19.2-10 COMPUTER RECREATION AND CRYSTALLOGRAPHIC TEACHING: NUCLEATION AND GROWTH, MISCELLANIES AND ORDERING, RESOLVED IN SPACE AND TIME.

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A paper by S. Hayes (Scientific American, Dec. 1983, 24-30) and an earlier one by P. Laves (Die Chemie 57, 1889-1944, 30-33, reprinted in Z. Krist., 151, 1980, 21-29) stimulated us to develop "electronic spreadsheets" for computer simulations and visualization of a variety of crystallographic phenomena. An electronic spreadsheet is a 2-dimensional matrix of cells, where the values of each cell can be made to depend on any other cell or group of cells.

Sohncke's (1879) Principle (stating that repeated next neighbour symmetry leads to long range order) is thus easily visualized. Exercises revolving space and time are printed out showing the development of microstructures step by step, by modifying the operating, starting and boundary conditions of the computer program, the influences of various parameters of assignable physical meaning can be made visible for better understanding and teaching. Most instructive are electronic spreadsheets with sequential print-out for demonstrating nucleation and growth and resulting microstructures under varying conditions such as type and rate of nucleation, random or local seeding, isotropic or anisotropic growth. Microstructures are quickly evaluated for fluctuations, grain size distributions, inter-molecular distances, etc. Other applications of electronic spreadsheets with series of print-outs are the visualisation of fluctuations in solid solutions with a range of composition, order-disorder transitions, formation of antiphase domain boundaries, etc.

19.2-11 CRYSTALLOGEOCHEMICAL CLASSIFICATION OF SILICATES: AN EXHIBITION.

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Since Bragg (Z. Krist. 1930) it is common practice to classify silicates according to the way [SiO₄] tetrahedra are linked with each other. The discovery of many new silicate structures since then induced several extensions of the Bragg classification. At present the following parameters are used in classifying crystalline silicates (numbers in parentheses are possible and, in italics, observed values):

\[ n \] : number of different silicate anions

\[ \text{a} (1, 2, 3, \ldots) \]

\[ \text{CN} \] : coordination number of silicon

\[ (\ldots, 4, 5, 6, \ldots) \]

\[ L \] : linkedness of [SiO₄] polyhedra, i.e. the number of oxygen atoms shared between two [SiO₄] : \( 0 \) : isolated, \( 1 \) : corner-shared, \( 2 \) : edge-shared, \( 3 \) : face-shared

\[ G \] : connectedness of [SiO₄] polyhedra, i.e. the number of element \( G \) (corners, edges or faces) : one [SiO₄] polyhedron shares with others [SiO₄] polyhedra [SiO₄] tetrahedra, \( 0, 1, 2, 3, 4, 5, 6 \) for [SiO₄] octahedra

\[ B \] : branchended of silicate anions (unbranch., open-branch., loop-branch., mixed-branch., hybrid) (Liebmann, Review in Mineralogy 1980, 5, 1)

\[ D \] : dimensionality of silicate anions, i.e. the number of dimensions of infinite anion extension (0 for terminated and cyclic anions, 1 for chains, 2 for layers, 3 for frameworks)

\[ M \] : multiplicity of silicate anions is the