MS22.02.05 DATABASES AND PREDICTION OF NEW INORGANIC COMPOUNDS. N.N. Kiselyova, A.A.Baikov Institute of Metallurgy of Russian Academy of Sciences

Application of artificial intelligence (AI) methods to processing large information volumes of databases (DB) on substance and material properties allows to find the regularities in data and to use of found regularities for the prediction of the possibility of forming inorganic compounds and for the estimation of their properties.

DB on inorganic ternary compounds' properties, DB on phase diagrams of the systems with intermediate semiconducting phases, and DB on crystals with acousto-, electro- and nonlinear optical properties are discussed.

The advantages of AI methods (a possibility of processing large information volumes, the search for complicated and multidimensional regularities and so on) are illustrated by the example of predicting the new ternary compounds and estimating some their properties. The method of computer learning (the method of concept formation in pyramidal networks) was used for processing information of DB inorganic ternary compounds' properties. The examples of known compounds, taken from DB, were used for computer learning. Each ternary compound was described in computer memory as set of component (chemical elements and/or binary compounds) property values with indication of information about belonging to one of the considered class of compounds. The search for regularities is based on formation and analysis of the semantic pyramidal network which receptors are the component property values. The prediction requires only the knowledge of the values of the component properties. The comparison of these predictions with the new experimental data shows that the average reliability of predicted ternary phases exceeds 80 percent.

The information-predicting system is developing for the data retrieval on the known compounds and for automation of the prediction of inorganic compounds, not yet synthesized, and the forecasting of its properties. This system will employ the DB on inorganic compounds properties, AI system, DB on elements properties, knowledge base, conversational processor and monitor.

MS22.02.06 MATERIALS CHARACTERISATION AND DATABASES. Jo Daams, Philips Research, Prof. Holstlaan 4, 5656 AA Eindhoven, The Netherlands

In an industrial research environment where precise and fast characterisation of materials is essential, databases are widely used. Especially in our Materials Analysis Department these databases, providing chemical and physical data, are used on a daily basis. The structure analysis group, consisting of X-Ray Diffraction (XRD) and Electron Microscopy (TEM and SEM), uses databases like the Powder Diffraction Files from the ICDD and there is access to crystallographic databases like CRYSTMET.

In studies involving "new materials", however, these databases are more or less incomplete and to a certain extent not up-to-date. Especially those databases which contain, from an user point of view, perfect data, have the tendency to run some years behind the literature. Therefore, they are as such not very useful in our particular type of research environment. So it is common practise in our work to make our own or to update the existing databases. This part of our work searching for and collecting crystal structural information is rather time consuming due to the fact that for crystallographic data more then a hundred scientific journals have to be scanned. In the presentation some aspects of using databases in materials science will be presented. For example, in some ternary systems about 60 compounds are published (including the elements, binary and ternary compounds). For about 45 of these compounds the crystal structure data has also been published. In the powder diffraction files, however, only 30 powder patterns found in this system are included. Meaning that users, working in this system, have to calculate the other powder patterns in order to make their database complete. In conclusion databases are essential tools in material science especially in a characterisation group. The applicability of the existing databases is, however, strongly hindered by a number of obstacles. It is therefore necessary that the IUCr (representing the users of databases) starts a cooperation with database "manufacturers" in order to obtain up-to-date, correct and easy accessible databases.

MS22.02.07 VOIDS, ELECTRONS, AND HIERARCHICAL ORDER IN INORGANIC COMPOUNDS. Reinhard Nesper, Lab. of Inorganic Chemistry, ETHZ, Universitatstr. 6, CH-8092 Zurich, Switzerland

Quick access to inorganic structure data bases does not only allow for a fast generation of different structure models, but consecutively to analyse interactively the structures in terms of geometrical, electrostatic, and quantum mechanical means.

Using hitherto available analytical tools consistency checks of retrieved structures e.g., space filling criteria (localization of voids [1]), site potentials, and electronic properties (electron localization function [2]) can easily be generated and together with the geometrical information be displayed.

Experimental data (e.g. electron densities) and symmetry representations (periodic nodal surfaces, PNS [3]) may be added to yield deeper understanding of structure property relations. Relations between PNS and structures as well as hierarchical structure series [4] may effectively be analysed by combined use of data bases and sophisticated 3D grafics.

Selected examples are given in the paper.

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