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The Texture of Single Crystals of Brucite

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X-ray studies of single crystals of tabular brucite give no evidence of irregularities in the stacking sequence of the hexagonal layers of the structure. Rotation diagrams show both sharp spots and extended Debye–Scherrer arcs. They indicate a texture having a range of orientations of the c axis relative to the morphological c axis but with no rotation of the a axes around the c axis. Such a texture could arise from bending of the crystal lattice about $\langle 1\bar{2}10\rangle$ directions and may be produced by a type of edge dislocation arising from additional planes of unit cells parallel to $\{10\bar{1}0\}$.

1. The structure of brucite

The structure of brucite, $Mg(OH)_2$, first determined by Aminoff (1919) (see also Bragg, 1937, p. 107), is a close-packed hexagonal layer structure consisting of layers of hydroxyl ions with magnesium ions in octahedral positions between alternate hydroxyl layers. A re-examination of the structure was undertaken with a view to determining if faults occurred in the stacking of the layers similar to those found in other hexagonal layer structures such as micas, chlorites, graphite, cobalt. Some fine single crystals of brucite from Wood's Mine, Texas (Pa.) were kindly made available from the British Museum collection, (B. M. 33222), by Dr G. F. Claringbull. These crystals are of tabular habit, a description of which, with chemical analysis, is given by Palache, Berman & Frondel, (1944, vol. 1, p. 636). For X-ray analysis, crystals about 0·2 mm. in size were selected and about a dozen were examined by rotation about the hexagonal a, c and $\langle 10\bar{1}0\rangle$ axes using a 6 cm. diameter camera and filtered Cu $K\alpha$ radiation. No evidence was obtained for any departure of the structure from a regular layer sequence.

2. The texture of brucite

Rotation photographs of tabular brucite, examples of which are reproduced in Fig. 2, show a number of sharp spots, but the majority of reflexions are streaked along Debye–Scherrer arcs by amounts which depend on the indices of the reflexions and on the crystal examined. Miss Ali, in this laboratory, had previously observed these effects with brucite crystals. They suggest that the crystallites or mosaic elements forming a single crystal have a characteristic texture. Garrido (1936) has already studied the texture of fibrous forms of brucite but there appears to have been no previous discussion of a texture in tabular varieties.† It is probable that other layer-lattice structures show similar effects.

The observations may be summarized as follows:

(i) Reflexions of type ($hki0$) appear as sharp spots in rotations about a axes and $\langle 10\bar{1}0\rangle$ axes, but show marked extension in c axis rotations.

(ii) General reflexions, ($hkil$), are extended over Debye–Scherrer arcs in all rotation photographs.

Measurements of the lengths of the arcs, obtained with a Bernal $\xi\,\zeta$ chart, when represented in a reciprocal-lattice diagram, show that the texture can be described as arising from a variation in direction of the c axes of the crystallites about the morphological c axis, but with little or no rotation of the a axes around the c axis. Fig. 1 shows schematically the effect of this texture on the reciprocal lattice. Points along the c^* axis (corresponding to $000l$ reflexions) are spread over areas which are circular in outline; points in the a^*a^* plane (corresponding to $hki0$ reflexions) develop arcs perpendicular to the plane; points in general positions (corresponding to $hkil$ reflexions) give rise to elliptical areas which tend towards the linear or circular extremes as the reciprocal vector d^* tends towards the a^*a^* plane or the c^* axis. It is evident from Fig. 1 that sharp $hki0$ reflexions will be

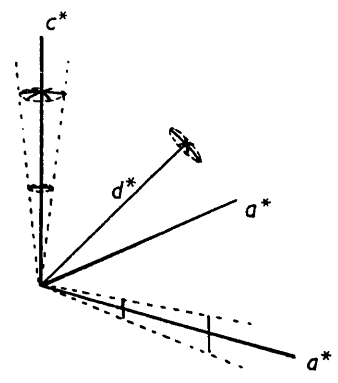

Fig. 1. To illustrate the effect on reciprocal-lattice points of small rotations of the lattice about a-axis directions.

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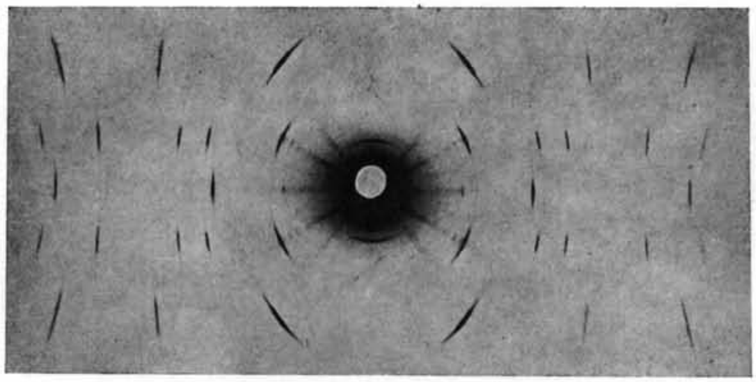
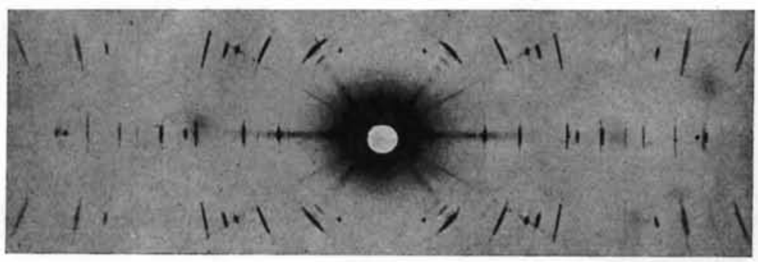
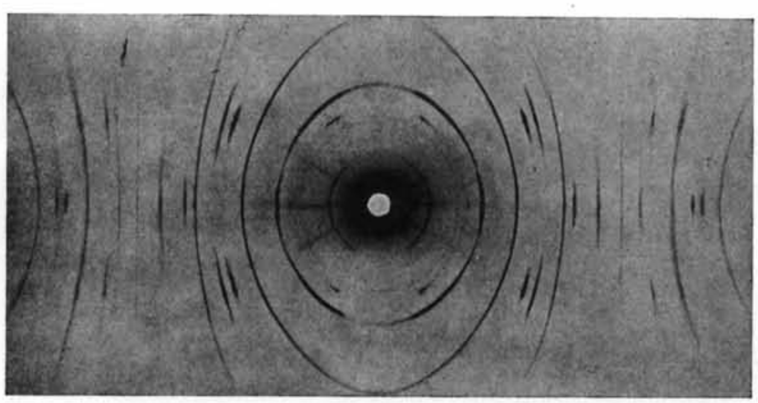
† We have since found that Megaw (1933), in an X-ray study of the thermal expansion of brucite crystals from the same locality, has commented on the disorientation within these crystals.



(a)



(b)



(c)

Fig. 2. Rotation photographs of brucite crystals (*a*) about the *c* axis, (*b*) about an *a* axis, (*c*) about an *a* axis, but for a different crystal showing greater misalignment of crystallites.

recorded only by a rotation about a direction lying in the a^*a^* plane.

The range of mosaic orientations is derived most directly from $000l$ arcs in a-axis or $\langle 10\bar{1}0 \rangle$-axis rotations and from $hki0$ arcs in c-axis rotations. The numerical values vary considerably from crystal to crystal; in the best crystals we have examined, the c axes of the crystallites lie within a cone having a semi-vertical angle of a few degrees. The angle is about 4° for the crystal which provided Figs. 2(a) and (b). In other crystals the angular range of the c axes is considerable (cf. Fig. 2(c)). In the more perfect crystals, the number of crystallites may be relatively small and the Debye–Scherrer arcs then tend to break up into separate spots with roughly equal separations; this can be seen in Fig. 2(b). It suggests a polygonization effect. In the less perfect crystals, the arcs are very extended and tend to be quite smooth, which suggests a large number of crystallites.

3. Possible origin of the texture

It is of interest to consider briefly how the observed texture may occur. It can be pictured as arising from small rotations of the crystallites about the three morphological a axes. Such rotations could be produced, as in metal structures, by sets of edge dislocations arising from the insertion of additional planes of atoms or of unit cells parallel to the a axes. It is necessary to consider if a plausible model is possible in the brucite structure. The shear caused by the introduction of an edge dislocation into an otherwise perfect lattice is concentrated into a plane perpendicular to the inserted atomic plane. Such a shearing may easily occur between the layers of the brucite structure which are held together with weak secondary valencies and which give rise to the perfect basal cleavage. As regards the disposition of the hydroxyl ions across the shearing plane, a model is suggested by the extended half-dislocation concept used by Heidenreich & Shockley (1948, p. 57) in discussing screw dislocations in face-centred cubic lattices which have a close-packed array of atoms on (111) planes and also by Christian (1951) in connection with the hexagonal–cubic transformation of cobalt. In Fig. 3(a), the open and black circles represent, respectively, sheets of hydroxyl ions above and below the shearing plane with an additional line (or plane) of ions accommodated parallel to an a axis in the upper sheet, as indicated by the arrows. At the two sides of the diagram the ions have their normal close-packed arrangement and there will be continuity of structure across the shearing plane; this is also indicated schematically in Fig. 3(b). The effect of the dislocation will be to bend the structure about the a axis in the manner shown in Fig. 3(b). If dislocations of this type occurred frequently throughout a crystal, diffraction effects of the kind obtained with cobalt would be expected. No direct evidence of this kind has been obtained so far, possibly because the number of dislocations is too small. In drawing Fig. 3(a) the black circles were placed in undisturbed positions and the array of white circles was then added in such a way as to accommodate the extra line of circles; actually both layers should be disturbed, as we have shown in Fig. 3(b). Extended dislocations of the type considered would be expected to occur equally with respect to the three a axes, thereby producing the type of texture which is observed.

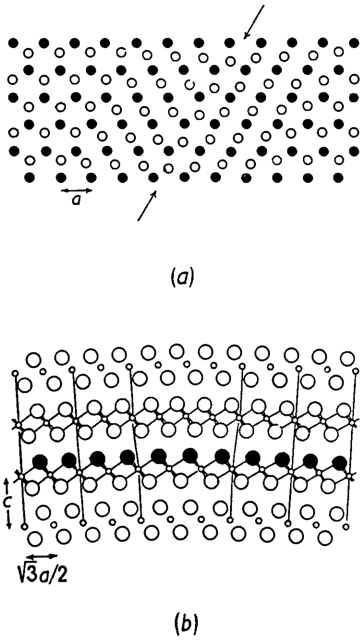


Fig. 3. To illustrate the bending of a layer lattice due to edge dislocations. (a) Projection on the basal plane of the hydroxyls above (open circles) and below (black circles) the plane of shear, with an additional line (or plane) of atoms indicated by the arrows. (b) Projection on a plane normal to the line of arrows. Small circles represent magnesium ions.

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References

Aminoff, G. (1919). *Geol. Fören. Stockh. Förh.* **41**, 407.

Bragg, W. L. (1937). *Atomic Structure of Minerals*. London: Oxford University Press.

Christian, J. W. (1951). *Proc. Roy. Soc.* A, **206**, 51.

Garrido, J. (1936). *Z. Krystallogr.* **95**, 189.

Heidenreich, R. D. & Shockley, W. (1948). *Conference on Strength of Solids* (Bristol). London: The Physical Society.

Megaw, H. D. (1933). *Proc. Roy. Soc.* A, **142**, 198.

Palache, C., Berman, H. & Frondel, C. (1944). *Dana's System of Mineralogy*. New York: Wiley.