X-RAY DIFFRACTION STUDY OF OLIVINE SOLID SOLUTION SERIES

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ABSTRACT

Lattice constants of sixteen analyzed olivines fit a linear relation against mole % forsterite within about 5 mole % forsterite. Using calculated lattice constants and atomic coordinates estimated from Gibbs' structures of two olivines, spacings and intensities of powder patterns were synthesized for the whole solid solution series.

Olivine $(Mg,Fe)_2SiO_4$ is a mineral which forms continuous solid solutions between forsterite Mg_2SiO_4 and fayalite Fe_2SiO_4. The Mg/Fe ratio in the mineral can be estimated by measuring certain physical constants such as refractive indices, optic angle, or the density of the mineral (Poldervaart, 1950; Bloss, 1952). It is also possible to determine the composition from the X-ray diffraction powder data. Yoder and Sahama (1957) found the following relationship between the interplanar spacing of the (130) reflection and the amount of forsterite substitution (Fo%) in the mineral:

$$\text{Fo(mole \%)} = (4233.91 - 1494.59\, d(130) \pm 3\text{–}4\% \qquad (1)$$

In this work new relationships have been established between the lattice

TABLE 1. OLIVINE DATA

References	a (Å)	b (Å)	c (Å)	v (Å^3)	Fo(mole %)
Yoder & Sahama (1957)	4.817	10.477	6.105	308.1	0
ASTM 7-164	4.816	10.482	6.095	307.7	6
ASTM 7-163	4.808	10.452	6.080	305.5	15
ASTM 7-158	4.799	10.393	6.063	302.4	41
Heckroodt (1958)	4.789	10.330	6.041	298.9	53
ASTM 7-157	4.783	10.335	6.031	298.1	54
ASTM 7-73	4.787	10.332	6.035	298.5	56
ASTM 7-159	4.784	10.318	6.027	297.5	64
Heckroodt (1958)	4.768	10.242	6.004	293.2	79
Heckroodt (1958)	4.760	10.236	6.003	292.5	80
Heckroodt (1958)	4.760	10.219	5.994	291.6	88
ASTM 7-156	4.763	10.225	5.993	291.9	88
ASTM 7-75	4.760	10.223	5.992	291.6	90
ASTM 7-74	4.758	10.207	5.988	290.8	96
Yoder & Sahama (1957)	4.756	10.195	5.981	290.0	100
Swanson & Tatge (1953)	4.76	10.20	5.99	290.8	100

constants as well as the X-ray intensities of certain reflections versus the Mg/Fe ratio in the series.

The lattice parameters and the unit-cell volumes of 16 chemically analyzed olivines, reported in the literature, are listed in Table 1. Graphs constructed from this data are shown in Figure 1. These graphs show the existence of linear relationships (within the limits of error) between these

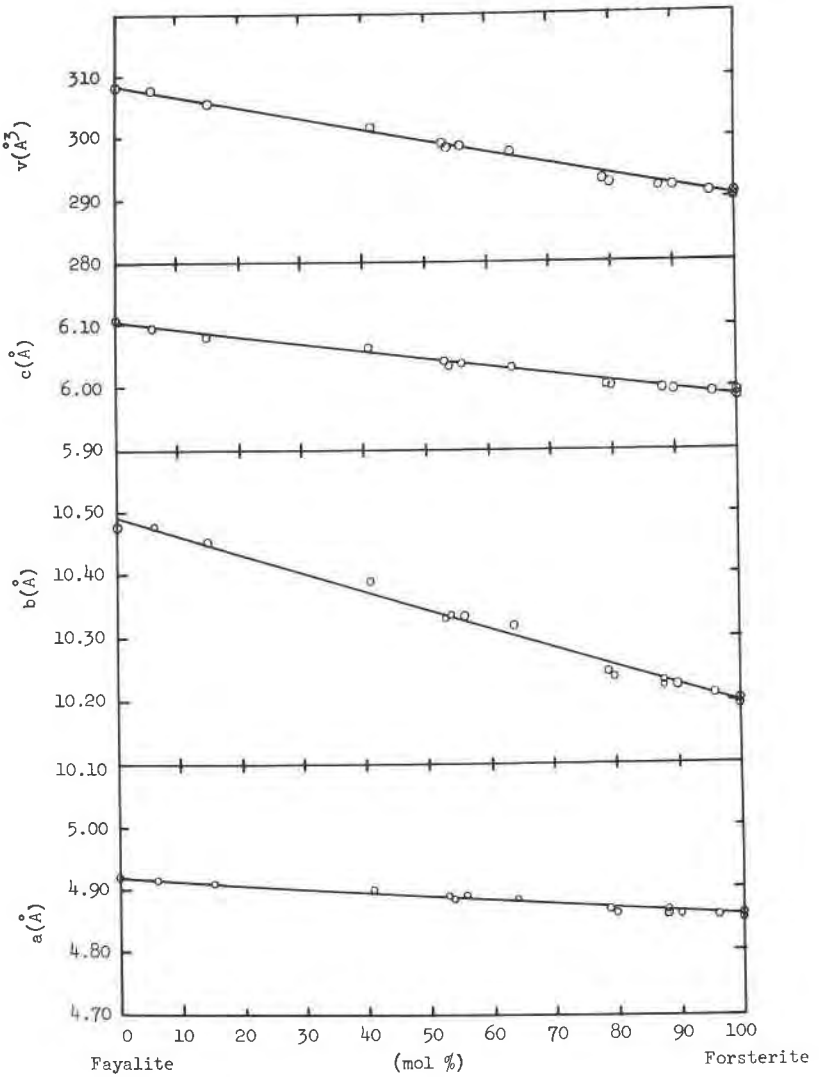

FIG. 1. Unit cell parameters versus composition in olivines.

parameters and the composition. Eliseev (1958), however, found small deviations from linearity in both a- and *b*-axes functions. Eliseev's conclusion was based on fewer samples and the compositions were determined only by their refractive indices. Therefore, this slight discrepancy may be due to the inaccuracy of his chemical data.

The following equations, obtained with a least-squares technique from the data of Table 1, can be used to determine the amount of forsterite substitution (Fo%) from the unit cell parameters in unanalyzed olivines.

$$\begin{aligned} \text{Fo(mole \%)} &= (7288.27 - 1511.77a) \pm 5.8\% \\ \text{Fo(mole \%)} &= (3417.44 - 325.53b) \pm 3.8\% \\ \text{Fo(mole \%)} &= (4977.01 - 815.40c) \pm 3.7\% \\ \text{Fo(mole \%)} &= (1625.96 - 5.265V) \pm 3.6\% \end{aligned} \qquad (2)$$

Table 2 demonstrates the good agreements (within the limits of error) between the results obtained with the relationships established in this work and those obtained by other methods of analysis.

TABLE 2. RESULTS ACCORDING TO VARIOUS METHODS—Fo (mole%)

References to the samples	Chemical analysis	This work[a]	From Yoder & Sahama's equation
ASTM 7-74	96	94.8	96.9
ASTM 7-156	88	89.0	92.1
ASTM 7-73	56	54.0	53.5
ASTM 7-163	15	17.8	17.7
ASTM 7-164	6	6.5	4.7
Yoder & Sahama (1957)	100	99.3	100
Yoder & Sahama (1957)	0	2.4	0

[a] Average of the four values obtained from equations (2).

The X-ray powder patterns of six members of the olivine series between forsterite and fayalite (with intervals of 20 percent forsterite) have been calculated by a computer program prepared by the author.[1] This program differs from Deane Smith's[2] program only in that it modifies the intensities for the anomalous scattering of the constituent atoms. These patterns are listed in Table 3 and can be used as standards for the X-ray

[1] Materials Research Laboratory, Pennsylvania State University.

[2] Smith, Deane K. (1963). A Fortran program for calculating X-ray powder diffraction patterns. UCRL-7196, Lawrence Radiation Laboratory, Livermore, California.

TABLE 3. CALCULATED X-RAY POWDER PATTERNS OF OLIVINES—CuKα-RADIATION

			Forsterite[1]		Chrysolite[2]		Hyalosiderite[3]		Hortonolite[4]		Ferro-Hortonolite[5]		Fayalite[6]	
h	k	ℓ	d	I*	d	I*	d	I*	d	I*	d	I*	d	I*
0	2	0	5.096	20	5.126	16	5.157	13	5.187	11	5.217	10	5.248	9
1	1	0	4.310	1			4.338	1	4.352	3	4.366	6	4.380	9
0	2	1	3.879	64	3.899	44	3.919	29	3.939	20	3.959	14	3.979	9
1	0	1	3.722	22	3.734	15	3.746	10	3.758	7	3.770	5	3.782	3
1	1	1	3.497	15	3.509	26	3.521	36	3.534	45	3.546	53	3.558	60
1	2	0	3.477	14	3.491	11	3.506	9	3.521	8	3.535	7	3.550	6
1	2	1	3.006	6	3.018	6	3.031	5	3.043	5	3.056	5	3.068	5
0	0	2	2.991	18	3.003	14	3.015	11	3.027	9	3.039	7	3.051	6
1	3	0	2.764	62	2.778	71	2.791	78	2.805	85	2.818	91	2.831	96
0	2	2	2.579	1	2.591	5	2.603	11	2.614	18	2.626	24	2.638	31
0	4	0			2.563	1	2.578	3	2.594	5	2.609	8	2.624	11
1	3	1	2.509	80	2.521	75	2.533	71	2.545	68	2.557	65	2.568	62
1	1	2	2.457	100	2.466	100	2.476	100	2.485	100	2.494	100	2.504	100
2	0	0			2.384	2	2.391	6	2.397	9	2.404	12	2.411	14
0	4	1	2.344	12	2.358	13	2.371	13	2.384	13	2.397	14	2.410	15
2	1	0	2.316	10	2.322	9	2.329	9	2.336	9	2.342	9	2.349	9
1	2	2	2.267	44	2.277	33	2.286	26	2.295	20	2.305	16	2.314	13
1	4	0	2.246	30	2.258	25	2.269	20	2.281	17	2.293	15	2.305	13
2	1	1	2.160	20	2.166	16	2.173	13	2.179	11	2.186	9	2.192	8
1	3	2	2.030	5	2.039	5	2.048	6	2.057	6	2.066	6	2.076	6
2	2	1					2.041	1	2.048	1	2.055	1	2.061	1
2	3	0	1.948	3	1.955	2	1.963	1	1.970	1				
0	4	2	1.940	3	1.950	3	1.960	3	1.970	2	1.980	2	1.990	2
1	5	0	1.874	7	1.884	6	1.894	5	1.904	4	1.914	3	1.925	3
2	0	2	1.861	2	1.867	1	1.873	1	1.879	1	1.885	1	1.891	1

1. Mg_2SiO_4
2. $(Mg_{.80}Fe_{.20})_2SiO_4$
3. $(Mg_{.60}Fe_{.40})_2SiO_4$
4. $(Fe_{.60}Mg_{.40})_2SiO_4$
5. $(Fe_{.80}Mg_{.20})_2SiO_4$
6. Fe_2SiO_4

*Integrated intensities.

powder patterns of olivines. In the calculation of these patterns the crystallites composing the powder were assumed to be uniform in size and randomly oriented. These patterns are for copper radiation. The intensities reported are integrated intensities and have not been corrected for absorption. Therefore, these patterns can best be used in conjunction with diffractometer studies. The lattice constants for these patterns were obtained from equations (2) and their atomic coordinates and temperature factors were estimated by interpolation and extrapolation of two members of the olivine series: forsterite $Fo_{90}Fa_{10}$ and hortonolite $Fo_{47}Fa_{53}$ refined by Gibbs *et al.* (1964) and Gibbs[1]. The variation of calculated intensities with composition for several of the reflections are illustrated in Figure 2. These graphs can greatly enhance the reliability of determination of the forsterite substitution in unanalyzed olivines.

The method described in this paper, based on X-ray diffraction, possesses many advantages. It can be used to determine the composition of single grains of olivine removed from thin or polished sections. It can also be used to study the compositional variations in zoned olivine crystals, and to determine the average composition of a powder sample.

[1] Gibbs, G. V. (1964). Private communication.

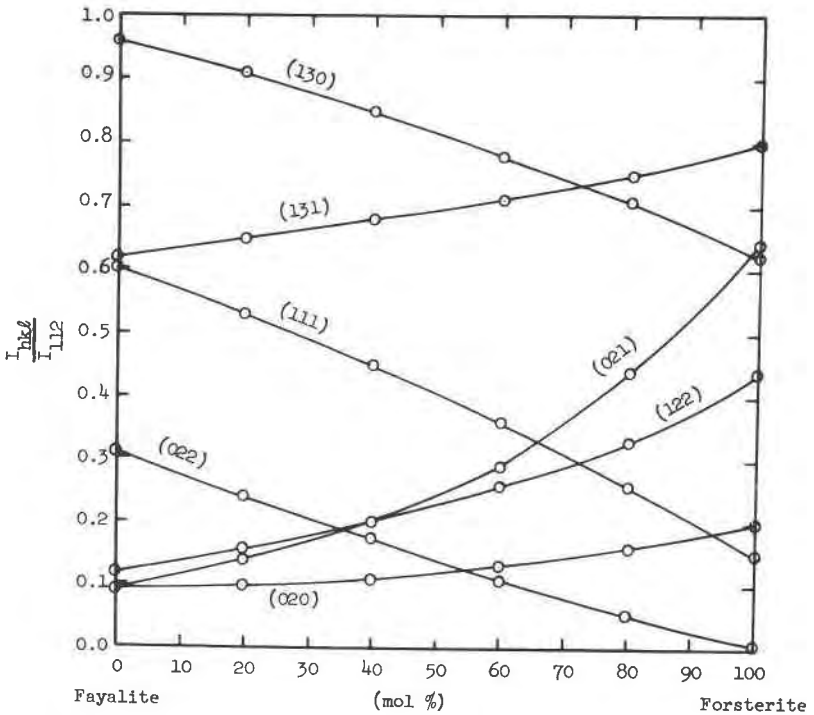

FIG. 2. Variation of the calculated intensity ratios with composition, for several of the reflections in olivines.

ACKNOWLEDGMENTS

Special thanks are due Dr. Tibor Zoltai for his guidance and suggestions during this work. Dr. Gerald Johnson, Jr. is also acknowledged for reading the manuscript critically.

This work was in part supported by The Joint Committee on X-ray Powder Diffraction Standards (Grants Nos. 2212–2112).

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Manuscript received, June 20, 1968; accepted for publication, September 21, 1968.