

ON AN UP-TO-DATE MODIFICATION OF THE CONCEPT OF MINERAL SPECIES

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SUMMARY

The modernization of the earlier concept of mineral species, which has become obsolete in the first place, from the point of view of crystal chemistry, seems to be an ever increasing necessity. Taking as a basis the initiative of A. N. Winchell, the author proposes to define the individuality of the natural solid phase by the crystal lattice type. That would not only inhibit the unnecessary increase of the number of mineral names, but lead also to significant simplifications on systematics.

In the present state of the development of science, we are in possession of an enormous bulk of knowledge concerning the extremely variable multitude of natural crystal compounds, the minerals. This bulk can—just as in the other branches of natural science—be mastered and ordered only by appropriate systematizing. With the increasing amount and progressing evaluation of knowledge, this drive towards systematizing has, in the course of the history of science, gone necessarily through several stages of evolution. The basic unit of systematics being the species, the development of science has inevitably brought about some changes in the delimitation and definition of the concept of mineral species as well.

It is known that in the age of A. G. W e r n e r the minerals were chiefly distinguished by their external features. The requirement of physical and chemical homogeneity first came to the foreground in the work of R. J. H a ü y, resulting in the elimination of rocks and "petrefacts", frequently named among minerals in previous enumerations. Some time later, J. J. B e r z e l i u s considered the minerals to be identical with or analogous to laboratory-made compounds, which has led to a quite significant and none too advantageous turn in the development of the specimen concept. It was only around the middle of the last century that the concept of the mineral species was defined by combining the chemical composition with the correlate physical properties and morphic features. This definition was, up to the last decades, found to be sufficient for delimiting the individualities of minerals. Progress in the applied methods of investigation has led to the elimination of a significant part of formerly given mineral names, based upon incomplete determination of the nature of the mineral; and to a number of simplifications by condensing and identifying minerals formerly relegated to different species.

However, in the light of our present knowledge the definition of a mineral species is dependent on somewhat different conditions, so that a new definition of the species concept seems to be warranted. In the first place, it is necessary to be aware of the fact that a mineral is a natural crystalline phase whose

chemical composition, valued as its principal property, is necessarily subject to variations, and whose chemical as well as physical properties will be variable in dependence on structural properties. Therefore, as contrary to previous definitions, the mineral is not a simple molecular compound in which the quality and quantity relations of the constituting atoms is throughout and invariably identical, as expressed by the — customary — chemical formula.

A lattice structure is a set of geometrically defined points. Within this set, there are sub-sets of points of identical position. Theoretically, a filling of geometrically identical points by chemically identical atoms is postulated. It is well known that this ideal case is almost never attained in solids of natural origin. It is not only that geometrically identical points are occupied by chemically different atoms, but that there occur in the lattice positions also atoms not mentioned at all in the formula, and, moreover, with varying valences, without destroying the original structural framework. At the same time, however, all the properties of the natural solid phase depend much more on the lattice positions of the atoms than on the chemical nature of the same. It is proven by a number of examples that the physical properties of a compound can be widely different in spite of strictly identical chemical composition. It is sufficient to quote the diamond-graphite or the disthene-sillimanite pairs.

It is an unavoidable consequence of what has been said above that the introduction of new points of view to the definition of the mineral species is imperative. The first of these is that the individuality of the mineral, the independence of the crystalline phase rests with the *lattice type*. It was A. N. Winchell who first called attention to the fact that the mineral species concept is rather obsolete, being based more or less on traditions and manifesting itself only in mineral nomenclature.* He was led to this statement by the construction of his well-known and useful diagrams showing the variations of physical properties in dependence on variations of chemical composition. Since that time, there were several authors who, in some form or other, expressed the necessity of modernizing the species concept. Among our Hungarian colleagues, it was E. Nemečz** who most determinedly advocated modernization, applying some new ideas to the systematic treatment of silicates and some of the oxide minerals.

In mineral systematics, up-to-date modification of the species concept would lead to significant changes, mostly to simplifications. The sequences of chemical compounds which were formerly considered to be separate minerals formed by the mixing of two or more molecules, will be to-day classed as belonging to one and the same structural type and, consequently, to one and the same mineral species, with the original minerals regarded eventually as varieties of the new one. We may cite as an example the series of rhombic pyroxenes, varying (theoretically) from the composition $Mg_2Si_2O_6$ to the composition $Fe_2Si_2O_6$; it is usual to mention in this series the well-known names enstatite, bronzite and hypersthene. This example shows clearly that the natural unit of systematics must necessarily be the common denominator of this sequence, namely the structure, in which the silicate framework is

* A. N. Winchell—H. Winchell: Elements of optical mineralogy, 4. Edit. Part II. London, 1951.

** Nemečz E.: Szilikátásványok és azok teleptana (Silicate minerals and their paragenesis), *Veszprém*, 1954.

neutralized by Mg^2 and Fe^2 cations in varying proportions: the formation of a "pure", one-cation mineral, the so-called "minal" is never formed. Therefore, to express the application of a new specimen concept, let us accept the suggested term "enstenite", formed by condensation out of the three original names. In this sense, the three former minerals are subspecies or varieties of the new one, defined by arbitrary limits. Another well-known example is that of the garnet family, where there occurs no chemically "pure" phase, either. However, within the populous group formed by combinations of substitution there emerge two sub-groups of more closely related population, differing from each other in lattice dimensions as well as in other properties: *pyralspite* (the population of Al-garnets, pyrope, almandite and spessartite) and *ugrandite* (the population of Ca-garnets: uvarovite, grossularite and andradite). Within the categories of systematizing, it is not even necessary for most of the species serving as bases of systematics to apply nomenclatural modifications of this kind. It is sufficient to refer to the term tourmaline, being a collective structural name for a given group of compounds. In this case the individual varieties (elbaite, dravite, schoerl) were quite correctly, though not always consciously, regarded and treated as varieties of the species. Also worth mentioning is one of the most intensely studied rock-forming mineral groups, that of plagioclases. Here, not only the extreme members *Ab* and *An* were taken for separate mineral species, but especially in earlier times, also the intermediery varieties, although the definitions of the component ratios have, since the time of G. Tschermak (1864), undergone quite frequent changes. When considering recent investigations, it would be essential to define the plagioclase sequence systematically by a single lattice type and to distinguish within that the single-cell (albite, oligoclase, andesine) and double-cell (labradorite, bytownite, anorthite) subspecies by their more continuous substitution, with the ancient names considered as varieties.

Let us quote as a special example that of the multiple oxides of spinel lattice. Here, the specimen concept cannot be brought to bear by giving names as was done above, as the rather predominant occurrence of the R^3 cations, situated in exchangeable positions, defines in itself some subspecies which contain further varieties according to the accompanying bivalent cation. Therefore, we have to apply the term "spinel-lattice minerals" or simply, "spinel", utilizing and generalizing the name of one of the subspecies.

Of course, when deliberating on the independence of the structural type as a basic unit of systematics, it is nevertheless necessary to keep in mind and correctly evaluate crystal chemical relations of other kinds. Types of identical lattice, built up by identical atoms, which can pass into each other by continuous structural changes, with only the residual differences vanishing by sudden rearrangement, will have to be termed homootype modifications, just as before, instead of subspecies (as e. g. the SiO_2 structures).

There are some further structure types, built up likewise by identical atoms in identical coordination, which exhibit, nevertheless, some specific geometrical differences in the relative position of their bonds. In such cases the problem whether we have to deal with a separate mineral species will depend on the magnitude of the deviation from the ideal structure. There occur some characteristic examples in the family of layer lattices. The structural variations of graphite or the micas could be mentioned, in which, as is well known, the relative position of one layer relative to another is characterized

by a certain amount of geometrical displacement, with identical position occurring only at greater intervals. This mild form of structural polymorphy does not necessarily imply that the structures with a layering sequence differing from the ideal one should be regarded as separate species. However, if the differences in the layering sequence are greater, as in the case of the kaolinite-dickite-naerite group, and especially if a random disorganization arises (halloysite), it is warranted to consider the different structures as independent species.

For a new, up-to-date rearrangement of our knowledge it is a basic requirement to accentuate, as far as made possible by the present state of mineralogy, the points of view of the new specimen concept. Beside that, it can be expedient or even justified to distinguish subspecies and varieties by appropriate names.

These points of view, if not in exactly the same form, can readily be recognized in the new attempts at systematization, as e. g. in one of the most up-to-date and most widely known works, the "*Tables*" by H. Strunz,* where most of the "series" (*Reihe*) defined within the smallest categories are simultaneously structural types to be separated as new mineral species according to the new concept.

A mineral system reconstructed by applying the above-said ideas would, beside meeting the requirements of our time by presenting an application of the principles of crystal chemistry, also offer some other theoretical and practical advantages. For one, the number of mineral species would significantly decrease, and a better understanding of the chemical and physical interrelations of the varieties belonging to one lattice type would be reached at, instead of the lexicographical heap of data presented up to now. On the other hand, such a rearrangement would be a valuable asset in grouping the minerals according to united crystal chemical-geochemical principles — which is likewise most timely — and thus would gradually lead to the building-up of greater categories out of the common traits of the smaller ones, and thus to a necessary construction of the whole mineral system.

* H. Strunz: Mineralogische Tabellen 3. Aufl. Leipzig, 1957.