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CONFIRMATION OF THE CRYSTAL STRUCTURE OF PENTLANDITE

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Because of the comparative weakness of the powder method to give symmetry information, and because of its absolute inability to provide adequate intensity data for structures having many of the merohedral symmetries, there is always doubt as to the validity of a complicated structure based upon data derived by the powder method. The structure of pentlandite was proposed by Lindqvist, Lundqvist, and Westgren[1] (herein referred to as LLW) on the basis of powder diffraction data. For this reason it was thought desirable to check it by a single-crystal method.

Professor Clifford Frondel of Harvard University kindly furnished us with a sample of pentlandite from the Creighton Mine, Sudbury, Ontario. While the material consisted of fragments, one of the smaller pieces had the form of a plate with two parallel plane surfaces, and appeared to be a possible single crystal. Assuming this to be the case, it was mounted for the precession camera so that the normal to the plane surface was the precessing axis. The resulting precession photographs had the appearance of being based upon a single crystal, and showed plane symmetry *6mm* for the zero level and *3m* for the upper levels.

A cone axis photograph taken with the same fragment showed a period along the precessing axis of 17.56 Å. Because of the trigonal symmetry of the axis it was a candidate for the direction [111] of an isometric crystal. If so, the period along [100] is $17.56/\sqrt{3} = 10.14$ Å. Since this value is close to the value for a given by LLW, namely 10.02 Å, this correlation of the precessing axis with [111] was tentatively accepted as correct.

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[1] Lindqvist, Märta, Lundqvist, Dick, and Westgren, A., The crystal structure of Co_9S_8 and of pentlandite $(Ni, Fe)_9S_8$: *Svensk. Kemisk. Tidskrift*, **48**, 156–160 (1936).

Accordingly the crystal was remounted so that [100] became the precessing axis, and a series of precession photographs was taken for the levels 0, 1, 2, 3, and 4. The cell edge, computed from measurements on the zero level, was found to be $a = 10.03$ Å, as compared with 10.02 Å of LLW.

The plane symmetry of each of the levels proved to be $4mm$. This information combined with the symmetry $3m$ of the [111] axis, shows that the diffraction effects of the crystal have symmetry $4/m\ \bar{3}\ 2/m$, which is consistent with any of the three crystal classes $4/m\ \bar{3}\ 2/m$, $\bar{4}3m$, or 432. The lattice proved to be face-centered, and there were no extinctions other than those required by the face-centered lattice. This fixes the space group as one of the three $F4/m\ \bar{3}\ 2/m$, $F\bar{4}3m$, or $F432$. The symmetry adopted by LLW was the first of these.

The cell and symmetry of the structure proposed by LLW are therefore consistent with our findings by single crystal methods. It remained to check the particular structure proposed by LLW. This is in space group $F4/m\ \bar{3}\ 2/m$, with the 36 Fe and Ni atoms distributed at random over equipoints $4b$ and $32f$, with $x = \frac{1}{8}$, and the 32 S atoms distributed over equipoints $8c$ and $24e$, with $y = \frac{1}{4}$. We computed the amplitudes to be expected from such a structure, squared them, and multiplied by the Lorentz-polarization factor appropriate to the various levels of the precession photographs. These computed intensities were then compared with the degrees of blackness of the various corresponding spots on the precession photographs. All-around satisfactory agreement was found. From this it was concluded that the structure proposed by LLW for pentlandite is essentially correct.

A NOTE ON THE CALCITE-WOLLASTONITE EQUILIBRIUM

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The equilibrium pressure and temperature conditions of the reaction:

$$\text{Calcite} + \text{Quartz} = \text{Wollastonite} + \text{Carbon Dioxide}$$
$$CaCO_3 + SiO_2 = CaSiO_3 + CO_2$$

are important in limiting the conditions of formation of some broad groups of metamorphic rocks. Goldschmidt's original calculations have recently been improved by Danielsson (1) by the application of more recent thermodynamic data. At the time of Danielsson's calculations *P-V-T* data for carbon dioxide were not available for much of the region of interest. Kennedy (2) has recently published such data up to 1400 bars and 1000° C. and these data have been used to check the calculations further.