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REDETERMINATION OF ORIENTATION OF COHERENT INTERFACE BOUNDARIES BETWEEN α- AND α'_H-PHASES IN DICALCIUM SILICATE

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ABSTRACT

Principal distortions (η_i) of the α-to-α'_H lattice deformation for pure Ca_2SiO_4 at 1738 ± 15 K were $\eta_1 = 0.984 < 1$, $\eta_2 = 0.997 \sim 1$, and $\eta_3 = 1.057 > 1$. These meet the general requirements for the occurrence of coherent interphase boundaries between the two phases. The boundaries, the orientation of which was found from calculation by matrix algebra analysis, intersect $(001)_\alpha$ at 29.3 ± 0.3°. This is compatible with 27 ± 3°, determined experimentally for Ca_2SiO_4 solid solution. The reverse transition, α'_H-to-α, was also expected to be accompanied by the formation of coherent boundaries, which intersect $(001)_{\alpha'H}$ at 27.6 ± 0.3°. © *1998 Elsevier Science Ltd*

Introduction

When crystals of Ca_2SiO_4 solid solutions (C_2Sss) are cooled from the stable temperature region of the trigonal α-phase, a polymorphic phase transition occurs, leading to the formation of orthorhombic α'_H-phase lamellae within the host α-phase. The lamella orientation has been experimentally determined from combined use of X-ray diffractometry and optical microscopy (1). The results showed that there were six sets of crystallographically related lamellae, each of which occurred in parallel with $<210>_\alpha$ and formed an angle of 27 ± 3° with $(001)_\alpha$.

When lamellae and the host have similar structures, a good lattice matching usually occurs across the interface (2). With pure Ca_2SiO_4 (C_2S), Fukuda and Maki (3) assumed perfect coherency at the boundaries between α- and α'_H-phases, to find the orientation from calculation by matrix algebra analysis. This requires cell parameters of both phases. Their calculation was based on the cell parameters determined at different temperatures; 1773 K for the α-phase and 1573 K for the α'_H-phase.

Recently, Remy et al. (4) have determined the temperature dependence of cell parameters for pure C_2S by high-temperature X-ray diffractometry. This has enabled us to determine the cell parameters of both α- and α'_H-phases at the transition temperature. In the present study,

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TABLE 1
Cell parameters of α- and α'_H-Ca_2SiO_4 at the transition temperature (1738 ± 15 K).

Phase	Crystal System	*a* (Å)	*b* (Å)	*c* (Å)
α	Trigonal	5.519 ± 0.001*	9.560 ± 0.003*	7.297 ± 0.004
α'_H	Orthorhombic	5.610 ± 0.001	9.589 ± 0.003	6.901 ± 0.002

* An orthohexagonal cell ($\sqrt{3}a = b$) is taken for the α-phase.

the author redetermined the orientation of coherent interfaces using these cell parameters and demonstrated a good compatibility with the lamella orientation, as determined experimentally.

Results and Discussion

Cell Parameters at the Transition Temperature

Remy et al. (4) detected the α-to-α'_H transition between 1723 K and 1753 K. Thus the author assumed the transition temperature to be at 1738 ± 15 K. The cell parameters for both phases at that temperature (Table 1) were found from extrapolation of the linear regression of their cell-parameter variations (Fig. 1). Though their experiments were performed during heating, significant hysteresis in cell parameters between heating and cooling is unlikely because the sample temperatures were high enough (above 1445 K) to eliminate the thermal hysteresis during the measurement.

Description of the α-to-α'_H Transition

In the matrix algebra analysis, the α-to-α'_H transition is described by two mathematical terms, lattice deformation and rigid-body rotation. If we take an orthohexagonal cell for the a-phase ($\sqrt{3a_\alpha} = b_\alpha$) to define an orthonormal relationship, the former is represented by a diagonal matrix (**B**) as follows:

$$\mathbf{B} = \begin{bmatrix} \eta_1 & 0 & 0 \\ 0 & \eta_2 & \eta_3 \\ 0 & 0 & 0 \end{bmatrix}$$

where η_1 ($=a_{\alpha'H}/a_\alpha$), η_2 ($=b_{\alpha'H}/b_\alpha$), and η_3 ($=c_{\alpha'H}/c_\alpha$) are the principal distortions along the a_α-, b_α-, and c_α-axes, respectively.

For complete coherency at the boundaries, one of the principal distortions must be equal to unity and the others must be smaller and larger than unity (5). From the observation that the lamellae were parallel to the b_α-axis (1), η_2 must be unity. Substituting η_i for the cell-parameter values in Table 1, we obtain $\eta_1 = 0.9838 \pm 0.0003$ (<1), $\eta_2 = 0.9970 \pm 0.0001$ (~1), and $\eta_3 = 1.0574 \pm 0.0003$ (>1). As a result, the present lattice deformation satisfies the requirement for the occurrence of the coherent boundaries.

The subsequent rigid-body rotation (**R**) of the product α'_H-phase lattice realizes the perfect

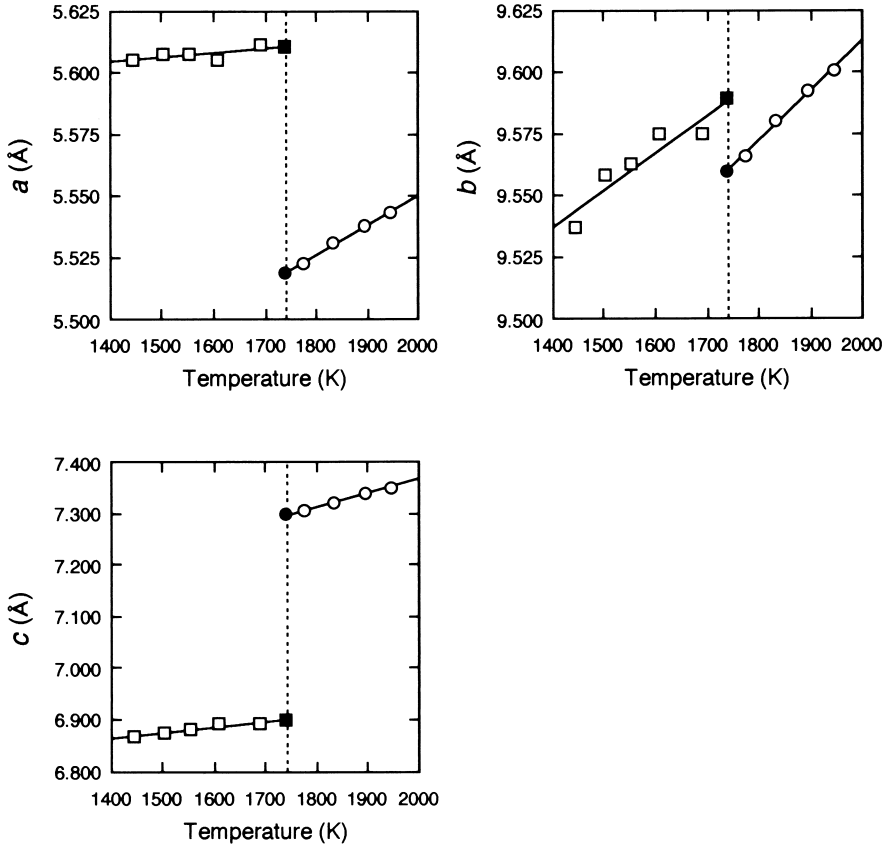

FIG. 1.
Unit-cell parameters of the α (●) and α'_H (■) phases at the transition temperature of 1738 ± 15 K. Cell-parameter variation with temperature of the α (○) and α'_H (□) phases was determined by Remy et al. (4).

lattice matching across the interface (2,3). The overall α-to-α'_H transition is thus represented by **RB**. The orientation of the interface boundaries as well as the rigid-body rotation angle is determined from the equation det $\mathbf{RB} - \mathbf{I} = 0$, where **I** is unit matrix.

Coherent Interphase Boundaries

Figure 2 shows the coherent interface boundary between the α- and α'_H-lattices in the *ac*-planes at 1738 K. The α'_H-phase lattice is rotated by 1.73 ± 0.01° anti-clockwise to fit with the parent α-phase lattice across the interface. The interface forms an angle of 29.3 ± 0.3° with $(001)_\alpha$. This is compatible with 27 ± 3°, determined experimentally for C_2Sss (1). The deviation of 2.3° (= 29.3 − 27) may arise in part from the difference in cell parameters, especially *a*- and/or *c*-axis lengths, between pure C_2S and C_2Sss at the transition temperatures. The trigonal symmetry of the parent α-phase produces six symmetrically equivalent sets of interfaces, which correspond to the six sets of the α'_H-phase lamellae observed

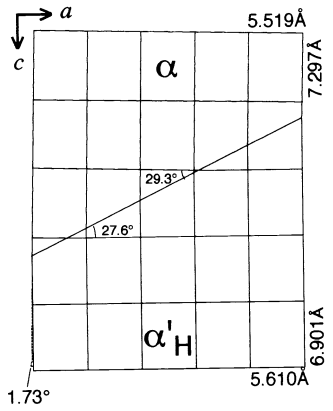

FIG. 2.
Lattices of the α- and α'_H-phases fitted together at the coherent interface at 1738 K. The interphase boundary forms an angle of 29.3° with $(001)_\alpha$ and that of 27.6° with $(001)_{\alpha'H}$.

microscopically (1). The α'_L-to-β transformation usually occurs during subsequent cooling and leads to the formation of polysynthetic twinning at the submicroscopic level within each lamella (1).

The reverse α'_H-to-α transition, described by $R^{-1}B^{-1}$, is also expected to be accompanied by the formation of coherent boundaries, which intersect $(001)\alpha'_H$ at 27.6 ± 0.3° (Fig. 2). Because of the symmetry change from orthorhombic to trigonal, two sets of interfaces related by rotation around the $b_{\alpha'H}$-axis should be formed within the parent α'_H-phase.

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