

MS22.02.02 DISPLAY OF 3D CRYSTAL STRUCTURES OVER THE INTERNET USING VRML, FOR INORGANIC DATABASES. A.W. Hewat, ILL, BP 156X Grenoble Cedex 9, 38042 FRANCE

3D crystal structures can be displayed on all types of computer, even inexpensive home machines connected to the Internet, using the new Virtual Reality Modelling Language (VRML). Ball-and-stick, co-ordination polyhedrae, and space-filling models can be rotated in real time and zoomed to examine details of the structure. Structural chemists might search the ICSD database, and display and compare the resulting inorganic structures on-line, just as structural biologists have already done with the Protein Data Bank and 'RasMol'. No special application like RasMol is needed with VRML, since the 3D viewer is a simple extension of Netscape and other WWW applications, and freely available.

The VRML file describing the 3D structure is simple ASCII, and as such can be saved, edited, forwarded by email, and transferred to any other computer for display. This file would be constructed on the remote server, following current ideas that WWW viewers need not even use complete computers.

Apart from the obvious interest to professional researchers, who will of course also continue to use commercial applications like BioSym/MSI's Cerius, this should help educate young people about chemistry and the importance of crystallography.

Anyone with a home computer and a telephone modem will be able to understand immediately the common structural elements of oxide superconductors, or the difference between alpha- and beta-quartz.

In this contribution, I will demonstrate how this might work in practice for the Inorganic Crystal Structure Database (ICSD). A demonstration database has already been set up for example, for superconductors, on the WWW at http://www.ill.fr/dif/3D_crystals.html.

MS22.02.03 DYNAMISM FOR MATERIALS DESIGN AFTER INFORMATION FUSION. Shuichi Iwata, RACE, The University of Tokyo 4-6-1 Komaba, Meguro-ku, Tokyo 153 Japan

Trials and errors to design materials for structural, opto-electric and electro- magnetic applications are reported so as to develop a set of software tools for materials research and developments. Fusion of relevant information is the first step and three types of information, namely, (1)calculated data by different models with explicit semantics on the basis of underlying principles and mechanisms, (2)a set of structure-related data of phase diagrams, crystallographic data, basic intrinsic properties, diffraction data and microstructural images, and (3)engineering data for different applications, are tried to be integrated on a workbench to find out solutions. In general problem solutions do not follow one deterministic way and trials and errors are the normal case. Therefore the software tools need to have an adaptability to any changes in the process of materials design so that we are designing the functions of the software tools by using the following five aspects.

(1)Establish Intentions : De fact driven approaches by taking advantage of VRML and other browsers are proposed on the basis of the following considerations. How to get a new idea emerged and to discover multi-variate patterns through the mining of data;browsing of continuous, heterogeneous information via filtering/focusing/erasing/selecting/reasoning to extract useful information, with fluctuating/changing viewpoints.

(2)Establish View : How to define, reduce dimension of, and represent design space to visualize solutions using indices, structure/properties/functional/process/etc. maps based upon focus

attributes. Parameters describing structural stability, band structures and microstructural images are the keys for the above applications.

(3)Establish Concepts and Categories : How to enable in situ process discovery, classify/organize design and/or control space into sub-spaces and/or sub- processes searching for feasible solutions and/or regularities to include problem decomposition based upon multi-variate criteria/guidelines/heuristics.

(4)Establish Associatively and Causality : How to create design 'windows' for unique linear combinations of material properties, e.g., strength, temperature, stress, creep rate, corrosion, etc. for applications involving high temperature.

(5)Establish a Paradigm : How to implement and combine geometric reasoning and analytic models with discrete optimization methods in available computing resources for the simultaneous design of material, shape and process.

These latter three aspects are mixed up to form a "virtual production line" to verify each candidate material until we get a suitable material in the reality by replacing all parts of the "virtual production line" by a "real" line, tactics and strategies of which are proposed in the presentation.

MS22.02.04 NIST WORKSHOP ON CRYSTALLOGRAPHIC DATABASES. Vicky Lynn Karen, Alan Mighell, Materials Science and Engineering Laboratory, National Institute of Standards and Technology, Gaithersburg, MD 20899 USA

The NIST Workshop on Crystallographic Databases was one in a series of NISTsponsored workshops each addressing a particular type of data. A main goal of the Workshop was to foster interactions between providers of crystallographic databases and various user communities. Workshop proceedings will be made available to the general scientific community in a special issue (May/June, 1996) of the NIST Journal of Research (to request a copy, e-mail karen@tiber.nist.gov). The organization of the journal issue parallels that of the meeting, with manuscripts from the speakers organized into three major sections followed by a discussion on the adequacy of current crystallographic data activities. The first section covers formal data activities; the second, scientific usages; and the third, data transfer. In this talk, the status of the crystallographic data efforts will be briefly discussed. Currently, the crystallographic community is being well served. The Data Centers have built evaluated databases covering all classes of compounds and they have developed theories and scientific programs for standardizing, evaluating and searching the data. Nevertheless, the manuscripts from the workshop clearly reveal that the data field is in a period of dynamic transition that is being driven by many factors including a greatly increased user demand for information. This talk will also outline some of the future directions which may include the cross-linking of entries in crystallographic and related chemical/materials databases, the evolution of unified systems for searching a group of related databases, and the development of software to aid in materials design and properties prediction.