# THE SPACE-GROUP AND UNIT CELL OF SYLVANITE

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Faceted crystals of sylvanite from Cripple Creek, Colorado (kindly furnished by Prof. Charles Palache of Harvard University) and from Săcărâmbu (Nagy-Âg), Transilvania (kindly supplied by Dr. W. F. Foshag of the U. S. National Museum) were investigated by means of the Weissenberg $x$-ray goniometer. Rotation photographs were made around the principal zone-axis, also Weissenberg photographs of the equator and first and second layer-lines. Copper K- and chromium K-radiation was used. The Weissenberg photographs were analyzed graphically by the method of Schneider (1928). New crystallographic axes were chosen to conform with the arrangement of the symmetry elements assumed in the International Tables for the Determination of Crystal Structures. The dimensions of the structural unit cell, all determined by purely röntgenographic measurements, are $a_0=8.94$ Å, $b_0=4.48$ Å, $c_0=14.59$ Å, all $\pm 0.02$ Å; $\beta=145°\ 26'\pm 20'$. Diffraction effects were obtained from the following planes: $u00$, $g00$, $0u0$, $0g0$, $00g$, $0uu$, $0ug$, $0gu$, $0gg$, $u0g$, $g0g$, $ug0$, $gu0$, $gg0$, $uuu$, $uug$, $ugu$, $ugg$, $guu$, $gug$, $ggu$, $ggg$ where $u$ denotes any odd number and $g$ denotes any even number. No diffraction effects were obtained from the following: $00u$, $u0u$, $g0u$, $uu0$. Thus sylvanite belongs either to the space-group $Pc-C_s^2$ or to the space-group $P2/c-C_{2h}^4$, both of which are characterized by the absence of diffraction effects from $00u$, $u0u$, and $g0u$, due to the presence of a glide-plane parallel to 010 with a glide component $c/2$. Absence of diffraction effects from $uu0$ is not a characteristic of any monoclinic space-group and is a consequence of the special set of parameter values in the sylvanite structure. Faceted crystals of sylvanite have been studied with the reflection goniometer by several investigators. Projections of such crystals drawn by Koksharov, Schrauf, Vrba, and Palache and reproduced by Goldschmidt (1923) show the habit of sylvanite to be holohedral. Consequently the space-group of sylvanite appears to be $P2/c-C_{2h}^4$. The chemical analysis of crystallographically studied material made by Palache (1900) corresponds to the composition (Au, Ag) $Te_2$ with a ratio of gold to silver equal to 1.15. The density determined by Palache (1900) on three isolated crystals by means of the hydrostatic balance is 8.16. The density computed from the $x$-ray measurements on the assumption that the formula is $AuAgTe_4$ is 8.11; if the gold-silver ratio is taken as 1.15 instead of 1.00 and if, as appears probable, the slight

excess of gold is the result of replacement of silver atoms by gold atoms in the structure, the corresponding $x$-ray density would be 8.17. The agreement of the measured and calculated densities leaves no doubt that the number of "molecules" of $AuAgTe_4$ in the unit cell is two.

Sylvanite was first proved to belong to the monoclinic system by Koksharov (1866, 1888), who calculated the following axial elements from measurements made on one twinned crystal and determined the twin-plane:

$$a_K : b_K : c_K = 1.7732 : 1 : 08890, \quad \gamma_K = 55°21\tfrac{1}{2}';$$

here $a_K$ denotes the vertical axis, $b_K$ the clinodiagonal axis, $c_K$ the orthodiagonal axis, and $\gamma_K$ the angle which the clinodiagonal axis makes with the vertical axis. The directions of Koksharov's axes are those of possible structural axes, but to obtain the structural lattice the unit length of his $b$-axis (i.e. his clinodiagonal axis) must be multiplied by two. The corresponding values of the axial elements in terms of the present writers' axes are given in Table 1 for comparison with the values obtained by $x$-ray analysis.

TABLE 1. AXIAL ELEMENTS OF SYLVANITE

A comparison of the transformed axial elements of Koksharov and of Schrauf with those of Tunell and Ksanda

| | | $a$ : $b$ : $c$ | $\beta$ |
|---|---|---|---|
| Koksharov | (reflection goniometer) | 1.9947:1:3.2822; | 145°40′ |
| Schrauf | (reflection goniometer) | 1.9914:1:3.2679; | 145 33 |
| Tunell and Ksanda | ($x$-ray goniometer) | 1.9955:1:3.2567; | 145 26 |

An elaborate study of the morphology of sylvanite was made by Schrauf (1878) on numerous crystals from Transilvania (Siebenbürgen). The relationship between the axes chosen by the present writers for

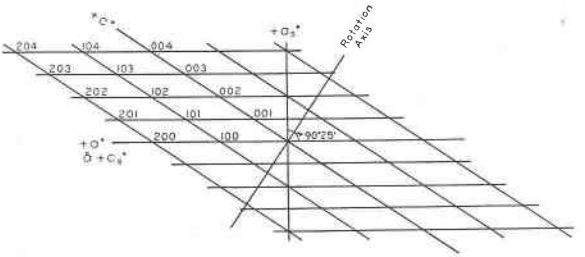


FIG. 1

purposes of structural analysis and those of Schrauf is indicated in Fig. 1, which is a section of the reciprocal lattice through the origin parallel to the symmetry plane. The reciprocal axes of Tunell and Ksanda are let-

tered $a^*$ and $c^*$; reciprocal axes corresponding to the linear axes of Schrauf are lettered $a_S^*$ and $c_S^*$. The linear axial elements of Schrauf do not correspond to the relative dimensions of a possible unit cell in the structure and for this reason were not retained for purposes of structural analysis. The axial elements calculated by Schrauf are:

$$a_S : b_S : c_S = 1.6339 : 1 : 1.1265; \ \beta_S = 90°25'.$$

The corresponding values of the axial elements in terms of the present writers' axes are given in Table 1 for comparison with the values obtained by $x$-ray analysis.

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