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LETTER

Symmetry analysis of the phase transition and twinning in $MgSiO_3$ garnet: Implications to mantle mineralogy

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Introduction

The (Mg,Fe)SiO_3 (majorite) garnet phase is considered to be a major constituent of the transition zone of the Earth's mantle between the 400- and 670-km discontinuities (Ringwood, 1967; Liu, 1977; Akaogi and Akimoto, 1977; Ito and Takahashi, 1987). The addition of Al to the $MgSiO_3$ system stabilizes the cubic ($Ia3d$) pyrope-type garnet, whereas for the $MgSiO_3$ composition, the symmetry is reduced to tetragonal ($I4_1/a$) primarily because of the ordering of the Mg and Si atoms in the octahedral sites (Kato and Kumazawa, 1985; Sawamoto, 1987). The $MnSiO_3$ garnet phase also shows tetragonal symmetry and nearly complete ordering of $^{[6]}$Mn and $^{[6]}$Si in the octahedral sites (sixfold coordination indicated by the superscript [6]; Fujino et al., 1986) (cf. $CaGeO_3$ and $GdGeO_3$ garnets, Prewitt and Sleight, 1969). Because of the geophysical importance of the $MgSiO_3$ garnet phase, a possible cubic to tetragonal phase transition in the $MgSiO_3$ garnet and the associated cation ordering in the octahedral sites are of great interest from the thermodynamic point of view. This transition also has important implications on the seismic velocities in the transition zone. Recently, tetragonal single crystals of $MgSiO_3$ garnet have been synthesized at 17 GPa and 1800 °C (Angel et al., 1989); these show partial $^{[6]}$Mg-$^{[6]}$Si ordering in the octahedral sites and two different types of twinning: (1) merohedric twinning with irregular twin boundaries and {110} as the reflection planes and (2) pseudomerohedric twinning with twin lamellae parallel to {110} related by a $\bar{3}$ rotation parallel to ⟨111⟩. Remarkably, both sets of twins are found in leucite ($KAlSi_2O_6$) crystals of volcanic origin, which have crystallized with the cubic ($Ia3d$) symmetry and subsequently undergone a sequence of closely spaced phase transitions, $Ia3d \rightarrow I4_1/acd \rightarrow I4_1/a$, at approximately 605 and 590 °C, respectively (see Lange et al., 1986). High-temperature electron-microscope experiments on leucite show that the pseudomerohedric {110} twins result from the cubic ($Ia3d$) to tetragonal ($I4_1/acd$) transition, where the $\bar{3}$ operation of the cubic point group is lost, and the merohedric twins result from the tetragonal ($I4_1/acd$) to tetragonal ($I4_1/a$) transition, where the diagonal mirror plane (110) of the high-temperature tetragonal phase is lost (Palmer et al., 1988; Heany and Veblen, 1988). That these twins in leucite are transformation twins and not growth twins is further confirmed by the fact that the tetragonal leucite crystals grown hydrothermally at 500 °C (considerably below the temperature of the phase transitions) show no signs of twinning (Friedel and Friedel, 1890; Wyart, 1940). On the basis of similar twinning found in $MgSiO_3$ garnet crystals, we suggest that as in leucite these are also transformation twins and that the $MgSiO_3$ garnet synthesized at 17 GPa and 1800 °C has undergone a cubic to tetragonal phase transition on cooling. In this letter, we analyze the cubic to tetragonal phase transition in $MgSiO_3$ garnet in terms of group theory. We consider the $^{[6]}$Mg-$^{[6]}$Si ordering in the octahedral sites as the primary order parameter, which drives the phase transition.

Order-parameter description

The phase transition in $MgSiO_3$ garnet from $Ia3d$ to $I4_1/a$ is driven by the onset of a primary order parameter at the transition temperature. From the tables of Stokes and Hatch (1988), it can be seen that a primary order parameter transforming according to the three-dimensional $\Gamma_4^+(T_{1g})$ representation of $Ia3d$ can induce the cubic to tetragonal transition being considered. The transformation is an *improper ferroelastic* transition, and thus the strain cannot serve as the primary order parameter. The cubic to tetragonal transition could be continuous since the representation satisfies the Landau and Lifschitz conditions and it results from the order parameter taking on the restricted form (η, 0, 0). In Table 1 we show the new basis vectors of the tetragonal phase as well as the location of the origin of this phase relative to the original cubic origin. The location (0, ½, 0) is expressed in terms of the basis vectors of the original cubic structure.

The transition $Ia3d \leftrightarrow I4_1/a$ is a *translationengleich* transition, i.e., no translations are lost at the transition. There are a number of ways of selecting the fourfold axis from $Ia3d$, and each selection determines an equivalent domain of $I4_1/a$. The number of such equivalent tetragonal domains for the lower-symmetry phase can be obtained by simply considering the change in the orders of

TABLE 1. The six possible domain orientations for the subgroup $I4_1/a$

Domain	Basis vectors	Origin	Generators	Direction vector
1	(0, 1, 0), (0, 0, 1), (1, 0, 0)	(0, ½, 0)	$(C_{4x}^{+}\|\frac{1}{4}, \frac{5}{4}, -\frac{1}{4})$, $(I\|0, 1, 0)$	$(a, 0, 0)$
2	(0, 1, 0), (0, 0, −1), (−1, 0, 0)	(½, ½, 0)	$(C_{4x}^{-}\|-\frac{1}{4}, \frac{5}{4}, \frac{1}{4})$, $(I\|-1, 1, 0)$	$(-a, 0, 0)$
3	(1, 0, 0), (0, 1, 0), (0, 0, 1)	(½, 0, 0)	$(C_{4z}^{+}\|\frac{5}{4}, -\frac{1}{4}, \frac{1}{4})$, $(I\|1, 0, 0)$	$(0, 0, a)$
4	(1, 0, 0), (0, −1, 0), (0, 0, −1)	(½, 0, ½)	$(C_{4z}^{-}\|\frac{5}{4}, \frac{1}{4}, -\frac{1}{4})$, $(I\|1, 0, 1)$	$(0, 0, -a)$
5	(0, 0, 1), (1, 0, 0), (0, 1, 0)	(0, 0, ½)	$(C_{4y}^{+}\|-\frac{1}{4}, \frac{1}{4}, \frac{5}{4})$, $(I\|0, 0, 1)$	$(0, a, 0)$
6	(0, 0, −1), (1, 0, 0), (0, −1, 0)	(0, 0, 0)	$(C_{4y}^{-}\|\frac{1}{4}, -\frac{1}{4}, -\frac{3}{4})$, $(I\|0, 0, 0)$	$(0, -a, 0)$

Note: The basis vectors, origin locations, and generators are specified relative to the high-symmetry $Ia3d$ phase. Order-parameter directions for each domain are also listed.

the point groups $m3m$ and $4/m$, which are 48 and 8, respectively. Thus there are six equivalent domains in the lower-symmetry phase, and all are orientational (twin) domains. Table 1 gives basis vectors of each of the domains, their origin locations, the generators of each corresponding equivalent symmetry subgroup, and the order-parameter direction for each domain.

From Tables 9 and 10 of Stokes and Hatch (1988), the free energy for the Γ_4^+ representation is easily obtained. The free energy is an expansion of the order parameter in invariant polynomial forms. The expansion to the fourth degree is

$$\Phi = a_1(\eta_1^2 + \eta_2^2 + \eta_3^2) + a_2(\eta_1^2 + \eta_2^2 + \eta_3^2)^2 + a_3(\eta_1^4 + \eta_2^4 + \eta_3^4). \quad (1)$$

A transition to $I4_1/a$ and the third domain would correspond to an order parameter value of $(0, 0, \eta)$. This value of η corresponds to a range of coefficients a_1, a_2, a_3 that makes Φ a minimum. Other equivalent domain orientations with the same subgroup symmetry would give the same value of Φ and are thus energetically degenerate with $(0, 0, \eta)$.

In Table 2 we show other subgroup possibilities and their description as given in Stokes and Hatch (1988). Phase transitions from cubic to trigonal, monoclinic, and triclinic phases are possible by parametric distortions of the Γ_4^+ parameter. For each phase, order-parameter directions are shown for one representative domain. A given phase will occur only if the coefficients of the free-energy expansion in Equation 1 are such that they minimize the free energy for that direction of the order parameter.

The primary order parameter $\eta = (0, 0, \eta)$ (domain three) determines the lower-symmetry phase $I4_1/a$. The subgroup is obtained by keeping all symmetry elements of $Ia3d$ that leave invariant the order parameter η (which transforms according to Γ_4^+). In most transitions, atomic distortions (either atomic displacements or atomic ordering) for more than one Wyckoff position transform according to Γ_4^+ and can contribute to the distortion allowed by Γ_4^+. Any one of these allowed distortions could be used as a primary order parameter. There are also additional distortions that could occur and that do not destroy the symmetry of the $I4_1/a$-subgroup phase. These secondary distortions, which we take as secondary order parameters, do not transform according to Γ_4^+ but will couple linearly to it. Since the coupling terms between the secondary and primary order parameters are linear in the secondary order parameter, distortions transforming according to the secondary order parameter must occur at the transition, even if they are small. For $I4_1/a$, the additional distortions are of the form $\mathbf{Q} = (q, 0)$, which arises from the two-dimensional irreducible representation $\Gamma_3^+(E_g)$, and $\mathbf{P} = (p)$, which arises from the one-dimensional irreducible representation $\Gamma_1^+(A_{1g})$. From symmetry considerations it follows that only these two irreducible representations can couple linearly with Γ_4^+. As can be seen from Table 4 of Stokes and Hatch (1988), certain strain components transform according to Γ_3^+ and Γ_1^+, but no strain components transform according to Γ_4^+. Specifically, the strain combination $(\epsilon_{11} + \epsilon_{22} + \epsilon_{33})$ transforms according to Γ_1^+, whereas the combinations $(\epsilon_{11} + \epsilon_{22} - 2\epsilon_{33}, \sqrt{3}\epsilon_{11} - \sqrt{3}\epsilon_{22})$ transform according to the two-dimensional Γ_3^+. Thus (1) a volume dilation (contraction) can appear at the transition because of coupling of Γ_1^+ with the primary order parameter and (2) a tetragonal and/or orthorhombic distortion can also appear because of the first and second component, respectively, of Γ_3^+. The distortions of Γ_1^+,Γ_3^+ resulting from coupling with the primary order parameter Γ_4^+ will be considered in more detail below.

MICROSCOPIC DISTORTIONS

In several previous publications, the method of induced representations has been discussed (Hatch et al., 1987; Hatch and Griffen, 1989; Ghose et al., 1989; Hatch and Ghose, 1989; Hatch and Stokes, 1989a, 1989b). The method determines which microscopic distortions (displacements, orderings, etc.) are consistent with order parameters appearing at the transition. For the $MgSiO_3$ garnets, the Wyckoff positions of the atoms and their site symmetry in the cubic phase are given in Table 3. From the tables of Putnam (1985) (or Kovalev, 1986), the possible orderings and/or displacements attributed to these atomic positions can be obtained. All orderings and/or displacements are defined relative to the (cubic) high-symmetry equilibrium distributions or positions. Table 3 presents those results. There, under column three, the induction frequency of a local displacive distortion from the cubic position is shown, followed by the induction frequency of an ordering distortion for each occupied cubic position of $MgSiO_3$. These two frequencies are separated by a hyphen. If a zero entry appears, it signifies that

TABLE 2. Possible subgroups obtained from the cubic *Ia3d* phase by the three-dimensional Γ_4^+ mode

Subgroup	Species	Direction	Basis	Origin
C_{4h}^6 (88) $I4_1/a$	ifs	(*a*, 0, 0)	(0, 1, 0), (0, 0, 1), (1, 0, 0)	(0, ½, 0)
C_{2h}^6 (15) $C2/c$	ifs	(*a*, *a*, 0)	(0, 0, −1), (−1, −1, 0), (−½, ½, ½)	(0, 0, 0)
C_{3i}^2 (148) $R\bar{3}$	ifs	(*a*, *a*, *a*)	(−1, 1, 0), (0, −1, 1), (½, ½, ½)	(0, 0, 0)
C_i^1 (2) $P\bar{1}$	ifs	(*a*, *b*, *c*)	(−½, ½, ½), (½, −½, ½), (½, ½, −½)	(0, 0, 0)

Note: Each subgroup results from a distinct direction of the order parameter indicated in column three. The subgroup basis and origin are specified relative to the high-symmetry *Ia3d* phase.

the local distortion is not allowed by Γ_4^+ for that Wyckoff position. Similar information is listed for the representations Γ_1^+,Γ_3^+. Of special importance is the information concerning the 16(*a*) sites. These positions *can* contribute an ordering mechanism to the phase transition that transforms as the Γ_4^+ representation. They cannot, however, contribute a displacement contribution. In the high-symmetry cubic phase, $^{[6]}$Mg and $^{[6]}$Si atoms are disordered on the 16(*a*) sites with equal probability. An ordering of the atoms on this Wyckoff position is consistent with a Γ_4^+ order parameter and could thus serve as the primary order parameter of transition. *We take this ordering as the primary distortion of the transition.*

As seen from Table 3, other atomic distortions are also consistent with the Γ_4^+ symmetry. For example, an ordering of atoms in the 24(*d*) sites or the 96(*h*) sites are also symmetry allowed by Γ_4^+. However, such ordering is not applicable in the structural change that we are considering. Notice that atomic displacements from the cubic equilibrium positions of atoms at the 24(*c*), 24(*d*), and 96(*h*) sites are also symmetry-allowed by Γ_4^+. It is expected that such displacements would occur in conjunction with the ordering process at the 16(*a*) sites.

We also expect secondary distortions from Γ_1^+ and Γ_3^+ to contribute to the lower-symmetry phase, particularly as we move farther away from the transition temperature. For ease of development, we focus on the ordering at the 16(*a*) sites even though we expect that a complete microscopic description of the distortions of the $I4_1/a$ phase would require considerations of additional microscopic distortions from Γ_4^+ as well as distortions from Γ_1^+ and Γ_3^+.

As we concluded above, ordering at the 16(*a*) sites will act as the primary order parameter of Γ_4^+ for the cubic to tetragonal transition. A local ordering would be described by the A_g representation of $\bar{3}$ at the (0, 0, 0) (*a*) site. The condition that the ordering transforms under Γ_4^+ puts stringent restrictions on the relative ordering at other equivalent (*a*) sites. Using projection-operator methods, we obtain the following $\phi(\mathbf{r})$ functions for the Γ_4^+ representation induced from the A_g representation of $\bar{3}$:

$$\begin{aligned}\phi_1 &= [1, 1, -1, -1, -1, -1, 1, 1],\\ \phi_2 &= [1, -1, -1, 1, 1, -1, 1, -1],\\ \phi_3 &= [1, -1, 1, -1, 1, -1, 1, 1].\end{aligned} \tag{2}$$

The elements of each basis function correspond to the eight equivalent non-body-centered (*a*) sites of *Ia3d* listed from top to bottom in the same order as the *International Tables for X-ray Crystallography* (1983), that is, (0, 0, 0), (½, 0, ½), (0, ½, ½), (½, ½, 0), (¾, ¼, ¼), (¾, ¾, ¾), (¼, ¼, ¾), and (¼, ¾, ¼). The basis-function elements are then repeated in the same sequence for the points obtained by adding the body-centering vector (½, ½, ½) to the above set. The elements of these functions give the relative weighting of the (*a*)-site ordering demanded by the Γ_4^+ representation. To be specific, if at (0, 0, 0) we take the ordering probability as $\rho = \rho_{Mg} - \rho_{Si}$, then in the *Ia3d* phase, $\rho = 0$. At the transition (to the third domain corresponding to ϕ_3 in Eq. 2) ρ becomes nonzero at (0, 0, 0), the opposite nonzero ordering appears at (½, 0, ½), the same amount at (0, ½, ½), etc. Notice that for the transition from *Ia3d* to $I4_1/a$, only the single function ϕ_3 contributes for a transition to domain three (see Table 1).

A similar calculation for the grandite garnets was performed where the 16(*a*) sites of *Ia3d* were also considered (Hatch and Griffen, 1989). There, however, the cation ordering transformed according to the $\Gamma_5^+(T_{2g})$ representation. As can be seen by comparing Equation 2 with the results of Hatch and Griffen (1989), the relative ordering, as expected, is different for the two distinct representations.

DOMAIN-WALL FORMATION

As discussed above, the transition from *Ia3d* to $I4_1/a$ is driven by the primary order parameter Γ_4^+, which gives the $^{[6]}$Mg-$^{[6]}$Si ordering at the 16(*a*) sites. The Γ_4^+ representation can also couple with the Γ_1^+ and Γ_3^+ representations so that at the transition, additional distortions appear but they do not destroy the symmetry of the tetragonal $I4_1/a$ phase. Because of the linear-quadratic coupling between Γ_1^+ and Γ_4^+ and the linear-quadratic coupling between Γ_3^+ and Γ_4^+, contributions from strain must appear at the transition. The symmetry change at the transition and the spontaneous onset of strain will lead

TABLE 3. Assignment of atomic positions for $MgSiO_3$ in the *Ia3d* phase

Atoms	Position	Site symmetry	Γ_4^+ (T_{1g})	Γ_1^+ (A_{1g})	Γ_3^+ (E_g)
$^{[8]}$Mg	24(*c*)	222	3-0	0-1	1-1
$^{[6]}$Mg, $^{[6]}$Si	16(*a*)	$\bar{3}$	0-1	0-1	0-0
$^{[4]}$Si	24(*d*)	$\bar{4}$	2-1	0-1	1-1
O	96(*h*)	1	1-1	1-1	1-1

Note: The Wyckoff position and site symmetry for each distinct set of atoms are listed. In columns four, five, and six, the induction frequency for displacements followed by the induction frequency for ordering is listed for each Wyckoff position and each representation Γ_4^+, Γ_1^+, Γ_3^+.

to twinning in the lower-symmetry phase. There are six energetically equivalent domains for the phase $I4_1/a$ that can be viewed as resulting from the loss of the threefold axes along ⟨111⟩ (pseudomerohedric twins) and the loss of the diagonal mirror planes {110} (merohedric twins). Both types of twinning were observed through electron microscopy by Angel et al. (1989).

The loss of symmetry in going from the (cubic) $Ia3d$ phase to the low-temperature phase can be used to determine domain-wall orientations resulting from the minimization of elastic strain. The Γ_1^+ representation leads to a volume expansion or contraction and will not lead to orientational domains. The Γ_3^+ representation, however, leads to orientational domains, and their description can be broken into two parts. (1) The first symmetry change results from the loss of the ⟨111⟩ threefold axis. This symmetry change would be $m3m$ to $4/mmm$ and would be a ferroelastic change. From the work of Sapriel (1975), the domain walls are parallel to {110}. (2) The second part, the loss of the mirror planes, implies that the two domains are related by the lost symmetry element, i.e., the {110} mirror plane. This symmetry loss gives rise to the merohedric twinning.

Since the transition is improper ferroelastic and the coupling of the primary order parameter to elastic strain is linear-quadratic, there is no effect on the elastic constants of the cubic phase above the transition temperature, but there will be a decrease in selected elastic constants below the transition (Lüthi and Rehwald, 1981). The Γ_1^+ mode will affect the stiffness constants $c_{11} + 2c_{12}$, whereas the Γ_3^+ mode will affect $c_{11} - c_{12}$ in the tetragonal phase (Chan, 1988).

Conclusions

We suggest that the rapid Mg-Si ordering in the octahedral sites of $MgSiO_3$ (majorite) garnet during quenching from 17 GPa and 1800 °C results in a cubic to tetragonal phase transition. This implies that under mantle conditions the majorite garnet is cubic (with complete octahedral Mg-Si disorder) and not tetragonal as is currently believed.

Acknowledgments

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References cited

Akaogi, M., and Akimoto, S. (1977) Pyroxene-garnet solid-solution equilibria in the systems $Mg_4Si_4O_{12}$-$Mg_3Al_2Si_3O_{12}$ and $Fe_4Si_4O_{12}$-$Fe_3Al_2Si_3O_{12}$ at high pressures and temperatures. Physics of Earth and Planetary Interiors, 15, 90–104.

Angel, R.J., Finger, L.W., Hazen, R.M., Kanzaki, M., Weidner, D.J., Liebermann, R.C., and Veblen, D.R. (1989) Structure and twinning of single-crystal $MgSiO_3$ garnet synthesized at 17 GPa and 1800 °C. American Mineralogist, 74, 509–512.

Chan, S.K. (1988) The polymorphic transformations of zirconia. Physica, B150, 212–222.

Friedel, C., and Friedel, G. (1890) Actions des alcalis et des silicates alcalins sur le mica: production de la néphéline, de l'amphigène, de l'orthose. Bulletin de la Société française de Minéralogie et de Cristallographie, 13, 129–139.

Fujino, K., Momoi, H., Sawamoto, H., and Kumazawa, M. (1986) Crystal structure and chemistry of $MnSiO_3$ tetragonal garnet. American Mineralogist, 71, 781–785.

Ghose, S., Tsukimura, K., and Hatch, D.M. (1989) Phase transitions in ilvaite, a mixed-valence iron silicate. II. A single crystal x-ray diffraction study and Landau theory of the monoclinic to orthorhombic phase transition induced by charge delocalization. Physics and Chemistry of Minerals, 16, 483–496.

Hatch, D.M., and Ghose, S. (1989) A dynamical model for the $I\bar{1}$-$P\bar{1}$ phase transition in anorthite, $CaAl_2Si_2O_8$ II. Order parameter treatment. Physics and Chemistry of Minerals, 16, 614–620.

Hatch, D.M., and Griffen, D.T. (1989) Phase transitions in the grandite garnets. American Mineralogist, 74, 151–159.

Hatch, D.M., and Stokes, H.T. (1989a) Group theoretical description of phase transitions in solid bromoform. Journal of Physics: Condensed Matter, in press.

——— (1989b) Comment on "Silent soft mode in hexagonal barium titanate observed by hyper-Raman scattering." Physical Review, B, in press.

Hatch, D.M., Stokes, H.T., and Putnam, R.M. (1987) Symmetry analysis of the microstructure and phase transitions of a crystallographic space group: Applications. Physical Review, B35, 4935–4942.

Heaney, P.D., and Veblen, D.R. (1988) A transmission electron microscope study of the low–high leucite phase transition. Geological Society of America Abstracts with Programs, 20, 103.

International tables for X-ray crystallography. (1983) Vol. A. T. Hahn, Ed. D. Reidel, Dordrecht, Holland.

Ito, E., and Takahashi, E. (1987) Ultrahigh-pressure phase transformations and the constitution of the deep mantle. In M.H. Manghnani and Y. Syono, Eds., High-pressure research in mineral physics, Geophysical Monograph 39, 221–230. American Geophysical Union, Washington, D.C.

Kato, T., and Kumazawa, M. (1985) Garnet phase of $MgSiO_3$ filling the pyroxene-ilmenite gap at very high temperature. Nature, 316, 803–805.

Kovalev, O.V. (1986) Irreducible representations of the space groups. Gordon and Breach, New York.

Lange, R.A., Carmichael, I.S.E., and Stebbins, J.F. (1986) Phase transitions in leucite ($KAlSi_2O_6$), orthorhombic $KAlSiO_4$, and their iron analogues ($KFeSi_2O_6$, $KFeSiO_4$). American Mineralogist, 71, 937–945.

Liu, L. (1977) The system enstatite-pyrope at high pressures and temperatures and the mineralogy of the earth's mantle. Earth and Planetary Science Letters, 36, 237–245.

Lüthi, B., and Rehwald, W. (1981) Ultrasonic studies near structural phase transitions. In K.A. Müller and H. Thomas, Eds., Structural phase transitions I, p. 131–184. Springer-Verlag, New York.

Palmer, D.C., Putnis, A., and Salje, E.K.H. (1988) Twinning in tetragonal leucite. Physics and Chemistry of Minerals, 16, 298–303.

Prewitt, C.T., and Sleight, A.W. (1969) Garnet-like structures of high-pressure cadmium germanate and calcium germanate. Science, 163, 386–387.

Putnam, R.M. (1985) Subduction frequency calculations for site point-group representations in the representations of the 230 space groups. M.S. thesis, Brigham Young University, Provo, Utah.

Ringwood, A.E. (1967) The pyroxene-garnet transformation in the earth's mantle. Earth and Planetary Science Letters, 2, 255–263.

Sapriel, J. (1975) Domain-wall orientations in ferroelastics. Physical Review, B12, 5128-5140.

Sawamoto, H. (1987) Phase diagram of $MgSiO_3$ at pressures up to 24 GPa and temperatures up to 2200 °C: Phase stability and properties of tetragonal garnet. In M.H. Manghnani and Y. Syono, Eds., High-pressure research in mineral physics, Geophysical Monograph 39, 209–219. American Geophysical Union, Washington, D.C.

Stokes, H.T., and Hatch, D.M. (1988) Isotropy subgroups of the 230 crystallographic space groups. World Scientific, Singapore.

Wyart, M.J. (1940) Étude cristallographique d'une leucite artificelle. Structure atomique et symmétrie de minérale. Bulletin de la Société française de Minéralogie et de Cristallographie, 63, 5–17.

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