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Orientation of phase and domain boundaries in crystalline solids: reply

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In Fleet (1982) I showed that the habit plane orientations of all the common feldspar intergrowths, with the exception of the coarse-scale plate perthite, are consistent with minimization of lattice misfit and thereby demonstrated that the contribution of *anisotropic* elasticity to the orientations of these intergrowths is relatively insignificant. This contradicted the conclusions of Willaime and Brown (1974) and Brown and Willaime (1974), who argued that the coherent elastic theory results in unique explanations for the morphology of braid perthite and diagonal association perthite (complex or zigzag cryptoperthite). In their present discussion, Willaime and Brown (1985) suggest that the analysis of diagonal association perthite in Fleet (1982) is flawed by inappropriate selection of input lattice parameter data and incorrect calculation of elastic strain energy, and that too few data are presented to support the conclusions stated. Discussion of this perthite in Fleet (1982) was, of necessity, quite general, and I appreciate that the arguments in this section of the text are somewhat obscured by imprecise reporting and unqualified comments. In my reply, I shall introduce new observations and data into the discussion to permit a close comparison of the application of the lattice misfit and coherent elastic theories to complex cryptoperthite, to question the assumptions invoked by Willaime and Brown (1974, 1985), and to justify my selection of input lattice parameters.

As is well known, in approximate (001) section the habit plane of the coarse-scale diagonal association zigzag is inclined at angles of $\pm 18°$ to $\pm 32°$ to $(60\bar{1})$ (Willaime and Brown, 1974; Brown and Willaime, 1974; Lorimer and Champness, 1973), which correspond to the zone arcs $(63\bar{1})$ to $(66\bar{1})$ and $(\bar{6}31)$ to $(\bar{6}61)$ (Fig. 1). Throughout the present discussion paired zigzag interfaces will be regarded as being related by monoclinic symmetry and the interface with h negative will be referred to as "symmetry-related." Less frequently noted in the context of phase boundary analysis is that the actual interface between the fine albite twin lamellae and the K-rich matrix in both normal and zigzag cryptoperthites defines a second fine-scale zigzag (e.g., Brown and Willaime, 1974; Willaime et al., 1976; MacKenzie and Zussman, 1974; Fig. 2). Measurements on the jacket illustration of MacKenzie and Zussman (1974) reveal a bimodal distribution of habit plane orientations (Fig. 2b), with one mode at about $\pm 20°$ to $(60\bar{1})$ for fine-scale interfaces inclined away from the associated coarse interface, corresponding to poles near $(63\bar{1})$ and $(\bar{6}31)$, and a second mode at about $\pm 50°$ to $(60\bar{1})$ for fine-scale interfaces inclined toward the associated coarse interface, corresponding to $(36\bar{1})$ and $(\bar{3}61)$ (Fig. 1). The zigzag interface in Figure 2a should not be confused with the zigzag depicted in Figure 7 of Willaime and Gandais (1972). The latter represents the relative orientation of the albite-twinned triclinic $(60\bar{1})$ planes which have an *actual* zigzag orientation of about $\pm 2°$ to $(60\bar{1})$.

Additional lattice misfit minima and elastic strain energy minima for intermediate microcline-intermediate albite interfaces have been computed (Table 1) and, with selected data from Fleet (1982, Table 1), are compared with the observed habit plane orientations of cryptoperthite in Figures 1a and 1b, respectively. Lattice misfit minima for lattice parameters of monoclinic alkali feldspars and combinations of sanidine or intermediate microcline with anorthoclase, high or low albite lie on a zone arc that closely straddles the orientations of normal cryptoperthite and zigzag cryptoperthite (h positive). Moreover, lattice misfit minima for intergrowths with triclinic Na-rich phases (2a, 3b, 5b, Fig. 1a), computed with no ad hoc assumptions, are in good agreement with the $(36\bar{1})$ plane of the fine zigzag. Furthermore, an equivalent correlation exists between lattice misfit minima computed with albite-twinned anorthoclase or high albite lattice parameters (2Aa, 3Ab, Fig. 1a) and the symmetry-related interface orientation $(\bar{3}61)$.

In contrast, coherent elastic strain energy minima for sanidine-anorthoclase (2c, Fig. 5, Fleet, 1982), intermediate microcline-intermediate albite (5b, 5a, Fig. 1b) and maximum microcline-low albite (1c, 1b, 1a, Fig. 7, Fleet, 1982) lattice-parameter combinations are in overall poor agreement with the h positive habit plane of zigzag cryptoperthite.

All of the present calculations were made with program EPLAG (Fleet, 1982). EPLAG calculates coherent elastic strain energy using the misfit tensor rather than the three-dimensional strain tensor (as in the calculation of Willaime and Brown, 1974). Use of the misfit tensor is consistent with the ideal two-dimensional lattice coher-

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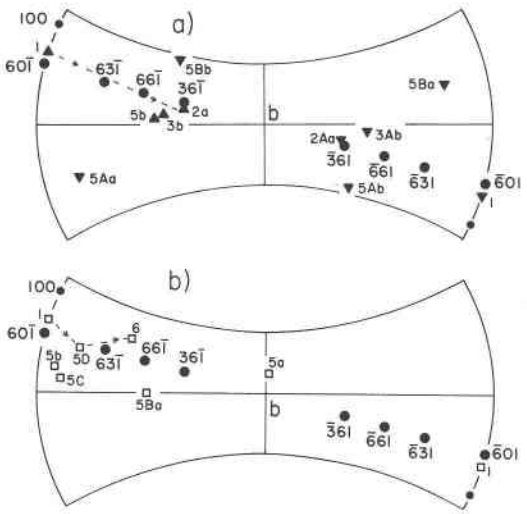

Fig. 1. Orientation of cryptoperthite intergrowths (circles) compared with (a) lattice misfit minima (triangles), and (b) coherent elastic strain energy minima (squares): stereographic projection terminated by 60° small circles about (001) and (00$\bar{1}$); labels on calculated data refer to Table 1 and Fleet (1982, Table 1).

Table 1. Calculated phase-boundary orientations for diagonal association perthite

No.	Model Intergrowth*	Data†	Lattice Misfit Minima h	k	ℓ	Strain Energy Minima h	k	ℓ	P_{max}/P_{min}
5 a	Int Mic(8)-Int Ab(12)	3	$\bar{1}0$	4	$\bar{5}$	0	9	$\bar{1}$	2.35
b			8	9	$\bar{3}$	7	1	$\bar{2}$	2.33
5Ba	Int Mic(8)-Int Ab(12,A)	3	$\bar{1}\bar{1}$	4	6	8	9	$\bar{3}$	2.32
b			7	11	2				2.31
5C	Int Mic(8)-Int Ab(12) MESE	3				7	1	$\bar{2}$	
5D	Int Mic(8)-Int Ab(12,WB)	3	9	0	$\bar{1}$	7	2	$\bar{1}$	4.32

* Abbreviations: Ab, albite; Int, intermediate; Mic, microcline; A, albite twin-related unit-cell parameters with $\alpha'=180-\alpha$, $\gamma'=180-\gamma$; MESE, mean strain energy of 5 and 5B; WB, albite-twinned-equivalent monoclinic cell, after Willaime and Brown (1974).

† Willaime and Brown (1974, Table 1).

ence model, since it restricts elastic strains to the plane of the interface. This condition requires coherency stress components outside of the interface plane and these contribute to the elastic strain energy. In contrast, use of the strain tensor assumes the two coherent lattices to be relaxed outside of the plane of the interface, and the resulting shear strains contribute to the elastic strain energy. Both approaches to coherent elastic strain energy calculation involve an arbitrary assumption. This dichotomy is a result of the elastic nature of crystalline solids. Fortunately, its quantitative effects are rather trivial for calculations on feldspar intergrowths and, contrary to the suggestion of Willaime and Brown, have no bearing on the present debate. For example, pole 6 in Figure 1b is (8.5,5.6,$\bar{1}$) by the Willaime and Brown (1974) calculation and (8.5,6.2,0.$\bar{8}$) by the present calculation (Fleet, 1982, Table 1). Similarly, pole 5D (Fig. 1b) is (7.8,2.5,$\bar{1}$) and (7.8,2.2,1.$\bar{1}$), respectively. The small discrepancies that do exist are attributable partly to uncertainty in interpolation of pole orientation within the 5° grid interval of the present calculation and partly to small differences in defining area misfit.

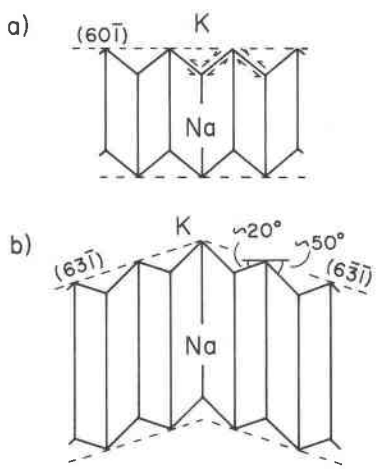

Fig. 2. Schematic representation of interface between fine albite-twinned Na-rich phase and K-rich phase in (a) normal cryptoperthite, and (b) complex (zigzag) cryptoperthite: approximate (001) section.

Willaime and Brown (1974) and Brown and Willaime (1974) have argued in favor of a common interface plane for both of the albite-twinned orientations in the Na-rich phase, noting agreement between the orientations of the strain energy minimum for maximum microcline and albite-twinned-equivalent-monoclinic low albite lattice parameters and the (66$\bar{1}$) habit plane (6, Fig. 1b). However, there are two important objections to this hypothesis.

1. The twinned triclinic unit cells only have dimensional correspondence in planes normal to the twin plane, (010). The effect of this may be illustrated using Figure 7 of Willaime and Gandais (1972). When an interface plane is constructed in general orientation, it becomes clear that the interface orientation of one twin individual is not twin-equivalent to the interface orientation of the other. Thus, two-dimensional coherence requires coherency stresses in two crystallographically-unrelated planes. The total coherent elastic strain energy should be obtained from the sum of the strain energy contributions of the separate twin orientations (e.g., 5C, Fig. 1b).

2. The *actual* interface between the two phases apparently would not have been the hypothesized common interface plane but the fine-scale zigzag (Fig. 2b). Coherence at the fine zigzag interface destroys one of the basic

assumptions of the coherent elastic model, that of homogeneous stress in each phase (e.g., Fig. 2a).

It could be argued that since the coherency stresses in complex intergrowths are expected to be very local the coherent elastic model is still applicable. However, minima calculated with this assumption (5a, 5b, 5Ba, 5C, Fig. 1b) are in poor agreement with the observed habit planes. It should be noted, in particular, that the coherent elastic model is not able to account for the symmetry-related habit planes without adopting the questionable hypothesis associated with modelling the minima 6 and 5D (Fig. 1b) and twinning the K-rich matrix.

Thus, while complex cryptoperthites do exhibit a high degree of diffraction coherence, it does not appear that the coherent elastic model of Willaime and Brown (1974) is physically the most realistic one for calculating their phase boundary orientations. Furthermore, the Willaime and Brown theory does not explain the development of sinuous (wavy) Na-rich lamellae within a *monoclinic* K-rich matrix (e.g., Spencer M cryptoperthite, Lorimer and Champness, 1973, Fig. 2).

The lattice misfit theory favors development of cryptoperthite textures at temperatures at which the K-phase is monoclinic or, at most, has just a small degree of triclinic distortion. The good correlation with the symmetry-related interface orientation exists only for sanidine-twinned anorthoclase and sanidine-twinned high albite lattice parameter combinations.

There is general agreement that the normal cryptoperthite intergrowth develops in the early stages of unmixing, when both phases are monoclinic. With relatively rapid cooling toward a quenched condition the Na-rich phase transforms through the albite-twin mechanism and the fine zigzag interfaces rotate away from $(60\bar{1})$ toward an optimal orientation consistent with sanidine-anorthoclase lattices.

Complex cryptoperthite develops with slower cooling. As the Na-rich phase in normal cryptoperthite begins to transform, subtle changes from ideal monoclinic unit-cell parameters induce coordinated clockwise and counterclockwise rotation of the interfaces in the [106] zone. At this stage in development the interface may remain continuous (wave-like). At a later stage with further rotation from $(60\bar{1})$ the coarse zigzag cryptoperthite with discontinuous interfaces develops. The K-rich phase may also be twinned at this time but this is not essential to the reconstruction. The fine albite twin lamellae form subsequently within the preexisting coarse twins, with concomitant readjustment of the interfaces with the K-rich phase. Since adjacent twin lamellae must be approximately of the same width, only one interface in each fine zigzag pair, that with similar orientation to the associated coarse-scale interface (Fig. 2b), is able to rotate to an optimal position. This reconstruction requires departure from the widely accepted view that fine albite twinning in cryptoperthite always develops directly from a monoclinic precursor. However, the amount of triclinic distortion being invoked is small, even in comparison to that of the anorthoclase lattice. Cooling of most cryptoperthites appears to have been sufficiently slow to transform the Na-rich phase to low albite. The apparent absence of an incipiently transformed triclinic Na-rich phase is not too surprising. The phase boundary orientations may be the only relic of its existence.

The lattice misfit theory does not indicate unequivocally that the fine albite twinning postdates development of the coarse zigzag, as I suggested in Fleet (1982). The reconstruction of Willaime et al. (1976), with early development of the fine albite twinning (and the fine-scale zigzag), is not excluded, although the associated misfit minima are not in such close agreement with the observed phase boundary orientations (e.g., poles 5Ab, 5 Bb, Fig. 1a). In this reconstruction, the periodic perturbation of the Na-rich lamellae of normal cryptoperthite is associated with the development of long-period twinning in the K-rich phase. One of the fine zigzag orientations in periodic regions of the interface becomes dominant. As the intergrowth coarsens the orientation of the corresponding coarse interface rotates progressively toward that of the dominant fine zigzag orientation.

Also, the development of the lozenge-shaped texture of Spencer N cryptoperthite (Lorimer and Champness, 1973) from a fine-scale albite twinned, coarse zigzag cryptoperthite (with a monoclinic K-rich matrix) is a definite possibility.

It is quite evident from Fleet (1982) that not all of the calculated misfit minima of alkali feldspars are associated with phase boundaries. Favored orientations correspond to regions of generally low elastic strain energy, but precise alignment of phase boundaries within these regions does appear to be determined by lattice misfit rather than by minimization of strain energy. Topological constraints may be a factor here, also.

Willaime et al. (1976) argue that early development of the fine-scale albite twinning in the Na-rich phase is favored by general uniformity of twin periodicity within individual zigzag and lozenge-shaped areas. Twin periodicity does correlate with average lamellar width in parallel cryptoperthite (Willaime and Gandais, 1972; McLaren, 1974) but there is little evidence that this correlation extends to the angular tips of the Na-rich areas. In Spencer M cryptoperthite, for example, which has matured only slightly from the normal cryptoperthite stage, twin periodicity remains constant through the tapered terminations of the Na-rich lamellae (Lorimer and Champness, 1973, Fig. 2a). Also, following the logic of the Willaime et al. (1976) reconstruction, twin periodicity would have to progressively increase with coarsening (as noted by McLaren, 1974). If this were possible, twin periodicity would be adjusted in the angular tips as well.

In summary, the coherent elastic theory does not yield unique explanations for the morphology of diagonal association perthite (and of braid perthite), and the conclusion of Fleet (1982) that anisotropic elasticity does not make a

significant contribution to the orientations of alkali feldspar intergrowths is reaffirmed. It is emphasized that the present theory does not deny the existence of coherency stresses in these intergrowths. The lattice misfit theory simply reproduces the observed habit plane orientations more precisely than the coherent elastic model. This agreement is not obtained by inappropriate selection of lattice parameter data. Since there is general agreement that normal cryptoperthite is associated with coexisting monoclinic lattices and that complex cryptoperthite develops from it, it seems appropriate to investigate the effects of coexisting sanidine-anorthoclase, sanidine-high albite and intermediate microcline-high albite lattices on intergrowth morphology before jumping discontinuously to maximum microcline-low albite lattices.

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