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Thermodynamics of Plagioclase II: Temperature Evolution of the Spontaneous Strain at the $I\bar{1} \leftrightarrow P\bar{1}$ Phase Transition in Anorthite

Simon A.T. Redfern and Ekhard Salje
Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge, CB2 3EQ, England

Abstract. The temperature dependence of the lattice parameters of pure anorthite with high Al/Si order reveals the predicted tricritical behaviour of the $I\bar{1} \leftrightarrow P\bar{1}$ phase transition at $T_c^* = 510$ K. The spontaneous strain couples to the order parameter Q° as $x_i \propto S^i_{xQ} Q^{\circ 2}$ with $S^1_{xQ} = 4.166 \times 10^{-3}$, $S^2_{xQ} = 0.771 \times 10^{-3}$, $S^3_{xQ} = -7.223 \times 10^{-3}$ for the diagonal elements. The temperature dependence of Q° is

$$Q^\circ = \left(1 - \frac{T}{510}\right)^\beta, \quad \beta = \tfrac{1}{4}.$$

A strong dependence of T_c^*, S^i_{xQ} and β is predicted for Al/Si disordered anorthite.

1. Introduction

The room temperature phase of anorthite, $CaAl_2Si_2O_8$, has triclinic symmetry with space group $P\bar{1}$. The crystal structure was determined by Kempster et al. (1962) and refined by Czank (1973) and Kalus (1978). At higher temperatures, a reversible phase transition from $P\bar{1}$ to $I\bar{1}$ was first discovered by Brown et al. (1963). The equilibrium transition temperature T_c^* is 510 K according to Wruck (1986). Before, material related anomalies in the diffuseness of critical reflexions (called "c" and "d") had been observed by Laves and Goldsmith (1954) and attributed to ordering of Ca domains. Much speculation about the transition mechanism led to confusion, and Laves et al. (1970) and Czank (1973) reported that the symmetry forbidden reflexions of the $I\bar{1}$ phase still exist up to 1,500° C. A clear distinction between the effect of dynamical and static X-ray and neutron scattering was made by Frey et al. (1977) however. These authors clearly showed that a phase transition takes place near $T_c^* = 510$ K and that residual scattering intensity at $T > T_c^*$ is due to inelastic scattering in fully Al/Si ordered anorthite. Their results on the temperature evolution of the scattering intensities at $T < T_c^*$ are in full agreement with our present findings and also with those of Adlhart et al. (1980).

In this paper we present experimental evidence for the predicted tricritical behaviour of the phase transition based on the observation of the temperature evolution of the spontaneous strain. Its understanding is based on a theoretical approach which has been published separately as paper I of this series (Salje 1987). There it is shown that the phase transition is entirely related to a critical behaviour of symmetry equivalent Z and Z' points on the Brillouin zone boundary. In fact it is interesting to note that anorthite is the only end member feldspar to show a zone boundary instability. The relationship between the Brillouin zones of the $I\bar{1}$ and $P\bar{1}$ phases is shown in Figure 1 of paper I. The transition is of special interest in that it is an example of improper ferroelastic behaviour, hence the transition mechanism cannot simply be due to the ordering of Ca in a double potential (as this would not give rise to the spontaneous strain we have observed). The concepts of Landau theory have been used to describe the thermodynamic behaviour of anorthite in paper I.

The description of the thermodynamic behaviour requires the use of two biquadratically coupled order parameters. One, Q°, corresponds to the rapid lattice distortion at the phase transition itself, the other, Q_{od}, corresponds to the degree of "frozen in"Al/Si order arising from the high temperature $C\bar{1} \leftrightarrow I\bar{1}$ symmetry reduction. Coupling between these two order parameters is strain-induced, a common and dominant coupling mechanism in ferroelastics. The influence of Q_{od} explains the dependence of the $I\bar{1} \leftrightarrow P\bar{1}$ transition on thermal history; annealing and quenching an anorthite will change the value of Q_{od}. Extrapolation of the data of Carpenter and Ferry (1984) indicates that the $C\bar{1} \leftrightarrow I\bar{1}$ transition occurs at between 2,000 K and 2,250 K which is above the melting point. Since the Al/Si disorder acts as a secondary order parameter to the $I\bar{1} \leftrightarrow P\bar{1}$ transition, this transition may be used as a tool for the study of the otherwise inaccessible high temperature transition. In addition the sensitivity of the transition to Na and other impurities, and to thermal history indicates the potential usefulness of the $I\bar{1} \leftrightarrow P\bar{1}$ transition for the thermodynamic characterisation of phases.

In order to understand the modifications of the transformation behaviour due to Al/Si disorder and Ca→Na substitution it is necessary to understand the critical behaviour of fully ordered, endmember anorthite. It is shown in paper I that the transition temperature for pure Ca-feldspar depends explicitly on the degree of Al/Si order. The phase transition would occur at a temperature T_c for fully Al/Si disordered anorthite ($Q_{od} = 0$) and is renormalized to an observed value T_c^* in partly or fully Al/Si ordered anorthite. Therefore in this paper we confine ourselves to the study of pure $CaAl_2Si_2O_8$, and focus on the behaviour of Q° in the "ideal" and simplest case. The results of lattice parameter refinements from X-ray powder patterns taken over a temperature range of about 700 K across the transition are

presented, and from these the temperature evolution of the spontaneous strain and the corresponding representation surface is calculated. The order parameter Q° is calculated for the temperature range considered and computed values of the coupling constants are given.

2. Experimental

Pure end member Ca anorthite from the Val Pasmeda locality, South Tyrolia, was used for this study. The anorthite content determined by electron microprobe varies between 99.5% and 100% An. This metamorphic anorthite is well ordered and is the same sample as that characterised by Carpenter et al. (1985), where details of the preparation and separation of the pure powder are given.

The powdered anorthite was mounted as a thin film in a Huber 632 heating Guinier powder camera. A bent quartz monochromator selected $CuK\alpha_1$ radiation and reduced background intensity. Heating was controlled by a Huber 633 temperature controller. A chromel/alumel thermocouple was used, and throughout the whole temperature range its position relative to the sample remained constant. This allowed a relative temperature stability of better than 1 K, although absolute accuracy was less. Any systematic error was constant however, and a correction was facilitated using the value of T_c^* from Wruck as a fixed point. The controller allowed automatic film movement between each exposure.

An internal Si standard was used to correct for film shrinkage. Powder lines were measured using a Nonius Guinier viewer, allowing measurement to within $0.01°(2\theta)$. Cell parameters were calculated by least squares refinement using about forty reflexions indexed with the help of the calculated powder patterns of Borg and Smith (1969).

The temperature evolution of the lattice parameters is shown in Figure 1. The data scatter gives an indication of the standard error. Above 600 K changes are linear, and due solely to thermal expansion. This thermal expansion has been extrapolated by linear regression from the high temperature $I\bar{1}$ phase to the $P\bar{1}$ low temperature phase. The dashed lines correspond to the lattice parameters to be expected in the absence of spontaneous strain arising from the transition. The dashed curves show the significant deviations in b, β^*, and γ which are observed below the transition temperature. It is remarkable that only the excess functions for these three lattice parameters show a measurable temperature dependence, whereas the excess functions for a, c, and α are zero within our experimental resolution. This behaviour is not related to any symmetry constraints of the phase transition process but appears as a result of the structural behaviour of anorthite. These results are interpreted in terms of the spontaneous strain which couples with the order parameter, Q°, of the transition.

3. The Spontaneous Strain of the Phase Transition $I\bar{1} \leftrightarrow P\bar{1}$

The concept of spontaneous strain was developed in the 1970s in connection with investigations of ferroelastic materials. It was first introduced into the description of structural phase transitions in feldspars by Salje (1985) and Salje et al. (1985). As Tolédano and Tolédano (1980) have already pointed out, we can expect ferroelastic phase transitions to constitute the major part of the ferroic phase transitions inferred possible in Landau theory, and they are very common in minerals. In the case of ferroelastics, a paraelastic phase exists above T_c^* which is defined as being free of strain. On passing below T_c^* the transition to the ferroelastic phase occurs giving rise to a spontaneous strain. The spontaneous strain may be represented by a symmetric second-rank tensor which vanishes by symmetry in the high symmetry paraelastic phase. It will be noticed that the description of the high symmetry paraelastic phase is important in ferroelastic phase transitions, since the spontaneous strain must be measured relative to the lattice parameters of the paraelastic phase. This is unlike ferroelectric of ferromagnetic phase transitions, where the occurence of spontaneous polarization or spontaneous magnetization depends only on the symmetry of the "ferro" phase. The spontaneous strain gives rise to anomalous behaviour of the thermal expansion, the lattice parameters deviating from the expected extrapolation of those in the paraelastic phase. Thus, by careful measurement of the lattice parameters in the low symmetry ferroelastic phase the evolution of the spontaneous strain may be determined.

The role of the spontaneous strain in the $P\bar{1} \leftrightarrow I\bar{1}$ transition is described in paper I. For experimental purposes the spontaneous strain is defined in a Cartesian coordinate system R_i $(i=1, 2, 3)$ where the deformation in the ferroelastic phase transforms a point R_i to r_i with an elastic displacement vector $u_i = r_i - R_i$. The components u_i can be expressed as a function of the initial coordinates in a Lagrangian form, and the state of deformation of the body can be characterized by the symmetric polar second-rank tensor (Bhagavantam 1966, Nye 1957). This linear Lagrangian strain tensor is defined as

$$x_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i}\right). \tag{1}$$

The underlying Cartesian coordinate system used for anorthite is

R_2: parallel to the crystallographic b axis
R_3: parallel to the crystallographic c^* axis
R_1: perpendicular to both.

The lattice parameters are related to the linear Lagrangian spontaneous strain tensor elements by the equations (Schlenker et al. 1978):

$$x_1 = x_{11} = \frac{a \sin\gamma}{a_0 \sin\gamma_0} - 1 \tag{2}$$

$$x_2 = x_{22} = \frac{b}{b_0} - 1 \tag{3}$$

$$x_3 = x_{33} = \frac{c \sin\alpha \sin\beta^*}{c_0 \sin\alpha_0 \sin\beta_0^*} - 1 \tag{4}$$

$$\tfrac{1}{2}x_4 = x_{23} = \frac{1}{2}\left(\frac{c\cos\alpha}{c_0 \sin\alpha_0 \sin\beta_0^*} - \frac{b\cos\alpha_0}{b_0 \sin\alpha_0 \sin\beta_0^*} + \frac{\cos\beta_0^*}{\sin\beta_0^* \sin\gamma_0} \cdot \left(\frac{\alpha\cos\gamma}{a_0} - \frac{b\cos\gamma_0}{b_0}\right)\right) \tag{5}$$

$$\tfrac{1}{2}x_5 = x_{13} = \frac{1}{2}\left(\frac{a \sin\gamma \cos\beta_0^*}{a_0 \sin\gamma_0 \sin\beta_0^*} - \frac{c \sin\alpha \cos\beta^*}{c_0 \sin\alpha_0 \sin\beta_0^*}\right) \tag{6}$$

$$\tfrac{1}{2}x_6 = x_{12} = \frac{1}{2}\left(\frac{a\cos\gamma}{a_0 \sin\gamma_0} - \frac{b\cos\gamma_0}{b_0 \sin\gamma_0}\right) \tag{7}$$

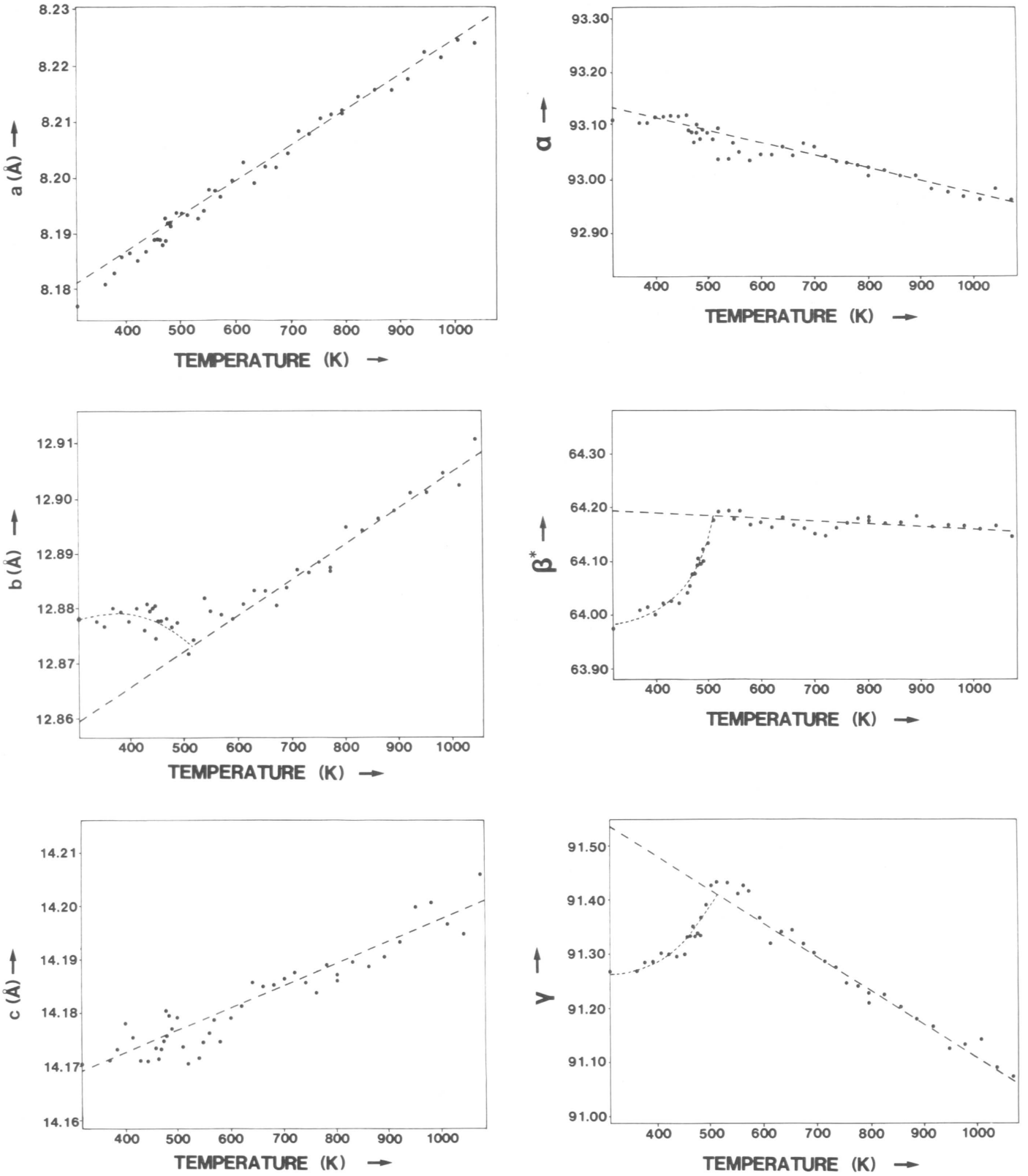

Fig. 1. Temperature dependence of the lattice parameters up to 1,070 K. The $I\bar{1}$ "background" is shown by the dashed lines, the deviations of b, β^*, and γ in the $P\bar{1}$ phase are indicated by the dotted lines

Where the subscript 0 denotes those parameters expected by extrapolation of those in the $I\bar{1}$ phase.

The temperature dependence of the six tensor elements $x_1 \ldots x_6$ is shown in Figure 2. Since strain is a symmetric tensor it may be referred to its principal axes, giving the principal strains. Each of the strain tensors calculated and shown in Figure 2 was diagonalised following the method of Jacobi in Ralston and Wilf (1960). The three principal strains, $\varepsilon_1, \varepsilon_2, \varepsilon_3$ are along the principal axes – three mutually perpendicular directions which remain perpendicular

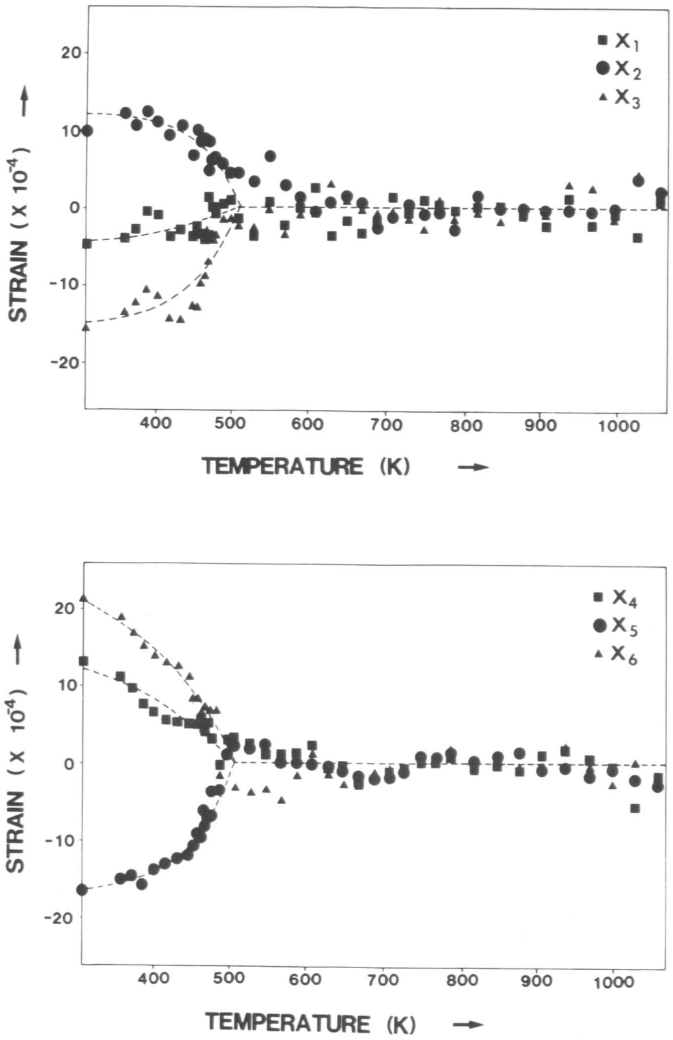

Fig. 2. Temperature evolution of the spontaneous strain tensor elements $x_1 \ldots x_6$

during deformation. These diagonal strain elements are shown in Figure 3. Within the limits of the experimental error ε_2 remains zero below the transition temperature, whereas ε_1 and ε_3 oppose one another.

The representation surface defined by the equation

$$x_{ij} R_i R_j = 1 \tag{8}$$

is a hyperboloid of revolution. Although the orientation of the strain ellipsoid defined by the equation

$$\frac{r_1^2}{(1+\varepsilon_1)^2} + \frac{r_2^2}{(1+\varepsilon_2)^2} + \frac{r_3^2}{(1+\varepsilon_3)^2} = 1 \tag{9}$$

could be an explicit function of temperature our experimental results clearly indicate that its principal axes remain constant. The $P\bar{1}$ cell is in a state of plane strain with respect to the $I\bar{1}$ cell, approximating to a pure shear along the direction of ε_2. This direction corresponds to approximately $[\bar{2}36]$ in the crystal and hardly changes with temperature. Structurally this behaviour indicates that the crystal structure of anorthite in its $I\bar{1}$ phase is not only changed in such a way as to give rise to the doubling of the unit cell in $P\bar{1}$ at $T < T_c^*$ but also to shear of the structure along roughly the $[\bar{2}36]$ direction. This orientation does not change with temperature although there are no symmetry constraints to prevent it from doing so. It is therefore likely that this stability is due to the internal topology of the crystal structure and *not* due to the mechanism of the phase transition process itself.

4. Thermodynamic Calculations and Discussion

The experimental results are now interpreted in terms of the order parameter treatment derived in paper I. Here the variation of the strain parameters is explained in terms of strain induced coupling between the order parameter of the $I\bar{1} \leftrightarrow P\bar{1}$ transition, Q°, and the order parameter of the

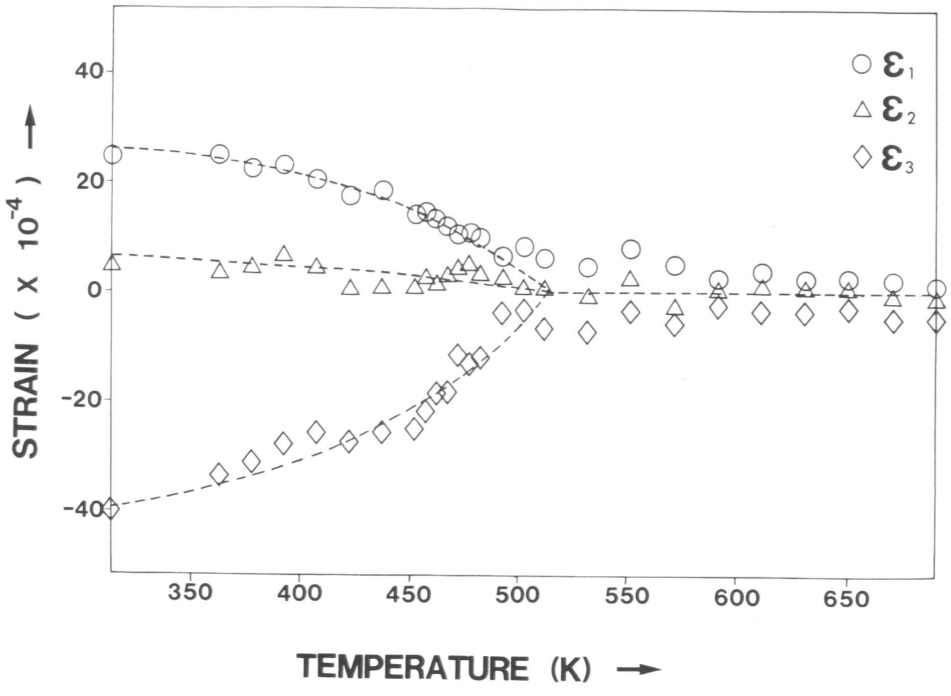

Fig. 3. Temperature dependence of the diagonalised strain tensor components $\varepsilon_1 \ldots \varepsilon_3$

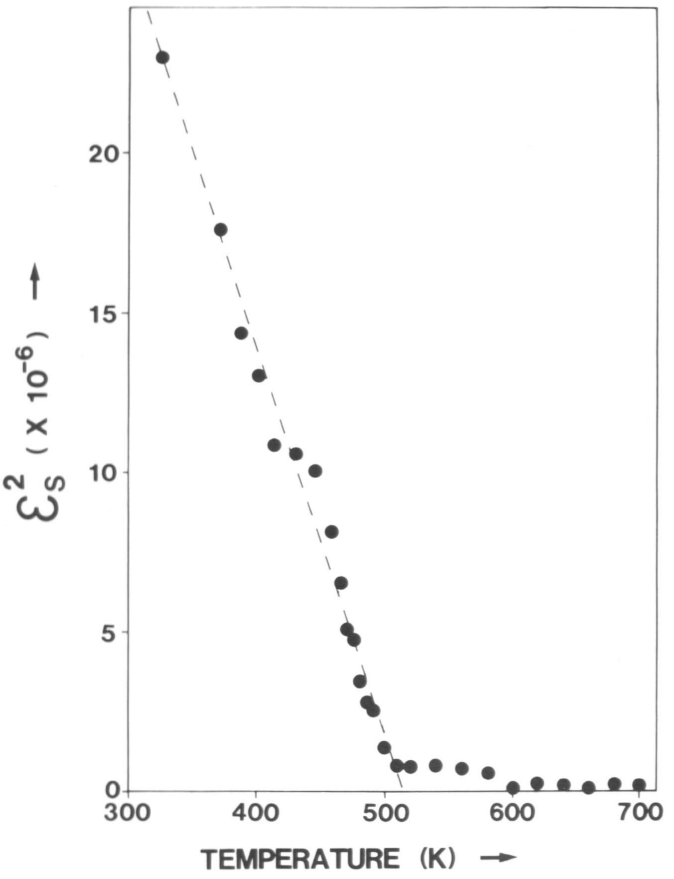

Fig. 4. Variation with temperature of the square of the spontaneous strain, which is proportional to $Q^{\circ 4}$. The linear dependence observed indicates $Q^{\circ} \propto (T_c^* - T)^{\frac{1}{4}}$ and reflects the tricritical nature of the phase transition

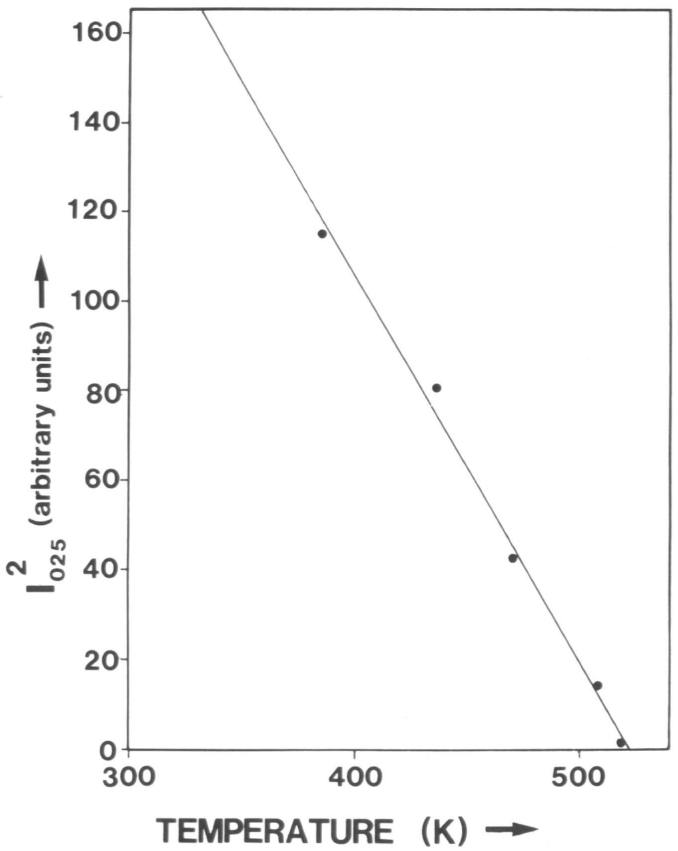

Fig. 5. Temperature variation of the square of the intensity of elastic scattering of the 025 reflexion (from the data of Adlhart et al. 1980)

$C\bar{1} \leftrightarrow I\bar{1}$ Al/Si ordering transition, Q_{od} (see equation 3 in paper I). This leads to the expression for strain in terms of both order parameters given in equation 30 of paper I:

$$x_i = (\Delta_i + S^i_{xQ\,od}) Q^2_{od} + (\delta_{i4} \Delta''_4 + \delta_{i6} \Delta''_6) Q_{od} + S^i_{xQ} Q^{\circ 2} \qquad (10)$$

Here the term in Q^2_{od} is due to the coupling arising from the high temperature $C\bar{1} \leftrightarrow I\bar{1}$ transition, with a "frozen in" degree of order Q_{od}. This transition occurs at around 2,100 K according to Carpenter and Ferry (1984). The term in Q_{od} is the additional strain due to the monoclinic-triclinic transition to be expected above the $C\bar{1} \leftrightarrow I\bar{1}$ transition, of the same form as in the $C2/m \leftrightarrow C\bar{1}$ transition in albite (Salje et al. 1985). The final term in the expression arises from the strain coupling to the $I\bar{1} \leftrightarrow P\bar{1}$ order parameter Q°.

Val Pasmeda anorthite is highly ordered material with small fluctuations in the degree of Al/Si order. We find that for this mineral $Q_{od} \simeq 1$, and within the temperature range studied this value of Q_{od} is frozen in and remains constant (due to the kinetic barriers to Al/Si ordering). Thus the only temperature dependent term in equation 10 is $S^i_{xQ} Q^{\circ 2}$. In other words, the effects observed in the behaviour of spontaneous strain through the transition reflect directly the behaviour of the order parameter for the $I\bar{1} \leftrightarrow P\bar{1}$ transition, Q°, and $x_i \propto Q^{\circ 2}$. However, it is important to note that this behaviour is not encountered for volcanic anorthite, or crystals containing Na (paper I). The critical exponent, β, of the order parameter may thus be obtained from the behaviour of the strain. Since $Q^{\circ} \propto (T_c^* - T)^{\beta}$, then $x_s \propto (T_c^* - T)^{2\beta}$. Here x_s is the scalar spontaneous strain defined in the form adopted by Aizu (1970). Thus

$$x_s = \sqrt{\sum_i x_i^2} \qquad (11)$$

Any physical property which transforms as x_i will show the same critical dependence including the diagonal strain elements with $\varepsilon_s = \sqrt{\sum_i \varepsilon_i^2}$ which is proportional to $(T_c^* - T)^{2\beta}$. The relationship between ε_s^2 and T is shown in Figure 4 where a linear dependence is evident. Since $\varepsilon_s^2 \propto (T_c^* - T)$ the critical exponent β is $\frac{1}{4}$ which indicates the tricritical nature of the $I\bar{1} \leftrightarrow P\bar{1}$ transition in Val Pasmeda anorthite. This result is in agreement with Wruck (1986) whose measurements of excess heat capacity on the same material also show a tricritical behaviour. Further evidence for tricritical behaviour is found in the neutron and X-ray scattering data of Frey et al. (1977), and Adlhart et al. (1980). Theoretically, the integrated intensities of elastic scattering show the same temperature dependence as strain, since $I \propto Q^{\circ 2}$ for critical c and d reflexions. Indeed, Figure 5 shows the linear temperature dependence of I^2_{025} which confirms the tricritical behaviour with $\beta = \frac{1}{4}$. The internal consistency of the data of Adlhart et al. and our findings is demonstrated in Figure 6 where the linear correlation between the spontaneous strain and the intensity of the 025

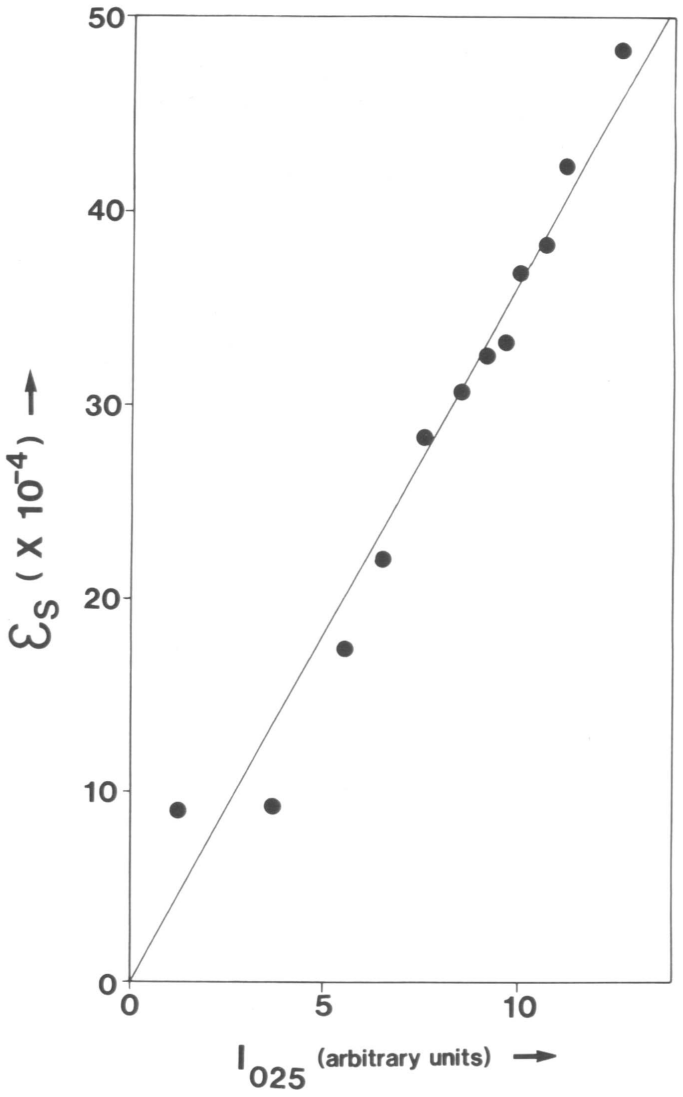

Fig. 6. The linear dependence of spontaneous strain on scattering intensity of a critical reflexion. This results from a shared proportionality to the square of the order parameter Q°

reflexion (which both reflect the same temperature evolution of $Q^{\circ 2}$) is shown.

At a tricritical point the fourth order term in the Landau expansion for free energy becomes zero. In equation 25 of paper I it is shown that for Val Pasmeda anorthite exhibiting tricritical behaviour the order parameter below T_c for the $I\bar{1} \leftrightarrow P\bar{1}$ transition becomes

$$Q^\circ = \left(\frac{a_0}{c}(T_c^* - T)\right)^{\frac{1}{4}} \tag{12}$$

Therefore, if we know T_c^* we are able to calculate the order parameter at any temperature. The value for T_c^* determined by Wruck (1986) is 510 K, which is in agreement with the results of Adlhart et al. (1980), Frey et al. (1977), and Staehli and Brinkmann (1974). Since $Q^\circ = 1.0$ at $T = 0$ K

$$\frac{c}{a_0} = T_c^* = 510 \text{ K} \tag{13}$$

and

$$Q^\circ = \left(1 - \frac{T}{514.5}\right)^{\frac{1}{4}} \tag{14}$$

which gives the final temperature dependence of Q°.

The coefficients S^i_{xQ} in equation 10 may be calculated from the slopes of x_i against $Q^{\circ 2}$, allowing the determination of x_i at all temperatures if Q_{od} is known;

$$x_1 = f_1(Q_{od}) - 0.765 \times 10^{-3}\, Q^{\circ 2}$$
$$x_2 = f_2(Q_{od}) + 1.381 \times 10^{-3}\, Q^{\circ 2}$$
$$x_3 = f_3(Q_{od}) - 2.907 \times 10^{-3}\, Q^{\circ 2}$$
$$x_4 = f_4(Q_{od}) + 2.062 \times 10^{-3}\, Q^{\circ 2}$$
$$x_5 = f_5(Q_{od}) - 3.471 \times 10^{-3}\, Q^{\circ 2}$$
$$x_6 = f_6(Q_{od}) + 4.072 \times 10^{-3}\, Q^{\circ 2}$$

where in each case

$$f_i(Q_{od}) = (\Delta_i + S^i_{xQ_{od}})Q^2_{od} + (\delta_{i4}\Delta''_4 + \delta_{i6}\Delta''_6)Q_{od}. \tag{15}$$

Similarly the diagonal strain elements may be described in terms of a function of $Q^{\circ 2}$ and Q_{od} analogous to equation 10 giving the following dependence on $Q^{\circ 2}$

$$\varepsilon_1 = f_1(Q_{od}) + 4.166 \times 10^{-3}\, Q^{\circ 2}$$
$$\varepsilon_2 = f_2(Q_{od}) + 0.771 \times 10^{-3}\, Q^{\circ 2}$$
$$\varepsilon_3 = f_3(Q_{od}) - 7.223 \times 10^{-3}\, Q^{\circ 2}$$

where in each case

$$f_i(Q_{od}) = (\Delta_i + S^i_{\varepsilon Q_{od}})Q^2_{od} + (\delta_{i4}\Delta''_4 + \delta_{i6}\Delta''_6)Q_{od}. \tag{16}$$

Using these equations it is now possible to determine the value of Q° in fully ordered anorthite end member feldspars at any temperature. Further studies of anorthites with varying degrees of Al/Si order will allow determination of the other coupling constants between the strain and Q_{od}, and in a forthcoming paper we will discuss the influence of $f_i(Q_{od})$ for slightly disordered anorthite.

The theoretical approach of paper I is thus seen to explain the behaviour of the spontaneous strain in anorthite below 510 K, predicting the observed tricritical behaviour and allowing the determination of quantitative relationships between the strain and the order parameter.

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