American Mineralogist, Volume 58, pages 792–793, 1973

MINERALOGICAL NOTES

X-Ray "Powder" Data for Chalcophyllite

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Abstract

A Gandolfi-type apparatus fabricated by the author has been used to obtain a simulated powder pattern from a single crystal of chalcophyllite [$Cu_{48}Al_2(AsO_4)_3(SO_4)_3(OH)_{27} \cdot 36H_2O$]. Pattern quality is greatly improved by the use of a technique which eliminates specimen grinding and concomitant structure damage.

Introduction

Chalcophyllite [$Cu_{18}Al_2(AsO_4)_3(SO_4)_3(OH)_{27} \cdot 36H_2O$] from Braden, Chile, has been described by Berry and Steacy (1947). It is rhombohedral and is (probably) in the space group $R\bar{3}m$. Unit cell dimensions based on hexagonal axes are: a = 10.77 Å, c = 57.52 Å.

Attempts to obtain a chalcophyllite powder pattern suitable for indexing were not successful when conventional specimen preparation was used. Diffraction lines were too broad and diffuse to permit accurate measurement. This fact, coupled with the apparently fragile structure revealed by the physical properties (H = 2; cleavage {0001}, perfect), suggested that chalcophyllite is highly susceptible to grinding damage.

Experimental Method and Results

A device for obtaining powder-like diffraction patterns from single crystals had been previously fabricated by the author. It employs simultaneous rotation and oscillation of a single crystal about two axes to randomize crystal orientation in a manner similar to that described by Gandolfi (1967). A small wrist watch movement is used to drive the inclined secondary axis.[2]

Previous use of the Gandolfi-type device with a variety of different mineral species had demonstrated its capacity for improving pattern quality, particularly at high θ angles. This indicated that a θ-dependent effect was being overcome by the use of the device, probably by avoiding the structure damage resulting from specimen grinding in the conventional powder method. Thus the device seemed appropriate for application to the chalcophyllite problem, where even low-θ lines appeared to be adversely affected by grinding damage.

A chalcophyllite single crystal of 0.3 mm average diameter from *El Teniente* Mine, Rancagua, Chile, was X rayed with the Gandolfi-type apparatus and a good quality "powder photograph" was obtained. Diffraction lines were much sharper than those produced by a normal powder mount. The film was calibrated with a quartz standard and the nine lowest-order lines were indexed by comparison with calculated d-spacings from a FORTRAN computer program by Shiono (1971). The resulting "powder" data for chalcophyllite are given in Table 1.

Conclusion

Chalcophyllite powder pattern quality is enhanced by the use of a method which eliminates specimen grinding from the experimental procedure. A Gandolfi-type apparatus would appear to have special application in cases where minerals are highly susceptible to structure damage.

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[2] The apparatus is described in an unpublished 1972 Univ. of Arizona M.S. thesis.

TABLE 1. X-Ray "Powder" Data for Chalcophyllite

I*	d(obs), Å	d(calc), Å	hkl
100**	9.47	9.59	006
18**	7.10	7.25	015
6	5.66	5.69	018
31	4.71	4.79	0,0,12
7	3.88	3.91	208
12	3.59	3.62	0,2,10
8	3.17	3.20	0,0,18
		3.18	0,1,17
5	2.98	3.01	2,1,10
3	2.83	2.85	0,2,16
5	2.73		
25	2.67		
48	2.58		
32	2.34		
(Plus 15 additional lines to d=1.47 Å)			

CuKα radiation, Ni filter
*Intensities visually estimated from calibrated film strip
**Split lines due to absorption

Acknowledgments

The author is indebted to Drs. John W. Anthony and W. John McLean for suggesting this study and for their helpful advice during its completion. Financial support was provided by a National Science Foundation Traineeship and by a scholarship from The Tucson Gem and Mineral Society, Incorporated.

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