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Fritz H. Laves – 100 years young

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This year Fritz Laves, professor for crystallography and petrography and head of the Mineralogical Department at the University and the Eidgenössische Technische Hochschule in Zurich from 1954 to 1976, an accomplished leading scientist and outstanding pioneer in crystal chemistry, would be 100 years old.

Fritz Laves was born 1906 in Hannover, studied mineralogy first in Innsbruck, then in Göttingen and obtained his Ph.D. in Zürich in 1929 under the guidance of Prof. Paul Niggli. His professional career led him again to Göttingen, then to Halle/Saale, Marburg/Lahn, Chicago and finally back to Zurich.

Following his unexpected death in 1978, two of his former collaborators wrote authoritative orbituaries (Jagodzinski, 1979; Hellner, 1980) where the very wide range and the high quality of Laves' scientific work was appropriately exposed and honoured.

The present memorial, more than a quarter of a century after Laves passed away, should concentrate on what has been left today from his great scientific legacy. This is not a very easy task, not alone due to the great quantity of ideas Laves had on different aspects of crystal chemistry, but also of later modifications and changes in notation, definition and content, required due to later new experimental and theoretical results. All scientists build upon the great work of their predecessors, but this is often done unconsciously. If the original work was done too many years ago or was slightly modified, some of the later writers do not remember and do not cite the source of their inspiration. This can make it difficult to properly judge the impact of previous scientific work.

All these considerations led me, the writer of this text, being myself an inorganic crystal chemist, to try to investigate how much I have been inspired – consciously or unconsciously – by ideas of Prof. Laves and his co-workers. It is obvious that this very personal approach cannot do proper justice to Prof. Laves' complete scientific legacy.

Laves' thesis was published in full in Z. Kristallographie (Laves, 1930). He presented a classification of crystal structures based on topological concepts and introduced construction formulae where heteronuclear and homonuclear contacts (Bauverbände) were properly differentiated. This concept (but in simpler notation without numerical distance values) was used after the war by Machatschki (1947) for his crystal chemical formulae. Parthé proposed in 1980 an extension of the crystal chemical formulae. In 1990 a slightly modified version of the crystal chemical formulae was accepted by a nomenclature subcommittee of the IUCr for the nomenclature of simple inorganic structure types (Lima-de-Faria, Hellner, Liebau, Makovicky, Parthé, 1990).

Laves and Witte (1935) proposed a geometrical principle for the formation of the so-called "Laves phases" $MgZn_2$, $MgNi_2$ and $MgCu_2$ having general composition AB_2. Ignoring the chemical bonding, they focused on the observation that two kind of spherical atoms A and B with a radius ratio of 1.2 to 1 can be closely packed very favourably forming polyhedra with unusual high co-ordination numbers. Concerning a discussion of the label "Laves phase", see Paufler and Schulze (1971).

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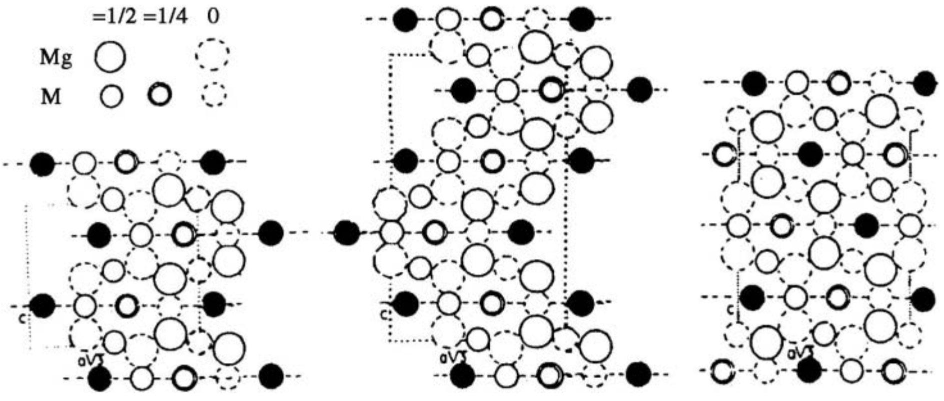

$MgZn_2$
-left-right-

$MgNi_2$
-left-left-right-right-

$MgCu_2$
-left-left-

Fig. 1. The relationship between $MgZn_2$, $MgNi_2$ and $MgCu_2$, interpreted as an intergrowth of a single kind of common slab (Parthé, 1996). The traces of the intergrowth planes are shown as dashed horizontal lines. The intergrowth plane contains only M atoms of which every second at $\pm^1/_4$ has been blackened. Connecting blackened circles to form a parallelograms, each slab appears in this projection as a succession of identical stuffed parallelograms which are "left-leaning" or "right-leaning", respectively, if the slab has been rotated for 180 degrees. The three structures differ in the sequence of rotated and non-rotated slabs.

Laves himself proposed the name Kasper polyhedra for the new co-ordination polyhedra. Some of these polyhedra with extreme high co-ordination number have recently become important for the interpretation of quasi-crystalline atom arrangements.

The structure types of the Laves phases and their geometrical relationships are these days basic textbook material. As shown in Fig. 1, the three structure types can be interpreted as an intergrowth of a common slab, which is either non-rotated or rotated for 180° around an axis perpendicular to the intergrowth plane.

Laves and Witte, after an evaluation of experimental results on Mg based alloys, suggested in 1936 that the different stackings of the three different Laves phases might be correlated with the valence electron concentration of the alloys (specifying that Ni atoms contribute nothing to the valence electron pool). This unusual idea proved to be fruitful. Some 40 years later, Komura and Kitano (1977) reported about a dozen of new, differently stacked Laves phases where the slab stacking depends on the value of the valence electron concentration of the compound.

Laves made an important contribution to topology. He evaluated the number of the possible tessellations of a plane with tiles which are all congruent and/or congruent by mirror-image (Laves, 1931). He derived the 11 possible so-called "Laves tilings". The Laves tilings are now cited regularly in books on tilings and patterns. In Fig. 2 are shown the 11 Laves tilings for the special case where the vertices of all tiles are regular. A tessellation of tiles where all vertices are regular has the following property. At every given corner of a tile where N tiles meet, the angle between the tile edges (leading to this tile corner) must be $360/N$ degrees for each one of these N tiles. As seen in Fig. 2, the tiles have 3, 4, 5 or 6 vertices and N has values of 3, 4, 6, 8 or 12.

Laves studied also the packing of spheres. Together with Heesch he published in 1933 a manuscript on the thinnest possible sphere packing. Each sphere has here three neighbours. The density of this packing is 0.056. In comparison, in the closest packing each sphere has 12 neighbours and the density is 0.740.

In 1956 Laves wrote a large paper on crystal structure and atomic size, where he introduced the space-filling parameter. The concept was actually known before, but the parameter had been called packing index (Fairbairn, 1943). Parthé (1961) picked up the idea of Laves and proposed space filling vs radius ratio diagrams based upon double-logarithmic co-ordinates to be used for the prediction of possible structure type changes under high pressure. However, the general applicability for this approach was limited because in this model the atoms are assumed to be rigid, excluding any possible change of electronic structure (and size) under pressure.

Laves had a long-standing interest in the feldspars too. In a 1954 publication written by Goldsmith and Laves an experimental aluminium-atom-avoidance rule for

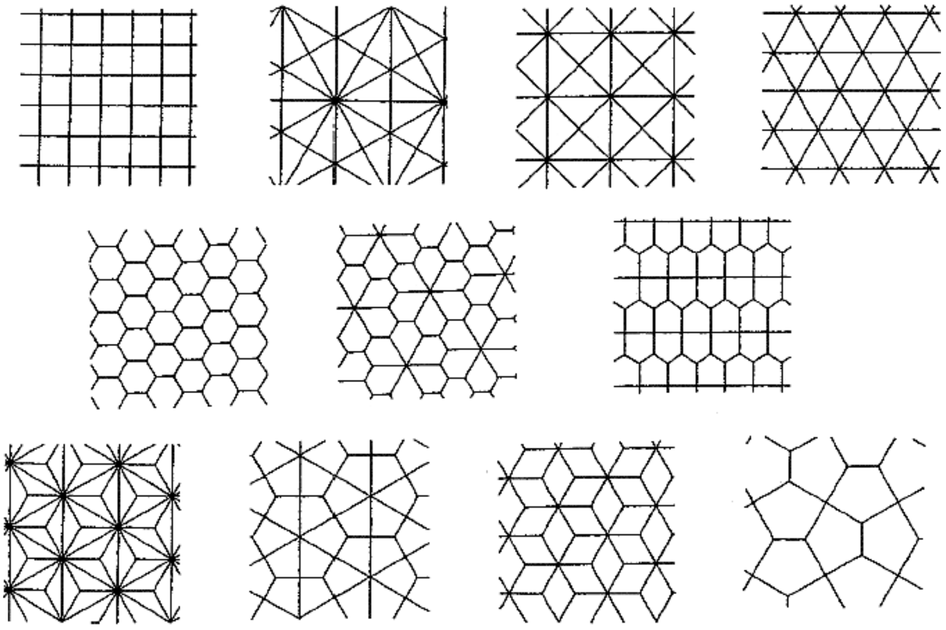

Fig. 2. The 11 Laves tilings for tiles with regular vertices.

feldspars was announced. This rule corresponds somewhat to the Loewenstein rule, which was published in the same year. In a feldspar anion complex no Al—O—Al linkages should occur. This rule was helpful to predict the Al and Si atom order in the feldspars. Thirty years later a similar avoidance rule was formulated for ternary intermetallic rare earth-transition metal-silicides by Parthé and Hovestreydt (1985). The trigonal prism waist-contact-restriction rule forbids prism waist contacts between transition elements themselves and between transition elements and rare-earth elements within the crystal structure. This avoidance rule proved to be important to find models for the correct atom order in complex ternary crystal structures with very large unit cells (see for example, Prots and Jeitschko, 1998).

Laves must also have felt that it might be useful, if crystal structure data would be described in some standardized way. Schwarzenbach, one of his co-workers, presented in 1963 some preliminary ideas how this might be done. It was some 20 years later, that Parthé and Gelato published their paper on crystal structure data standardization (1984) and three years later the corresponding STRUCTURE TIDY computer program (Gelato and Parthé, 1987).

The writer has presented here a few examples where he believes that he himself had been inspired, or at least influenced in some way (consciously or unconsciously), by the ideas of Prof. Laves and his research group. The reader should excuse omissions where the author himself has not come in contact with other works of Prof. Laves. The writer is convinced that every inorganic crystal chemist has inherited something useful from Prof. Fritz Laves scientific work, although not everyone might be aware of it.

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