THE COMPOSITION AND PHYSICAL PROPERTIES OF GARNET

Horace Winchell, Geology Department, Yale University

Diagrams relating physical properties to chemical composition are familiar to all mineralogists. An exhaustive list of citations to such diagrams would be impossible here, but would include such books as Troeger (1956) and Winchell (1951), and a great many shorter articles such as those of Sriramadas (1957), and Kennedy (1947). With only a few exceptions (as Ford, 1915), such charts show the physical properties such as one or more refractive indices, lattice constants, melting, inversion, and decomposition temperatures, specific gravity, etc., by means of contour lines drawn over diagrams in which the main coordinates are determined by chemical composition. Yet the commonest use of these charts is probably for determining composition from the physical measurements. The usual arrangement is clearly best if there are more physical parameters than chemical ones—but that condition is not necessarily satisfied, especially if physical parameters are limited to those that can be conveniently measured. An important example in which exchange of the dependent and the independent variables may be useful is the garnet system, where at least five chemical components should be determined, but the conveniently measured physical properties are only refractive index $n$, lattice constant $a$, and specific gravity $G$.

Garnet Diagram

Since the early work of Ford (1915) there have been several systematic efforts to estimate or measure the refractive index, $n$, specific gravity $G$, and lattice constant $a$, of the five principal components of the garnet system, grossularite (abbr. gro), andradite (and), almandite (alm), spessartite (sp), and pyrope (pyr); the latest seem to be those of Skinner (1956), on synthetic materials, and of Fleischer (1937) on analyzed natural materials, from which properties of the components were derived by extrapolation. Kennedy (1947) collected eight triangular diagrams showing all but two of the three-component subsystems possible in the five-component garnet system, with contour lines showing refractive indices and densities of the three-component compounds. Sriramadas (1957) used similar triangular diagrams but showed contours of indices and lattice constants, based on the more recent data of Skinner (1956). To utilize all combinations of the conveniently measurable data $a$, $n$, $G$, yet another set of similar diagrams would be needed, with contour lines of $G$ and $a$. Perhaps it would be better to add the $G$-contours to the diagrams of Sriramadas.
The implied assumption in these diagrams is that the physical properties represented on each triangle are additive functions of the molecular proportions of the compounds A, B, and C, at the corners; thus the refractive index of a sample would be

$$n = n_A x_A + n_B x_B + n_C x_C$$  \hspace{1cm} (1)

throughout the subsystem A-B-C, where $n_\Lambda$, etc., are the indices of the pure components, and $x_\Lambda$, etc., are their respective molecular proportions in the sample. This equation can be extended to include any number of additional components, as D, E, F, etc., but graphical presentation becomes increasingly difficult as more components are considered (Mertie, 1948). Fleischer (1937) proved empirically that this type of relationship is at least a very good approximation for natural garnets, although Zen (1956) shows that the relation for $a$ is at best only a first approximation to the truth if volume effects are additive.

Rather than trying to show the dependence of three physical properties on the five chemical components in the garnet system, it would seem reasonable to treat two of the properties as independent variables and show the several chemical compositions, and the third physical property, as functions of the two chosen properties. We concur with Sriramadas that the index and the lattice constant are probably the best-measured physical properties; hence we use these as ordinate and abscissa, respectively, in Figs. 1 and 2, and locate the points corresponding to each of the end-member components as summarized by Skinner (1956). To avoid excessive confusion of lines on the diagram, only four components (pyr, alm, gro, and and) are shown in Fig. 1, with straight lines connecting them in pairs to represent in conventional manner the chemical variations in the corresponding binary series. These straight lines outline four triangles, the faces of a skew tetrahedron, and contour lines on these triangular faces show the variations of the specific gravity $G$.

Fig. 2 shows the same four components, and a fifth (spessartite), with contour lines plotted on the six triangular fields that have spessartite as one corner. Using inks of several colors, it is possible to show all ten triangular fields on the same diagram without undue confusion, but here the data are better separated as in Figs. 1 and 2. The point representing uvarovite (uv) is shown, but the effect of that component on garnets in general is not indicated. Its properties $a=11.955$, $n=1.861$, $G=3.895$, were obtained by extrapolation from the data of Knorring (1951), with minor adjustments to maintain general self-consistency of all data used in Figs. 1 and 2. The form of these diagrams is analogous to that published by Ford (1915, Fig. 9), who plotted $n$ and $G$ as abscissa and ordinate, without drawing the composition triangles. Winchell (1951 and earlier editions) used the same basis to construct a diagram showing the
estimated properties of the pure components or "end-members," and drew sufficient networks of lines between them to enable the user to interpolate conveniently in the systems that are geologically most significant. In the accompanying Figs. 1 and 2 this scheme is carried out more fully,
with the best data now available. Short ticks at equal intervals along the boundaries of the several triangles show 10-percent increments of composition for each binary series; they can be connected by light lines to facilitate reading from the diagram the composition corresponding to any point within one of the triangles. In many cases the contoured specific
NOTES AND NEWS 599

gravity data resolve ambiguities due to overlap of the three-component composition fields, and in some cases the contours may even permit estimates to be made on the basis of the four-component composition regions enclosed by one of the tetrahedrons.

Thus, for example, if a garnet of unknown composition has \( a = 11.550 \), \( n = 1.770 \), and \( G = 3.880 \), its composition may be estimated by reference in Fig. 1 to the triangle pyr-alm-gro as mostly pyrsalma (found by drawing a line through the apex “gro” and the given point so as to cut the “pyr-alm” base of the triangle at pyrsalma), modified by about 17% of gro, i.e., pyrsalmagro. The contour lines show that such a garnet would have \( G = 3.894 \). Similarly in Fig. 1, the composition could also be (pyrsalma + 13% gro) and, or pyrsalmand, for which \( G = 3.808 \); Fig. 2 shows that the same point may also represent a garnet with composition pyrsalmaSp and \( G = 3.950 \). The measured value, \( G = 3.880 \), lies 0.84 of the way from pyrsalmand to pyrsalma and, and the composition may therefore be estimated as pyrsalma and, by adding .84 (pyrsalma and) and .16 (pyrsalmand). Alternatively, we find by similar reasoning the composition pyrsalmaSp and, in fact, there is a 5-component series between these two 4-component compositions, in every part of which the required \( a, n, \) and \( G \) would be the same. A geological mineralogist would use such other data as a qualitative test for Mn, and/or mineral associations in the rock, to fix this specimen at or very near the correct composition along such a series. It is hardly necessary to emphasize again the assumptions on which such use of Figs. 1 and 2 are based—(a) the accuracy of the data used in their construction, (b) the adequacy of “Vegard’s law” for the rather small ranges of values of physical properties involved, and (c) that for the specimen at hand, other components are insignificant compared to the five used in the calculation. With these limitations clearly in mind,—limitations that apply equally to other types of charts,—the two diagrams here presented may be used conveniently in place of the ten triangular diagrams representing faces of Mertie’s (1948) 4-dimensional hypertetrahedron, eight of which were given by Kennedy (1947), and by Sriramadas (1957). Levin (1950) has described an algebraic solution that he carries out on a desk-type electric computer in about 20 minutes per determination, using measured variables \( a, n, G, \) and the weight-percentage of MnO or of FeO.

BIBLIOGRAPHY

Fleischer, Michael (1957), The relation between chemical composition and physical properties in the garnet group, Am. Mineral., 22, 751.

Ford, W. E. (1915), A study of the relations existing between the chemical, optical, and other physical properties of the members of the garnet group, Am. J. Sci. (4)40, 33-49.

DAHLLITE PSEUDOMORPHS AFTER PYRITE CONCRETIONS FROM BIG HORN BASIN, WYOMING

RICHARD S. MITCHELL AND W. CULLEN SHERWOOD,
University of Virginia, Charlottesville, Virginia

The occurrence of spherulitic phosphate concretions in the basal part of the Thermopolis formation (Upper Cretaceous) in the Big Horn Basin, Wyoming has been known for over fifty years. Fisher (1906) described these concretions as consisting mainly of "phosphate of lime" and having the structure of marcasite, the mineral he believed the phosphate had replaced. McConnell (1935) published a thorough petrographic description of these concretions. In his work he determined they are composed primarily of dahllite, the carbonate-hydroxyapatite. The suggestion was made that the forms might represent replacement, but he was unable to find relicts of a replaced material. The purpose of this note is to present evidence that indicates these masses are actually pseudomorphs of dahllite after pyrite. The specimens used in this study were collected by the senior writer in the summer of 1955 near Rainbow Canyon on the eastern edge of the Big Horn Basin.

The concretions are spherical in shape, frequently have a rough external surface, and average slightly over one inch in diameter. In cross section the specimens always exhibit a radial structure and show a rather consistent arrangement of their mineral constituents. At the center of all the concretions studied is an irregular mass of iron oxide which is often stellate in shape. This oxide was determined to be primarily goethite in all but one instance where hematite was found to be predominant. From the iron oxide center gray-brown dahllite extends to the surface of the spheres and constitutes the major portion of the spherulites. The concre-