composition in Garnet

Halle Morrison

Department of Geology, The College of Wooster, Wooster, OH 44691

Faculty Sponsor: Lori Bettison-Varga, The College of Wooster

Zoë Brown

Department of Earth Sciences, Buffalo State College, 1300 Elmwood Avenue, Buffalo, NY 14222

Faculty Sponsor: Jill Singer, Buffalo State College

INTRODUCTION

The chemical composition of garnet in metamorphic rocks provides an invaluable tool to petrologists studying various conditions of metamorphism. The garnet mineral structure is a vast storehouse of many different elements, all of which have an effect on its properties. All of the major components in garnet can be easily measured, except for Fe^{3+} and Fe^{2+} ; only total iron can be determined by traditional microanalytical methods. Only with difficulty and/or time-consuming bulk analytical methods can Fe^{3+} be measured. As a result, the relationships between Fe^{3+} and unit cell volumes in garnet are poorly understood. The purpose of this study is to investigate the relationships between unit cell volumes of garnets and Fe^{3+} concentration, either measured or calculated.

ANALYTICAL METHODS

The Adirondack Mountains proved to be a good source in which to sample a variety of garnets and garnetiferous rocks with varying chemical compositions and physical properties. All garnets sampled were isolated from rocks collected in Adirondack Highland localities. Garnet localities at the Gore Mountain and Willsboro Wollastonite mines provided material for eight of the samples presented here, as they yielded excellent garnet crystals. All localities are shown on Figure 1.

From a collection of 13 samples, garnet was separated from the parent rock with the aid of a dissecting microscope and isolated for analysis. The garnets were pulverized, prepared by mixing with isopropyl alcohol, and placed on a microscope slide for x-ray diffraction to determine unit cell volumes. Grain mounts of the garnets were prepared by fastening the grains to a common microscope slide with epoxy glue and polished. The garnets were analyzed for major-element compositions (Table 1) using both SEM/EDS and XANES techniques. X-ray diffraction powder patterns were obtained with a Scintag XDS 2000 x-ray diffractometer with a scan time of one °/minute (total scan time of 68 minutes). Mineralogic compositions were determined with the Amherst College scanning electron microscope equipped with an EDS spectrometer, and the synchrotron X-ray microprobe to collect XANES spectra (beamline X26A, National Synchrotron Light Source, Brookhaven National Laboratory, Upton, New York).

Data collected in this study were combined with additional data from various sources contained in Deer *et al* (1961). These data were chosen on the basis of analysis for unit cell length, FeO and Fe_2O_3 , SiO_2 , Al_2O_3 , MgO , MnO , CaO , and no other oxides >0.1 wt. %. The resultant data set contains garnets with a wide range of compositions. Calculated cell volumes were obtained by multiplying mole percent compositions of each of the five garnet end-members (andradite, almandine, grossular, pyrope, and spessartine) by the cube of the a axis length, assuming ideal end-member mixing. "Misfit" was defined as the difference between the calculated and measured cell volume of each sample. Distinctions were made between the entire data set and that portion taken solely from the literature (Table 2).

PREDICTION OF UNIT CELL VOLUMES FROM MAJOR-ELEMENT COMPOSITION

Four methods of calculating unit cell volume were tested (Table 2):

1. *Using Fe^{3+} measured from wet chemistry or other techniques, including XANES.* Average Misfit of the unit cell volumes was initially calculated using $a = 12.056 \text{ \AA}$ (Deer *et al.*, 1961) -- a common value used in molar volume calculations for the andradite component. Misfit between measured and calculated molar volume was $2.194 \pm 10.797 \text{ \AA}^3$. Next, Misfit was recalculated using $a = 12.061 \text{ \AA}$ -- the value measured for the end-member andradite standard used at Brookhaven National Lab; Misfit was reduced to $1.952 \pm 10.669 \text{ \AA}^3$. Finally, the value of a for andradite that would correspond to zero Misfit was calculated to be 12.1012 \AA , suggesting that the actual unit cell length commonly reported in literature is too low and must be adjusted.

2. *Assuming all iron present is Fe^{2+} .* Average misfit between measured and calculated unit cell volumes