Acta Cryst. (1958). **11**, 323

A Possible Explanation of the δ_c Separations in Intermediate Plagioclase

By F. Chayes

Geophysical Laboratory, Carnegie Institution of Washington, Washington, D.C., U.S.A.

(*Received* 6 *August* 1957 *and in revised form* 5 *December* 1957)

The δ_c 'separation' in intermediate plagioclase varies with composition as the reciprocal of the average run length of the major constituent in a two-element random run sequence containing $N\alpha$ A's and $N\beta$ B's, where α is the proportion of tetrahedral sites occupied by Al. The case corresponds to virtually complete short-range disorder in at least one direction.

Empirical relations between δ_a, δ_b and δ_c

The subsidiary reflections of intermediate plagioclase are the subject of a careful, thorough study by Gay (1956), who has shown that the displacement of subsidiary from principal layer lines is virtually a linear function of composition in the range $20 < \text{An} < 75$. Following terminology already established, Gay designates the 'separation' of a subsidiary layer line from the next underlying principal layer line along a crystallographic axis by δ_a, δ_b or δ_c, depending upon the axis in question. He records the average 'separations' in degrees of reciprocal space, and an examination of his tables and graphs indicates that the interrelationship of these distances is both close and simple.

In 19 specimens Gay was able to measure both δ_a and δ_b, in 23 he obtained both δ_a and δ_c, and for 21 he records both δ_b and δ_c. He concludes that '... δ_a and δ_b are linearly dependent on δ_c', but gives no reason for choosing δ_c as independent. In any case, the linear correlation between all three pairs of subsidiaries is extraordinarily high.

The purpose of this note is to point out that the variation of the spacing of δ_c—the best resolved or most frequently observed of the subsidiaries—is about what would be expected if it were controlled by the average run lengths of Al and Si at complete short-range disorder.

It is at first sight rather puzzling to find that one of these closely correlated subsidiaries follows such a rule while the other two do not. In some experimental work stimulated by Gay's data I have found that subsidiary reflections do indeed occur in diffraction patterns of masks representing disordered or short-range-ordered distributions of stacking faults in layered structures, and that the locations of the subsidiaries differ greatly in the two cases (Abelson, 1957). These masks are not adequate models of the Al–Si situation in feldspar, but it may be pointed out that in the run model the existence of a certain level or type of ordering in one direction imposes no restrictions on (and conveys no information about) ordering in any other direction. There is no reason for all three subsidiaries to behave similarly unless ordering is the same along the three principal directions.

The run model of short-range disorder

Suppose that the points of an ordered point lattice are to be populated with A's and B's, the number of points being N, of A's $N\alpha$, and of B's $N\beta$, $\alpha < \beta = 1-\alpha$. The distribution is to be random in the sense that the probability of any site being taken by an A is α, and, similarly, $\Pr(B) = \beta$. Defining a 'run' as a sequence of like items bounded at each end by an unlike item, information about the distribution of A's and B's on the lattice may be summarized in terms of the number of runs, the distribution of run lengths in A and B, and the average run lengths in A and in B.* It is these averages which can be used to predict the δ_c separations.

Average run length at disorder

Since N is always very large we can take advantage of some simple large-sample approximations.

For N sufficiently large, the probability of a run of length i in A is (Hald, 1952, pp. 343–4)

$$\Pr(r_{Ai}) \cong \beta\alpha^{i-1}. \qquad (1)$$

The expected number (d_{Ai}) of such runs is

$$E(d_{Ai}) \cong N\beta^2\alpha^i, \qquad (2)$$

* Readers acquainted only with discussions of short-range ordering based on 'interpenetrating lattices' may like to know that the number of runs is the same as the number of 'right pairs' of the more usual formulation, that every run of length i contains $(i-1)$ 'wrong pairs', so that, if $f_a(i)$ is the frequency of runs of length i in A, the number of wrong pairs in A is $\Sigma(i-1)f_a(i)$, and similarly for B. Proceeding in this fashion one finds that at complete disorder there are $N\alpha^2$ wrong pairs in A, $N\beta^2$ wrong pairs in B, and $2N\alpha\beta$ right pairs. At perfect short-range order, defined, as usual, by the absence of wrong pairs in A, there are $N(1-2\alpha)$ wrong pairs in B and $2N\alpha$ right pairs. The order parameter most similar to that used in the model based upon interpenetrating sublattices is the proportion of runs of A which are of length 1, a quantity which varies from β at complete disorder to 1 at perfect short-range order. In the run model there is no *a priori* relation between long- and short-range ordering.

and the expected number of runs of all lengths in A is

$$E(d_A) \cong N\beta^2 \sum_1 \alpha^i \cong N\beta\alpha . \qquad (3)$$

Since $N\alpha$ A's are to be distributed among an expected number $N\beta\alpha$ of runs, the average or expected run length in A will be $1/\beta$. From symmetry we also have $1/\alpha$ as the expected run length in B.

α, β and $\bar{i}$ for Al and Si in disordered plagioclase

In pure albite one-fourth and in pure anorthite one-half of the tetrahedral sites are taken by Al. Letting Al = A and Si = B of the preceding section, and designating the composition of any plagioclase by the mol fraction An calculated from its analysis, we have that

$$\alpha = (\mathrm{An}/2)+(1-\mathrm{An})/4 = (\mathrm{An}+1)/4 .$$

Accordingly, $E(\bar{i}_B) = \alpha^{-1} = 4/(\mathrm{An}+1)$ at complete disorder.

Gay records δ_c in degrees of reciprocal space, but as runs, run lengths, etc., are more readily thought of in direct space, we convert by finding $360\delta_c^{-1}$ for each specimen. The results compare with $E(\bar{i}_{Si})$ calculated

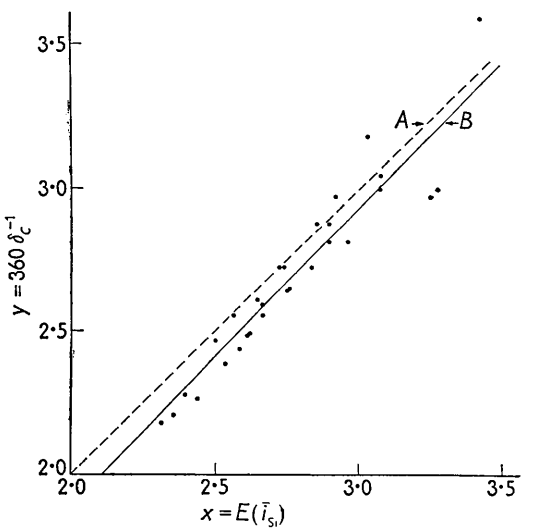

Fig. 1. δ_c separations as a function of Si run length. $X = E(\bar{i}_{Si}) = \alpha^{-1}$, $Y = 360\delta_c^{-1}$. (Line A: $\hat{Y} = X$; line B: line of best fit calculated from Table 1, $\hat{Y} = 1{\cdot}052X - 0{\cdot}222$.)

from the analyses as shown in Table 1 and Fig. 1. If the quantities $360\ \delta_c^{-1}$ and $E(\bar{i}_B)$ were estimating the same parameter, the line of best fit would be characterized by an intercept not differing significantly from zero and a slope not differing significantly from unity. The equation calculated from the data is $\hat{Y} = 1{\cdot}052X - 0{\cdot}222$, and in fact neither constant differs significantly from its expected value. Considering the difficulty of making measurements of this sort, the ever present uncertainties about analysis, and the possibility that some of the discrepancies are real, the fit is on the whole excellent. To a remarkable extent the 'repeat distance' calculated from the δ_c spacing behaves as if it were governed by the same rules which determine average run lengths in a run sequence characterized by short-range disorder.

Table 1. *Gay's data* (An, δ_c), α, $E(\bar{i}_{Si})$ *and* $360\ \delta_c^{-1}$ *for intermediate plagioclase*

An	δ_c	α	$E(\bar{i}_{Si})=\alpha^{-1}$	$360\delta_c^{-1}$
73	165	0·4325	2·312	2·182
70	163	0·4250	2·353	2·209
67	157	0·4175	2·395	2·278
64	159	0·4100	2·439	2·264
60	146	0·4000	2·500	2·466
58	151	0·3950	2·532	2·384
56	141	0·3900	2·564	2·553
55	148	0·3875	2·581	2·433
53	145	0·3825	2·614	2·483
53	145	0·3825	2·614	2·483
51	138	0·3775	2·649	2·609
50	141	0·3750	2·667	2·553
50	139	0·3750	2·667	2·590
47	132	0·3675	2·721	2·727
46	132	0·3650	2·740	2·727
45	136	0·3625	2·759	2·647
45	136	0·3625	2·759	2·647
41	132	0·3525	2·837	2·727
40	125	0·3500	2·857	2·880
38	128	0·3450	2·898	2·812
38	125	0·3450	2·898	2·880
37	121	0·3425	2·920	2·975
35	128	0·3375	2·963	2·812
32	113	0·3300	3·030	3·186
30	118	0·3250	3·077	3·051
30	120	0·3250	3·077	3·000
23	121	0·3075	3·252	2·975
22	120	0·3050	3·279	3·000
17	100	0·2925	3·419	3·600

In most cases the observed repeat distance is a little less than the average run length. The average discrepancy could be eliminated by supposing that the arrays are in fact not completely disordered. In the region for which data are available the required shortening of the expected repeat distance would be produced by an increase in the numbers of runs and, accordingly, in the numbers of right pairs, of some 6% over that characteristic of complete disorder.

References

ABELSON, P. H. (1957). Annual Report of the Director of the Geophysical Laboratory for the year 1956–7. *Carnegie Inst. of Wash. Year Book* No. 56.

GAY, P. (1956). *Miner. Mag.* **31**, 21.

HALD, A. (1952). *Statistical Theory with Engineering Applications*. New York: Wiley.