

DETERMINATION OF STRUCTURAL STATE OF CALCIC  
PLAGIOCLASES BY AN X-RAY POWDER TECHNIQUE

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Abstract

$B(2\theta_{(1\bar{1}1)} - 2\theta_{(\bar{2}01)})$  versus  $\Gamma(2\theta_{(131)} + 2\theta_{(220)} - 4\theta_{(1\bar{3}1)})$  for calcic plagioclases determined from X-ray powder data distinguishes among structural states and provides a rough estimate of plagioclase composition. A linear relationship between  $B$  and  $\Gamma$  for plagioclases of a particular structural state is related to the apparent linear relationships between  $\beta^*$  and composition  $\gamma^*$  and composition for these feldspars.

Introduction

Structural states and compositions of plagioclase feldspars are basic data required by petrologists studying the thermal histories and chemistries of igneous rocks. During the 1950's, J. V. Smith (1956), J. V. Smith and Gay (1957) and J. R. Smith and Yoder (1956) developed X-ray powder techniques that could be used to determine the structural state of a plagioclase, providing the chemical composition of the plagioclase was known. For plagioclases with compositions between  $An_0$  and  $An_{70}$ , variations of the gamma function [ $\Gamma = (2\theta_{(131)} + 2\theta_{(220)} - 4\theta_{(1\bar{3}1)})$ ], given by Smith and Gay (1957, p. 749), has provided a good estimate of structural state. For plagioclases in the range from  $An_{70}$  to  $An_{100}$ , the beta function [ $B = (2\theta_{(1\bar{1}1)} - 2\theta_{(\bar{2}01)})$ ] of Smith and Gay (1957, p. 754) has been used.

This paper attempts to demonstrate that an X-ray powder technique can provide significant information about the order-disorder of calcic plagioclases in the absence of independent compositional information. In addition, this technique can yield a petrologically useful estimate of the composition of such plagioclases.

Data and Experimental Procedure

Smith and Gay (1957) measured the angular separations  $B(2\theta_{(1\bar{1}1)} - 2\theta_{(\bar{2}01)})$  and  $\Gamma(2\theta_{(131)} + 2\theta_{(220)} - 4\theta_{(1\bar{3}1)})$  for 111 natural plagioclase feldspars that had been classified into five groups on the basis of their field occurrences. Data on synthetic feldspars and on natural specimens that had been subjected to heat treatments are also described in the same paper. Figure 1 from Smith and Gay's data is a plot of  $B$  versus  $\Gamma$  for 22 natural and five synthetic calcic plagioclases that had  $\Gamma$  values greater than  $1.00^\circ 2\theta$ . Plagioclases that had  $\Gamma$  values less than  $1.00^\circ$  were not plotted because the clear separation of ordered from disordered plagioclases breaks down in this range (less than

about  $An_{65}$ ). On Figure 1, Smith and Gay's data are supplemented by nine analyses of quickly quenched volcanic plagioclases from submarine volcanic ash layers (see also Table 1).

Samples of plagioclase phenocrysts from the submarine ashes that were analyzed in this laboratory were ground in acetone in a mortar and pestle for several minutes. The compositions were estimated by fusing about 15 representative phenocrysts per sample and measuring the refractive indices of the resulting glass beads (Schairer *et al.*, 1956). A Norelco diffractometer with a monochromator was programmed to make repeated scans between  $21.50$  and  $23.30^\circ 2\theta$  and between  $28.30$  and  $31.80^\circ 2\theta$ . The following X-ray settings were used: scan speed:  $1/8^\circ 2\theta/\text{min}$ ; chart speed:  $1/4''/\text{min}$ ; divergence and receiving slits  $1^\circ$  and  $0.1$  mm, respectively; and time constant 10 seconds. Usually, at least four measurements of  $B$  and  $\Gamma$  were made. These peak separations were measured to the closest  $0.001^\circ 2\theta$ . For the nine samples, the average standard deviations of the means of  $B$  and  $\Gamma$  were  $0.003$  and  $0.004^\circ 2\theta$ , respectively. It was found that at least three milligrams of powdered feldspar were needed to keep the standard deviations of  $\Gamma$  and  $B$  to an acceptable level (less than about  $0.005^\circ$ ). If the calculated standard deviations were too high, more measurements were made.

Structural States and Compositions of Calcic  
Plagioclases

It is evident from Figure 1 that a plot of  $B$  versus  $\Gamma$  clearly separates plagioclases of different structural states and hence of different thermal histories. Three dominant groupings of plagioclases with similar structural states are present: the highly disordered synthetic plagioclases; the volcanic plagioclases with intermediate ordering; and the well ordered plagioclases from very slowly cooled igneous and metamorphic rocks. Plagioclases from hypabyssal rocks, which have had cooling histories intermediate between those from relatively quickly cooled volcanic rocks and those from very slowly cooled plutonic igneous and metamorphic rocks, may have slightly more disordered structural states than those from the

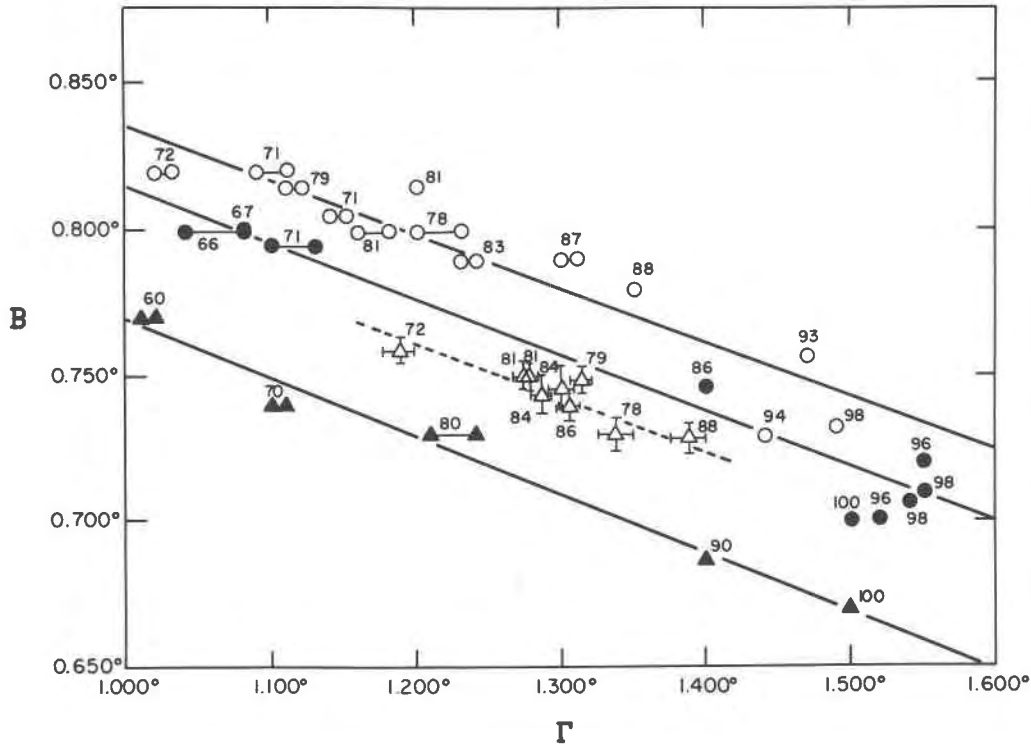


FIG. 1. A plot of  $B(2\theta_{(1\bar{1}1)} - 2\theta_{(\bar{2}01)})$  versus  $\Gamma(2\theta_{(131)} + 2\theta_{(220)} - 4\theta_{(131)})$  for calcic plagioclases. The feldspars have been grouped into 4 groups on the basis of their origin, with the following symbols:  $\circ$  (hypabyssal, plutonic, pegmatitic, metamorphic, charnockitic, and those from large basic igneous complexes);  $\bullet$  (volcanic);  $\triangle$  (volcanic ash layers); and  $\blacktriangle$  (synthetic). All data, except for the data on volcanic ash layers, was taken from Smith and Gay (1957). Diagonal lines represent regression lines through the various groups of data. Vertical and horizontal lines drawn through symbols for volcanic ash plagioclases represent plus and minus two standard deviations on the means of B and  $\Gamma$ , respectively. Horizontal lines connecting two symbols represent those samples for which more than one  $\Gamma$  value was given by Smith and Gay. Numbers above symbols denote wt percent  $An_{(An+Ab)}$ .

most slowly cooled rocks (see Smith and Gay, 1957, Figure 2). More data on calcic plagioclases with such thermal histories are required to verify this. The data for plagioclases from submarine volcanic ash layers suggest that they may constitute a group that occupies a position intermediate between synthetic and true volcanic plagioclases. Evidently, this disordered and metastable structural state was frozen into these plagioclases when they were explosively ejected near liquidus temperatures into sea water.

The composition of all the plagioclases plotted is also shown on Figure 1. In general, for feldspars of a particular structural state, the more An-rich plagioclases are associated with larger  $\Gamma$  and smaller B values. This is particularly evident for the synthetic feldspars. For more ordered plagioclases, the same relationship apparently holds, although there are exceptions. Nevertheless, it appears that an An com-

position of a calcic plagioclase may be estimated to within about 5 percent solely on the basis of its X-ray powder pattern. Rough estimates of this sort are particularly useful in the study of the calcic plagioclases of fine-grained igneous rocks.

### Discussion

J. V. Smith (1972) has recently shown that a plot of  $\beta^*$  versus  $\gamma^*$  clearly distinguishes between different structural states of calcic plagioclases. Since  $\Gamma$  depends on the reciprocal lattice angle,  $\gamma^*$  (Smith and Gay, 1957), and B depends on  $\beta^*$  (Brown, 1967), the covariance of B and  $\Gamma$  for plagioclases of a particular structural state is expected. Furthermore, Jackson (1961) demonstrated a linear relationship between  $\Gamma$  and composition ( $An_{60-83}$ ); in addition, Smith and Gay's (1957, Figure 2) data indicate an approximate linear relationship between B and com-

TABLE 1. B and  $\Gamma$  values for plagioclase phenocrysts of submarine volcanic ash layers (Cu  $K_{\alpha}$  radiation).

Core No.	Depth in core (cm)	Ave. % An	B	$\sigma_B$	$\Gamma$	$\sigma_{\Gamma}$
6709-20	725-728	81	0.749*	0.002*	1.277*	0.005*
6709-20	1099-1101	81	0.750*	0.002*	1.275*	0.003*
6709-20	1120-1121	86	0.740*	0.003*	1.305*	0.003*
6808-7	432-434	84	0.743*	0.004*	1.286*	0.001*
6808-7	530-532	79	0.749*	0.003*	1.313*	0.003*
6609-6	0-3	84	0.745*	0.005*	1.298*	0.005*
6601-1	260-262	78	0.730*	0.003*	1.337*	0.006*
6601-1	310-312	72	0.758*	0.002*	1.187*	0.005*
T9	0-4	88	0.728*	0.003*	1.386*	0.006*

position of calcic plagioclases of a particular structural state. Since B and  $\Gamma$  also depend on composition, it is not surprising that a plot of B versus  $\Gamma$  for calcic plagioclases of the same structural state should provide information about their compositions.

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#### References

- BROWN, G. M. (1967) Mineralogy of basaltic rocks. In H. H. Hess and A. Poldervaart, Eds. *Basalts*. Interscience, New York. pp. 103-162.
- JACKSON, E. D. (1961) X-ray determinative curve for some plagioclases of composition  $An_{60-83}$ . *U. S. Geol. Surv. Prof. Pap.* **424-C**, 286-288.
- SCHAIRER, J. F., J. R. SMITH, AND F. CHAYES (1956) Refractive indices of plagioclase glasses. *Carnegie Inst. Washington Year Book*, **1953** 195-197.
- SMITH, J. R., AND H. S. YODER, JR. (1956) Variations in X-ray powder diffraction patterns of plagioclase feldspars. *Amer. Mineral.* **41**, 632-647.
- SMITH, J. V. (1956) The powder patterns and lattice parameters of plagioclase feldspars. I. The soda-rich plagioclases. *Mineral. Mag.* **31**, 47-68.
- (1972) Critical review of synthesis and occurrence of plagioclase feldspars and a possible phase diagram. *J. Geol.* **80**, 505-525.
- , AND P. GAY (1957) The powder patterns and lattice parameters of plagioclase feldspars. II. *Mineral. Mag.* **31**, 744-762.