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Discussion on the anorthite superstructure. By FRITZ LAVES and JULIAN R. GOLDSMITH, *Department of Geology, University of Chicago, Chicago 37, Illinois, U.S.A.*

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In an important paper on the plagioclases, Cole, Sörum & Taylor (1951) discussed the problem of the anorthite structure. They found no evidence for structural changes induced by heat treatment, but did not work above 1100°C. The present authors (Goldsmith & Laves, 1951; Laves & Goldsmith 1951*a, b, c*) observed a strong influence of heat treatment on the structure, and briefly published the results of a large amount of experimental work in abstract form. We included a description of a pattern which is called 'the *D* pattern' by Gay & Taylor (1953) who state that it was 'not previously described'. This statement gives the impression that the '*D* pattern' as well as their interpretation of this pattern differs from our observations and conclusions. Fortunately this is not the case.

Gay & Taylor regret the fact that our results were published only in abstract form. Abstracts were published because we felt that our observations, previously overlooked by others, had a bearing on the problems of the plagioclase feldspars, yet we postponed more detailed publication (even though a large body of data was on hand) in order to obtain more measurements on the shape and intensities of the diffuse areas in reciprocal space as a function of temperature. Gay & Taylor state our reasons quite well when they write 'A complete understanding of the nature of the order-disorder change, and of the relationship between anorthite and albite, awaits high-accuracy structure-analysis of minerals showing the different types of pattern' and '... the nature of the disordering transition involving the Ca ions, which is responsible for the observed variations in the anorthite structure, remains obscure pending the completion of the accurate analysis of an ordered material'.

Inasmuch as the abstracts, with one exception (1951*c*), are somewhat difficult to obtain, and because we feel that in some respects they contain more actual information (albeit highly condensed) on anorthite than the paper of Gay & Taylor, we here reproduce two of them.

Short-range order in anorthite*

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Anorthite ($\text{CaAl}_2\text{Si}_2\text{O}_8$) has a unit cell four times as large as the other feldspars, albite ($\text{NaAlSi}_3\text{O}_8$) and orthoclase (KAlSi_3O_8). Using the accepted orientation for feldspars, in anorthite the *c* axis is doubled, and the 'base centering' of the *a b* plane is lost. Therefore, X-ray photographs of anorthite show additional reflections (first observed by Taylor) as compared with the other feldspars. The reflections that are common to all feldspars will be called 'main' reflections (type (*a*)), the additional ones are called 'subsidiary' reflections.

In this investigation it has been found that the main reflections are always sharp (and on the average, strong) whereas the subsidiary reflections (weak, on the average)

can be diffuse. The degree of diffuseness depends on the history of the formation and on the heat treatment of the anorthite crystals. It is also to be noted that the subsidiary reflections are of two different types (*b*) and (*c*), the diffuseness of which is affected differently by heat treatment. Type (*c*) spots are generally much more diffuse than type (*b*), and the degree of diffuseness appears to be a continuous function of the temperature at which the crystal is treated. The (*c*) spots are rather sharp at 1100°C., and very diffuse (and elongated in the direction of the *b* axis) at 1500°C. Equilibrium is apparently established in less than one hour. The type (*b*) reflections are not affected in this manner; although sharpened by heat treatment, attempts to make them diffuse again at high temperature have been unsuccessful.

The indices of the three types of reflection are:

Type (*a*) (main spots): (*hkl*) with *l* even and (*h+k*) even;

Type (*b*): (*hkl*) with *l* odd and (*h+k*) odd;

Type (*c*): (*hkl*) with (*h+k+l*) odd.*

As will be discussed, these observations are best explained by assuming that the (*a*) spots are due to a fundamental feldspar structure. The subsidiary spots (*b*) and (*c*) are a consequence of order-disorder relations with Al and Si ions controlling the (*b*) reflections, Ca ions the (*c*) reflections.

The experimental evidence that the degree of diffuseness of types (*b*) and (*c*) is different and independent of each other favors the assumption that there are two types of short-range order with different order-disorder coefficients and different 'domain sizes'. In discussing some types of order-disorder relations a schematic model of the special case of anorthite will be proposed.

On the superstructure of gallium- and germanium-containing anorthites†

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The X-ray reflections from anorthite, divided into (*a*), main spots, and (*b*) and (*c*), subsidiary spots, are discussed in the preceding abstract. As an aid in the interpretation of the data obtained from natural and synthetic anorthites, partial replacements of the Al and Si atoms by Ga and Ge were made in synthetic crystals so as to change the scattering powers of the Al and the Si positions in the structure. Three compounds were crystallized and studied: (*a*) anorthite with three-eighths of the Al replaced by Ga, (*b*) anorthite with three-eighths of the Si replaced by Ge, and (*c*) anorthite with three-eighths of the Al and three-eighths of the Si replaced by Ga and Ge. The angular geometry of the Ga- and Ge-containing anor-

* In Laves & Goldsmith (1951*c*) the type (*c*) reflections were further subdivided, and the entire classification is precisely the same as that now published by Gay & Taylor.

† Reprint of Goldsmith & Laves, 1951.

* Reprint of Laves & Goldsmith, 1951*b*.

thites is virtually the same as in normal anorthite, differences being less than 20'. As would be expected, the cell dimensions differ slightly.

The main reflections are thus virtually identical to those in anorthite. The intensity relations of the (b) subsidiary spots are greatly different in Ga-containing anorthite, Ge-containing anorthite, and normal anorthite. However, the general intensity relations of the Ga- and Ge-containing anorthite are much like those of normal anorthite. It is thus obvious that the (b) subsidiary reflections are controlled by Al and Si positions. The (c) type subsidiary reflections appear the same in all of the synthetic compounds, including normal anorthite. It is thus concluded that the Ca atoms are those influencing the (c) type subsidiary reflections.

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Variations in the anorthite structure: a note. By P. GAY and W. H. TAYLOR, *Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England*

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The publication, in the preceding note by Laves & Goldsmith (1954), of abstracts (originally dated 1951) of their work on anorthite is very convenient. We still feel some regret that the authors have not yet published details of their work on this very complex problem.

We are glad to re-emphasize that our own findings are in no way in conflict with what we have gathered of the significance of the work of Laves & Goldsmith; this was made quite clear in our earlier publication (Gay & Taylor, 1953) where we refer three times to the 'similar observations' and 'similar ideas' of Laves & Goldsmith appearing in their publication, to which full and complete references were given by us.

Laves & Goldsmith quote the phrase 'not previously described' used by us in reference to the *D* pattern. Read in context in our paper, we hope it is clear that the phrase refers to the fact that whereas Cole, Sörum & Taylor (1951) discussed the *S* and *A* patterns, the *D* pattern was not previously described by them, for the remark appears in a section devoted to brief recapitulation of experimental

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The crystal structures of ZrBeSi and ZrBe₂. By J. W. NIELSEN and N. C. BAENZIGER, *Department of Chemistry, State University of Iowa, Iowa City, Iowa, U.S.A.*

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ZrBeSi

During an attempt to prepare a barium-beryllium alloy, reaction with a zirconium silicate crucible took place. The small cluster of crystals formed in the reaction product did not provide sufficient sample for quantitative chemical analysis. The composition of the crystals was determined primarily from X-ray diffraction data together

References

- COLE, W. F., SÖRUM, H. & TAYLOR, W. H. (1951). *Acta Cryst.* 4, 20.
 GAY, P. & TAYLOR, W. H. (1953). *Acta Cryst.* 6, 647.
 GOLDSMITH, J. R. & LAVES, F. (1951). A. C. A. Meeting, Chicago, October 1951. (Abstract, p. 11.)
 LAVES, F. & GOLDSMITH, J. R. (1951a). International Congress of Crystallography, Stockholm, June 1951. (Abstract.)
 LAVES, F. & GOLDSMITH, J. R. (1951b). A. C. A. Meeting, Chicago, October 1951. (Abstract, p. 10.)
 LAVES, F. & GOLDSMITH, J. R. (1951c). Mineralogical Society of America Meeting, Detroit, November 1951. (Abstract; also *Amer. Min.* (1952), 37, 295.)

observations made in this laboratory, in a paragraph dealing with Gay's recent work, and in a sentence which compares this with the results of Cole *et al.*, mentioned in the line above. We realize, after reading the note by Laves & Goldsmith, that it is possible to misunderstand our wording at this place. We regret this, but would point out that if the whole paper is read, and that of Gay (1953) on which our discussion is based, it is abundantly clear that we have in no way underestimated the value of Laves & Goldsmith's researches.

References

- COLE, W. F., SÖRUM, H. & TAYLOR, W. H. (1951). *Acta Cryst.* 4, 20.
 GAY, P. (1953). *Miner. Mag.* 30, 169.
 GAY, P. & TAYLOR, W. H. (1953). *Acta Cryst.* 6, 647.
 LAVES, F. & GOLDSMITH, J. R. (1954). *Acta Cryst.* 7, 131.

with a few qualitative chemical tests. Synthesis of the compound further verified the composition as ZrBeSi.

Zero- to fourth-layer Weissenberg diagrams, using Cu *K* radiation, were obtained from one of the crystals, and the dimensions of the hexagonal cell were determined from a powder diagram. Final intensity comparisons were made on the basis of the powder diagrams. The unit cell dimensions are