C - 44819. DATA RETRIEVAL AND CRYSTALLOGRAPHIC TEACHING

PRESENTATION OF NON-COMMERCIAL 19.2 - 9CRYSTALLOGRAPHIC TEACHING AIDS.

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A dozen teaching aids demonstrating a variety of crystallographic principles by using self-constructed parts or commercial toy items and suitable for teaching individually large groups will be presented, namely:

- a simple polaroscope to show homogeneity and anisotropy, an etched silicon single crystal polyhedron
- to show plane symmetry on crystal surfaces, wooden blocks and re-usable tape to show _
- point group symmetry and multiplicity, a magnet tree with branches and leaves to
- show space group symmetry elements, Kugeli, a children's toy, to show space group symmetry and cubic crystal structures,
- an assembly of a plate, rods, discs and spheres to build crystal structure models and surfaces of different orientations,
- Coloredo, a children's toy, to show 2-dimens-ional crystal structure projections, sheets of postage stamps of different count-ries (translational symmetry of perforation)
- to show moirés, incommensurate arrays, etc,
- a reciprocal structure model to show correlations between geometric structure factors in diffraction theory, - bath room tiles to show auto-radiography,
- a swing-o-graph to show anisotropic tempera-
- ture factors, glass tubelet cuttings, 2 by 4 mm, (bushings for insulating lead-in wires through metal sockets) to show liquid crystallinity with domains, grain boundaries and defects.

19.2 - 10COMPUTER RECREATION AND CRYSTALLOGRAPHIC TEACHING: NUCLEATION AND GROWTH, MISCIBILITY AND ORDERING, RESOLVED IN SPACE AND TIME. By G. Pöppel and <u>H. von Philipsborn</u>, Universität, D-8400 Regensburg.

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

Sohncke's (1879) Principle (stating: repeated next neighbour symmetry leads to long range order) is thus easily written in computer language. Sequences resolving 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 speadsheets 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-nuclei distances, etc.

Other applications of electronic spreadsheets with series of print-outs are the visualization of fluctuations in solid solutions with a range of composition, order-disorder transitions, formation of antiphase domain boundaries, etc.

1974-1984 : TEN CRYSTALLOGRAPHIC COURSES AT 19.2-11 ERICE. By Lodovico Riva di Sanseverino, Istituto di Mineralogia, Pza Porta S. Donato 1, Univ. Bologna, Italy

The tenth anniversary since crystallographic courses started at the Ettore Majorana Centre for Scientific Culture, Erice, Italy, has stimulated the presentation of some data on content, participants, planning and outcome for the ten courses held in this decade.

Erice is an ideal site for 7-to-14 days meetings with limited number of participants and its facilities have now been checked and appreciated by scientists belonging to more than eighty disciplines for twentyone years.

Between 1974 and 1984 the crystallographic courses hawe dealt with 9 out of the 23 categories in which the scientific content of the present congress has been divided: "synchrotron radiation" will be added in 1986. The international character results from the total number of crystallographers (927), representing more than fifty countries: the italian presence has been limited to an ave rage of 11%. "Off-set" lecture notes or properly printed proceedings are the permanent scientific heritage from the courses.

After a short, but qualifying Directorship by Professor Dorothy Hodgkin, Professor T.L. Blundell has recently taken up the responsability for the scientific planning: at the moment titles and dates of prospective meetings are defined till 1989. However, proposals for the future will be welcomed at any time.

With a special attention for crystallographic frontier topics, the aim of this activity is to stimulate a fruitful exchange of ideas, mutual collaboration and an overnational human feeling.

19.2-12 CRYSTALLOCHEMICAL CLASSIFICATION OF SILICATES : AN EXHIBITION. By F. Liebau and G. Bissert, Mineralogisches Institut der Universität, 2300 Kiel, Germany.

Since Bragg (Z. Krist. (1930) 74, 237) it is common practice to classify silicates according to the way $[SiO_4]$ 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 classi-fying crystalline silicates (numbers in parentheses are possible and, in italics, observed values) :

N : number of different silicate anions

(1,2,3,...) CN : coordination number of silicon

В

D

- L
- : coordination number of Silicon (...,4,5,6,...) : linkedness of [SiO₁] polyhedra, i. e. the number of oxygen atoms shared between two [SiO₁] (0: isolated, 1: corner-shared, 2: edge-shared, 3: face-shared) : connectedness of [SiO₁] polyhedra, i. e. the number of elements (corners, edges or faces) one [SiO₁] polyhedron shares with others (0,1,2,3ⁿ,4 for [SiO₄] tetrahedra, 0,1,2,3,4,5,6 for [SiO₆] octahedra) : branchedness of silicate anions (unbhan-ind) s
- : branchedness of silicate anions (unbranched, open-branched, loop-branched, mixed -branched, hybrid) (Liebau, Review in Mi-
- neralogy (1980) 5, 1) dimensionality of silicate anions, i. e. the number of dimensions of infinite an-ion extension (0 for terminated and : extension (0 for terminated and ion cyclic anions, 1 for chains, 2 for layers, for frameworks)

: multiplicity of silicate anions is the Μ