A NEW METHOD OF BUILDING CRYSTAL STRUCTURE MODELS

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The construction of models of crystal structures presented no very great difficulties as long as the investigated structures were relatively simple, commonly cubic ones. One method was to slide metal rods into a heavy base board and to fasten beads or balls on these rods at proper intervals. Later more attractive models were made with wooden balls held together by metal rods which at the same time represented the coordinate valency bonds. The difficulty in constructing such models lies in the drilling of holes in the wooden balls at proper angles and in the centering of the balls during the drilling. Besides, with the coming of more complicated structures this method became so difficult and expensive that it is practically prohibitive now.

Sir William H. and Professor W. L. Bragg have introduced a new method of construction for complex structures.[1] In these models the valency coordinates are represented by thin glass tubes which are strung on copper or brass wires. Since such construction lacks support the most important positions of atoms are held in place by black metal rods stuck into a wooden base board. The centers of atoms at the intersections of the glass tubes are represented by balls of colored wax or other plastic material.

There are two objections to this construction. (1) The black supporting rods cause the already complex structures to appear even more so, and (2) the glass tubes are easily broken.

The writer thinks that he has a new method of construction which eliminates these objectionable features without introducing new ones. Brass rods are used to represent the valency bonds. These rods are soldered together. The junction points are positions of atoms and, therefore, are covered by balls after the completion of soldering. The balls are made from "plastic wood."[2] After the plastic wood has set the balls are painted, preferably with an enamel. These models are very rigid even when of large size.[3] The

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[1] Stereoscopic photographs of crystal models, edited by Sir William and Professor W. L. Bragg: Adam Hilger, Ltd., *London*, **1929**, and **1930**.

[2] Manufactured by Addison Leslie Company, Canton, Massachusetts.

[3] The writer has constructed one with 300 atomic positions.

most convenient scale seems to be $1\text{Å} = 30$ mm. If a smaller scale is used difficulty is experienced in reaching some of the positions inside of the model during the process of constructing the balls. The brass rods should be about 3/32 of an inch thick which is a standard size, carried in stock. It can easily be bent in sharp angles if pliers are used.

In the building of a model, for example, of sillimanite,[4] the following procedure may be adopted: A model of a unit cell of sillimanite with dimensions $a = 7.43\text{Å}$, $b = 7.58\text{Å}$, and $c = 5.74\text{Å}$, will be about $22 \times 23 \times 17$ cm. in size. It is advisable to construct one which extends beyond the limits of one unit cell in order to show the interesting double chain bonds of SiO_4 and AlO_4 described by the writer.[5] A plan of the atomic positions must be constructed first with the aid of the coordinate table by Taylor.[6] The elevation of each atom above the plane of the paper (measured along the c axis) is written under each atom. Since Taylor gives the positions of the atoms of only one "molecule," the positions of those of the other three "molecules"—there are four in the unit cell—must be found by applying the operations of symmetry for the space group V_h^{16} of sillimanite. A side elevation may be constructed in the same manner.

Now the coordinate bonds, that is the positions of the brass rods, are drawn on the plan. In sillimanite each Si is linked to the nearest four O. Half of the Al are linked to six nearly equidistant O, the other half to four O. An excellent check on the positions of the atoms in practically all oxygen compounds is the fact that O positions can not be closer than 2.5Å to each other. The distance between O and Si should be not smaller than 1.5Å.

It will be noticed in the plan that some of the atoms are linked in such a way that they lie in a plane parallel to the plane of the paper. These bonds can be bent from one piece of brass rod by taking the dimensions and angles directly from the plan. The angles and dimensions of other bonds are obtained by projecting the positions of the atoms on to the planes in which their bonds—and therefore the brass rods—are located. In this manner computations of angles and of directions can be avoided entirely. It is advisable to connect certain atoms which are really not linked together by

[4] Taylor, W. H., The structure of sillimanite and mullite: *Zeit. f. Krist.*, vol. **68**, pp. 503–521.

[5] Gruner, J. W., Structures of some silicates: *Am. Mineral.*, vol. **16**, p. 445, 1931.

[6] *Op. cit.*, p. 512.

auxiliary brass rods during the time of construction. These rods can be easily cut away before the plastic wood is applied.

The soldering presents no difficulties even in places where four or more rods are to be joined if a good flux[7] is used. Sometimes after a number of connections have been soldered it is found that certain rods can not be joined together on account of a slight cumulative error in angles or lengths of rods. It is, of course, very easy to un-solder some of the joints and correct the errors.
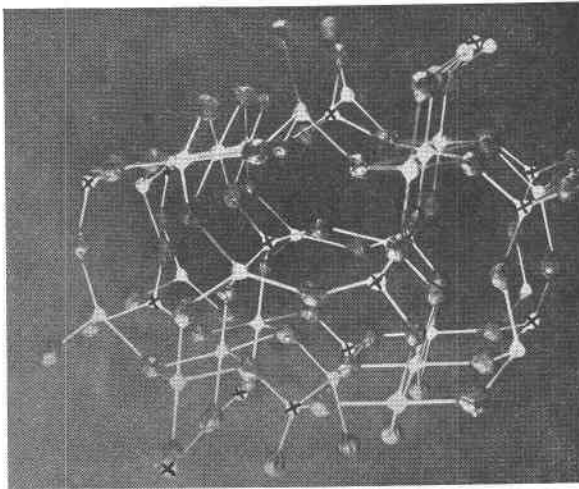

Fig. 1. Model showing the structure of sillimanite Al_2SiO_5. Large balls are O, small white ones are Al, small ones with X are Si.

For best results the plastic wood should be put on in layers and not all at once for each ball. It would be almost impossible to make these balls perfectly spherical, but even imperfect ones look well after painting. The writer makes each element a different size. A brilliant red or some other bright color should be used for the most common atom—in silicates for oxygen—in the models. It adds to attractiveness and to visibility in a lecture room. Fig. 1 is a model of sillimanite as seen approximately in the direction of the c axis. The large balls are O ions. The small white ones with a black x are Si ions. On account of the reflection of light some of the brass rods appear much heavier than others in the photograph.

[7] The writer found a solution of zinc chloride and denatured alcohol in the ratio of 1:1 very satisfactory.