

**Zeitschrift:** Schweizerische mineralogische und petrographische Mitteilungen = Bulletin suisse de minéralogie et pétrographie

**Band:** 47 (1967)

**Heft:** 1: Feldspäte

**Artikel:** The lattice constants and related parameters of "plagioclases (low)". Part IV of laboratory investigations on plagioclases

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**DOI:** <https://doi.org/10.5169/seals-36957>

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# The Lattice Constants and Related Parameters of "Plagioclases (low)"

(Part IV of Laboratory Investigations on Plagioclases)

By *H. U. Bambauer* (Münster)\*, *E. Eberhard* and  
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With 5 figures and 1 table in the text

## Zusammenfassung

Von 36 Plagioklasen werden genaue Gitterkonstanten bestimmt und daraus Achsenverhältnis und  $\sigma$ -Winkel des Rhombischen Schnittes berechnet. Die Werte werden graphisch dargestellt und daraus wird versucht, den Verlauf der Grenzkurven für die Reihe „Plagioklas (tief)“ anzugeben. Die Kurven zeigen Diskontinuitäten bei  $An_{1,3}$ ,  $An_{16}$ ,  $An_{33}$ ,  $An_{50}$  und  $An_{76-80}$ . Ferner wird ein Diagramm zur Indizierung von Plagioklas-Pulveraufnahmen für den Bereich  $2\theta = 13^\circ-54^\circ$  (Cu  $K\alpha_1$ ) mitgeteilt.

## Abstract

The unit cell dimensions of 36 plagioclases are determined; using these values the axial ratios and the  $\sigma$ -angles of the rhombic section are calculated. The variations in all these parameters have been correlated with the chemical composition of the specimens. An attempt is made to determine the boundary curves, representing the series "plagioclase (low)". Such curves exhibit discontinuities at  $An_{1,3}$ ,  $An_{16}$ ,  $An_{33}$ ,  $An_{50}$  and  $An_{76-80}$ . In addition, a new diagram is presented as an aid to indexing powder patterns of plagioclases in the  $2\theta$ -range  $13^\circ-54^\circ$  (Cu  $K\alpha_1$ ).

## I. INTRODUCTION

The variation of the positions of the lines in the powder patterns of plagioclases, discussed in the accompanying paper (BAMBAUER et al.,

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1967), necessarily depends upon the variation of lattice constants that differ on account of changes in chemical composition and structural state. Therefore, a determination of the six lattice constants should give additional information on the variability of plagioclase-states. The numerous lattice constants to be found in the literature are not used in this investigation for the following reasons: It was felt that at this stage "relative" values are more indicative than "absolute" ones. As different investigation-methods may have different limits of error, especially if chemical analyses are considered, the same X-ray method and the same analytical method were used to determine the properties of all the plagioclases in this investigation. As to the chemical composition of plagioclases described in the literature the following may be said: Frequently the An-content was determined indirectly (e. g. optical methods). Further, all the analyses reported in the literature are bulk analyses, which do not take into consideration the inclusions of other minerals or the anti-perthitic potash feldspar. In some cases the An-content has been inferred from the bulk Ca-content alone.

Whereas in earlier papers (BROWN, 1960; CLAISSE, 1950; DOMAN et al., 1965; GOODYEAR and DUFFIN, 1955; SMITH and YODER, 1956; SMITH, 1956, 1958) values e. g.  $2\theta_{131}-2\theta_{\bar{1}\bar{3}1}$  or  $\gamma^*$  already lead to interesting conclusions regarding the behaviour of plagioclases with respect to their chemical composition, a determination of all the cell constants should be more indicative. Therefore, 36 of the feldspars used by CORLETT and RIBBE (1967) and by BAMBAUER et al. (1967) were selected for this investigation. In addition the knowledge of all the cell constants would make it possible to calculate other values of geometrical interest, e. g.  $\sigma$ , the angle of the "rhombic section". The term "plagioclase (low)" is here used to mean the series of plagioclases which extend from albite (low) to antorthite (primitive) and is in a "most ordered" state as far as nature provided it. Both the end members have maximum ordered Al/Si-distributions (RIBBE et al., 1962; MEGAW et al., 1962).

## II. EXPERIMENTAL

### *A. Material investigated*

The following specimens (36) were selected for the determination of lattice constants from those listed by CORLETT and EBERHARD (1967):

- a) A representative number (25) of those specimens which were used to draw the boundary curves "plagioclases (low)" in the  $\Delta(\theta)$ -diagrams of BAMBAUER et al. (1967).
- b) A few other specimens (11) which were interesting because of their higher Or-content or their anomalous  $\Delta(\theta)$ -values.

The data for the 36 specimens are summarised in Table 1.

### *B. The determination of lattice constants*

#### a) X-ray method

Powder photographs were taken using an AEG-Guinier camera and  $\text{Cu K}\alpha_1$ -radiation. Silicon ( $a = 5.4305 \text{ \AA}$ ) was used as an internal standard.

#### b) Measurement

As far as possible the same films were used from which the  $\Delta(\theta)$ -values (BAMBAUER et al., 1967) were determined. A few poorly exposed photographs were retaken.

All the lines in the approximate  $2\theta$ -range  $20^\circ$ — $50^\circ$  with sufficient intensity were measured (accuracy of measurement  $2 \times 10^{-3} \text{ mm}$ ). Depending on the sharpness and intensity of the photographs, this corresponds to between 40 and 120 lines per photograph. The reproducibility of the positions of the lines in especially sharp photographs is better than  $1 \times 10^{-2} \text{ mm}$ .

The influence of film shrinkage and camera radius on line positions were corrected by means of the standard substance. During the calculations it was found that no difficulties arose from the relatively long intervals between the powder lines of the standard substance.

#### c) Calculations

The prerequisite for calculating the lattice constants was a satisfactory indexing of the powder pattern. This was accomplished in the following way: The positions of the powder lines of an albite pattern given by SMITH (1956) were marked on the abscissa of Fig. 1. The positions of the corresponding lines of many plagioclases were marked at the appropriate values on the ordinate, which correspond to the different compositions. The points having the same indices are joined by lines (Fig. 1)<sup>1</sup>). The refinement of the lattice constants was carried out with

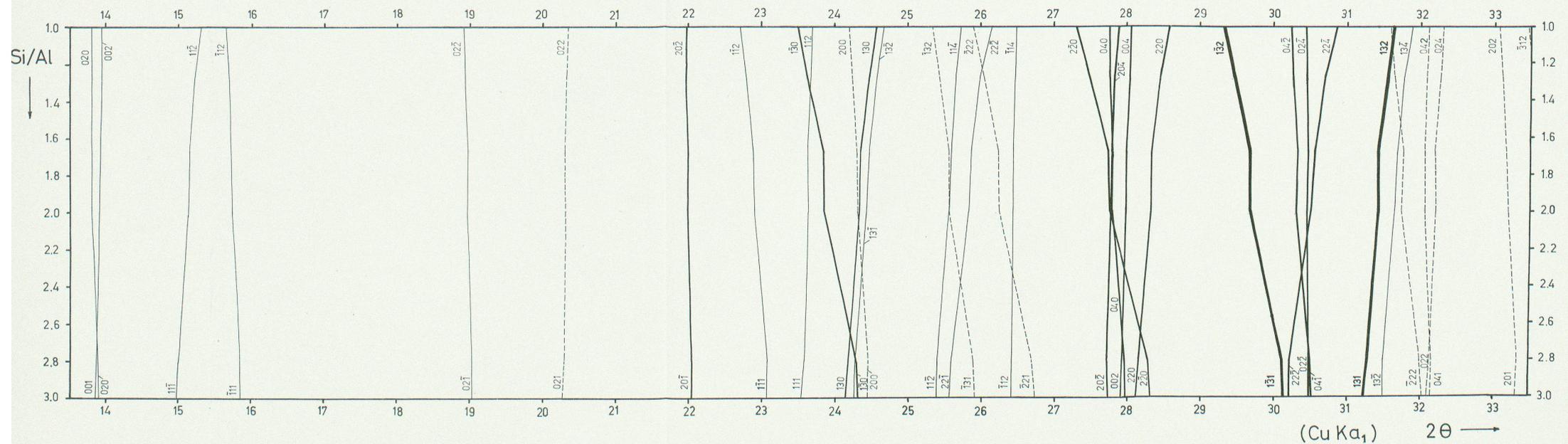
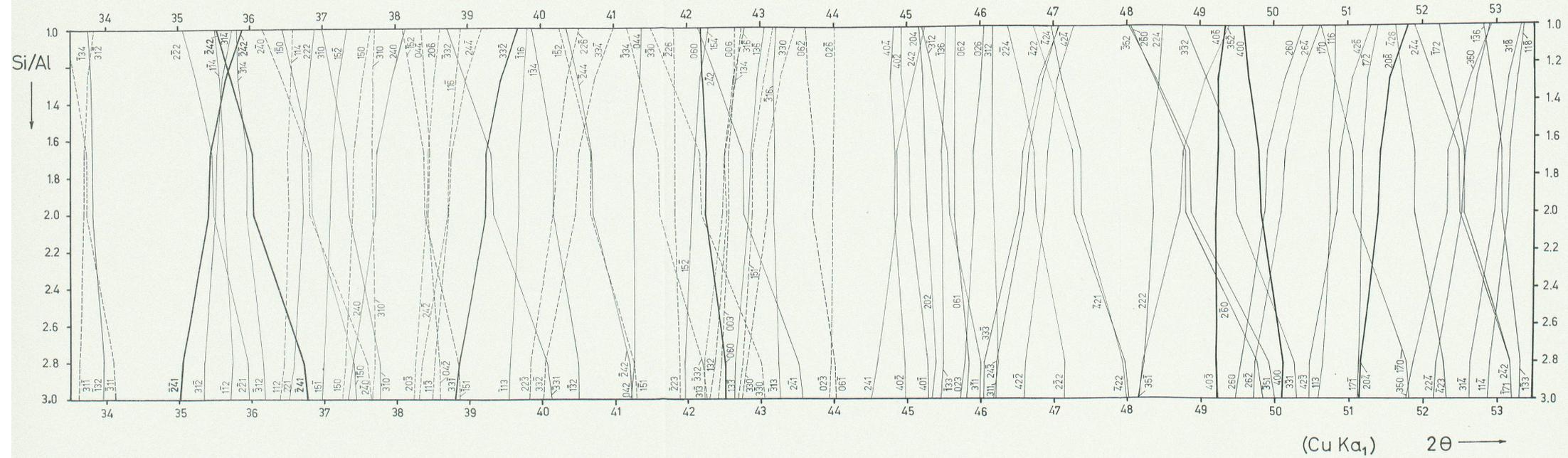
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<sup>1</sup>) An-rich plagioclases have a doubled ( $\sim 14 \text{ \AA}$ )  $c$ -dimension. Since it is difficult to determine in powder photographs the boundary of the superstructure region, the superstructure reflexions are omitted.

Table 1. Lattice constants and related parameters of 36 plagioclases

Nr.	Si/Al	An	Or	a	b	c	$\alpha$	$\beta$	$\gamma$	$a^*$	$b^*$	$c^*$	$\alpha^*$	$\beta^*$	$\gamma^*$	V	a:b	c:b	$\sigma$	Nr.
194	3.0	0.0	0.3	8.141	12.786	7.159	94.25	116.59	87.69	0.1374	0.078428	0.1565	86.40	63.50	90.45	664.5	0.6367	0.5599	32.70	194
191	2.98	0.5	1.2	8.141	12.785	7.159	94.26	116.59	87.69	0.1374	0.078433	0.1565	86.39	63.50	90.46	664.5	0.6367	0.5599	32.12	191
167	2.97	0.7	0.2	8.139	12.782	7.157	94.29	116.60	87.69	0.1374	0.078457	0.1566	86.36	63.49	90.43	663.9	0.6367	0.5599	32.25	167
163	2.935	1.7	0.6	8.139	12.785	7.158	94.20	116.61	87.76	0.1374	0.078426	0.1566	86.43	63.47	90.40	664.2	0.6366	0.5599	32.03	163
110	2.845	11.1	1.4	8.148	12.798	7.156	94.20	116.57	87.85	0.1372	0.078351	0.1566	86.37	63.51	90.31	665.6	0.6367	0.5592	30.70	110
278	2.55	13.0	0.5	8.149	12.804	7.142	94.07	116.52	88.45	0.1372	0.078300	0.1568	86.22	63.52	89.70	665.1	0.6365	0.5578	22.38	278
84	2.43	16.5	0.7	8.151	12.814	7.138	94.01	116.50	88.63	0.1371	0.078224	0.1569	86.21	63.53	89.53	665.4	0.6361	0.5571	19.77	84
171	2.41	17.2	0.6	8.154	12.826	7.137	93.94	116.48	88.74	0.1370	0.078153	0.1569	86.22	63.54	89.45	666.5	0.6358	0.5564	18.48	171
2	2.405	17.6	0.9	8.153	12.824	7.134	93.95	116.46	88.84	0.1370	0.078167	0.1569	86.17	63.55	89.33	666.1	0.6358	0.5563	16.88	2
104	2.39	17.9	0.5	8.155	12.834	7.130	93.88	116.45	89.07	0.1370	0.078108	0.1570	86.13	63.55	89.11	666.4	0.6354	0.5555	13.60	104
67	2.37	18.5	0.9	8.158	12.831	7.137	93.94	116.45	88.80	0.1369	0.078128	0.1569	86.20	63.57	89.38	667.2	0.6358	0.5562	17.30	67
162	2.33	20.2	3.9	8.162	12.827	7.137	93.88	116.46	88.85	0.1369	0.078146	0.1569	86.23	63.56	89.35	667.3	0.6363	0.5564	17.00	162
288	2.31	21.0	0.9	8.161	12.836	7.131	93.89	116.45	89.01	0.1369	0.078095	0.1570	86.14	63.56	89.16	667.3	0.6358	0.5556	14.30	288
166	2.29	21.5	1.2	8.153	12.830	7.134	93.90	116.43	88.94	0.1370	0.078126	0.1569	86.17	63.58	89.24	666.7	0.6355	0.5560	15.47	166
114	2.23	23.9	0.3	8.154	12.847	7.120	93.79	116.42	89.45	0.1370	0.078031	0.1572	86.05	63.55	88.73	666.3	0.6347	0.5543	7.88	114
170	2.19	25.3	1.0	8.159	12.843	7.127	93.80	116.41	89.28	0.1369	0.078048	0.1570	86.11	63.58	88.91	667.3	0.6353	0.5549	10.53	170
193	2.185	25.6	1.0	8.158	12.837	7.124	93.80	116.40	89.26	0.1369	0.078085	0.1571	86.12	63.59	88.94	666.7	0.6355	0.5550	10.83	193
101	2.125	28.0	0.8	8.163	12.853	7.124	93.71	116.36	89.38	0.1368	0.077980	0.1570	86.16	63.62	88.85	668.1	0.6351	0.5542	9.25	101
136	1.96	35.3	0.4	8.161	12.859	7.116	93.66	116.30	89.71	0.1367	0.077948	0.1571	86.07	63.66	88.52	667.9	0.6346	0.5534	4.25	136
5	1.91	37.4	4.2	8.171	12.862	7.119	93.59	116.30	89.68	0.1366	0.077925	0.1570	86.15	63.67	88.58	669.2	0.6353	0.5535	1.73	5
94	1.82	41.8	0.4	8.170	12.869	7.114	93.42	116.28	89.06	0.1366	0.077882	0.1571	86.16	63.67	88.24	669.1	0.6348	0.5528	-0.87	94
212	1.79	43.2	0.4	8.167	12.856	7.113	93.60	116.27	89.71	0.1366	0.077962	0.1571	86.13	63.69	88.55	668.1	0.6353	0.5533	4.38	212
237	1.78	43.7	1.3	8.172	12.865	7.116	93.60	116.27	89.66	0.1365	0.077906	0.1571	86.15	63.70	88.60	669.4	0.6352	0.5531	5.07	237
91	1.705	47.8	0.2	8.166	12.851	7.113	93.61	116.26	89.64	0.1366	0.077992	0.1571	86.15	63.70	88.61	667.9	0.6354	0.5535	5.27	91
74	1.605	53.8	1.0	8.173	12.855	7.110	93.58	116.23	89.79	0.1365	0.077968	0.1572	86.11	63.73	88.47	668.5	0.6358	0.5531	3.18	74
81	1.605	53.7	0.8	8.169	12.862	7.108	93.58	116.22	89.81	0.1365	0.077931	0.1572	86.10	63.74	88.44	668.4	0.6351	0.5527	2.75	81
48	1.595	54.3	1.0	8.172	12.861	7.107	93.52	116.22	90.03	0.1365	0.077941	0.1572	86.07	63.73	88.23	668.5	0.6355	0.5526	-0.48	48
96	1.53	58.1	1.2	8.180	12.870	7.109	93.52	116.20	90.04	0.1363	0.077883	0.1571	86.06	63.75	88.22	670.0	0.6356	0.5523	-0.53	96
11	1.51	59.8	0.2	8.173	12.862	7.107	93.56	116.19	89.98	0.1364	0.077937	0.1572	86.04	63.79	88.27	668.8	0.6355	0.5526	0.23	11
45	1.37	68.7	0.2	8.175	12.865	7.102	93.50	116.14	90.31	0.1363	0.077927	0.1572	85.95	63.79	87.93	668.9	0.6355	0.5521	-4.42	45
103	1.37	69.0	0.7	8.179	12.869	7.102	93.49	116.16	90.36	0.1363	0.077904	0.1573	85.93	63.76	87.88	669.2	0.6355	0.5519	-5.10	103
61	1.31	73.1	0.6	8.181	12.870	7.099	93.41	116.10	90.55	0.1362	0.077898	0.1573	85.93	63.81	87.71	669.5	0.6356	0.5516	-7.75	61
36	1.26	77.0	0.3	8.180	12.869	7.096	93.38	116.13	90.63	0.1363	0.077908	0.1574	85.92	63.78	87.63	668.8	0.6356	0.5514	-8.83	36
300	1.23	80.0	0.2	8.179	12.868	7.093	93.34	116.08	90.80	0.1363	0.077923	0.1574	85.89	63.82	87.47	668.7	0.6356	0.5512	-11.0	300
299	1.21	81.9	0.0	8.181	12.871	7.096	93.34	116.10	90.79	0.1363	0.077904	0.1573	85.90	63.80	87.48	669.1	0.6356	0.5513	-10.83	299
116	1.07	93.1	0.0	8.179	12.873	7.090	93.21	115.97	91.11	0.1362	0.077895	0.1573	85.88	63.91	87.19	669.3	0.6353	0.5507	-15.13	116

Nr.: specimen number given by CORLETT and EBERHARD; Si/Al: Si/Al-ratio derived from An-content; An: mol-% An from microprobe analyses by CORLETT and RIBBA; Or: mol-% Or in the matrix; a, b, c: cell edges given in Å-units. The standard deviation is usually  $\pm 0.001$  Å;  $a^*$ ,  $b^*$ ,  $c^*$ : reciprocal cell edges given in Å<sup>-1</sup>;  $\alpha$ ,  $\beta$ ,  $\gamma$ : cell angles in degrees. The deviation is mostly within 0.01°;  $\alpha^*$ ,  $\beta^*$ ,  $\gamma^*$ : reciprocal cell angles; V: Volume of the cell, calculated from the lattice constants;  $\sigma$ : angle of the rhombic section.



-----: These lines are not readily visible; however they are marked in the  $2\theta$ -range  $13^\circ$ — $45^\circ$ .

————: The pair  $131/\bar{1}\bar{3}1$ , which is important diagnostically.  
 ————: All other readily visible lines in the  $2\theta$ -range  $13^\circ$ — $54^\circ$ .

Fig.1. Relations between  $2\theta$  ( $\text{Cu K}\alpha_1$ ) and chemical composition (given as Si/Al-ratio) in the powder patterns of "plagioclase (low)".

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the help of the CDC-1604-A-computer, using the lattice constants refinement programm ZH=LCLS<sup>2)</sup>. For every sample approximate lattice constants, inferred from literature data, were used as input. It was usually observed that after the completion of only two cycles the standard deviation did not exceed  $\pm 0.0015 \text{ \AA}$  for lattice edges and  $\pm 0.01^\circ$  for lattice angles. In a very few cases the punched cards for some lines had to be removed because of unusually large differences between the calculated and the measured values. These discrepancies may be due to false measurement or false indexing. From Fig. 1 can be seen that such errors in indexing are possible for certain reflexions near the points of intersection of lines. The refined lattice constants and other parameters calculated from these lattice constants are given in Table 1 and the data are presented graphically in Figs. 2, 3 and 5. For the construction of the boundary curves for "plagioclases (low)", shown in the figures, only the 25 points, which satisfied the condition II A a), were considered. Because of the scatter of the plotted data, the drawing of these curves presented some difficulty. Since the behaviour of a few points (e. g. 36 and 84) was always "good" the curves could be drawn using them as reference points. The behaviour of a point is supposed to be "good", if it shows the same deviation (in all the figures) from the general trend (i. e. an average line) indicated by all the other points.

### III. RESULTS

According to BROWN (1960) a nearly linear relation between the lattice constants and Si/Al-ratios is to be expected: Thus Figs. 2, 3 and 5 have the Si/Al-ratio as abscissa. The following relations are observed in the diagrams:

1. In general the lattice constants of "plagioclases (low)" vary with increasing An-content in the following ways:

- a)  $a$  and  $b$  increase,  $c$  decreases; the corresponding  $a^*$ ,  $b^*$  and  $c^*$  behave in the opposite way (no diagrams are given for these parameters).
- b)  $\gamma$  increases and  $\beta$  decreases; the corresponding  $\gamma^*$  and  $\beta^*$  vary in the opposite way;  $\alpha$  and  $\alpha^*$  behave differently: both of them decrease.
- c) The angles  $\gamma$  and  $\gamma^*$  vary much more than the other lattice angles.

<sup>2)</sup> We thank Dr. Charles W. Burnham who made available to us his programm LSLSQ and Dr. M. Fehlmann for rewriting it to suit the CDC-computer.

d)  $a : b$  varies very little, but  $c : b$  shows a distinct decrease. The data available in the literature generally show the same trends (see e. g. SMITH, 1956; BROWN, 1960).

2. There are discontinuities in the lattice-constant/ $An$  relations (Figs. 2 and 3) analogous to those of the  $\Delta(\theta)/An$  curves presented by BAMBAUER et al. (1967). The distinctness of these discontinuities is different for different lattice constants. In Fig. 3 for example,  $\gamma^*$  shows distinct breaks at  $Si/Al=2.02$  and  $1.67$ , whereas the  $\beta^*$ -curve shows an almost

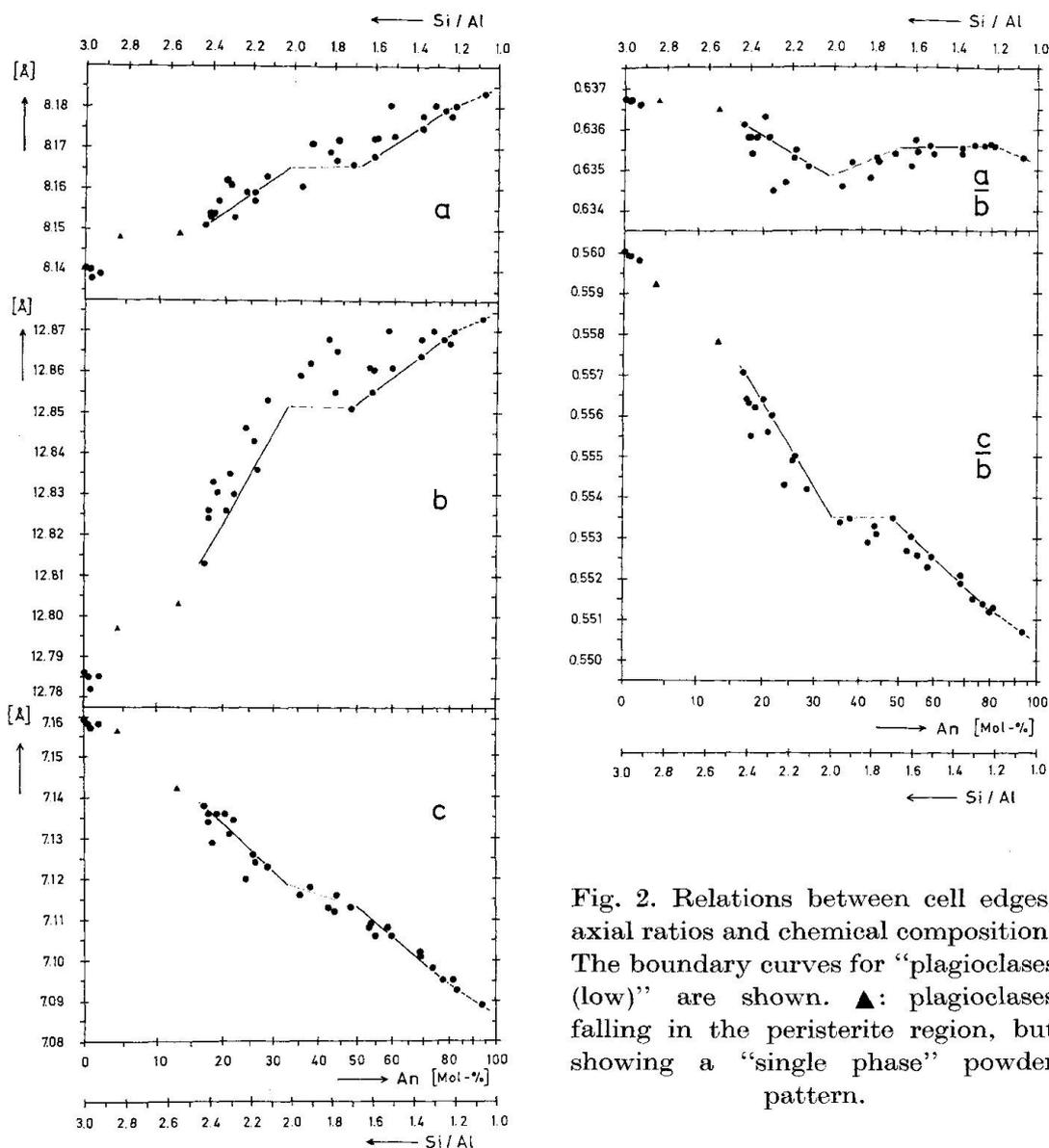


Fig. 2. Relations between cell edges, axial ratios and chemical composition. The boundary curves for "plagioclases (low)" are shown.  $\blacktriangle$ : plagioclases falling in the peristerite region, but showing a "single phase" powder pattern.

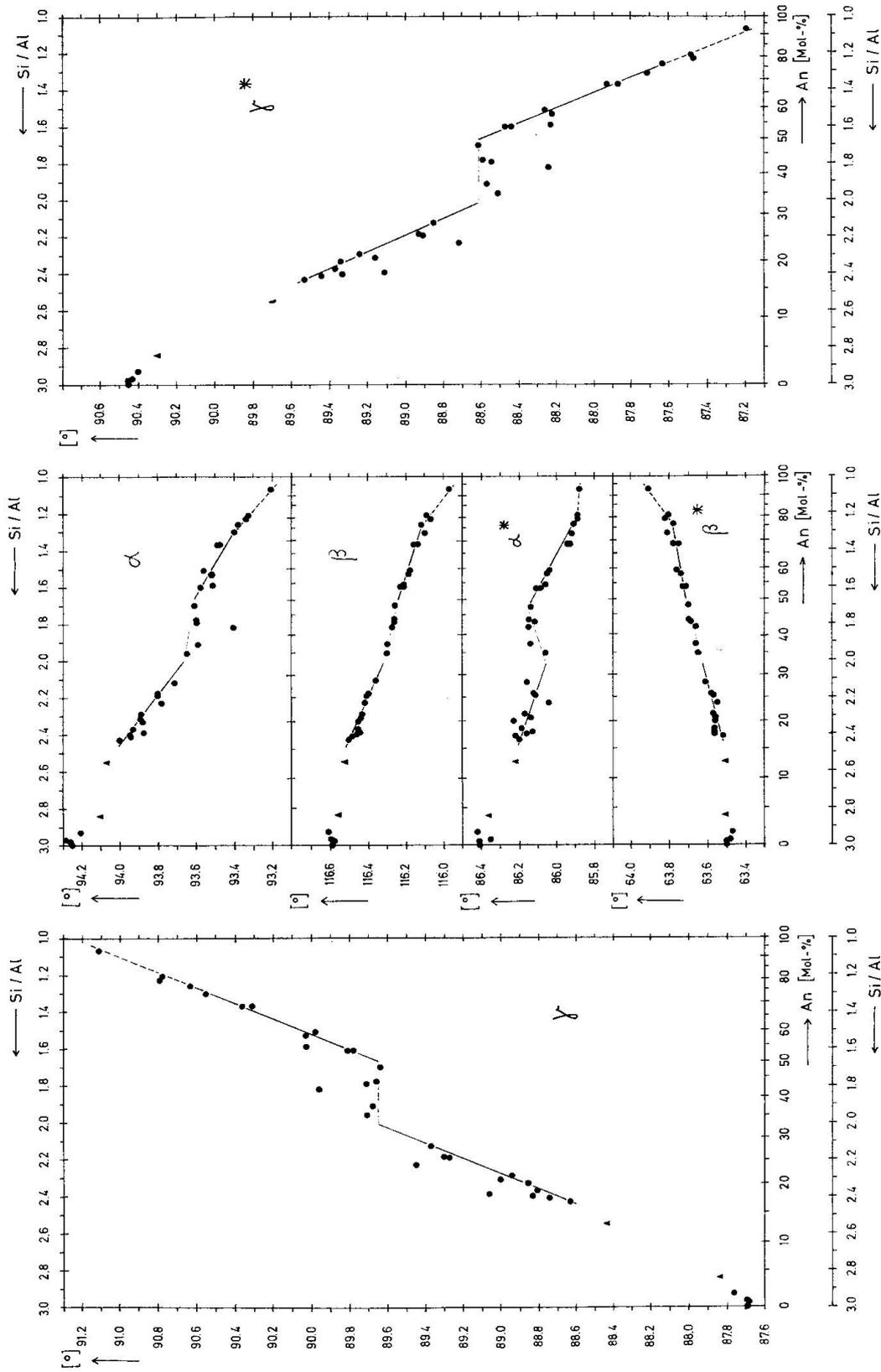


Fig. 3. Relations between lattice angles and chemical composition. The boundary curves are for "plagioclases (low)".  $\blacktriangle$ : see Fig. 2.

linear behaviour in this range. Considering Figs. 2 and 3 the boundary curves can be subdivided into parts corresponding to:

- a)  $\text{Si}/\text{Al} = 3.0$  to appr. 2.97 ( $\text{An}_{0.0-1.3}$ ): Range of albite (low).
- b)  $\text{Si}/\text{Al} = 2.97-2.45$  ( $\text{An}_{1.3-16}$ ): Peristerite gap.
- c)  $\text{Si}/\text{Al} = 2.45-2.02$  ( $\text{An}_{16-33}$ ): Linear within the limits of experimental error.
- d)  $\text{Si}/\text{Al} = 2.02-1.67$  ( $\text{An}_{33-50}$ ): As in the case of  $\Delta(\theta)$ -values uncertainties still exist.
- e)  $\text{Si}/\text{Al} = 1.67-1.25$  ( $\text{An}_{50-76}$ ): Linear within the limit of experimental error.
- f)  $\text{Si}/\text{Al} = 1.25-1.00$  ( $\text{An}_{76-100}$ ): No comments can be made about this region at this stage.

3. The Or-content has the greatest effect on  $a$  and on  $a^*$ . This suggests an analogy to the alkali feldspars. However, due to the insufficient data, no precise information can be given on such a correlation.

4. The determination of the lattice constants of both components of peristerites seems to be but rarely possible by the powder method. Among the intense lines which may be indexed with certainty only the pairs  $131/\bar{1}\bar{3}1$  and  $\bar{2}41/\bar{2}\bar{4}1$  are resolved. Peristerites are, as hitherto, best determined either by single crystal methods (LAVES, 1954; BROWN, 1960) or by electron microscopy (RIBBE, 1960; FLEET and RIBBE, 1965).

Among the investigated specimens there were occasionally plagioclases whose  $\Delta(\theta)$ -values fell on the interpolated plagioclase (low)-curve in the peristerite-gap. The powder patterns of such specimens could not be differentiated from those of homogeneous phases. The lattice constants were determined for two such specimens (Nrs. 110 and 278). One of them seems to be a peristerite because of its bluish-white schiller. In Figs. 2 and 3 the values of its lattice angles fall rather exactly on to the line interpolated between  $\text{An}_{1.3}$  and  $\text{An}_{16}$ , while those of its lattice edges deviate from this line.

5. Using the lattice constants derived from Figs. 2 and 3 the following quantities were calculated:

- a) Relations between  $2\theta \text{Cu K } \alpha_1$  and An-content to check Fig. 1. This diagramm was originally intended for indexing the powder patterns of the series "plagioclases (low)". However, plagioclases show the puzzling phenomenon that the lattice constants of a "high" or "intermediate"

plagioclase are approximately the same as those of a "plagioclase (low)" having a different An-content. This means that a powder pattern of any plagioclase, whether "high" or "intermediate" must be almost the same as that of a plagioclase (low); (ignoring the differences in the intensities of the lines). Therefore this diagram can serve to index powder patterns of plagioclases of all compositions and structural states. The best way to index the powder patterns is to measure the value  $2\theta_{131} - 2\theta_{1\bar{3}1}$  in it. Using this value the corresponding Si/Al-ratio given by the boundary curve for "plagioclases (low)" in the diagram (Fig. 5) of BAMBAUER et al. (1967) must be sought. For the Si/Al-value so obtained, Fig. 1 gives the indices along the abscissa in the order of increasing  $2\theta$ .

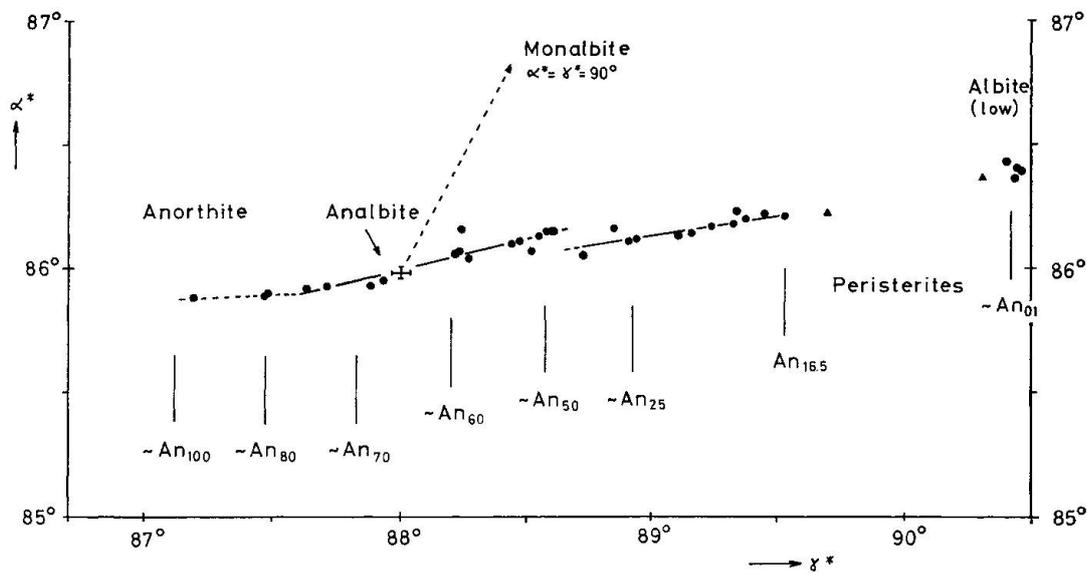


Fig. 4. Relations between  $\alpha^*$  and  $\gamma^*$ . The An-calibration is valid only for "plagioclases (low)".  $\blacktriangle$ : see Fig. 2.

b) Relations between  $\Delta(\theta)_1$ ,  $\Delta(\theta)_2$  and An-content. The agreement between the calculated and observed values of  $\Delta(\theta)_1$  and  $\Delta(\theta)_2$  appears to be rather good considering the accuracy obtainable by the methods of this investigation. In addition an attempt was made to calculate  $\Delta(\theta)$ -curves for an Or-content of 4 mol-% using the lattice constants of microcline (low), and assuming that Vegard's law is approximately applicable for mixed crystals plagioclase (low)-microcline (low). The agreement between the calculated and observed values is satisfactory in the case of  $\Delta(\theta)_1$  but poor for  $\Delta(\theta)_2$ , as can be seen from Figs. 5 and 6 of BAMBAUER et al. (1967).

c) The angle  $\sigma$  of the rhombic section using the relation  $\text{ctg } \sigma = \frac{\cos \alpha^*}{\text{ctg } \gamma}$ . Fig. 5 shows the curves for "plagioclases (low)" and "plagioclases (high)". The curve "plagioclase (high)" was calculated from lattice constants, determined for synthetic specimens of EBERHARD (1967).

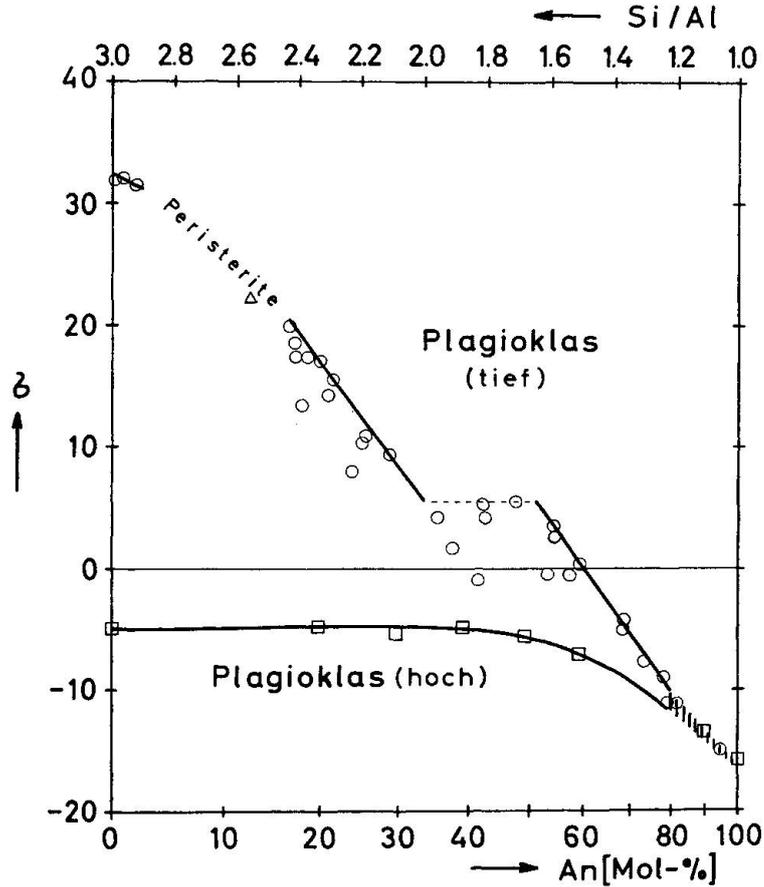


Fig. 5. Relation between the  $\sigma$ -angle of the rhombic section and chemical composition for natural "plagioclases (low)" and synthetic "plagioclases (high)".

#### IV. DISCUSSION

##### A. The shape of the curves

The position of the curves cannot be given with certainty in the region  $\text{Si/Al} = 3.0\text{--}2.97$  (Figs. 2—4); therefore they were omitted. However general trends are recognizable.

It is found that the values for "plagioclases (low)" and "plagioclases (high)" nearly coincide in the range  $\text{An}_{76\text{--}100}$  (Fig. 5). Therefore it may

be difficult to distinguish between these two series by powder-diagrams if the An-value is larger than appr. An<sub>75</sub>. Further additional complications may arise because of the variety of domain-order/disorder states described by BROWN et al. (1963). Thus the curves An<sub>76-100</sub> have not been extended to An<sub>100</sub>, and are shown only as dotted lines. Future corrections are not expected to affect the main trend of the curves, but amendments in details may be possible.

While the limiting curves for "plagioclases (low)" of the range An<sub>16-33</sub> and An<sub>50-76</sub> are considered to be good approximations to straight lines, uncertainties exist for the interval An<sub>33-50</sub>. Therefore, in Figs. 2, 3 and 5, dotted lines represent an interpolation of our data in this region. Future investigations of additional material are necessary.

### *B. Comparison with data in the literature*

It is assumed that the material, which was selected for this investigation from about 300 specimens is representative for the most ordered state of "plagioclase (low)" produced by nature. Some of the published values of the lattice constants for plagioclases show very good agreement if plotted in Figs. 2 and 3; other values deviate considerably to both sides of the curves presented. An explanation of this fact cannot be given at this stage. Perhaps the scatter may be due to inhomogeneities of the material investigated. The bulk composition of a "crystal" may not be representative of the homogeneous "host"-phase which is responsible for the position of the powder lines measured. As is now well known the relation of the powder data of the "plagioclases (low)" to the An-content exhibits discontinuities. Such discontinuities became obvious with varying distinctness in the data published by CLAISSE (1950) at An<sub>30-40</sub>; by GOODYEAR and DUFFIN (1954, 1955) at An<sub>30</sub> and An<sub>70-80</sub>; by SMITH and YODER (1956) at An<sub>30-40</sub> and by SMITH and GAY (1958) at An<sub>35-40</sub> and An<sub>50</sub>.

A comparison between literature data and those presented in this investigation is possible in certain cases. GOODYEAR and DUFFIN (1955) show breaks in the  $\gamma^*$ -curve at about An<sub>30</sub> and An<sub>70</sub>. The data of SMITH (1956) refer mainly to the region An<sub>16-33</sub>. The data of BROWN (1960) reveal some interesting features. However, since the precession method and the bulk An-content (without Or) were used in this work, the resolution of his data with respect to boundary curves was less than that of the data presented in this investigation. If the smooth curves drawn by

BROWN (relating  $\gamma^*$  and  $(010) \wedge (\bar{1}01)$  with chemical composition) are reexamined, there are strong indications of discontinuities at  $An_{30}$  and  $An_{50-60}$ . His  $\alpha^*/\gamma^*$  diagram is very similar to Fig. 4 in this investigation.

Until now the most detailed information on structural discontinuities in the series "plagioclases (low)" is from DOMAN et al. (1965). Relating  $\gamma^*$  (determined from single-crystal photographs) with An-content (determined mainly by refractive indices), these authors found that  $\gamma^*/An$ -values group themselves along more or less parallel, mutually displaced lines. Their diagrams indicate discontinuities at about  $An_3$ ,  $An_{16}$ ,  $An_{33}$ ,  $An_{50}$  and  $An_{92-96}$ . Neglecting indications found during this investigation<sup>3)</sup> that  $An_{1.3}$  is a maximum value for the An-content in albite (low) and that the upper limit of the peristerite gap occurs at  $An_{16}$ , there is a relatively good agreement between the present values and those of DOMAN et al. However, whereas DOMAN et al. observed mutually displaced "segments" in the pertinent curves, we only observed "breaks" in them. Further work appears to be necessary for clarifying the situation. In addition, there are the following differences between the results of DOMAN et al. and those of this investigation:

a) DOMAN et al. find a discontinuity at appr.  $An_{94}$  whereas our data indicate such a discontinuity at appr.  $An_{75}$  (it should be noted that within the An-rich region the  $\gamma^*/An$ -diagram of DOMAN et al. is hardly indicative).

b) There is no agreement in the region  $An_{33-50}$ . In this range our  $\gamma^*$ -values are always  $\bar{\approx} 88.61^\circ$  and the  $\gamma^*$ -values found in the literature are always  $\bar{\approx} 88.69^\circ$ . DOMAN et al. however show an isolated line in this region, which runs more or less parallel to the general trend of the  $\gamma^*/An$ -relations from  $\gamma^* = 88.22^\circ$  ( $An_{52}$ ) to  $\gamma^* = 89.08^\circ$  ( $An_{34}$ ). It should be taken into consideration that all the points on this curve with  $\gamma^* > 88.75^\circ$  are determined by the use of one, perhaps inhomogeneous, plagioclas specimen (GD 1805) from a ferrogabbro. This specimen appears to be of considerable interest, as no similar values of  $\gamma^*$  have been obtained by us for plagioclases of this range. (As according to our experience, plagioclases from such rocks are likely to have a high Or-content which cannot be determined optically, it would be of interest to examine the specimen GD 1805 of DOMAN et al. with a microprobe analyser for any "impurities" that may be present in the matrix in solid solution.)

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<sup>3)</sup> This value is based on an analysis of the Ab-rich phase of a peristerite using the electron microprobe analyser.

*C. Significance of the discontinuities*

The reasons for the discontinuities, found and depicted in Figs. 1—5, are still unknown. Structure determinations (as far as Al/Si-distributions are concerned) of chemically intermediate "plagioclases (low)" are very desirable. In addition, electron microscopy (LAVES et al., 1965) and very high resolution X-ray techniques developed by JAGODZINSKI and KOREKAWA (1965) may lead to a better understanding of the variety of feldspar structures. This variation appears to be due to their Al/Si distributions, the significance of which was first envisaged by BARTH (1934). A mathematical treatment of the possibilities of Al/Si order under the assumption that no Al-tetrahedra have common oxygen corners is given by NIGGLI (1967) in an accompanying paper.

*Acknowledgements*

This investigation was partly supported by a "Schweizerisches Bundesstipendium" (K. Viswanathan). We thank Professor F. Laves for his interest in this investigation and take the opportunity of thanking Dr. Mabel Corlett for microprobe analyses and Dr. M. Fehlmann and Miss H. Wulf for their help in the computer (CDC of the ETH) calculations.

## REFERENCES

SMPM = Schweiz. Mineralogische und Petrographische Mitteilungen

- BAMBAUER, H. U., CORLETT, M., EBERHARD, E., VISWANATHAN, K. (1967): Diagrams for the determination of plagioclases using X-ray powder methods. SMPM 47/1, 333—349.
- BARTH, T. F. W. (1934): Polymorphic phenomena and crystal structures. Amer. Sci., 27, 273—286.
- BROWN, W. L. (1960): Lattice changes in heat treated plagioclases. Z. Krist. 113, 297—329.
- (1960): The crystallographic and petrologic significance of peristerite unmixing in the acid plagioclases. Z. Krist. 113, 330—344.
- CLAISSE, F. (1950): A roentgenographic method for determining plagioclases. Amer. Min 35, 412—420.
- CORLETT, M. und EBERHARD, E. (1967): Das Material für chemische und physikalische Untersuchungen an Plagioklasen. SMPM 47/1, 303—316.
- CORLETT, M. and RIBBE, P. H. (1967): Electron probe microanalysis of minor elements in plagioclase feldspars. SMPM 47/1, 317—332.
- DOMAN, R. C., CINNAMON, C. G. and BAILEY, S. W. (1965): Structural discontinuities in the plagioclase feldspar series. Amer. Mineral. 50, 724—740.
- EBERHARD, E. (1967): Zur Synthese der Plagioklase. SMPM 47/1, 385—398.

- FLEET, S. G. and RIBBE, P. H. (1965): An electron-microscope study of peristerite plagioclases. *Mineral. Mag.* 35, 165—176.
- GAY, P. (1962): Sub solidus relations in the plagioclase feldspars. *Norsk. Geol. Tidsskr.* 42, 2, 37—56.
- GOODYEAR, J. and DUFFIN, W. J. (1954): The identification and determination of plagioclase feldspars by the X-ray powder method. *Mineral. Mag.* 30, 306—326.
- (1955): The determination of composition and thermal history of plagioclases by the X-ray powder method. *Mineral. Mag.* 30, 648—656.
- JAGODZINSKI, H. und KOREKAWA, M. (1965): Supersatelliten im Beugungsbild des Labradorits. *Naturwiss.* 23, 640.
- LAVES, F. (1954): The coexistence of two plagioclases in the oligoclase composition range. *J. Geol.* 62, 409—411.
- LAVES, F., NISSEN, H. U., BOLLMANN, W. (1965): On schiller and submicroscopical lamellae of labradorite. *Naturwiss.* 14, 427—428.
- MEGAW, H. D., KEMPSTER, C. J. E., and RADOSLOWICH, E. W. (1962): The structure of anorthite,  $\text{CaAl}_2\text{Si}_2\text{O}_8$ . II. Description and discussion. *Acta Cryst.* 15, 1017—1035.
- NIGGLI, A. (1967): Die Ordnungsmöglichkeiten der Al-Si-Verteilung in Plagioklasen. *SMPM* 47/1, 279—287.
- RIBBE, P. H. (1960): An X-ray and optical investigation of the peristerite plagioclases. *Amer. Min.* 45, 626—644.
- RIBBE, P. H., FERGUSON, R. B. and TAYLOR, W. H. (1962): A three-dimensional refinement of the structure of low albite. *Norsk Geol. Tidsskr.* 42, 2, 152—157.
- SMITH, J. R. and YODER, H. S. (1956): Variation in X-ray powder patterns of plagioclase feldspars. *Amer. Min.* 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.
- (1958): The powder patterns and lattice parameters of plagioclases feldspars. II. *Mineral. Mag.* 31, 744—762.

Manuscript received September 30th, 1966.