from 3·986 A. at 0° C. to 3·975 A. at the lowest temperature reached before the second transition occurs in the neighbourhood of −90 to −100° C. (see Fig. 1). Geometrically, since $a = c$ and $\beta = 90°$, this lattice has orthorhombic symmetry, with the diagonals of the (010) face of the pseudo-monoclinic cell forming the new a and c axes (Megaw, 1946).

The individual subcrystallites of this low-temperature mosaic structure are inclined to one another at small angles of 25' with orientations in the orthogonal directions. Because of the breakdown into a mosaic structure dielectric measurements can only represent average values in the respective crystal directions.

At the second transition near −90° C., there is a further change in the axial parameters. In all cases investigated the crystal changes to a mosaic structure at this temperature with a unit cell having axes

$$a = b = c = 3\text{·}999\ \text{A.}, \quad \text{with} \quad \beta = 90° \ 14'.$$

The structure at this second transition is thus almost cubic with a slight distortion from true orthogonality.

Optical observations with the polarizing microscope showed that the transition from one phase to another, as the temperature was lowered gradually through either of the transitions, occurred discontinuously. The new phase seemed either to creep across the crystal as a consequence of a series of very minute jumps, or to appear suddenly over large sections of the crystal. Microscope observations in polarized light show the low-temperature mosaic structure as consisting of sets of ill-defined dark lines, approximately parallel to the original a and b axes of the room-temperature tetragonal structure. Extinction was poor at approximately 45° to these axes. In all cases, the crystals returned to their original structure, or a similar one, when reheated to room temperature.

A full account of this work will be published later.

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Hydroxyl groups in afwillite. By HELEN D. MEGAW, *Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England*

The mineral afwillite (Parry & Wright, 1925) has the empirical formula $Ca_3Si_2O_{10}H_6$. An investigation of its structure, undertaken with the particular purpose of finding the part played in it by the hydrogen, has now been completed, though further work is needed to determine the atomic parameters exactly.

Experimental data were obtained from single-crystal oscillation and Weissenberg photographs, and used to construct Patterson projections and Patterson bounded projections. No *a priori* assumptions were made about the location of the hydrogen atoms. For this reason, the term 'oxygen atom' is used to include O^{2-}, and OH^-, H_2O groups; the distinction between them follows in the final stages of the determination of the structure.

The main features of the structure can be described by considering one formula-unit, $Ca_3Si_2O_{10}H_6$. The silicon atoms occur in SiO_4 groups, each sharing one edge and two corners with the oxygen polyhedra surrounding neighbouring calcium atoms. The two silicon atoms and two of the three calcium atoms are thus, linked up in a densely packed belt continuous throughout the structure. The polyhedron surrounding the third calcium atom shares two opposite edges with neighbouring calcium polyhedra of two adjacent belts. Each silicon atom is at the centre of a fairly regular tetrahedron; each calcium atom has six close oxygen neighbours, and two others not quite so close.

The novel and most interesting feature of the structure is the environment of some of the oxygen atoms. Of the four oxygens of each silicon tetrahedron, each of the two which do not form part of the shared edge has only one other cation neighbour, a calcium atom. The sum of the Pauling bond strengths is $\frac{2}{8} + \frac{4}{4} = 1\frac{1}{4}$, as compared with the value 2 required by O^{2-} for electrical neutrality; it suggests that these atoms are OH^-. Further, the oxygen atom has the two cation neighbours on the same side, and on its other side only oxygen neighbours—an arrangement which suggests the occurrence of hydroxyl bonds.

The two oxygen atoms not directly linked to silicon have one near calcium neighbour, and two rather more distant, again in a very one-sided arrangement with oxygens adjoining on the other side; they also seem to be OH groups. Detailed consideration of the system of hydroxyl bonds must wait till the refinement of the structure has been completed.

The remaining four oxygen atoms form the shared edges of the silicon tetrahedra and calcium polyhedra; they also partake in shared edges between two calcium polyhedra in the alternate layers. Thus they have each one silicon and three calcium neighbours, tetrahedrally arranged, and the sum of the bond strengths is

$$\frac{4}{4} + \frac{3 \times 2}{8} = 1\frac{3}{4};$$

they may reasonably be identified as O^{2-}.

There is another argument proving that at least *some* of the atoms directly linked to silicon are OH. This follows inevitably from the empirical formula $Ca_3Si_2O_{10}H_6$, once the existence of the SiO_4 groups is established. There are only two oxygen atoms not required for the SiO_4 groups, and they cannot accommodate more than four hydrogen atoms, unless, as seems very improbable, OH_3^+ ions should be present. This argument is quite independent of the details of the environment of the oxygen atoms considered in the previous paragraphs.

This direct linkage of silicon to OH is a new observation, which has not, to the best of the author's knowledge, been established in any published work on silicate structure. It may very well throw light on other problems of hydroxyl-containing silicates.

Further work is in progress, and it is hoped to publish fuller details later. I wish to express my thanks to Dr P. J. G. de Vos for his help with the experimental work, and to Prof. C. E. Tilley for providing the material.

I also wish to thank Sir Lawrence Bragg for his interest in the work.

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Note on the structure of uranium.

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The structure of the low-temperature, or alpha, phase of uranium has been studied by Wilson (1933) and by Jacob & Warren (1937). In both investigations, the powder technique was used. Wilson reports a monoclinic cell with the following constants

$$a = 2 \cdot 829, \quad b = 4 \cdot 887, \quad c = 3 \cdot 308 \, \text{A.}, \quad \beta = 63° \, 26' \, (116° \, 34').$$

Jacob & Warren observed additional lines and deduced an orthorhombic cell with

$$a = 2 \cdot 852, \quad b = 5 \cdot 865, \quad c = 4 \cdot 945 \, \text{A.}$$

The space group is D_{2h}^{17}–$Cmcm$. Atoms are in the $4(c)$ position, and satisfactory intensity agreement was found with the y parameter equal to $0 \cdot 105 \pm 0 \cdot 005$.

Because of the uncertainties inherent in the interpretation of powder photographs of low symmetry, it was felt advisable to confirm the structure using single crystals. Rotation and Weissenberg photographs are consistent with the cell and space group of Jacob & Warren.

Intensities are in substantial agreement with those calculated from the suggested structure. No refinement of the parameter is possible because of the high absorption. As a typical example, calculation gives

$$002 \gg 006 > 004,$$

whereas it is observed that

$$006 \ggg 002 > 004.$$

The apparent reversal is due to the fact that, for copper radiation, 006 is a high-theta reflection and is relatively unaffected by absorption.

It is of interest to note that the cell deduced by Wilson can be considered as contained in that of Jacob & Warren. The axial relations can be expressed as follows

$$- a_{\text{mono.}} = a_{\text{ortho.}}, \quad b_{\text{mono.}} = c_{\text{ortho.}}, \quad c_{\text{mono.}} = \tfrac{1}{2}(a_{\text{ortho.}} + b_{\text{ortho.}}).$$

The monoclinic angle, β, is that between the a axis and the $a + b$ direction.

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Reflexion method for projecting crystal-structure models.

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Parallel-light devices (see, for example, Low & Waldram, 1949) are in use in several laboratories for obtaining projections of wire crystal-structure models and for correlating models and two-dimensional Fourier syntheses. A sheet of plate glass is almost as satisfactory for the first purpose, and can be used for the second, though less conveniently. Its simplicity may, however, recommend it. Relatively large and robust models may be used; the high cost of large parabolic reflectors restricts the size of those used with parallel-light devices.

The point of projection is obtained by moving the eye until the atom and its reflexion coincide. It may be recorded in various ways, depending on the purpose for which it is wanted: (1) the point of projection may be marked on the glass with a suitable pencil; (2) its Cartesian co-ordinates may be read off on a sheet of graph paper placed beneath the glass; (3) its fractional co-ordinates may be read off on a scale drawing of the unit cell with its edges divided into tenths or twentieths. The accuracy obtained (0·005–0·01 of the cell edge) is

sufficient for many purposes. For the first method it is convenient to place a sheet of black paper beneath the glass; the reflexion of the model is then easily seen with ordinary lighting. For the other two methods, and for the correlation of the model with trial Fourier syntheses placed beneath the glass, the model should be illuminated from the side, the lamp being shaded so that the paper beneath the glass is not too bright.

We have used the method only with single projections. There seems no reason, however, why it should not be used for two or three simultaneously, suitable stands being used to support vertical or inclined glass sheets. A lamp mounted in a cocoa tin pointing roughly along the cell diagonal would probably suffice to illuminate the model without throwing too much light on the glass sheets.

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