Crystal Structure of an Anisotropic Pyrope Garnet That Contains Two Cubic Phases

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Abstract: The crystal structure of two different samples of pyrope garnet, ideally Mg$_3$Al$_2$Si$_3$O$_{12}$, from South Africa was refined using the Rietveld method, space group $Ia$3$_d$ and monochromatic synchrotron high-resolution powder X-ray diffraction (HRPXRD) data. Sample 1 from Wesselton Mine is a single cubic phase and is optically isotropic. Electron-probe microanalysis (EPMA) provided an average composition [Mg$_{2.30}$Fe$_{2+0.26}$Ca$_{0.42}$Mn$_{2+0.02}$]$_2$[Al$_{1.73}$Fe$_{3+0.06}$Cr$_{3+0.01}$Ti$_{2+0.01}$Fe$_{2+0.12}$]$_2$Si$_3$O$_{12}$, which contains a significant amount of Cr cations. The unit-cell parameter (Å) and bond distances (Å) are $a$ = 11.56197(1) Å, average <Mg-O> = 2.2985, Al-O = 1.9101(4), and Si-O = 1.6343(3) Å. Sample 2 from De Beers Diamond Mine has an average composition [Mg$_{2.33}$Fe$_{2+0.33}$Ca$_{0.33}$Mn$_{2+0.01}$]$_2$[Al$_{1.77}$Fe$_{3+0.12}$Cr$_{3+0.06}$Ti$_{2+0.05}$Fe$_{2+0.05}$]$_2$Si$_3$O$_{12}$ and is a fine-scale intergrowth of two cubic phases. The weight percentage, unit-cell parameter (Å), and bond distances (Å) for phase 2a are 62.2(1)%, $a$ = 11.56185(1) Å, average <Mg-O> = 2.3006, Al-O = 1.9080(4), Si-O = 1.6334(4) Å. The corresponding values for phase 2b are 37.8(1)%, $a$ = 11.53896(1) Å, average <Mg-O> = 2.2954, Al-O = 1.9020(6), and Si-O = 1.6334(6) Å. The two cubic phases in sample 2 cause the crystal to be optically anisotropic because of strain induced birefringence. The unit-cell parameter and bond distances for sample 1 are similar to those in phase 2a.

Keywords: garnet; pyrope; intergrowth of two cubic phases; Rietveld refinements; synchrotron high-resolution powder X-ray diffraction (HRPXRD); crystal structure

1. Introduction

Garnet-group minerals, general formula $X_3Y_2Z_3O_{12}$, are of interest in various research fields (solid-state physics, materials science, inorganic chemistry, and geology). They are important in laser technology. Li-stuffed garnet (e.g., Li$_3$La$_5$Zr$_2$O$_{12}$, where the sum of cations is 12 instead of 8) are currently attracting attention because of their possible use in rechargeable batteries for the automotive industry [1]. Silicate garnets are one of the major constituents in the Earth’s crust, upper mantle, and transition zone. These minerals are commonly found in many igneous and metamorphic rocks, as well as in beach sands and in some sedimentary rocks. Investigations of the structural, physical, and thermodynamic properties of garnets are important for understanding various Earth and technological processes. Garnets occur as complex solid solutions, but the most significant and common member in the upper mantle is pyrope, Mg$_3$Al$_2$Si$_3$O$_{12}$, which requires high pressure to form. Investigations of the structural, physical, and thermodynamic properties of pyrope and majorite are important for understanding the Earth’s mantle. Pyrope is also used as an indicator mineral for finding diamonds.

Diffraction peaks from garnets showing splitting are known and were interpreted as arising from different phases (e.g., [2–9]). In the case of majorite, [Mg$_3$]([MgSi])Si$_3$O$_{12}$, the split reflections were interpreted as arising from a garnet with tetragonal symmetry [10–16]. Intergrowth of two or three cubic garnet phases was observed with synchrotron high-resolution powder X-ray diffraction (HRPXRD) data; all such garnets show splitting of reflections. It is important to correctly identify the origin of split reflections in garnet samples because of their thermodynamic implications. This study reports split reflections from unusual pyrope that arise from two different cubic phases and give rise to strain-induced birefringence [17–23].
The crystal structure of many members of the garnet group has been refined [24–28]. The general formula for garnet is \( [8] \text{X}_3[6] \text{Y}_2[4] \text{Z}_3[4] \text{O}_{12} \), where the eight-coordinate dodecahedral X site contains Mg, Ca, Mn, or Fe\(^{2+}\) cations, the six-coordinate octahedral Y site contains Al, Cr\(^{3+}\), Fe\(^{3+}\), Ti\(^{4+}\), or Zr\(^{4+}\) cations, and the four-coordinate tetrahedral Z site contains Si, Fe\(^{3+}\) or Al cations, or \((\text{O}_3\text{H}_4)\) groups (e.g., the work of [29]). The structure of garnet consists of alternating ZO\(_4\) tetrahedra and YO\(_6\) octahedra with X atoms filling cavities to form XO\(_8\) dodecahedra. The eight O atoms in the XO\(_8\) dodecahedron occur at the corners of a distorted cube (Figure 1).

The Mg atom is too small for the X dodecahedral cavity size (that is, the Mg-O bond length is too long), so the bond-valence sum for Mg is less than 2 vu in pyrope, and more than 2 vu for Ca in grossular, Ca\(_3\)Al\(_2\)Si\(_3\)O\(_{12}\) [27,30–33]. This anomaly implies the possibility of positional (static) disorder or large thermal vibration (dynamic disorder) of the Mg atoms in pyrope. The dynamic disorder may be interpreted as the atom having an effectively larger size than if no disorder is present. Structural studies of pyrope have reported anomalously large atom displacement parameters (ADPs) of the Mg atom where \( U_{\text{Mg}} > U_{\text{O}} \) [27,30–33]. There have been debates as to whether the Mg atom shows positional disorder [34–37] or dynamic disorder [30–33,38–42].

This study examines the crystal structure of two pyrope samples using HRPXRD data that show a two-phase intergrowth in sample 2 and a single phase for sample 1. This study also shows that \( U_{\text{Mg}} < U_{\text{O}} \), so no anomaly was observed for the Mg ADPs, but the bond valence for the Mg atom is less than 2 vu.

2. Materials and Methods

2.1. Sample Description

The dark-red pyrope samples were obtained from the Royal Ontario Museum (ROM). Sample 1 (ROM #M29463) is from Wesselton Mine, Kimberley, Cape Province, South Africa, and sample 2 (M29466) is from De Beers Diamond Mine, Kimberley, Cape Province, South
Africa. The pyrope crystals occur as well-rounded grains (≈5 mm in diameter) that were derived from weathered kimberlites and deposited as gravels. One 5 mm grain from each sample was broken, and a few fragments were used in this study. Sample 1 is isotropic and is a single cubic phase (Figure 2a), whereas sample 2 is birefringent and contains two cubic phases (Figure 2b,c).

Figure 2. Thin-section images of pyrope: (a) plane-polarized light (PPL) image for sample 1, (b) PPL with the corresponding cross-polarized light (XPL) image (c) for sample 2, which is anisotropic and contains two cubic phases. The scale bars represent 100 µm.

2.2. Electron-Probe Microanalysis (EPMA)

Quantitative chemical compositions were collected with a JEOL JXA-8200 WD-ED electron-probe microanalyzer (EPMA) (JXA-8200, JEOL, Mitaka, Japan). The JEOL operating program on a Solaris platform was used for ZAF (atomic number, Z; absorption, A; fluorescence, F) correction and data reduction. The wavelength-dispersive (WD) analyses were conducted quantitatively using an accelerated voltage of 15 kV, a beam current of 20 nA, and a beam diameter of 5 µm. Relative analytical errors were 1% for major elements and 5% for minor elements. Various standards were used [almandine-pyrope (MgKα), grossular (CaKα), almandine (FeKα, AlKα, SiKα), rutile (TiKα), spessartine (MnKα), and chromite (CrKα)]. The samples appear homogeneous based on EPMA results of 12 spots from different areas of a crystal with a diameter of about 2 mm. The EPMA data were analyzed using the method and spreadsheet developed by Locock [43], and the average chemical composition is given (Table 1).

### Table 1. Average EPMA results for two different pyrope samples.

| Oxide (wt. %)       | Sample 1    | Sample 2    |
|---------------------|-------------|-------------|
| SiO₂                | 41.67(11)   | 42.17(12)   |
| TiO₂                | 0.15(2)     | 0.85(2)     |
| Al₂O₃               | 18.05(6)    | 20.65(13)   |
| Cr₂O₃               | 6.95(5)     | 0.98(5)     |
| FeO/FeO₉otive       | 5.44(8)     | 8.37(8)     |
| MnO                 | 0.35(2)     | 0.23(2)     |
| MgO                 | 21.40(12)   | 21.95(15)   |
| CaO                 | 5.42(5)     | 4.32(4)     |
| ∑                   | 99.93       | 99.52       |
| Recalc. (wt. %)     |             |             |
| Final FeO           | 4.52(31)    | 6.29(17)    |
| Final Fe₂O₃         | 1.03(31)    | 2.31(21)    |
| ∑ (calc.)           | 99.54       | 99.75       |
| Cations for 12 O atoms |           |             |
| Mg²⁺                | 2.297       | 2.328       |
| Ca²⁺                | 0.418       | 0.329       |
Table 1. Cont.

| Oxide (wt. %) | Sample 1 | Sample 2 |
|--------------|----------|----------|
| Fe$^{2+}$    | 0.264    | 0.329    |
| Mn$^{2+}$    | 0.021    | 0.014    |
| ΣX           | 3.000    | 3.000    |
| Al$^{3+}$    | 1.532    | 1.731    |
| Cr$^{3+}$    | 0.396    | 0.055    |
| Fe$^{3+}$    | 0.056    | 0.123    |
| Fe$^{2+}$    | 0.008    | 0.045    |
| Ti$^{4+}$    | 0.008    | 0.045    |
| ΣY           | 2.000    | 2.000    |
| Si$^{4+}$    | 3.000    | 3.000    |
| ΣZ           | 3.000    | 3.000    |

End-member mole %

|                        | Sample 1 | Sample 2 |
|------------------------|----------|----------|
| Pyrope *               | 69.86    | 77.59    |
| Almandine              | 6.01     | 8.49     |
| Morimotoite            | 0.81     | 4.51     |
| Andradite              | 0.00     | 3.69     |
| Uvarovite              | 13.13    | 2.76     |
| [Fe$_3$][Fe$_2$]Si$_3$O$_{12}$ | 2.78    | 2.49     |
| Spessartine            | 0.71     | 0.46     |
| Knorringite            | 6.66     | 0.00     |
| Quality Index          | Superior | Superior |

*The dominant end member is pyrope (bold). End-members with mole % < 0.05 are not reported.

2.3. Synchrotron High-Resolution Powder X-ray Diffraction (HRPXRD)

The two pyrope samples were studied with HRPXRD that was performed at beamline 11-BM, Advanced Photon Source (APS), Argonne National Laboratory (ANL). A small fragment (about 2 mm in diameter) of the sample was crushed to a fine powder using a corundum mortar and pestle. The crushed sample was loaded into a Kapton capillary (0.8 mm internal diameter) and rotated during the experiment at a rate of 90 rotations per second. The data were collected at 23 °C to a maximum 2θ of about 50° with a step size of 0.001° (2θ) and a step time of 0.1 s per step. The HRPXRD traces were collected with a multi-analyzer detection assembly consisting of twelve independent silicon (111) crystal analyzers and LaCl$_3$ scintillation detectors that reduce the angular range to be scanned and allow for rapid acquisition of data. A silicon (NIST 640c) and alumina (NIST 676a) standard (ratio of 1/3 Si:2/3 Al$_2$O$_3$ by weight) was used to calibrate the instrument and refine the monochromatic wavelength used in the experiment (see Table 2). Additional details of the experimental setup are given elsewhere [44–46]. The experimental techniques used in this study are well established [47–52].

Table 2. HRPXRD data and Rietveld refinement statistics for two pyrope samples.

| Miscellaneous | Sample 1 | Sample 2 |
|---------------|----------|----------|
|               | Single Phase | Phase 2a | Phase 2b |
| wt. %         | 100       | 62.2(1)  | 37.8(1)  |
| a (Å)         | 11.56197(1) | 11.56185(1) | 11.53896(1) |
| Δa (Å)        | 0         | -        | 0.0229   |
| Reduced χ²    | 1.508     | 1.121    |          |
| *R (F²)       | 0.0421    | 0.0658   |          |
| N$_{obs}$ †   | 542       | 1286     |          |
| λ (Å)         | 0.41383(2) | 0.41387(2) |          |
Data points    | 47994     | 47990    |          |

*R (F²) = Overall R-structure factor based on observed and calculated structure amplitudes = $\left[ \sum (F_o^2 - F_c^2) / \sum F_o^2 \right]^{1/2}$. N$_{obs}$ † is the number of observed reflections. 2θ range = 2°–50°.
2.4. Rietveld Structural Refinement

The HRPXRD data were analyzed with the Rietveld method [53], as implemented in the GSAS program [54], and using the Expgui interface [55]. Scattering curves for neutral atoms were used. The starting atom coordinates, cell parameter, and space group, \( Ia\overline{3}d \), were taken from Novak and Gibbs [27]. The background was modeled using a Chebyshev polynomial (eight terms). In the GSAS program, the reflection-peak profiles were fitted using a type-3 profile (pseudo-Voigt; [56, 57]). A full-matrix least-squares refinement was carried out by varying the parameters in the following sequence: a scale factor, unit-cell parameter, atom coordinates, isotropic displacement parameters, and site occupancy factors (sofs) using the dominant atom in the X, Y, and Z sites.

Examination of the HRPXRD trace for sample 2 shows the presence of two separate phases with different unit-cell parameters as indicated by the splitting of the diffraction peaks. The two separate phases were refined together. Toward the end of the refinement, all the parameters were allowed to vary simultaneously, and the refinement proceeded to convergence.

The cell parameters and the Rietveld refinement statistical indicators for the two samples are listed in Table 2. Atom coordinates, isotropic displacement parameters, and sofs are given in Table 3. Bond distances are given in Table 4.

| Table 3. Atom coordinates *, isotropic displacement parameters \( U (\text{Å}^2) \), and sofs for two pyrope samples. |
|---------------------------------------------------------------|
| Site | Miscellaneous | 1. Single | 2. Phase 2a | 2. Phase 2b | 2a–2b |
|------|---------------|-----------|-------------|-------------|--------|
| Mg(X) | \( U \) | 0.0080(1) | 0.0081(1) | 0.0088(2) |
| Al(Y) | \( U \) | 0.0033(1) | 0.0033(1) | 0.0035(1) |
| Si(Z) | \( U \) | 0.0024(1) | 0.0029(1) | 0.0028(1) |
| O | \( x \) | 0.03396(3) | 0.03409(3) | 0.03403(5) |
| | \( y \) | 0.04953(5) | 0.04930(4) | 0.04990(5) |
| | \( z \) | 0.65390(3) | 0.65375(4) | 0.65350(5) |
| Mg(X) | sof | 1.164(1) | 1.176(2) | 1.155(2) | 0.021 |
| Al(Y) | sof | 1.122(1) | 1.107(2) | 1.039(2) | 0.068 |
| Si(Z) | sof | 0.925(1) | 0.926(1) | 0.928(2) | −0.002 |
| Mg(X) | EPMA sof | 1.203 | 1.206 |
| Al(Y) | EPMA sof | 1.202 | 1.123 |
| Si(Z) | EPMA sof | 1.000 | 1.000 |
| \( x^1 \) | \( \Delta \) (sof) | −0.039 | −0.030 | −0.051 |
| \( y \) | \( \Delta \) (sof) | −0.080 | −0.016 | −0.084 |
| \( z \) | \( \Delta \) (sof) | −0.075 | −0.074 | −0.072 |
| \( x^1 \) | \( \Delta e \) | −0.47 | −0.36 | −0.62 |
| \( y \) | \( \Delta e \) | −1.04 | −0.21 | −1.10 |
| \( z \) | \( \Delta e \) | −1.05 | −1.04 | −1.01 |

* X at (0, 1/4, 1/8) with Mg dominant, Y at (0, 0, 0) with Al dominant, and Z at (3/8, 0, 1/4) with Si dominant.

† \( \Delta \) (sof) = sof (HRPXRD refinement) − sof (EPMA).

‡ \( \Delta e = \) electrons (HRPXRD refinement) − electrons (EPMA); both \( \Delta \) (sof) and \( \Delta e \) are based on the assumption that both phases have the same composition. The isotropic displacement parameters (\( U \)) for phase 2a and 2b in sample 2 were not constrained to be equal because both phases occur in significant quantities. The refinement shows that the \( U \) values for the same sites are nearly equal to each other, as expected. Moreover, the \( U \) values for phase 2a and 2b are similar to those of sample 1.

| Table 4. Selected distances (Å) and angles (°) for two pyrope samples. |
|---------------------------------------------------------------|
| Bond | Multiplicity | 1. Single | 2. Phase 2a | 2. Phase 2b | 2a–2b |
|------|--------------|-----------|-------------|-------------|--------|
| Z-O | \( \times 4 \) | 1.6343(3) | 1.6334(4) | 1.6334(6) | 0.0000 |
| Y-O | \( \times 6 \) | 1.9101(4) | 1.9080(4) | 1.9020(6) | 0.0060 |
| X-O | \( \times 4 \) | 2.2227(3) | 2.2240(4) | 2.2211(5) | 0.0029 |
| X-O | \( \times 4 \) | 2.3742(3) | 2.3771(4) | 2.3696(5) | 0.0075 |
| \(<X-O> \times 8\) | \( \times 4 \) | 2.2985 | 2.3006 | 2.2954 | 0.0052 |
| \(<D-O> \times 4\) | \( \times 4 \) | 2.0353 | 2.0365 | 2.0315 | 0.0041 |

* \( <D-O> = (Z-O) + (Y-O) + (X-O) + (X-O)/4 \), which is the average distance for the four-coordinated O atom.
3. Results

The single-phase sample 1 has a chemical composition that is similar to sample 2, which contains two cubic phases (Table 1). The two cubic phases in sample 2 occur as an intergrowth on a finer scale (Figure 2c). In other birefringent garnets, the different cubic phases also occur as a fine-scale mixture [17–22]. The average composition for sample 1 is \( \text{[Mg}_{2.30}\text{Fe}^{2+}_{0.26}\text{Ca}_{0.42}\text{Mn}^{2+}_{0.02}]_3 \text{[Al}_{1.53}\text{Fe}^{3+}_{0.06}\text{Cr}^{3+}_{0.40}\text{Ti}_{0.01}\text{Fe}^{2+}_{0.01}]_2\text{Si}_{3}\text{O}_{12} \), which contains more \( \text{Cr}^{3+} \) and less \( \text{Al}^{3+} \) cations in the Y site. Sample 2 average composition is \( \text{[Mg}_{2.33}\text{Fe}^{2+}_{0.33}\text{Ca}_{0.33}\text{Mn}^{2+}_{0.01}]_3 \text{[Al}_{1.73}\text{Fe}^{3+}_{0.12}\text{Cr}^{3+}_{0.06}\text{Ti}_{0.05}\text{Fe}^{2+}_{0.05}]_2\text{Si}_{3}\text{O}_{12} \). The Y-O distance is expected to be longer for sample 1 because the radius of \( \text{Cr}^{3+} = 0.615 \) Å is larger than \( \text{Al}^{3+} = 0.535 \) Å [58]. The average <X-O> and Z-O distances are expected to be similar in both samples containing about 70% mole of the pyrope molecule, which is about the maximum mole % for most natural pyrope samples [59]. A notable exception is a nearly pure pyrope from the Dora Maira Massif, Western Alps, Italy [31,60–62]. The studied compositions (Table 1) correspond to pyrope in line with the garnet nomenclature [63] and the IMA-CNMNC rules [64]. This study builds on our previous work on garnet-group minerals [65–73].

Sample 1 is a single phase, but sample 2 contains two cubic phases. The same reflections are compared for the two samples (Figures 3 and 4). The sharp diffraction peaks (e.g., (400)) in Figure 3a represent a single cubic phase, whereas those in Figure 3b are split into two, indicating the presence of two different cubic phases. It is of interest to compare the insert in Figure 3b to the XRD traces obtained for majorite by other researchers [11,15]. However, those studies used tetragonal symmetry to refine the crystal structure of majorite, whereas a recent study shows that the previously observed splitting arises from cubic majorite and a completely different phase [74]. However, for sample 2, two different cubic phases were used to fit the trace in Figure 3b. Figure 4 shows an expanded 2θ scale for both samples, and the splitting of reflections is clearly observed in Figure 4b. Splitting of reflections was also observed in several other minerals [75–79].

The reduced \( \chi^2 \) and overall R (\( F^2 \)) Rietveld refinement values are 1.121 and 0.0658, respectively, for sample 2 (Table 2). The site occupancy factors (sofs) obtained from the refinement are similar to those calculated from the EPMA results (Table 3).

The unit-cell parameter for phase 2a is \( a = 11.56185(1) \) Å, whereas sample 1 has \( a = 11.56197(1) \) Å, which is similar to phase 2a. Two cubic phases and splitting of the reflections were not previously observed in pyrope, but they are easily observed in this study and other garnet-group members [17–22]. Simon et al. [62] described a prograde-zoned pyrope from the Dora Maira massif, the western Alps, with the Mg content increasing from the core to the rim of the crystal, where near end-member pyrope composition occurs. It is possible that such a pyrope may be a two-phase sample, or the diffraction peaks may be broad compared to those observed in this study. Further diffraction work is needed for such a sample.

In comparing the bond distances for sample 2 (Table 4; Figure 5), the difference is most for the Y-O distance, followed by the difference in average <X-O> distance. Therefore, subtle changes of cations on both the X and Y sites are responsible for the two different phases in sample 2. However, the difference in sofs from the refinement is significantly different for the Y sites in the two phases, whereas the sofs for the X and Z sites are nearly the same, so atoms in the Y site are responsible for the two different phases in sample 2. Sample 1 contains more \( \text{Cr}^{3+} \) cations, so the Y-O distance is longer for sample 1 (Table 4; Figure 5). The other distances are similar for both samples. Sample 1 and phase 2a have similar unit-cell parameters and bond distances. In Figure 5, these distances are plotted between the garnet series from pyrope to almandine and extend toward spessartine. The <D-O> data points for samples 1 and 2 fall on the linear trend line (Figure 5b). However, the other data points show more scatter but are close to the trend lines (Figure 5a,c,d). The less scatter of the <D-O> data points indicate that proper coordination of the O atoms is most important in garnet-group minerals.
pyrope composition occurs. It is possible that such a pyrope may be a two-phase sample, or the diffraction peaks may be broad compared to those observed in this study. Further diffraction work is needed for such a sample.

Figure 3. Full HRPXRD traces for both pyrope samples together with the calculated (continuous line) and observed (crosses) profiles. The difference curve ($I_{obs} - I_{calc}$) is shown at the bottom. The short vertical lines indicate allowed reflection positions. The intensities for the trace and difference curve that are above 20° 2θ are multiplied by 4. Inserts show that the (400) reflection is not split in sample 1 in (a) but clearly split into two in sample 2 in (b).
Figure 4. Expanded part of the HRPXRD traces showing no splitting of sharp reflections for sample 1 in (a), but splitting of sharp reflections into two for sample 2 in (b). The reflections in (a) are from a single phase, whereas those in (b) are from two cubic phases.
Sample 1 contains more Cr\(^{3+}\) cations, so the Y-O distance is longer for sample 1 (Table 4; Figure 5). The other distances are similar for both samples. Sample 1 and phase 2a have similar unit-cell parameters and bond distances. In Figure 5, these distances are plotted between the garnet series from pyrope to almandine and extend toward spessartine. The <D-O> data points for samples 1 and 2 fall on the linear trend line (Figure 5b). However, the other data points show more scatter but are close to the trend lines (Figure 5a,c,d). The less scatter of the <D-O> data points indicate that proper coordination of the O atoms is most important in garnet-group minerals.

Figure 5. Structural variations across the pyrope (Prp)-almandine (Alm) series extended toward spessartine (Sps). The Y-axis interval (0.046 Å) is set the same in (a–d). Linear solid trend lines are fitted to the open circle data points from Antao et al. [80]. Other data from the literature are shown as triangles (a = 11.457 Å (Prp)) from Merli et al. [61]; a = 11.459 Å (syn. Prp) and a = 11.531 Å (Alm) from Novak and Gibbs [27]; a = 11.526 Å (Cr-Prp) from Novak and Meyer [81], and black * (a = 11.452 for syn. Prp and a = 11.525 Å for syn. Alm from Armbruster et al. [30]). The red open diamond denotes a synthetic Prp from Antao et al. [74].
4. Conclusions

This study describes the crystal structure of two different pyrope samples. One sample is a single cubic phase and is optically isotropic. The other sample contains an intergrowth of two different cubic phases that have slightly different structures and compositions. Because this sample contains two cubic phases, it is optically anisotropic, as was observed in many recent studies on garnet-group minerals.

Previous structural studies of pyrope have reported anomalously large atom displacement parameters (ADPs) for the Mg atom where $U_{Mg} > U_O$ [27,30–33]. This study shows that $U_{Mg} < U_O$, so no anomaly was observed. The chemical analyses show that the X and Y sites contain several different cations.

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