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Internet-Accessible Electronic Materials Database System

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Abstract—The Electronic Materials Database System described in this paper incorporates the Diagramma Database (phase diagrams of semiconductor systems) and the Kristall Database (substances with special acoustooptic, electrooptic, and nonlinear optical properties). The database system is available in the Internet on the Web site http://phase.imet.ac.ru. The technology of integrating dissimilar databases of substances and materials is discussed, and the possibilities of using database systems in the fields of inorganic chemistry and materials research are examined.

INTRODUCTION

Advances in electronics, the most rapidly developing area of high technology, are highly dependent on the use of new materials. A critical issue in this context is information exchange between designers and users of electronic materials. Conventional ways of reporting research results (articles, books, handbooks, etc.) are unacceptable in electronics, where basic components are updated about every two years. Necessary information may be difficult to find because it is dispersed over numerous sources differing in scope. Modern information systems for researchers and engineers in electronic materials must ensure rapid updating, reliability, and completeness of data and must be Internet-accessible. It is these principles that form the basis of the Electronic Materials Database System, designed at the Baikov Institute of Metallurgy and Materials Science (IMET), Russian Academy of Sciences (RAS).

DATABASES OF ELECTRONIC MATERIALS PROPERTIES

Databases of the properties of inorganic substances and materials are being designed in all developed countries [1–19]. The great expenses for the creation of information systems amply repay themselves owing to the decrease in the information search and systematization time and lesser amount of unjustified research duplication. The recent increase in the number of databases has been due to the advent of powerful, convenient database management systems and high-performance computers. The table lists a number of databases close in subject matter to the IMET Databases.

IMET ELECTRONIC MATERIALS DATABASE SYSTEM

One of the general trends in designing information systems is the integration of existing databases into a single information system. Available data can be fully integrated into a set of databases—a single information system for users, operators, and administrators. This approach offers the advantages of lowering the expenses for managing databases and reducing information duplication. However, databases of substances and materials are, as a rule, designed at different institutions or even in different countries (table). Full integration of such databases is impossible because of differences in data quality and involves organizational difficulties since most information systems are used commercially or are accessible for users in only a limited number of countries or institutions. In such a case, it is reasonable to integrate databases using hypertext links and/or reference databases containing lists of properties and substances included in different information systems. Reference databases serve the function of a dispatcher and authorize access to information resources in different databases. This "virtual" integration of databases implies that individual subsystems develop independently. Nevertheless, the user gains access to the entire information about a particular substance or material available in the databases of the virtual integrated system. This approach was used in integrating the IMET Databases, since further expansion is planned to include databases developed at other Russian institutions.

At present, the IMET Database System includes the Diagramma Database (phase diagrams of semiconductor systems) and the Kristall Database (substances with special acoustooptic, electrooptic, and

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Databases of properties of inorganic electronic materials

Name	Institution	Contents	Ref.
Inorganic Crystal Structure Database (ICSD)	FIZ (FRG), National Institute of Standards and Technology (NIST) (USA)	Crystal structures of inorganic compounds	[1]
CRYSTMET	National Research Council (Canada)	Crystal structures of intermetallics	[2]
Crystal Data (CD)	NIST (USA)	Crystal structures of inorganic compounds	[3]
Electron Diffraction Database (EDD)	NIST, Sandia Nat. Lab. (USA)	Powder x-ray patterns, crystallographic data, electron diffraction data	[4]
Structural Phase Transitions Database	Institute of Low Temperatures and Structural Investigations (Poland)	Structural phase transitions in crystals	[5]
Pauling File on Binary Systems	Japan Science and Technology Corporation (Japan), Material Phases Data System (Suisse)	Phase diagrams of binary systems, crystal structures and physical properties of binary inorganic compounds	[6]
NISTCERAM	NIST, Gas Research Institute (GRI) (USA)	Thermal and mechanical properties of silicon carbide and silicon nitride	[7]
Surface Structure Database (SSD)	NIST (USA)	Structure of inorganic and organic surfaces	[8]
Powder Diffraction File (PDF)	International Center for Diffraction Data (ICDD) (USA)	Powder x-ray patterns of inorganic and organic substances	[9]
Properties of Electronic Materials Database (SMET)	Institute of Inorganic Chemistry, Siberian Division, RAS	Physical, thermodynamic, and structural properties of semiconductor materials	[10, 11]
Physicochemical Properties of High-Purity Substances Database	Institute of Chemistry of High-Purity Substances, RAS	Physicochemical properties of high-purity substances determining the efficiency of purification processes, impurity distribution coefficients in two-phase equilibria	[11, 12]
EPIDIF	Institute of High Temperatures, RAS	Interdiffusion coefficients of components in vapor-phase epitaxy of semiconductor materials	[13]
Database of Processes for Liquid-Phase Epitaxy of Semiconductor Heterostructures	Lomonosov State Academy of Fine Chemical Technology (Russia)	Parameters of liquid-phase epitaxy of semiconductor heterostructures	[11, 14]

nonlinear optical properties). The key features of these databases are

(1) reliable information (derived from numerous sources and validated by experienced experts);

(2) rapid data updating;

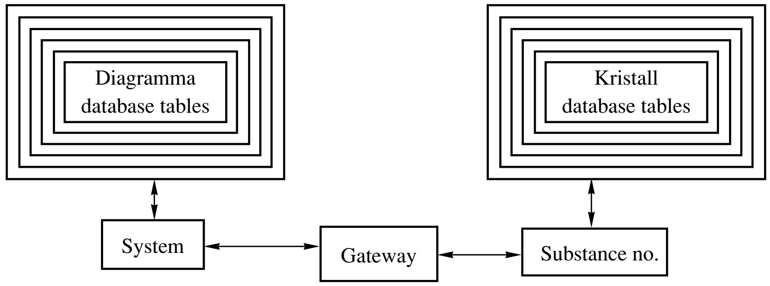
(3) full coverage of the field owing to the advanced structure and integration;

(4) ease of use owing to the carefully configured software and convenient interfaces;

(5) rapid access to information via the Internet owing to the high-speed optical fiber communication system and the powerful database server and IMET Web Server.

Diagramma Database: phase diagrams of semiconductor systems. The information in this database [15–17] is presented mainly in the form of tables and has been validated by experts. The tables contain experimental data on the lines of multi-, mono-, and invariant equilibria and singular points, similar data after statistical treatment or thermodynamic optimization, phase diagrams, and other graphical information. In addition, the database includes data on the crystal structures of phases, thermodynamic properties of phases and systems, calculated models, and analytical reviews of phase diagrams presented by experts, which contain additional information not included in the tables. The design of this database was described in detail earlier [15]. At present, the database contains information about several tens of binary and ternary systems, extracted from about 2000 publications.

In developing the Diagramma Database, particular attention was paid to assessing the reliability of phase-diagram data. The data were collected and evaluated by experts from RAS, research institutes, and institutions of higher education experienced in studies of semiconductor systems. Five quality levels corresponding to different experimental uncertainties were used by experts to assess the reliability of each data point (composition, temperature, pressure, etc.). The information about the error proposed by the expert is available at the



Structure of the IMET Electronic Materials Database System.

user's request while examining the tables containing information about phase equilibria.

Phase diagrams can be examined in both static and dynamic modes. In the former case, phase diagrams can be displayed, printed, or copied in the jpeg format. The dynamic mode requires the Macromedia Flash (current versions of MS Explorer maintain this software) and offers the possibility of determining the coordinates of points in *T*–*x* phase diagrams and expanding the scale, which allows the phase region of interest to be marked, looked through, and printed.

In addition to tables and graphic displays, the database provides access to most recent English-language publications. References to such publications are indicated in analytical reviews for the corresponding systems.

Kristall Database: substances with special acoustooptic, electrooptic, and nonlinear optical properties. The Kristall Database contains, in the form of tables, experimental data on the properties of acoustooptic, electrooptic, and nonlinear optical substances, together with information about experimental uncertainty, measuring techniques, preparation conditions, etc. [18, 19]. An important point is that most of the information in this database was collected and evaluated by Russian specialists involved in the design and practical use of such materials. The tables are supplemented by analytical reviews, which outline the preparation procedure and potential applications of the substance, describe special properties not included in the table, and, present, if available, critical evaluation of the data present in the database.

At present, the database contains data for tens of the most important substances: composition, melting point, density, hardness, heat capacity, solubility, Curie temperature, crystal structure, lattice parameters, thermal expansion, thermal conductivity, dielectric permittivity, dielectric losses, piezoelectric properties, electromechanical coupling coefficients, elastic constants, optical window, refractive indices, Selmeier coefficients, electrooptic properties, nonlinear optical properties, piezo- and elastooptic coefficients, sound velocities and attenuation, and acoustooptic properties under different conditions. The database includes extensive graphical information about the dependences of properties on different parameters (more than 1000 plots). The database provides access to most of the recent English-language publications represented in the tables.

Just as in the Diagramma Database, a large number of search parameters can be used in the Kristall Database. For example, information can be displayed about all electrooptic substances in a given crystallographic system that melt congruently below the preset temperature and whose particular linear electrooptic coefficient at the preset wavelength has a value in the preset range. To this end, the user enters the necessary search parameters into a form.

At present, both Russian- and English-language versions of the Kristall Database are available.

Integration of the Diagramma and Kristall Databases. The integration of the Diagramma and Kristall Databases made it possible to create a database system of the most promising electronic materials since the data on some substances (chalcogenides, pnictides, and others) in these databases are complementary. The user gains the most comprehensive picture of the properties of substances and their response to different influences. The databases are integrated using hypertext links.

To connect to the databases, the user should have access to the Internet and appropriate browsing software, e.g., Internet Explorer (version 4.0 or higher) or Netscape Navigator (version 4.5 or higher). Owing to the convenient interface and menu-driven navigation system, the database system is easy to handle even for a beginner.

To gain access to Diagramma or Kristall, one should be registered and have a login and password. The database security system involves multilevel protection based on Web server, Windows 2000, and database management system options. Either database has its own protection options, which makes it possible to prevent unauthorized access. The design features of Diagramma and Kristall and the use of the multilevel security system posed serious difficulties in integrating these databases. To obviate those difficulties, a system of gateways was designed.

The main function of such gateways is to ensure the transition from the data set on a particular substance in Kristall to the information available in Diagramma about the system composed of the same set of elements as the substance of interest, and vice versa (figure). For example, viewing the information about the Ga–As system, the user will also be provided with access to the data on the piezoelectric and nonlinear optical properties of GaAs. Thus, the gateway extends the access rights of users, permitting them to use a database to which they are not connected. At the same time, the user of Kristall will not gain access to the data on other systems, and the user with authorized access to Diagramma will not gain access to information about substances differing in the set of elements from the corresponding semiconductor system.

The high degree of integration is also ensured by the CrystalAdmin administrator system, designed to support the databases, convert information from earlier developed, local databases and view and edit tables in the Internet. The administrator system is a versatile means of managing the database: it is easy to customize to suit to any database management system and is simple to manage. In essence, this system is a versatile application client for remote access to any relational databases. The transition from one database to another must be authorized by the administrator or operator.

CONCLUSIONS

The Electronic Materials Database System, available in the Internet on the Web site http://phase.imet.ac.ru, can be used to supply information for basic and applied research in the fields of solid-state physics and chemistry; physicochemical analysis; and the physics and chemistry of semiconducting, acoustooptic, electrooptic, nonlinear optical, dielectric, ferroelectric, laser, piezoelectric, and pyroelectric materials and also in resolving a wide range of problems encountered in designing and characterizing materials for electronic, radio engineering, acoustoelectronic, hydroacoustic, microelectronic, optoelectronic, high-power electronic, infrared, quantum-electronic, and other devices and instruments. One important feature of the integrated database is the possibility of searching for potentially attractive, multifunctional electronic materials, e.g., those combining semiconducting and nonlinear optical properties.

The integration of databases of the properties of substances and materials, ensuring rapid and comprehensive information service, is not the only trend in the development of modern information systems. When systematized in databases, the wealth of information accumulated to date in chemistry and materials research will offer the possibility of elucidating the mechanisms relating the properties of substances to those of their components and the preparation and processing parameters. Such relationships can be used in designing materials with controlled properties [20–22].

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