Russian Chemical Reviews **79** (2) 145 – 166 (2010)

DOI 10.1070/RC2010v079n02ABEH004104

Computer information resources in inorganic chemistry and materials science

N N Kiselyova, V A Dudarev, V S Zemskov

Contents

Abstract. Information systems used in inorganic chemistry and materials science are considered. The following basic trends in the development of modern information systems in these areas are highlighted: access to information *via* the Internet, merging of documental and factual databases, involvement of experts in the evaluation of the data reliability, supplementing databases with information analysis tools on the properties of inorganic substances and materials. The bibliography includes 126 references.

I. Introduction

Collection, analysis and classification of data are essential steps of scientific cognition. For long, consolidated information has been traditionally published in handbooks and monographs.† However, at present the science is progressing so rapidly that handbooks go out of date when in the printing houses. A dramatic increase in amount of scientific and technological information, which was called 'information explosion', led to the situation where chemists and materials scientists spend from 25% to 33% of the working time for the search for necessary information. Computers, convenient database management systems (DBMS) and, especially, rapid propagation of the Internet promoted the creation and active use of a novel, progressive form of information resources, namely, computer databases. Their major advantages include rapid updating of content as new data become available, automated search for necessary data and the possibility to almost instantaneously receive the required information at any point of the world. It is databases that become the main source of information for the army of researchers. At present, many traditional handbooks have electronic versions.

To solve the problem of finding necessary information, chemists and materials scientists have created and manage a variety of databases on the properties of inorganic substances and materials. In this review we briefly outline the electronic information resources in this field and the trends in their development. We believe that the material presented here will help researchers in their search for data sources.

II. The structure of databases

Usually, a database is an array of interrelated multipurpose data, controlled by a DBMS. Information stored in the database is organized in one or another way, which implies that the description, storage and manipulation of data obey some general rules. The database provides integration of logically related data with minimum duplication. However, in some cases the term 'database' is only applied to interrelated data tables in an information system, which also includes a DBMS, a network access subsystem, as well as hardware and software for solving problems in particular subject areas (user applications), *etc*.

The main goals of a database are to ensure a rapid updating of information stored and to provide users with convenient data retrieval methods. When reaching the second goal, an essential role is played by the database design, especially the design of the database structure, which can be represented by a set of different-level data models listed below.

N N Kiselyova, V A Dudarev, V S Zemskov A A Baikov Institute of Metallurgy and Materials Science, Russian Academy of Sciences, Leninsky prosp. 49, 119991 Moscow, Russian Federation.
Fax (7-499) 135 86 80, tel. (7-499) 135 25 91, e-mail: kis@imet.ac.ru (N N Kiselyova), vic@80port.ru (V A Dudarev), tel. (7-499) 135 86 30, e-mail: zemskov@imet.ac.ru (V S Zemskov)

Received 14 September 2009
Uspekhi Khimii **79** (2) 162 – 188 (2010); translated by A M Raevskiy

† Many generations of inorganic chemists and materials scientists use fundamental series of handbooks by Gmelin and Landolt – Börnstein (*Gmelin Handbook of Inorganic and Organometallic Chemistry* Springer, 1924 – 2010; Landolt – Börnstein. *Numerical Data and Functional Relationships in Science and Technology* Springer, 1883 – 2010). Hundreds of handbooks on various fields of inorganic chemistry and materials science (see. *e.g.*, Refs 1 – 9) are desk books for researchers working in these fields.

A conceptual data model includes knowledge of physical and logical objects and their interrelations. The conceptual design involves analysis of the properties and characteristics of the subject area under study and the description of the database structure, usually in the form of a graph whose nodes and arcs characterize objects in the subject area and relations between them, respectively. The conceptual data model is problem-oriented and system-independent, being in no sense dependent on the choice of particular DBMS, operating system and the type of the computer.

A logic data model is obtained from the conceptual data model. This model is DBMS-oriented. In modern databases the logic data model is represented by a set of relational tables.

A physical data model defines the procedure for data storage in a particular DBMS and is based on the logic data model.

The design of the database structure for chemical science, especially on the conceptual and logic levels, is a fundamental problem. Successful solution to this problem requires the involvement of skilled personnel (chemists and materials scientists) who can reveal interrelations between parameters of objects and processes. In most cases, incorrect design of the database structure precludes automation of the data retrieval process. An example is provided by the database [10] on the phase diagrams of inorganic systems (http://www.matport.com/phase-diagram-center).‡ It contains huge arrays of data on the crystal chemical, thermochemical and other physical properties of various phases, but the admissible search quires are to a great extent limited by the specification of components of a particular chemical system. In this situation the user has to pass through the whole array of available data in order to find, *e.g.*, compounds with a specified type of the crystal structure.

From the standpoint of the information storage types, databases can conditionally be divided into two classes, *viz.*, documental databases and factual ones. In the documental databases, the storage units are mainly text documents (articles, patents, manufacturing documentation, *etc.*); in most cases, they are characterized by a set of key words for acceleration of the search for relevant information. Relational tables of factual databases contain factual data (numerical values of the properties, parameters of processes, *etc.*). Databases containing graphic information (cartographic databases, spectral databases, *etc.*) as well as the multimedia databases containing video and audio data form specific classes of databases. In these cases, object-specific data retrieval procedures are available.

The documental information resources in chemistry are organized in large databases, *e.g.*, 'ScienceDirect' (http://www.sciencedirect.com), 'Wiley' (www.wiley.com), 'Springer' (www.springer.com), 'American Chemical Society' (www.acs.org), 'Chemical Abstract Service' (www.cas.org), 'STN' (www.stn-international.de); a number of patent databases, *e.g.*, 'United States Patent and Trademark Office' (www.uspto.gov) or 'Questel' (www.qpat.com) *etc.*, and domestic information systems 'VINITI' (www2.viniti.ru), 'e-library' (www.elibrary.ru), *etc.* Usually, these databases contain electronic copies of published articles and books and can be accessed for fee *via* the Internet. The advantages of the electronic form include rapid delivery of information to users (often, the electronic versions are published on the Internet earlier than appear in the printed form) and the possibility of automated search for necessary information using the key words in the electronic documents. Recent progress in hardware and software also has made full-text search possible. A key problem in the design and operation of documental databases is to provide search for relevant information. Possible methods of solution to this problem are associated with the use of artificial intelligence concepts.[11]

A recent trend is 'interdiffusion' of the documental and factual databases, *i.e.*, traditional document systems are supplemented with tables containing factual information,[12] while factual systems include extensive text information and relevant tools for context search as well as the subsystems of full-text documents in the pdf or html formats.[13–22]

III. Databases on the properties of inorganic substances and materials

A large number of databases on the properties of inorganic substances have been developed to date. The list given below covers only a small proportion of information systems in inorganic chemistry and materials science. During the last five years, the number of databases in these subject areas has more than doubled. Traditionally, factual information systems accumulating data on the thermodynamic and thermophysical properties (Fig. 1) rank first. Databases containing crystallographic and crystal chemical data are also intensively developed and widely used in basic and applied research and in industry. Recently, the number of databases containing data on the mechanical (strength, fatigue characteristics, creep, *etc.*) and electrical properties of inorganic substances and materials increased by a factor of three.

Numerous factual databases on the properties of materials are designed and/or distributed by the U.S. National Institute of Standards and Technology (NIST), the National Institute of Materials Science (NIMS, Japan), the

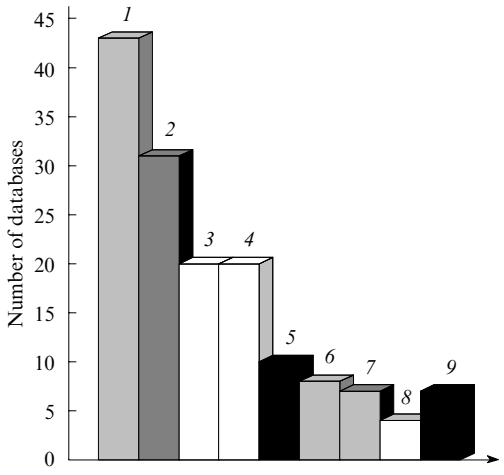

Figure 1. Distribution of databases on the properties of inorganic substances and materials with respect to subject areas.
Thermodynamic or thermophysical properties (*1*), mechanical properties (*2*), crystallographic and crystal chemical properties (*3*), electrical and electronic properties (*4*), corrosion properties (*5*), optical properties (*6*), phase diagrams (*7*), magnetic properties (*8*), other properties (*9*).

‡ Electronic addresses are as of end 2009.

German Scientific and Technological Information Network (STN) and the Scientific Group THERMODATA Europe (SGTE). A significant role in the co-ordination of activity of the database developers is played by the international Committee on Data for Science and Technology (CODATA).

The total number of computer information resources can characterize the scientific and industrial potential of a country. The world leader in this field, the USA, ranks first among the database developers (Fig. 2) mainly due to the development of information systems at the NIST. In the last decade, the number of information resources in Japan has continuously increased. Russia ranks third. Co-operation of researchers from different countries in creating so costly and hi-tech products (modern databases on the properties of substances and materials) should be pointed.

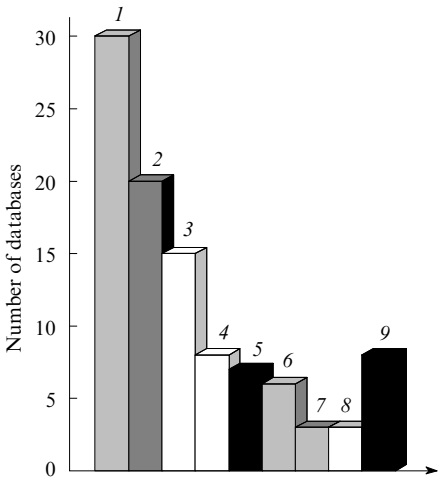

Figure 2. Geographic distribution of databases on the properties of inorganic substances and materials.
USA (*1*), Japan (*2*), Russia (*3*), France (*4*), Germany (*5*), United Kingdom (*6*), Canada (*7*), China (*8*), other countries (*9*).

Most databases considered in the review (see also Appendix) are factual ones. Due to a complex and quite 'rigid' structure these databases provide an almost 100% relevance of information retrieved. However, the preset structure of the factual databases usually restricts the set of parameters whose values are stored in the database tables.

In the text below we will briefly outline various databases on the properties of inorganic substances and materials, which were designed in different institutes. Criteria for database selection included the being in demand and the availability of information about the databases in publications and on the Internet. In addition to publications in periodicals, we used the description of databases at the STN, NIST, CODATA and NIMS Web-sites as well as information from a monograph.[23]

More detailed information on the databases on the properties of inorganic substances and materials can be retrieved from the database on information resources on inorganic chemistry designed at the A A Baikov Institute of Metallurgy and Materials Science (IMET), Russian Academy of Sciences (http:\\iric.imet-db.ru).

1. Databases on the thermodynamic and thermophysical properties of inorganic substances and materials

Most databases on the thermodynamic and thermophysical properties of inorganic substances and materials include software for thermodynamic simulation. Models include data on phases in chemical systems and their thermodynamic parameters, conditions for attainment of equilibrium, *etc*. The information systems are also supplemented with physicochemical models of phases in a chemical system (equations of state or functional dependences of the characteristic functions of phases on their compositions and on the thermodynamic parameters of the system). To obtain exact results, the primary data on the thermodynamic properties of substances are critically analyzed and checked for self-consistency.

a. Databases at the Joint Institute for High Temperatures, Russian Academy of Sciences

'IVTANTHERMO' is a database on the thermodynamic properties of inorganic substances under standard conditions.[24,25] It is based on the well-known handbook 'Thermal constants of substances'[§] and includes numerical data on the thermodynamic properties of individual substances in a wide temperature range. All data are self-consistent in the framework of the main laws of thermodynamics. The measurement errors of all recommended values are also given. Currently, the database includes data on the properties of more than 3000 substances formed by almost all elements of Mendeleev's periodic system. A distinctive feature of IVTANTHERMO is that the data accumulated in the system were obtained by the developers after critical analysis and processing of all published primary data using the methods developed at the Joint Institute for High Temperatures rather than taken from handbooks or other databases. The Internet version of the database can be accessed for free.

'THERMAL' is a mixed bibliographic/factual database on the thermophysical, thermodynamic and related elastic, electrical, magnetic, optical properties of inorganic and simple organic substances.[26,27]

'EPIBIB' is a bibliographic database, which is first of all aimed at simulating (i) gas transport processes in microelectronics and (ii) heat and mass transfer in the gas path of power stations.[28]

b. The NIST databases

The **'NISTTHERMO'** database includes information on the thermochemical properties of organic and inorganic substances;[29]

the **'NIST/TRC Ideal Gas'** database contains data on the thermophysical and thermodynamic properties (enthalpies, Gibbs free energies, heat capacities, *etc*.) of organic and other compounds in the ideal gas state;[30]

the **'IL THERMO'** database contains information on the chemical, thermophysical, thermodynamic and transport properties of ionic liquids;

the **'REFPROP'** database contains data on the thermodynamic and transport properties of pure gases and liquids as functions of the temperature and pressure;[31]

§ *Termicheskie Konstanty Veshchestv* (Thermal Constants of Substances) Nos 1–10 (Ed. V P Glushko) (Moscow: Izd. VINITI, 1965–1982).

the **'JANAF'** (Joint Army Navy Air Force) database contains data on the thermochemical properties of organic and inorganic substances.[32]

In the framework of the Standard Reference Data (SRD) programme the NIST acts as a successor of the traditions set up in the 1920s upon the issue of 'International Critical Tables' and continues to obtain reliable thermochemical data. The database at URL http://webbook.nist.gov contains data on the properties of thousands of organic and inorganic substances (enthalpy of formation, heat of combustion, heat capacity, entropy, phase transition enthalpies and temperatures, vapour pressure, *etc.*). The list of databases given above does not exhaust the NIST information resources in thermal physics. For instance, the NIST Structural Ceramics Database (WebSCD) contains data on the thermophysical, mechanical and physical properties of oxide, boride, carbide, nitride and oxynitride ceramic materials.

c. THERMODATA association databases

THERMODATA, a non-profit association from France,[33] created the following information systems.

'THERMDOC', a documental database containing tens of thousands of bibliographic references to publications in the field of thermodynamics of elements, alloys and solutions.

'THERMALLOY' contains thermodynamic data necessary for construction of models for industrially important binary, quasi-binary, ternary and quasi-ternary metallic, oxide and salt systems.

'THERMOCOMP' contains information on the thermodynamic properties of elements and pure substances and their reactions.

'NOBL Metals' contains thermodynamic data for systems with noble metals.

'Nuclea' contains data on the thermodynamic properties of materials for nuclear power plants *etc.*

'MOX-TDB' contains thermodynamic data on metallic and oxide systems containing plutonium (the database is a counterpart of the 'Nuclea' system).

d. SGTE databases

A consortium of scientific centres called the Scientific Group Thermodata Europe (SGTE) has been founded in the EU for the development of high-quality thermodynamic databases for inorganic systems and solving applied problems.[34, 35]

At present, in addition to the NOBL Metals and Nuclea databases (see above) the SGTE combines the following databases on the thermophysical properties.

'PURE' (National Physical Laboratory, UK), a database on the properties of chemical elements, which accumulates data on the thermochemical properties of all stable and many metastable states of elements in the temperature range from 298.15 K to vaporization temperatures.

'SSUB' (Institute National Polytechnique de Grenoble, France) contains data on the thermodynamic properties of more than 4000 gaseous and solid substances.

'SSOL' (National Physical Laboratory, UK) is a database on the thermodynamic properties of solutions containing data on the chemical elements, on binary and ternary systems and on the properties of certain more complex systems.

'SALT' (National Physical Laboratory, UK) is a database containing data on the thermodynamic properties of molten binary, ternary and multicomponent salt systems.

'SLAG' (Arcelor Research, France) is a database for thermodynamic calculations of equilibria in metallurgical slags.

'G35' (Institute National Polytechnique de Grenoble, France) is a database containing thermodynamic data for binary systems with $A^{III}B^{V}$ semiconductor phases.

e. THERMO-CALC databases

The Thermo-Calc information system was created to perform thermodynamic calculations and to construct the phase diagrams. This system was created in Sweden in the 1980s at the Royal Institute of Technology.[36–38] In 1997, the Thermo-Calc Software, Inc. company was founded to provide with information and software in the field of thermodynamics and diffusion.[38] Particular subject areas (chemistry, metallurgy, materials science, geochemistry, *etc.*) can be 'tuned' by selecting a corresponding database containing the necessary information:

SSUB — thermodynamic properties of substances;

SSOL — thermodynamic properties of solutions;

TCFE — thermodynamic properties of iron-based steels and alloys;

TCNI — thermodynamic properties of nickel-based alloys;

TTAL — thermodynamic properties of aluminium-based alloys;

TTTI — thermodynamic properties of titanium-based alloys;

TTTIAL — thermodynamic properties of TiAl-based alloys;

TTMG — thermodynamic properties of magnesium-based alloys;

COST2 — thermodynamic properties of light alloys;

NSLD and USLD — thermodynamic properties of solders;

SNOB — thermodynamic properties of alloys containing noble metals;

TTZR — thermodynamic properties of zirconium-based alloys;

CCC — thermodynamic properties of sintered carbides;

SEMC — thermodynamic properties of semiconductors;

STBC — thermodynamic properties of coatings for thermal barriers;

SLAG2 — thermodynamic properties of iron-based metallurgical slags;

ION — thermodynamic properties of ionic solutions;

NOX — thermodynamic properties of oxides;

SALT — thermodynamic properties of molten salts;

TCMP and TCES — information for calculations in metallurgy;

TCAQ and AQS — thermodynamic properties of aqueous solutions;

NUMT — thermodynamic properties of radioactive isotopes;

NUOX — thermodynamic properties of radioactive element oxides;

TCNF — thermodynamic properties of systems used in engineering of nuclear fuels; and

GCE — thermodynamic properties of minerals.

f. Databases at other institutions

The **MTDATA** system is a software suite for calculations of phase equilibria in multicomponent systems, which also includes a database containing data on the thermodynamic properties of materials in a wide range of changes in parameters.[39, 40]

DETHERM is an information system containing thermophysical data important for the design of various processes in chemical industry.[41] It contains the description of the properties of pure compounds and mixtures for tens of thousands of organic and inorganic substances. The database includes two subsystems, a factual and a bibliographic one. The former contains data on the thermodynamic, electrical, transport and electrochemical properties and on the phase equilibria for pure substances and mixtures. The documental subsystem contains bibliographic descriptions of journals, proceedings of conferences, handbooks, theses, reports, standards and information sheets.

TPRC/TPMD contains data on the thermophysical (thermal conductivity, heat capacity, thermal expansion, *etc*.), mechanical, electrical, physical and other properties of metals, alloys, nonmetals, gases, minerals, composites, coatings, *etc*.[42]

MALT2 (Materials-oriented Little Thermodynamic Database for Personal Computers)[43, 44] contains data on the thermodynamic properties of individual substances and software for calculations of the equilibrium composition and solution to problems in materials science. The database was created by a working group organized by the Japan Society of Calorimetry and Thermal Analysis. MALT2 contains the standard enthalpies of formation, standard Gibbs energies, standard entropies, heat capacities, heats of phase transitions, changes in enthalpies of phase transitions, *etc*. This database is aimed to analysis of production of ceramics, semiconductors, nuclear fuels, materials for production of nuclear reactors, analysis of plasmachemical processes, *etc*.

F*A*C*T. The F*A*C*T (Facility for the Analysis of Chemical Thermodynamics) software suite was designed as a result of collaboration between two universities, the McGill University and Ecole Polytechnique de Montreal.[45] The project began in 1976 for the design of software for manipulation of thermodynamic data and for solving problems in metallurgy. To keep the project alive and to use the F*A*C*T software suite in scientific research and education, the Centre de Recherche en Calcul Thermochimique/Centre for Research in Computational Thermochemistry (CRCT) was founded at Ecole Polytechnique in 1984. The F*A*C*T-Web provides free access to data on the thermodynamic properties of individual substances and chemical reactions and allows one to calculate the equilibrium compositions of thermodynamic systems.

2. Databases on the phase diagrams of inorganic systems

The phase diagrams are convenient and informative form of representation of equilibria in inorganic systems. Many databases on the thermophysical properties of substances (MTDATA, F*A*C*T, ADAMIS, *etc*.) include subsystems for storage of data on the phase diagrams and their graphic images. This feature and the development of convenient tools for input and output of graphic information gave an impetus to the development of specialized databases on the phase diagrams. A salient feature of such databases is the need for storage of not only tables, but also graphic information.

The phase diagrams can be represented in different manner:[13]

— using thermodynamic models for elements of diagrams with subsequent visualization of the calculated curves;

— using different approximating mathematical models for elements of diagrams (usually, polynomials) followed by visualization of the calculated curves;

— using data tables and splines for interpolation of data between nodes of the tables (coordinates of points from the table and splines are used for visualization of the phase diagram);

— using graphic methods, which involve the input of a phase diagram in a computer *via* an appropriate device (digitizer, scanner, *etc*.) followed by transformation to a format suitable for data storage in computer systems; an inverse transformation transforms data to the graphic form.

A recent trend in the design of databases on phase diagrams is a wide use of graphic techniques, which dominate all other methods in technological effectiveness and provide exact reproduction and a unified description of phase diagrams, a minimum amount of information necessary for storage of the output file, a convenient Web interface for manipulation of the graphic image of the phase diagram using conventional browsers, *etc*.

Now we will consider a number of databases on the phase diagrams.

The **Diagram** database includes the phase diagrams of systems containing semiconductors as well as the description of the crystal structure data and the semiconducting and thermodynamic properties of phases.[13, 14, 16, 17, 22, 46]

The **ACerS-NIST** database contains data for many (tens of thousands) oxide, chalcogenide, boride, carbide, pnictide, phosphate and other inorganic systems.

The **ASM** database is an electronic version of the known handbook on binary systems edited by Massalski[6] and a ten-volume handbook on ternary systems (*Handbook of Ternary Alloy Phase Diagrams* (Eds P Villars, A Prince, H Okamoto) (Materials Park, OH: ASM Int., 1995).

ADAMIS is a thermodynamic database on the properties of alloys for micro-soldering. It contains thermodynamic data (Gibbs potentials, activity, heats of mixing, heats of formation, *etc*.) on systems containing Ag, Bi, Cu, In, Pb, Sb, Sn and Zn, as well as the phase diagrams of these systems calculated using software based on the CALPHAD concepts.[47–49]

Pauling File. A local version of this database on the phase diagrams of binary systems and on the crystal structure of binary compounds is distributed on compact discs. It was developed by an international team including researchers from Switzerland, Germany, Japan and USA[12, 50] in the late 1990s. At that time, Pauling File was probably the best in completeness, quality of graphics and convenience of use among the databases on phase diagrams. More recently, an Internet version of this database appeared, also containing data on more complex systems. However, this version is much poorer than the local version in the quality of graphics and convenience of use.

MSIT PDC (Materials Science International Team Phase Diagram Center) is an information system containing data on a few thousands of phase diagrams for mainly metallic systems.[10] Data for this were assessed by specialists from different countries. The system also contains data on the isothermal, isobaric and polythermal sections, tables of invariant equilibria, $\log P - 1/T$ diagrams, schemes of phase

reactions, tables with crystal structure data, thermodynamic data, and data on the properties of substances and fields of their applications.

The data stored in this information system are used by the 'Springer' publishing house in compiling the series of handbooks (Landolt – Bornstein. *Numerical Data and Functional Relationships in Science and Technology. New Series. Group IV: Physical Chemistry. Ternary Alloy Systems Phase Diagrams*), which are available *via* the Internet at URL http://www.springer.com. The quality of the material and the convenience of information retrieval are much better compared to the MSIT PDC information system.

The **TAPP** database contains extensive information on the thermophysical properties (free energy of formation, thermal conductivity, viscosity, vapour pressure, enthalpy, entropy, *etc.*) of inorganic substances in the solid, liquid and gaseous states and the phase diagrams of the systems.[51] The main data sources for TAPP are the JANAF, DIPPR, TRC, *etc.* information systems.

3. Databases containing crystal structure data for inorganic substances

Databases containing crystallographic and crystal chemical data belong to the key information resources for chemists and materials scientists. Information on the crystal structure can be retrieved from most databases on the properties of inorganic substances and materials. However, specialized crystallographic databases contain detailed structural data, namely, the crystal system, space group, unit cell parameters, atom coordinates, thermal factors, crystal morphologies, methods of synthesis and investigation, graphic images of crystals, *etc.* For users of crystallographic databases, a main goal consists in identification of crystalline phases by comparing them with the available data. A severe difficulty in the development of information systems in this field is that the material on the subject is spread over different-type publications including literature on chemistry, physics, mineralogy, metallurgy, *etc.*

The **ICSD** (Inorganic Crystal Structure Database) is currently the largest database in the field of inorganic crystal chemistry and crystallography.[52–57] It contains data on the crystal structures of tens of thousands of inorganic compounds, including ceramics, minerals, pure elements and intermetallics. Information accumulated in the database covers structural data published in periodicals since 1913 up to date. An ICSD record includes a reference to a particular information source (article, monograph, *etc.*) and the corresponding data on the crystal structure including the name of a compound, chemical formula, synthesis conditions, crystallographic characteristics of the structure (crystal system, Pearson symbol, space group, unit cell parameters, atom coordinates, thermal factors, *etc.*). The database is updated twice a year; the amount of information in the database increases by about 2000 records upon each updating. ICSD is distributed by the NIST (USA) and the STN network (Germany).

NIST/Sandia/ICDD EDD is a database on electron diffraction, which contains chemical and crystallographic data (chemical formula, space group, unit cell parameters, *etc.*, and references to original publications) for tens of thousands of minerals, metals, intermetallics and other inorganic compounds, as well as software for identification of micro- and macrocrystalline materials.[58–61]

NIST CD is a database on the crystal structures. It contains data on the chemical, physical and crystallographic properties of hundreds of thousands of inorganic and organic substances[62] (chemical formula, name, structural type, crystal system, unit cell parameters and volume, space group, number of formula units in the unit cell, ratios of crystallographic axes, density, method of investigation, some physical properties, such as melting points, phase transformation temperatures, optical parameters, *etc.*), as well as references to information sources.

The **NSD** database accumulates the crystal structure data for metals, intermetallics, alloys and minerals, extracted from publications appeared before the year 1995. Data were assessed by experts from the NIST and the National Research Council of Canada.

The **CRYSTMET** database[63–65] has been developed since 1960 at the Los Alamos laboratory and more recently at the NRC Canada Institute for Scientific and Technical Information (NRC-CISTI). Since 1996, the database is distributed and managed by the Toth Information Systems. It contains information on the crystal structures of tens of thousands of intermetallics and minerals. The following data are available: reference to information source, chemical formula and name, structural type, the Pearson symbol, space group, crystal system, number of formula units, density (calculated and experimentally measured), unit cell parameters, atom coordinates, methods of investigation, *R*-factor, *etc.* The search depth is more than 80 years.

The **MINCRYST** database includes data on natural and synthetic minerals, their structural analogues (inorganic compounds with the structure of a mineral, *e.g.*, spinel, garnet, perovskite), simple substances and simple oxides.[66,67] The following information on substances is available: name; specification with respect to the useful property, composition, structure, parameters of synthesis; crystal chemical formula; space group; number of formula units (Z); unit cell volume (calculated); molar volume (calculated); density (calculated); the linear and mass attenuation coefficients (calculated); *R*-factor and the number of reflections included in structure solution; linear and angular unit cell parameters; number of atomic positions in the unit cell; X-ray wavelength for calculations of characteristics of polycrystalline substance; angular range for calculated X-ray diffraction pattern of the polycrystalline substance. In addition, the database contains data on the parameters of basic atomic positions, *hkl* indices, interplanar distances, relative integrated intensities, graphic image of the crystal structure, graphic image of line diagram of X-ray powder patterns of polycrystalline substances, references to original publications and references to publications in other databases.

The **PDF** is a database on the powder X-ray diffraction patterns,[68,69] which includes X-ray diffraction data, crystallographic data and bibliographic information on inorganic and organic substances. In addition to tabulated data for powder X-ray diffraction patterns of particular phases (characteristic interplanar distances and corresponding relative intensities), the synthesis and measurement conditions, and the data on other physical and crystallographic properties are given. To fulfill the demands of different groups of users, a number of different versions of the database were designed and are now distributed:

— 'PDF-2' is a product of collaboration between International Center for Diffraction Data (ICDD), Fachinformationszentrum Karlsruhe (FIZ Karlsruhe) and NIST. This is a database for analysis of inorganic materials. To accel-

erate the identification of materials, the database was filled by ICDD with data on many simple organic substances.

— 'PDF-4+' is an improved database ['PDF-2' is supplemented with the data that became available as a result of co-operation between ICDD and the Material Phases Data System (MPDS) (see 'Pauling File')]. This database was created for both identification of materials and quantitative analysis according to Rietveld, by the reference intensity ratio (RIR) method and by the full-profile method. The database contains digital X-ray diffraction patterns, molecular graphics and atomic parameters. This additional information is included in 'PDF-4+' to extend the possibility of using the data for quantitative analysis by the three methods mentioned above.

— 'PDF-4/Minerals' is based on the 'PDF-4+' and contains the same additional information on minerals and related substances.

— 'PDF-4/Organics' is a joint project of the ICDD and the Cambridge Crystallographic Data Centre (CCDC). This database is used for identification of organic and organometallic compounds. It contains data on a few thousands of inorganic substances, mostly fillers used in pharmaceutical industry.

The **CSD** database contains information on the crystal structures of many (hundreds of thousands) organic and organoelement compounds.[70–72] It includes X-ray diffraction and gas-phase neutron diffraction data and numerical values of some physical properties. Data for each substance stored in the database can be divided into three types (subsystems) with respect to their 'dimensionality'.

One-dimensional information includes bibliographic description, information on the crystal structure and data on the unit cell parameters, space group, polymorphism, biological activity, *etc*.

Two-dimensional information includes the molecular structure.

Three-dimensional information includes the three-dimensional representation of the molecular structure, atomic coordinates, bond lengths and bond angles, covalent radii, *etc*.

The three subsystems are linked to one another. It should be noted that the accuracy and relevance of the content of this database were thoroughly assessed by experts (some errors in publications were disclosed).

4. Databases on other physical properties of inorganic substances and materials

As mentioned above, databases containing thermophysical and crystallographic data belong the to the information systems which are traditionally used most often by chemists and materials scientists. Recently, the number of databases containing information on the mechanical, corrosion, electrical, optical, magnetic and other properties of inorganic substances and materials, which determine the possibility of their practical application (see Appendix) has increased dramatically. Large companies, research centres and universities create and support the information systems, on the one hand, to provide researchers with the data necessary for investigations and on the other hand to advertise their R&D and products. Particular attention should be paid to the databases on the properties of industrially important substances maintained by the U.S. National Institute of Standards and Technology (WebHTS, NISTCERAM, *etc*.), the DIPPR suite maintained by the U.S. Design Institute for Physical Property Data (DIPPR),[73–77] the CompoTherm, Structural Materials DB, Diffusion DB, Database System for Pressure Vessel Materials, *etc*. databases maintained by the National Institute of Materials Science (Japan),[78] and the database system developed by the IMET (Diagram, Phases, Cristal, Elements, BandGap).[13–17,21,22,46]

Data on the mechanical properties (strength, fatigue, creep, impact viscosity, hardness, *etc*.) are most often included in the databases for materials. Most databases contain information on the mechanical properties of ferrous materials and non-ferrous metals and alloys, first of all steels (ASMDATA, DMPME, MATADOR, CETIM-BDM, METALCREEP, MARTUF, JSSR DB, *etc*.), aluminum alloys (METALCREEP, AAASD, ALFRAC, *etc*.), composites (ASMDATA, CETIM-BDM, MSDRD, *etc*.) and ceramic materials (NISTCERAM, MSDRD, *etc*.).

The databases containing information on the electrical properties of substances (conductivity, dielectric and piezoelectric properties, the forbidden band width, *etc*.), namely, 'Cristal', 'BandGap', 'Elements', EMIS (bibliographic database), MPMD, Functional Ceramic Materials Database, COPPERDATA, Information system of rare earths, HYDROGENE DATA, INTERGLAD, *etc*. are also widely used.

Information on the corrosion properties of metals and alloys is available from the ASMDATA, COPPERDATA, DMPME, MAT-DB, MARTUF, *etc*. databases.

The number of databases filled with information on the optical and magnetic properties of inorganic substances and materials is much smaller. There are the 'Cristal' (transparency band, refractive indices, Sellmeier coefficients and the acousto-optical, electro-optical, piezo-optical, elasto-optical and nonlinear optical properties of substances), MPMD (refractive indices of materials for microelectronics), 'Elements' (magnetic susceptibility of chemical elements), the 'Information system of rare earths' (refractive indices and magnetic properties of rare-earth elements), INTERGLAD and 'SciGlass' (optical properties of glasses).

5. IMET databases on the properties of inorganic substances and materials

Consider the structure, principles of operation and main trends in the development of modern databases on the properties of inorganic substances and materials taking the databases developed by Russian specialists as examples.

The development of such databases at the IMET began in the 1980s[18] based on a BESM-6 mainframe. Even the first-generation personal computers allowed one to design readily transferable databases.[14,19,79] The evolution of the Internet and powerful personal computers gave an impetus to the design of modern databases.[13,15–17] Databases on the properties of inorganic substances and materials developed at the IMET can be divided into two groups, *viz*., databases containing brief information on the key properties of inorganic substances ('Phases' and 'Elements') and those containing detailed information on the properties of industrially important substances and materials ('Cristal', 'Diagram', 'BandGap').

All databases at the IMET can be accessed *via* the Internet in line with a key trend of the development of modern information systems in the field of materials science. The database content is updated weekly.

Software design was based on a distributed client–server model, according to which data processing is shared between the database server and the user's personal computer. Software for each database includes two subsystems,

namely, a system for remote access *via* the Internet and a remote administration system, which allows one to input and edit data and to manage the correct operation of the database.

The system of access to the database is based on the classical three-component model 'database server – Web-server – user'.

The database server controls the data and data storage. Data tables in the 'Phases', 'Cristal', 'Elements' and 'BandGap' databases are stored under control of the DBMS Microsoft SQL Server (Windows Server operating system), while data storage in the 'Diagram' database is under control of the Oracle DBMS (Solaris operating system).¶

The Web-server provides access to the database *via* the Internet and presentation of data in a user-friendly form. The Web-server is the Internet Information Server (IIS) running on the Windows Server platform. It supports the ISAPI (Internet Server Application Programming Interface) and ASP (Active Server Pages) technologies. The Web-server contains ASP-documents (pages) and ISAPI-applications, which are used for transfer of user queries to the database server. Data from the database server are represented in the form of html-pages and are sent to users. The Web-server and the database server are integrated using the ActiveX Data Objects interface.

Each IMET database has its own dialog administration system on the operator's or database administrator's computer connected to a local network or to the Internet.

'Phases', a database on the properties of inorganic compounds. This database contains data on more that 45 000 ternary and 15 000 quaternary inorganic compounds. Information was extracted from 24 000 publications.[13, 16, 17, 20, 79] The structure of the subsystem for the ternary compounds is shown in Fig. 3. The structure of the subsystem containing data on the quaternary compounds differs only in that additional information on the studied sections of the quaternary systems is available.

Information for filling the 'Phases' database is collected from periodicals, handbooks, monographs, reports and abstract journals. Analysis of the literature has shown that the most often used characteristics of inorganic compounds are as follows: crystal system, space group and number of formula units in the unit cell, melting type and point, decomposition temperature of a compound in the solid or gaseous phases and boiling point.

The 'Phases' database contains brief information on compounds. More detailed data on substances important for electronics is contained in the specialized databases 'Diagram', 'Cristal' and 'BandGap'.

'Diagram', a database on the phase diagrams of systems containing semiconductors. The 'Diagram' database[13–17, 46] contains information on the $P-T-x$-diagrams of semiconductor systems and on the physicochemical properties of phases formed in these systems. To date, the database contains detailed information on a few tens of systems, extracted from more than 2000 publications. This database provides an example of practical implementation of a trend in the development of modern information systems, *viz.*, assessment of the reliability of information stored in the system. Usually, all data included in the databases on the properties of inorganic substances and materials are

¶ The free test versions of the DBMS are used.

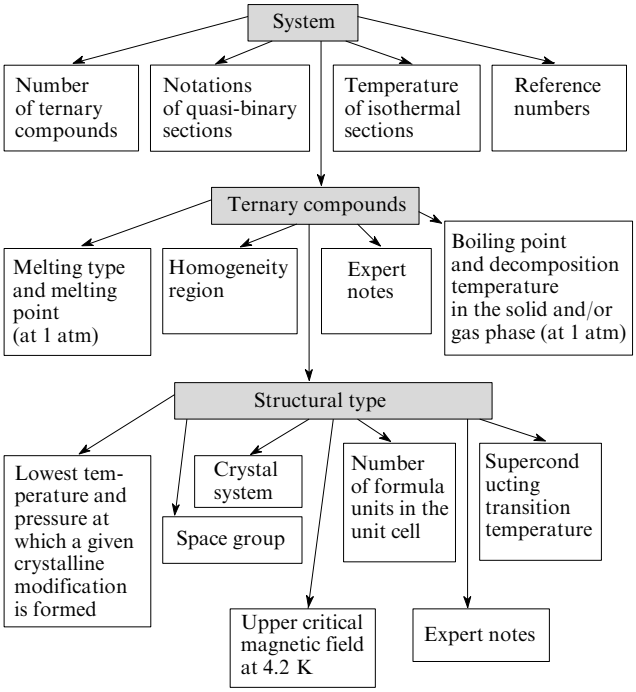

Figure 3. Conceptual structure of a block of data on the properties of compounds: 'Phases' database.

'cleared' from explicit errors and typos. However, assessment of the correctness and/or accuracy of the data reported in original publications requires high-skilled personnel. Databases similar to the 'Diagram' database, which contain information collected and assessed for reliability by high-skilled personnel, form a kind of 'gold information resources' with respect to the quality of data stored and to expenses for their development. However, these expenses are completely paid out because users get the critically assessed recommended values suitable for solving practical problems rather than raw data.

The development of databases on the phase diagrams of systems containing semiconductor phases began with collecting data for binary and ternary systems. The most important information stored in the database is shown in Figs 4 and 5. Of particular value are the analytical reviews on the phase diagrams written by experts. They, in particular, contain additional information on the systems, which is not included in the relational tables. In essence, these reviews are mini-monographs concerning particular systems and characterizing the state-of-the-art in this field.

In the Diagram database, the phase diagrams are stored in the form of bitmap (jpg format) and vector (swf format) images, which ensures, on the one hand, the desired accuracy of the output of portions of a diagram, and, on the other hand, scaling of images and determination of coordinates of points on the $T-x$-projections and isothermal sections.[13] Images are visualized using a conventional Internet browser and Adobe Flash Player (free option). The use of only conventional Web browsers (Microsoft Internet Explorer, Opera, Mozilla Firefox, Google Chrome, *etc.*) advantageously distinguishes the Diagram database from other related systems, *e.g.*, a database on metallic systems,[10] which requires a few megabytes of extra software to be loaded. It should be noted that the use of standard software as user interface is typical of all databases on the properties

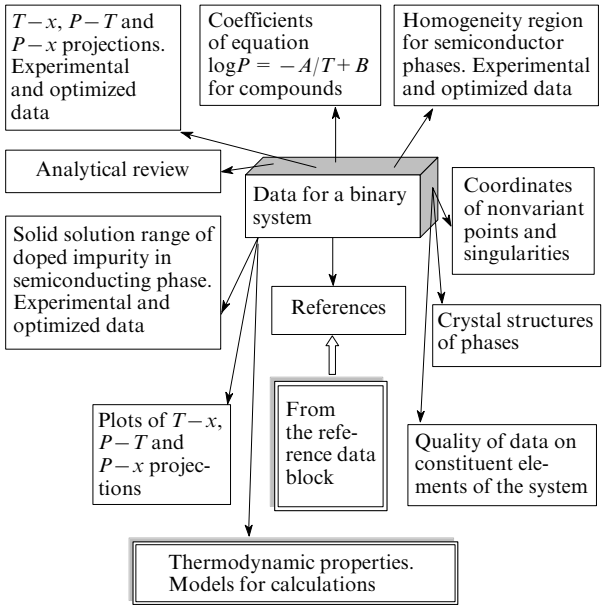

Figure 4. Conceptual structure of the data subsystem on binary systems: 'Diagram' database.

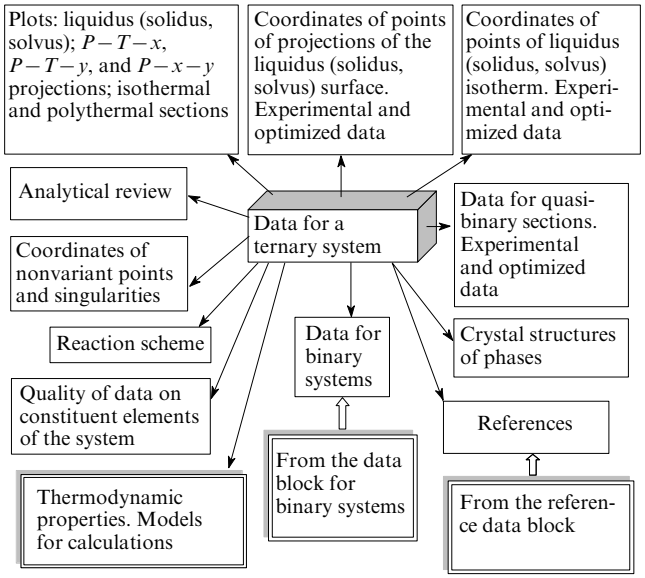

Figure 5. Conceptual structure of a block of data on ternary systems: 'Diagram' database.

of inorganic substances and materials developed at the IMET.

The system of data input, storage and visualization of graphic information is basic to the Diagram database; however, analytical reviews and special tables contain analytical models constructed as a result of thermodynamic self-consistency or statistical optimization of phase diagrams or their elements using different methods. Users can apply these models in their own calculations by substituting the parameters listed in the analytical reviews or stored in the corresponding tables of thermodynamic properties and theoretical models in the database. In addition, the corresponding tables contain the assessed and self-consistent numerical data for elements of phase diagrams.

'Cristal', a database on the properties of acousto-optical, electro-optical and nonlinear optical substances. The Cristal database [13, 16, 17, 21, 22, 46] contains data tables on the properties of acousto-optical, electro-optical and nonlinear optical materials including not only the known, but also new, potentially promising substances. The database structure and the list of the properties are shown in Fig. 6. Tabulated information on each substance is supplemented with an analytical review, which briefly outlines the method of synthesis, possible fields of application, specific properties of substances not covered due to the rigid structure of the database; if possible, an expert assessment of the data stored is given. It is important that information stored in the database was mainly collected and assessed by domestic researchers who designs and uses the materials in question.

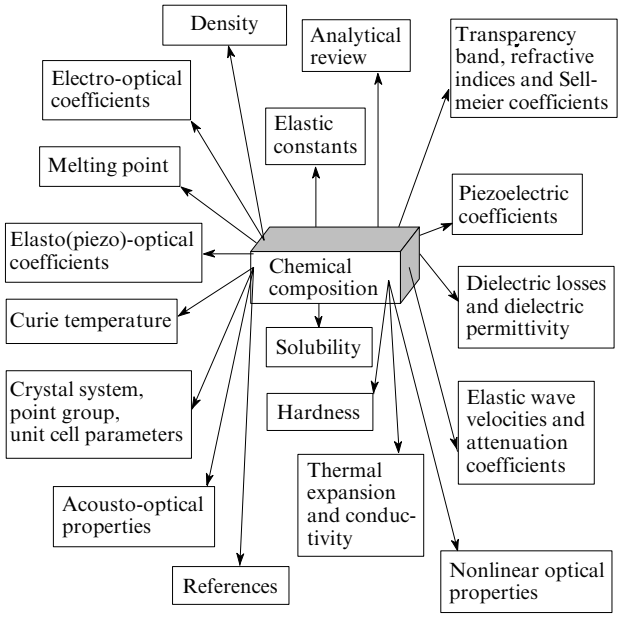

Figure 6. Conceptual structure of a block of data on the properties of substances: 'Cristal' database.

The database contains a large number of plots in the gif format.

Currently, the 'Cristal' database contains data for more than a hundred substances, extracted from 3000 publications. Two versions of this information system, in Russian and in English, are available; registered users can access both of them on the Internet.

'BandGap', a database on the forbidden band width in inorganic substances. The system of databases on the properties of electronic materials includes the 'BandGap' database, which contains information on the forbidden band width in more than four thousands of inorganic substances (Fig. 7).[16, 17] Not only data tables, but graphic information is also present. Only an English-language version of this information system has been developed; registered users can access it on the Internet.

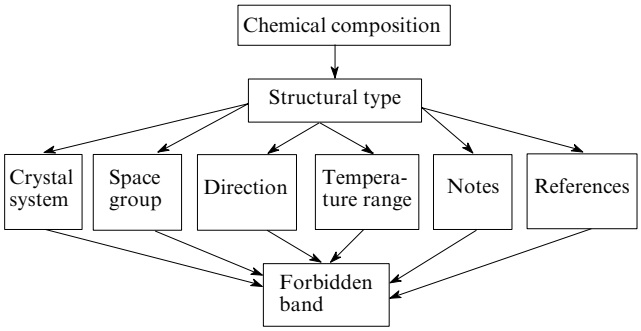

Figure 7. Conceptual structure of a block of data on the properties of substances: 'BandGap' database.

IV. Integration of databases as a trend in development of modern information systems in materials science

Among databases on the properties of inorganic substances and materials, none can provide complete information on all properties of a particular substance or material. Very often, researchers have to browse tens of databases in order to find necessary parameters of a given substance. A possible method of solution to this problem is integration of information sources to provide users with as complete as possible information on inorganic substances.

1. Database integration approaches

There are two strategies of database integration. One of them implies merging of all data into a single information system and serves as a basis for the 'extract, transform, load' (ETL) database integration methodology.[80] In this case, data from different databases are unified, 'cleared' from errors and then loaded into a specialized megabase, referred as 'Data Warehouse'. Creation of such a huge database looks quite attractive, but the unification of data characterized by different accuracy, accumulated in databases created in different institutions and/or countries, using different languages, hardware and software is a very complicated technological and management problem; in addition, the design and management is too expensive.

The second strategy involves virtual integration of databases on the properties of inorganic substances and materials and development of a nonuniformly distributed information system. It is this way that makes it possible to ensure independent development of particular databases and to provide users with access to the whole array of data on a particular substance or material, thus reaching the main goal of integration.[16, 17, 81]

Two main technological approaches are possible in the case of virtual integration of databases: 1) enterprise information integration (EII)[82] and 2) enterprise application integration (EAI).[83]

The former case involves the development of a date access software interface for retrieval of necessary data from different databases; namely, a central information system is built, which interacts with distributed data sources, retrieves information from different databases and sends consolidated data on the desired substance to the user.

The use of the second approach (EAI) is appropriate if databases are supplemented with applied programs. Practical implementation of this strategy involves integration of the user interfaces to access the computational subsystems rather than databases themselves. The role of such interfaces can be played by the Web-applications of corresponding information systems.

In connection with the fact that databases on the properties of inorganic substances and materials can contain identical data of different quality (reliability and completeness) for certain properties of substances there is a need for information quality assessment subsystem in databases to be integrated. Expert assessment should be performed by high-skilled personnel who assess the quality of data in different information systems to be integrated. Thus, if data for a certain property of a substance are available from a number of integrated databases, the system should not only retrieve the data, but also characterize their reliability calculated from the results of expert evaluation. The design of such a data assessment subsystem is one of the most complex organizing problems in database integration.

For skilled users, the results of expert assessment done by colleagues sometimes cast some doubt. In this connection, databases on the properties of inorganic substances and materials should provide hyperlinks to full texts of original publications used as data sources.

2. Integrated database system on the properties of inorganic substances and materials at the IMET

Experience in integration of information resources in inorganic materials science [16, 17] showed that none of the existing approaches is suitable for solving all problems in the integration of data sources and software applications in databases on the properties of inorganic substances and materials. Therefore, a unique complex strategy was proposed, which combines the enterprise information integration (EII) and enterprise application integration (EAI) technologies and can thus be denoted as (EII + EAI).[16, 17, 81] This strategy provides both the possibility of access to current user interfaces and free migration between them (EAI) and a rich potential for data extraction and aggregation obtained from different sources of data on the properties of substances, within EII approach. This methodology was used for integration of databases on the properties of inorganic substances and materials developed at the IMET. This provides powerful instruments for virtual integration of information resources created using different computer platforms, operating systems, DBMS and programming languages and characterized by different reliability of data and other parameters.[16]

At present, the integrated database system on the properties of inorganic substances and materials includes all information systems designed at the IMET ('Phases', 'Elements', 'Diagram', 'Cristal' and 'BandGap' databases) (Fig. 8) and the system for prediction of the properties of inorganic compounds.[84] A feature of this integrated system is that all databases were created using different DBMS and run on the fundamentally different computer platforms, *viz*., Sun ('Diagram' database) and Intel (other databases) under different operating systems, *viz*., Sun Solaris ('Diagram' database) and Microsoft Windows Server (other databases).

Database integration should imply the possibility of retrieving data for a substance selected by the user, if such data are stored in other databases. Thus, there is a need for some coordination unit, which knows what type of information is stored in each database. In other words, there should exist a 'handbook', which in some sense character-

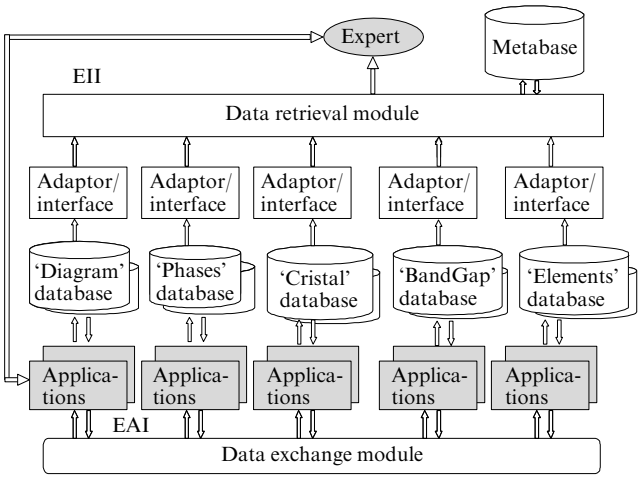

Figure 8. Structure of integrated database system on the properties of inorganic substances and materials at the IMET.

izes the data contained in the integrated databases. This function is executed by a metadata database (metabase)[16,17] (see Fig. 8), which is a special-purpose database containing reference data on the content of the integrated databases, namely, on the chemical systems (which can be identified based on the set of the constituent chemical elements) and substances (which are identified from the ratio of the constituent chemical elements) and on the corresponding properties. These data are sufficient for the search for relevant information on the properties of substances and materials.

When working with an integrated system, registered users enter the database at URL http://www.imet-db.ru. Having chosen a necessary compound in the, *e.g.*, 'BandGap' database, the user works with a menu containing links to other databases opened in separate browser windows. Upon clicking the link the user automatically arrives at a system ('Diagram' database) or a substance ('Cristal' database) containing the same elements as the compound chosen. Of course, such 'jumps' are only possible if the databases include information on related substances.

Currently, integration of databases on the properties of substances and materials is the mainstream of the development of information resources in materials science. It is integration that will allow anyone to get information infrastructure in chemistry and materials science, which will provide researchers with reliable and complete data on the properties of substances and materials and deliver consolidated data at any point of the world *via* the Internet.

V. Information calculating and information analytical systems

The main goal underlying the creation and maintenance of databases is to provide researchers with information service. However, the possibilities of data manipulation are much wider that those seeming at first glance. Traditionally, data retrieved from databases on the properties of inorganic substances and materials are used in thermodynamic and crystal structure calculations. Examples of integrated information calculating systems comprising databases and software for thermodynamic calculations are provided by the F*A*C*T,[45] MALT2,[45–47] MTDATA,[34,35] Thermo-Calc systems,[43,44] *etc*. A characteristic feature of information calculating systems is 'good' analytical description of dependences; in this case, the user should only enter a system command to retrieve necessary data from the database and transfer them to a particular model.

However, most practical problems in chemistry and, especially, materials science, can poorly be formalized using those simple algebraic structures which are used in, *e.g.*, thermodynamics. In particular, such problems include design of novel substances with preset properties, interpretation of spectral information, selection of substances to be used as materials for particular applications, elaboration of optimum processes for production of materials, separation and identification of substances, *etc*. At present, researchers most often solve these problems based on their experience and intuition. To solve poorly formalizable problems, information analytical systems[85] combining databases on the properties of inorganic substances and materials with data analysis subsystems[84] are designed.

Information analytical systems are widely used in business and management for automation of decision making process. Usually, a data analysis subsystem includes tools for data aggregation, processing of complex multicriteria quieries and software for the simplest statistical analysis and visualization of results. In more powerful systems designed to search for complex regularities in large data arrays, data are analyzed using the artificial intelligence software. It is this information analytical system created to search for regularities in databases on the properties of inorganic substances and materials and to use the regularities found for prediction of the possibility of formation of inorganic compounds yet not synthesized and for assessment of their properties has been developed at the IMET.[84,86]

Information analytical systems for the design of inorganic compounds (Fig. 9) include not only an integrated database system and a subsystem for data analysis and prediction (computer learning software),[87,88] but also a

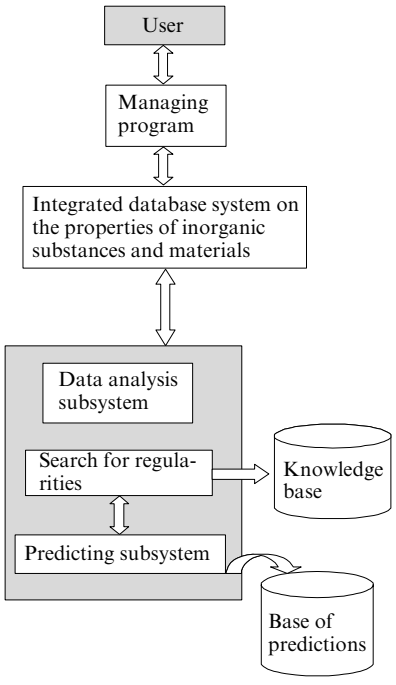

Figure 9. Block diagram of information analytical system for the design of inorganic compounds.

knowledge base and a base of predictions of the possibility of formation and the properties of the yet unknown inorganic compounds.

The information analytical system makes it possible to solve two important problems. First, it provides partially automated analysis of a huge body of experimental data accumulated by chemists to search for regularities followed by the design of novel compounds with predetermined properties. Second, it extends the possibilities of traditional databases on the properties of substances and materials by providing users with not only data on the known and studied substances, but also predictions for the substances not studied so far and their properties. A significant advantage of this information analytical system is the possibility of access *via* the Internet at URL http://ias.imet-db.ru. In this case the user can access 'live' data and regularities. Using the information analytical system, the properties of inorganic compounds not synthesized so far were predicted and some of them were assessed.[86]

VI. Conclusion

Databases on the properties of inorganic substances and materials are hi-tech products. It is not accidentally that the largest number of databases on the properties of inorganic substances and materials were designed and are maintained in the most developed countries including USA, Japan, Russian Federation, *etc*. Expenses for the design of databases on the properties of materials continuously increase, being, *e.g*., about USD 7,400,000 yearly in South Korea.[89] Only in 2009, the NIMS (Japan) was granted by more than USD 1,100,000 for the development of their information systems. In Russian Federation, there is almost no financial support for the design and development of domestic factual databases on the properties of inorganic substances and materials; this will undoubtedly lead to significant backlog in this hi-tech area. It should be noted that the main source of funds for most databases is the federal budget. However, reduction of expenses (i) for unsubstantiated duplication of research and (ii) for information search, as well as the possibility of obtaining reliable and complete data on the properties of substances would pay off the primary budget expenses.

Modern information systems based on computer technologies and containing reliable data can only formally be treated as the infrastructure of science and technology. Data collection and information analysis for databases on the properties of inorganic substances and materials is very often related to fundamental theoretical research and gives an impetus to novel experimental investigations. Usually, subsystems for calculations and prediction of the properties incorporated into many information systems accumulate the latest achievements in theoretical chemistry and materials science.

At present, *e.g*., identification of substances is unconceivable without electronic databases. Nevertheless, traditional mission of databases is to provide information service. Large databases have tens of thousands of users. The possibility of access to information *via* the Internet led to a dramatic increase in the number of users of databases on the properties of inorganic substances and materials. For instance, only in 2009 the information systems at NIMS (Japan) processed more than a 1,000,000 quieries made by about 45,000 researchers from 12,000 institutions.[90] In most cases, information was necessary for the design and investigations of novel materials.[90] The most demanded information concerns the mechanical, physical and chemical properties of substances.[91] Our experience in database management has shown that most users of information systems are researchers working in the field of design of novel substances and materials at academic institutions and universities. The number of users working in industry is still relatively small both in the Russian Federation and abroad.[90]

Analysis of the state-of-the-art in the field of design and maintenance of databases on the properties of inorganic substances and materials revealed the following key features of modern information systems:

— access to information *via* the Internet, which makes it possible to 'deliver' the necessary and most recent data immediately to the workplace of a chemist or materials scientist;

— expert assessment of information by high-skilled personnel which gets the recommended values rather than raw data;

— incorporation of data analysis tools from traditional thermodynamic calculations and statistical procedures to modern instruments of search for regularities in data arrays into databases to enable prediction of the behaviour of objects and ensure the decision making process; and

— integration of databases to provide users with complete information on the properties of particular substances and for further analysis of consolidated information on substances and materials.

International co-operation in database development and integration will allow one to preclude duplication of data and reduce expenses for the development of information systems. To initiate the process, one should overcome severe organizing difficulties, because many databases on the properties of inorganic substances and materials are managed on a commercial basis. However, information and software exchange will improve the marketability of information systems.

Future databases in inorganic chemistry and materials science are considered as a global integrated information system, which is accessible *via* the Internet and contains the expert assessed, recommended values of parameters of substances, references to full texts of original publications and supplemented with software for calculations and prediction of properties.

Databases containing the most demanded information in inorganic chemistry and materials science are briefly outlined in the Appendix, which also includes the following databases not mentioned above: (i) on thermodynamic properties — THERMOSALT,[92] THERSYST,[93] NEA-TDB,[94] TPDS,[95] *etc*., (ii) on the phase diagrams and physical properties — SSD,[97] SMET,[98] a database at the Institute of Chemistry of High-purity Substances, Russian Academy of Sciences,[99,100] EPIDIF,[101] SUPERCON,[102] a database on ceramic materials,[103] C and HTC-DATA,[104] AVOGADRO,[105] RADEN,[106] Gmelin-Online Datensystem,[107] MOGADOC,[108–110] COPPERDATA,[111] a database on amorphous materials,[112] HYDROGENE DATA,[113] SciGlass,[114–117] INTERGLAD,[118] MAT-DB,[119,120] SPTD1,[121] a database on imcommensurate phases,[122] Data-Free-Way,[123–125] and a database on nanocomposites.[126]

This review has been written with partial financial support from the Russian Foundation for Basic Research (Project Nos 09-07-00194, 08-07-00437, 08-01-90427 and 09-01-12060).

VII. Appendix

Table 1. Databases on the properties of inorganic substances and materials.

Database name and subject area	Organization	Country	Internet address [a]	Ref.	Note
IVTANTHERMO — a database on the thermodynamic properties of individual substances	Joint Institute for High Temperatures, Russian Academy of Sciences	Russia	www.chem.msu.su/rus/handbook/ivtan	24, 25	recommended thermophysical and thermodynamic properties of inorganic substances
THERMAL — a database on the thermophysical properties of pure substances	the same	"	www.thermophysics.ru	26, 27	
EPIBIB — a bibliographic database on the intermolecular potentials and transport properties of rarefied neutral gases	"	"	www.thermophysics.ru	28	
NISTTHERMO — a NIST database on the thermodynamic properties of inorganic and organic substances	National Institute of Standards and Technology	USA	www.nist.gov/srd/nist103b.htm; www.nist.gov/srd/nist103a.htm	29	
NIST Ideal Gas Database	the same	"	www.nist.gov/srd/nist88.htm	30	
IL Thermo — a NIST Ionic Liquids Database	"	"	www.nist.gov/srd/nist147.htm	see [b]	
REFPROP — a NIST database on the thermodynamic and transport properties of pure fluids	"	"	www.nist.gov/srd/nist23.htm	31	
Database on the thermophysical properties of gases used in the semiconductor industry	"	"	http://properties.nist.gov/fluidsci/semiprop	see [b]	
THERMODATA — a database on the thermodynamic properties of inorganic substances	THERMODATA, a non-profit association	France	http://thermodata.online.fr	33	bibliography concerning the thermodynamic properties of inorganic compounds and alloys, the thermophysical properties of inorganic compounds and alloys, and the phase diagrams
THERMALLOY — a database on the thermodynamic properties of inorganic substances	the same	"	http://thermodata.online.fr/theraloy.html	see [c]	
THERMOCOMP — a database on the thermodynamic properties of inorganic substances	"	"	http://thermodata.online.fr/anglais.html	see [c]	
MTDATA — a database and software for the calculation of phase equilibria and thermodynamic properties in multicomponent systems	National Physical Laboratory	UK	www.npl.co.uk/server.php&show=ConWebDoc.1226	38, 39	

Table 1 (continued).

Database name and subject area	Organization	Country	Internet address [a]	Ref.	Note
DETHERM — a database on the thermophysical properties of pure substances and mixtures	Gesellschaft für Chemische Technik und Biotechnologie e.V. (DECHEMA)	Germany	http://i-systems.dechema.de/detherm	41	available on the STN network
TPRC/TPMD — the Thermophysical Properties of Matter Database	Center for Information and Numerical Data Analysis and Synthesis of Purdue University	USA	https://cindasdata.com	42	
SGTE — a database on the thermodynamic properties of inorganic substances	The Scientific Group Thermodata Europe	EU	www.sgte.org	34, 35	
THERMO-CALC — a thermodynamic database and software for thermodynamic calculations	Thermo-Calc Software, Inc.	Sweden	www.thermocalc.com	36 – 38	
PPDS — a thermodynamic database and software for thermodynamic calculations	National Engineering Laboratory	UK	www.ppds.co.uk	see [c]	software for thermodynamic calculations and the database on the thermophysical properties of gases and liquids
MALT2 — a database on the thermodynamic properties of individual substances and software for calculation of the equilibrium compositions	Japan Society of Calorimetry and Thermal Analysis	Japan	www.kagaku.com/malt	43, 44	
F*A*C*T — a database on the thermodynamic properties of inorganic substances and software for thermodynamic calculations	Ecole Polytechnic de Montréal, McGill University, Centre de Recherche en Calcul Thermochimique/Centre for Research in Computational Thermochemistry	Canada	www.crct.polymtl.ca/fact	45	
ADAMIS — a database on the properties of alloys for micro-soldering	Tohoku University	Japan	–	47 – 49	thermodynamic properties of alloys for micro-soldering
THERMOSALT — a database on the thermodynamic properties of molten salt mixtures	Universite de Provence	France	–	92	
THERSYST — a database on the thermophysical properties of alloys magne-	Institute for Nuclear Energy and Energy Systems, University of Stuttgart	Germany	–	93	thermophysical and thermodynamic properties of solid aluminium, sium and titanium alloys
NIMS Thermodynamic Database	National Institute of Materials Science	Japan	www.nims.go.jp/cmsc/pst/database/periodic.htm		thermodynamic data and phase diagrams for binary systems
THERM PROP — a database on the thermodynamic properties of minerals	US Geological Survey, National Center for Thermodynamic Data of Minerals	USA		see [c]	

Table 1 (continued).

Database name and subject area	Organization	Country	Internet address [a]	Ref.	Note
NEA-TDB — a database on the thermophysical properties of actinide compounds and other substances for nuclear power engineering	Nuclear Energy Agency	France	www.nea.fr/html/dbtdb/	94	
TPDS — a database on thermophysical properties	National Metrology Institute of Japan, National Institute of Advanced Industrial Science and Technology, Keio University	Japan	http://riodb.ibase.aist.go.jp/TPDB/DBGVsupport/English/	95	thermophysical properties of inorganic and organic substances. The database is based on the *Japan Society of Thermophysical Properties; Thermophysical Properties Handbook* (2nd Ed.) (Tokyo: Yokendo, 2008)
NIST Chemical Kinetics Database	National Institute of Standards and Technology	USA	http://kinetics.nist.gov/kinetics/index.jsp	see [b]	gas-phase kinetic data
Diagram — a database on the phase diagrams of systems containing semiconductor phases	A A Baikov Institute of Metallurgy and Materials Science, Russian Academy of Sciences	Russia	http://diag.imet-db.ru	13 – 17, 46	phase diagrams of systems containing semiconductors; crystal structure data, the semiconducting and thermodynamic properties of phases
NIST Phase Equilibria Diagrams Database	National Institute of Standards and Technology, American Ceramic Society	USA	www.nist.gov/srd/nist31.htm	see [b]	phase diagrams of inorganic systems
Pauling File — a database on the phase diagrams of systems and the crystal structure of compounds	Japan Science and Technology Corporation, Material Phases Data System, National Institute for Materials Science	Japan, Switzerland	http://crystdb.nims.go.jp	12, 50	
MSIT-PDC — a database on the phase diagrams of inorganic systems	Materials Science International Services, GmbH	Germany	www.matport.com/phase-diagram-center/buy-online/purchase/selectElements	10	
The Phase Diagrams Database	American Society for Metals	USA	www.asminternational.org/asmenterprise/apd/help/About.aspx	see [c]	
FactSage — a phase diagrams database	Centre de Recherche en Calcul Thermochimique/Centre for Research in Computational Thermochemistry	Canada	www.crct.polymtl.ca/fact/	45, 96	
TAPP — a database on the phase diagrams and thermodynamic properties of inorganic substances	ESM Software	USA	–	51	
ICSD — a FIZ/NIST Inorganic Crystal Structure Database	Fachinformationszentrum Karlsruhe (FIZ Karlsruhe), National Institute of Standards and Technology	Germany, USA	www.nist.gov/srd/nist84.htm	52 – 57	
Electron Diffraction Database	National Institute of Standards and Technology, Sandia National Laboratory, International Centre for Diffraction Data	USA	www.nist.gov/srd/nist15.htm	58 – 61	

Table 1 (continued).

Database name and subject area	Organization	Country	Internet address [a]	Ref.	Note
NIST CD — NIST Crystal Data	National Institute of Standards and Technology	USA	www.nist.gov/srd/nist3.htm	62	
NIST Structural Database (NSD) — a database on the crystal structure of metals, intermetallics, alloys and minerals	National Institute of Standards and Technology	USA	www.nist.gov/srd/nist83.htm	see [b]	
CRYSTMET — a database on the crystal structures of intermetallics	TOTH Information Systems, Inc.	Canada	www.tothcanada.com	63 – 65	
MINCRYST — a crystallographic and crystal chemical database for minerals and their structural analogues	Institute of Experimental Mineralogy, Russian Academy of Sciences	Russia	http://database.iem.ac.ru/mincryst	66, 67	
PDF — a database on the powder X-ray diffraction data of inorganic and organic substances	International Center for Diffraction Data	USA	www.icdd.com	68, 69	
CSD — a database on the crystal structure of organic and organometallic substances	Cambridge Crystallographic Data Centre	UK	www.ccdc.cam.ac.uk	70 – 72	
NIST Surface Structure Database (SSD)	National Institute of Standards and Technology	USA	www.nist.gov/srd/nist42.htm	97	data on the surface structure of inorganic and organic substances
Phases — a database on the properties of inorganic compounds	A A Baikov Institute of Metallurgy and Materials Science, Russian Academy of Sciences	Russia	http://phases.imet-db.ru	13, 16, 17, 20, 79	
Cristal — a database on the substances possessing specific acousto-optical, electro-optical and nonlinear optical properties	the same	"	http://crystal.imet-db.ru	13, 16, 17, 21, 22, 46	
BandGap — a database on the forbidden band in inorganic substances	"	"	http://bg.imet-db.ru	16, 17	
Elements — a database on the properties of the chemical elements	"	"	http://phases.imet-db.ru/elements	17	
SMET — a database on the properties of materials for electronics	A V Nikolaev Institute of Inorganic Chemistry, Siberian Branch of the Russian Academy of Sciences	Russia	–	46, 48	physical, thermodynamic, semiconducting properties and crystal structure data for semiconductor materials
Database on the physicochemical properties of high-purity substances	Institute of Chemistry of High-Purity Substances, Russian Academy of Sciences	Russia	–	46, 99, 100	physicochemical properties of special purity substances determining the efficiency of purification processes; information on the impurity partition coefficients for two-phase equilibria

Table 1 (continued).

Database name and subject area	Organization	Country	Internet address [a]	Ref.	Note
EMIS — a bibliographic database on semiconductors and other materials for electronics	Institute of Electrical Engineers	UK	see [c]		
MPMD — the Microelectronics Packaging Materials Database	Center for Information and Numerical Data Analysis and Synthesis of Purdue University	USA	https://cindasdata.com/	37	data on the physical and physico-chemical properties of materials for electronics
EPIDIF — a database on the intermolecular potentials and diffusion coefficients for components of CVD processes in microelectronics	Joint Institute for High Temperatures, Russian Academy of Sciences	Russia	—	101	
NIST High-Temperature Superconducting Materials Database (WebHTS)	National Institute of Standards and Technology	USA	www.ceramics.nist.gov/srd/hts/htsquery.htm	see [b]	
SUPERCON — a database on the properties of superconducting materials	National Research Institute for Metals (part of the system of the National Institute of Materials Science databases)	Japan	http://supercon.nims.go.jp/English.html	102	
High magnetic field engineering and cryogenics database	National Institute of Materials Science	Japan	http://yuutsuzu.nims.go.jp/index_eng.html	see [e]	data on the thermal conductivity, electrical conductivity and superconducting properties of substances at low temperatures
ACDB — the Advanced Ceramics Database	Tsinghua University	China	—	see [c]	data on the mechanical and physical properties of silicon nitride and zirconia
NISTCERAM — a NIST Structural Ceramics Database	National Institute of Standards and Technology	USA	www.ceramics.nist.gov/srd/scd/scdquery.htm	see [b]	data on the thermophysical, mechani cal, corrosion properties and porosity of ceramic materials
Functional Ceramic Materials Database	University College London, Imperial College London, University of London, Regional Research Laboratory	UK, India	http://db.foxd.org	103	data on the dielectric permittivity, ion diffusion of oxides and other electroceramic materials. The database includes data mining software for assessment of parameters of particular materials
CERAB — a bibliographic database on the properties of ceramics	Cambridge Scientific Abstracts	USA	—	see [d]	available on the STN network
NIST Gas-Phase Infrared Spectra Database	National Institute of Standards and Technology	USA	www.nist.gov/srd/nist35.htm	see [b]	
C and HTC-DATA — a database on coatings and high-temperature corrosion	Universite de Provence	France	—	104	
AVOGADRO — a database for calculations in the field of physicochemical gas dynamics	Institute of Mechanics, M V Lomonosov Moscow State University	Russia	—	105	

Table 1 (continued).

Database name and subject area	Organization	Country	Internet address [a]	Ref.	Note
DIPPR — a database on the properties of engineering chemicals	Design Institute for Physical Property Data	USA	http://dippr.byu.edu/	73 – 77	temperature-dependent properties of industrially important chemicals
RADEN — a data bank on radiative and energy parameters for diatomic molecules	M V Lomonosov Moscow State University	Russia	www.elch.chem.msu.ru/cgi-bin/raden/raden.cgi	106	
Gmelin-Online Datensystem	Gmelin Institute for Inorganic Chemistry	Germany	–	107	physicochemical properties of inorganic and organometallic compounds. Available on the STN network
MOGADOC — a bibliographic database on the properties of substances in the gas phase	University of Ulm	Germany	www.uni-ulm.de/strudo/mogadoc/	108 – 110	bibliography on the structural, electrical and magnetic properties, electronic and microwave spectra of inorganic, organoelement and organic substances in the gas phase
ASMDATA — a database on the properties of materials	American Society for Metals	USA	http://asmcomm unity.asminternational.org/portal/site/www/MatInformation/OnlineDatabase	see [d]	data on the corrosion, mechanical, physical and other properties of composites, steels, metals, non-ferrous alloys and plastics
COPPERDATA — a bibliographic database on the properties copper and copper alloys	Copper Development Association Inc.	USA	www.csa.com/copperdata	see [d]	data on the mechanical, electrical, corrosion and thermal properties of copper and copper alloys
Information system on rare-earth metals	Changchun Institute of Applied Chemistry of Academia Sinica	China	–	111	data on the physicochemical properties of rare-earth metals and parameters of extraction processes
Amorphous Materials Database	Tohoku University	Japan	–	112	
HYDROGENE DATA — a database on the properties of hydrogen-containing materials	Centre National de la Recherche Scientifique/Centre d'Etudes de Chimie Metallurgique	France	–	117	data on the mechanical, electrical, electrochemical and magnetic properties of hydrogen-containing materials; information on hydrogen diffusion and solubility, on hydrogen storage materials, on the effects of surface, mechanical and heat treatment, structure, *etc*.
NRIM CDS — a database on creep	National Research Institute for Metals	Japan	–	see [c]	data on the creep, breaking strength and tensile strength of steels and alloys

Table 1 (continued).

Database name and subject area	Organization	Country	Internet address [a]	Ref.	Note
MATADOR — a database on the mechanical and physical properties of ferrous materials and non-ferrous metals	Motoren und Turbinen Union München GmbH	Germany	–	see [c]	
DMPME — a database on the mechanical properties of engineering materials	Shanghai Research Institute of Materials	China	–	see [c]	mechanical (including fatigue), physical, corrosion and other properties of ferrous materials and non-ferrous metals, steels and plastics
AAASD — a database on the properties and specifications of aluminium alloys	Aluminum Association, Inc.	USA		see [c]	
nSOFT FATIMAS MDM — a fatigue and cracking database	nCode International Ltd.	UK	www.ncode.com	see [c]	
CETIM-BDM — a database on the physical and mechanical properties of engineering materials	Centre Technique des Industries Mecaniques Centre d Information Technologique	France	–	see [c]	data on the mechanical and physical properties of ferrous materials and non-ferrous metals, steels, composites
SciGlass — a glass property information system	Thermex Company, ITC Inc.	Russia	www.sciglass.info	114 – 117	data on the mechanical, optical and electrical properties of glasses and the phase diagrams
INTERGLAD — a database on glass compositions and properties	New Glass Forum	Japan	http://61.194.5.20/interglad6/index.html	118	the same
Materials Strength Database	National Research Institute for Metals, Japan Information Center of Science and Technology	Japan	–	see [c]	data on the strength of steels, alloys and metals
MAT-DB — a database on the mechanical and physical properties of engineering alloys	Joint Research Centre of the European Commission — Institute for Energy	The Netherlands	–	119, 120	data on the mechanical, physical and corrosion properties of coatings, alloys and ceramics
A database on the properties of optical materials	Sandia National Laboratory	USA	–	see [c]	
FASMET — a database on the fatigue strength of metallic materials	Ritsumeikan University	Japan	–	see [c]	
CRAMET — a database on fatigue crack growth rates of metallic materials	the same	"	–	see [c]	
Fatigue DB — a steels fatigue database	National Institute of Materials Science		https://tsuge.nims.go.jp/top/fatigue.html	see [e]	
MSDRD — the Material Strength Database	Ritsumeikan University	"	–	see [c]	data on the mechanical properties of ceramics, composites and metals
JSSR DB — A database on springs	National Research Institute for Metals	"	–	see [c]	

Table 1 (continued).

Database name and subject area	Organization	Country	Internet address [a]	Ref.	Note
ALFRAC — a database aluminium fracture toughness	The Materials Properties Council, Aluminum Association, Inc., National Institute of Standards and Technology	USA	–	see [d]	strain fracture toughness data for 32 aluminium alloys
MARTUF — a database on the toughness of marine steels	The Materials Properties Council	"	–	see [d]	data on the mechanical, corrosion and other properties of steels
MDF — Metals DataFile, a database on the properties of ferrous alloys and non-ferrous metals	Cambridge Scientific Abstracts	"	–	see [d]	available on the STN network
METALCREEP — a database on the creep and rupture stress properties for aluminium alloys and steels	National Materials Property Data Network Inc.	"	–	see [d]	
SPTD1 — a database on structural phase transitions in crystals	Institute of Low Temperature and Structural Research, Polish Academy of Sciences	Poland	–	121	
ICSDB — The Incommensurate Structure Database	Universidad del Pais Vasco	Spain	www.cryst.ehu.es/icsdb/about.html		
A database of imcommensurate phases	Universite Catholique de Louvain	Belgium	www.mapr.ucl.ac.be/~crystal/index.html	122	
CompoTherm — a database and system for prediction of the thermophysical properties of composites	National Institute of Materials Science	Japan	http://composite.nims.go.jp	78	data on the thermophysical, thermodynamic and mechanical properties of composites
A Database System for Electronic Structures	Japan Science and Technology Corporation, National Institute of Materials Science	"	http://caldb.nims.go.jp/	see [e]	
CCT DB — a welding database system	the same	"	http://inaba.nims.go.jp/Weld/	see [e]	
Data-Free-Way — The Nuclear Materials Database	National Institute of Materials Science	"	http://dfw.nims.go.jp	123 – 125	
The Structural Materials Datasheet Online	National Institute of Materials Science, Japan Atomic Energy Research Institute, Japan Nuclear Cycle Development Institute	"	http://tsuge.nims.go.jp	see [e]	
Database System for Pressure Vessels Materials	National Institute of Materials Science	Japan	http://pvmdb.nims.go.jp/index_eng.html	see [e]	
The Diffusion Database	the same	"	http://diffusion.nims.go.jp/index_eng.html	see [e]	
A database on nanocomposites	D I Mendeleev University of Chemical Technology of Russia	Russia	–	126	

[a] The Internet addresses of the databases are as of December 2009. [b] Information from the website of the US National Institute of Standards and Technology (http://www.nist.gov). [c] Information from the CODATA website (www.codata.org). [d] Information from the STN website (www.stn.com). [e] A database maintained by the National Institute for Materials Science (NIMS, Japan) (http://mits.nims.go.jp/db_top_eng.htm).

References

1. M Hansen, K Anderko *Constitution of Binary Alloys* (New York: McGraw-Hill, 1958)
2. *Fiziko-Khimicheskie Svoistva Poluprovodnikovykh Veshchestv (Spravochnik)* [Physicochemical Properties of Semiconductors (Handbook)] (Eds A V Novoselova, V B Lazarev) (Moscow: Nauka, 1979)
3. *Fiziko-Khimicheskie Svoistva Elementov. Spravochnik* (Physicochemical Properties of Elements. Handbook) (Ed. G V Samsonov) (Kiev: Naukova Dumka, 1965)
4. R P Elliot *Constitution of Binary Alloys* (1st Suppl.) (New York: McGraw-Hill, 1965)
5. F A Shunk *Constitution of Binary Alloys* (2nd Suppl.) (New York: McGraw-Hill, 1969)
6. *Binary Alloy Phase Diagrams* Vols 1, 2 (Ed. T B Massalski) (Materials Park, OH: American Society for Metals, 1990)
7. *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* Vol. 3 (Eds P Villars , L D Calvert) (Metals Park, OH: American Society for Metals, 1985)
8. N A Toropov, V P Barzakovskii, V V Lapin, N N Kurtseva *Diagrammy Sostoyaniya Silikatnykh Sistem. Spravochnik. Dvoinye Sistemy* (State Diagrams of Silicate Systems. A Handbook. Binary Systems) (Moscow, Leningrad: Nauka, 1965) No. 1
9. L F Grigor'eva, G I Kosulina, M A Petrova, A I Sechnoi *Diagrammy Sostoyaniya Sistem Tugoplavkikh Oksidov. Spravochnik. Sistemy Keramicheskikh Vysokotemperaturnykh Sverkhprovodnikov* No. 6 (State Diagrams of Refractory Oxide Systems. Handbook. The Systems of Ceramic High-Temperature Superconductors) (Ed. R G Grebenshchikov) (St Petersburg: Nauka, 1997)
10. G Effenberg, in *The 6th International Scholl-Conference 'Phase Diagrams in Materials Science', 2001 (Technical Program and Abstracts)* (Kyiv: National Academy of Sciences of Ukraine, 2001) p. 1
11. *Intelligent Multimedia Information Retrieval* (Ed. M T Maybury) (Menlo Park, CA, Cambridge, MA: AAAI Press, The MIT Press, 1997)
12. P Villars, M Berndt, K Brandenburg, K Cenzual, J Daams, F Hulliger, T Massalski, H Okamoto, K Osaki, A Prince, H Putz, S Iwata *J. Alloys Compd.* **367** 293 (2004)
13. N N Kiselyova *Komp'yuternoe Konstruirovanie Neorganicheskikh Soedinenii. Ispol'zovanie Baz Dannykh i Metodov Iskusstvennogo Intellekta* (Computer Design of Inorganic Compounds. Application of Databases and Artificial Intelligence Techniques) (Moscow: Nauka, 2005)
14. V S Zemskov, N N Kiselyova, N N Kiselyov, V V Petukhov, E A Cheremushkin, L E Shelimova, N V Kravchenko, I N Belokurova *Neorg. Mater.* **31** 1198 (1995) [a]
15. Yu I Khristoforov, V V Khorbenko, N N Kiselyova, V V Podbel'skii, I N Belokurova, V S Zemskov *Izv. Vyssh. Uchebn. Zaved., Mater. Elektr. Tekh.* (4) 50 (2001)
16. V A Dudarev, N N Kiselyova, V S Zemskov *Persp. Mater.* (5) 20 (2006)
17. N Kiselyova, S Iwata, V Dudarev, I Prokoshev, V Khorbenko, V Zemskov *Int. J. Inform. Technol. Knowledge* **2** 366 (2008)
18. E M Savitskii, N N Kiselyova, B N Pishchik, N V Kravchenko, M S Golikova *Dokl. Akad. Nauk SSSR* **279** 627 (1984) [b]
19. N V Yudina, V V Petukhov, E A Cheremushkin, N N Kiselyova, V S Zemskov *Kristallografiya* **41** 490 (1996) [c]
20. N Kiselyova, D Murat, A Stolyarenko, V Dudarev, V Podbel'skii, V Zemskov *Inform. Res. Ross.* (4) 21 (2006)
21. Yu I Degtyarev, V V Podbel'skii, N N Kiselyova, V V Petukhov, O V Shekhanova, A A Bush, I N Belokurova, V A Pushko *Izv. Vyssh. Uchebn. Zaved., Mater. Elektr. Tekh.* (3) 35 (1999)
22. N N Kiselyova, I V Prokoshev, V A Dudarev, V V Khorbenko, I N Belokurova, V V Podbel'skii, V S Zemskov *Neorg. Mater.* **42** 380 (2004) [a]
23. *World Databases in Chemistry (World Databases Ser.)* (Ed. C J Armstrong) (East Grinstead, UK: Bowker-Saur, 1996)
24. L V Gurvich *Vestn. Akad. Nauk SSSR* (3) 54 (1983) [d]
25. G V Belov, V S Iorish, V S Yungman *CALPHAD* **23** 173 (1999)
26. M S Trakhtengerts *Nauchno-Tekhnich. Inform., Ser. 2, Inform. Protses. Sist.* (6) 30 (2006)
27. M S Trakhtengerts *Nauchno-Tekhnich. Inform., Ser. 2, Inform. Protses. Sist.* (7) 28 (2006)
28. V Yu Zitserman, G A Kobzev, L R Fokin, in *Teplogidravlicheskie Aspekty Bezopasnosti AEU s Reaktorami na Bystrykh Neitronakh. Mezhotraslevaya Tematicheskaya Konferentsiya (Tez. Dokl.)* [Heat-Hydraulic Aspects in Safety of Nuclear Energy Plants with Fast Reactors. Inter-Branch Thematic Conference (Abstracts of Reports)] (Obninsk: Leipunsky Institute for Physics and Power Engineering, 2005) p. 87
29. P Wang, D B Neumann *J. Chem. Inf. Comput. Sci.* **29** 31 (1989)
30. *NIST Standard Reference Database 88. NIST/TRC Ideal Gas Database. Version 2.0. Users' Guide* (Gaithersburg: NIST, 2006)
31. J G Kaufman, V J Drago *Model. Simul. Mater. Sci. Eng.* (1) 335 (1993)
32. M W Chase, C A Davies, J R Downey, D J Frurip, R A McDonald, A N Syverud *J. Phys. Chem. Ref. Data* **14** 1 (1985)
33. B Cheynet *CODATA Bull.* **58** 18 (1985)
34. P J Spencer *Z. Metallknd.* **87** 535 (1996)
35. A T Dinsdale *CALPHAD* **15** 317 (1991)
36. J-O Andersson, B Jansson, B Sundman *CODATA Bull.* **58** 31 (1985)
37. B Sundman, B Jansson, J-O Andersson *CALPHAD* **9** 153 (1985)
38. J-O Andersson, T Helander, L Hoglund, P Shi, B Sundman *CALPHAD* **26** 273 (2002)
39. R H Davies, A T Dinsdale, J A Gisby, J A J Robinson, S M Martin *CALPHAD* **26** 229 (2002)
40. Z Huang, P P Conway, R C Thomson, A T Dinsdale, J A J Robinson *CALPHAD* **32** 129 (2008)
41. U Westhaus, T Droge, R Sass *Fluid Phase Equil.* **158 – 160** 429 (1999)
42. C Y Ho, H H Li *J. Chem. Inf. Comput. Sci.* **33** 36 (1993)
43. H Yokokawa, S Yamauchi, T Matsumoto *Thermochim. Acta* **245** 45 (1994)
44. H Yokokawa, S Yamauchi, T Matsumoto *CALPHAD* **26** 155 (2002)
45. C W Bale, P Chartrand, S A Degterov, G Eriksson, K Hack, R Ben Mahfoud, J Melanqon, A D Pelton, S Petersen *CALPHAD* **26** 189 (2002)
46. V S Zemskov, F A Kuznetsov, V B Ufimtsev *Izv. Vyssh. Uchebn. Zabed., Mater. Elektron. Tekhn.* (3) 13 (1998)
47. I Ohnuma, X J Liu, H Ohtani, K Ishida *J. Electron. Mater.* **28** 1164 (1999)
48. X J Liu, I Ohnuma, C P Wang, R Kainuma, K Ishida, M Ode, T Koyama, H Onodera, T Suzuki *J. Electron. Mater.* **32** 1265 (2003)
49. X J Liu, K Oikawa, I Ohnuma, R Kainuma, K Ishida *JOM* **55** 53 (2003)
50. P Villars, N Onodera, S Iwata *J. Alloys Compd.* **279** 1 (1998)
51. *TAPP Database. Version 2.1* (Hamilton, USA: ESM Software Inc., 1991 – 1994)
52. G Bergerhoff, R Hundt, R Sievers, I D Brown *J. Chem. Inf. Comput. Sci.* **23** 66 (1983)
53. G Bergerhoff *Comp. Phys. Communs* **33** 79 (1984)
54. E Fluck *J. Res. NIST* **101** 217 (1996)
55. A Belsky, M Hellenbrandt, V L Karen, P Luksch *Acta Crystallogr., Sect. B* **58** 364 (2002)
56. M Hellenbrandt *Crystallogr. Rev.* **10** 17 (2004)
57. R Allmann, R Hinek *Acta Crystallogr., Sect. A* **63** 412 (2007)
58. M J Carr, W F Chambers, D Melgaard, V L Himes, J Stalick, A D Mighell *J. Res. NIST* **94** 15 (1989)
59. A D Mighell, V L Karen *J. Res. NIST* **101** 273 (1996)
60. D R Denley, H V Hart *J. Appl. Crystallogr.* **35** 546 (2002)
61. H V Hart *J. Appl. Crystallogr.* **35** 552 (2002)
62. S K Byram, C F Campana, J Fait, R A Sparks *J. Res. NIST* **101** 295 (1996)
63. G H Wood, J R Rodgers, S R Gough *J. Chem. Inf. Comput. Sci.* **33** 31 (1993)
64. G H Wood, J R Rodgers, S R Gough, P Villars *J. Res. NIST* **101** 205 (1996)

65. P S White, J R Rodgers, Y Le Page *Acta Crystallogr., Sect. B* **58** 343 (2002)
66. A V Chichagov, A B Belonozhko, A L Lopatin, T N Dokina, O L Samokhvalova, T V Ushakovskaya, Z V Shilova *Kristallografiya* **35** 610 (1990) [c]
67. A V Chichagov, D A Varlamov, in *Teoriya, Istoriya, Filosofiya i Praktika Mineralogii (Mater. IV Mezhdunar. Mineralogicheskogo Seminara)* [The Theory, History, Philosophy and Practice of Mineralogy (Proceedings of IVth International Mineralogy Seminar)] (Syktyvkar: Geoprint, 2006) p. 295
68. J Faber, T Fawcett *Acta Crystallogr., Sect. B* **58** 325 (2002)
69. S N Kabekkodu, J Faber, T Fawcett *Acta Crystallogr., Sect. B* **58** 333 (2002)
70. F H Allen, J E Davies, J J Galloy, O Johnson, O Kennard, C F Macrae, E M Mitchell, G F Mitchell, M Smith, D G Watson *J. Chem. Inf. Comput. Sci.* **31** 187 (1991)
71. D G Watson *J. Res. NIST* **101** 226 (1996)
72. F H Allen *Acta Crystallogr., Sect. B* **58** 385 (2002)
73. E Buck, E M Frankl *Chem. Eng. Progr.* **80** 82 (1984)
74. D A Palmer *AIChE Symp. Ser.* **86** 1 (1990)
75. Q Dong, A K R Dewan, K N Marsh *Int. J. Thermophys.* **202** 237 (1999)
76. G H Thomson, A H Larsen *J. Chem. Eng. Data* **41** 930 (1996)
77. W V Wilding, R L Rowley, J L Oscarson *Fluid Phase Equil.* **150**–**151** 413 (1998)
78. Y Xu, M Yamazaki, H Wang, K Yagi *Mater. Trans.* **47** 1882 (2006)
79. N N Kiselyova, N V Kravchenko, V V Petukhov *Neorg. Mater.* **32** 636 (1996) [a]
80. R Kimball, J Caserta *The Data Warehouse ETL Toolkit: Practical Techniques for Extracting, Cleaning, Conforming, and Delivering Data* (London: Wiley, 2004)
81. V Kornyushko, V Dudarev *Int. J. Inform. Theor. Applic.* **12** 121 (2006)
82. J P Morgenthal *Enterprise Information Integration: a Pragmatic Approach* (Morrisville: Lulu.com, 2005)
83. J P Morgenthal *Enterprise Applications Integration with XML and Java* (New York, Sydney, London: Prentice Hall PTR, 2000)
84. N Kiselyova, A Stolyarenko, V Ryazanov, V Podbel'skii *Int. J. Inform. Theor. Applic.* **15** 345 (2008)
85. V V Korneev, A F Gareev, S V Vasyutin, V V Raikh *Bazy Dannykh. Intellektual'naya Obrabotka Informatsii* (Databases. Intellectual Processing of the Information (Moscow: Izdatel' Molgacheva S V, 2001)
86. G S Burkhanov, N N Kiselyova *Usp. Khim.* **78** 615 (2009) [*Russ. Chem. Rev.* **78** 569 (2009)]
87. Yu I Zhuravlev, V V Ryazanov, O V Sen'ko *'Raspoznavanie'. Matematicheskie Metody. Programmnaya Sistema. Prakticheskie Primeneniya* ('Recognition'. Mathematical Methods. Programme System. Practical Applications) (Moscow: FAZIS, 2006)
88. V P Gladun *Protsessy Formirovaniya Novykh Znanii* (Process of Formation of new Knowledge) (Sofiya: Pedagog, 1995)
89. B K Kim, Y M Rhyim, in *Proceedings of the International Symposium on Materials Database (MITS 2008)* (Tsukuba: NIMS, 2008) p. 68
90. M Yamazaki, in *Proceedings of the International Symposium on Materials Database (MITS 2009)* (Tsukuba: NIMS, 2009) p. 7
91. Y Xu, in *Proceedings of the International Symposium on Materials Database (MITS 2009)* (Tsukuba: NIMS, 2009) p. 4
92. M Gaune-Escard, J-P Bros, Y Fouque, P Gaune, G Hatem, P Juhem *Metaux* **64** 208 (1988)
93. A M Zahra, C Y Zahra, R Castanet, G Jaroma-Weiland, G Neuer *J. Therm. Anal.* **38** 781 (1992)
94. E Östhols, H Wanner *The NEA Thermochemical Data Base Project* (Issy-les-Moulineaux: OECD Nuclear Energy Agency, 2000)
95. T Baba, Y Yamashita, A Nagashima *J. Chem. Eng. Data* **54** 2745 (2009)
96. A D Pelton *Rare Met.* **25** 473 (2006)
97. M A Van Hove, K Hermann, P R Watson *Acta Crystallogr., Sect. B* **58** 338 (2002)
98. S A Magarill, S V Borisov, N V Podberezskaya, E N Ipatova, V A Titov, F A Kuznetsov *Zh. Strukt. Khim.* **36** 559 (1995) [e]
99. G G Devyatykh, I D Kovalev, V A Krylov, K K Malyshev, L I Osipova *Izv. Vyssh. Uchebn. Zaved., Mater. Elektr. Tekhn.* (3) 44 (1998)
100. G G Devyatykh, Yu A Karpov, L I Osipova *Vystavka-Kollektsiya Veshchestv Osoboi Chistoty* (Exhibition-Collection of Special Substances Purity) (Moscow: Nauka, 2003)
101. L Fokin, V Popov, A Kalashnikov, L Zarkova, P Pirgov, I Petkov *Int. J. Thermophys.* **22** 1497 (2001)
102. Y Asada, E Nakada, T Yokokawa, Y Kurihara, A Yoshikawa *J. Mater. Sci. Soc. Jpn.* **24** 199 (1988)
103. D J Scott, S Manos, P V Coveney, J C H Rossiny, S Fearn, J A Kilner, R C Pullar, N McN Alford, A-K Axelsson, Y Zhang, L Chen, S Yang, J R G Evans, M T Sebastian *J. Chem. Inf. Model.* **48** 449 (2008)
104. S Komornicki, R Streiff *J. Phys. IV* **3** 1013 (1993)
105. E A Kovach, S A Losev, A L Sergievskaya *Metally* (4) 70 (1993)
106. L A Kuznetsova, E A Pazyuk, A V Stolyarov, in *Khimiya MGU* (The Chemistry of Moscow State University) (Moscow: Moscow State University, 1994) p. 53
107. A Nebel, U Tolle, R Maass, G Olbrich, R Deplanque, P Lister *Anal. Chim. Acta* **265** 305 (1992)
108. A Lohr, B Mez-Starck, H-G Schirdewahn, D-G Watson *J. Mol. Struct.* **97** 57 (1983)
109. J Vogt *J. Mol. Spectrosc.* **155** 249 (1992)
110. J Vogt, B Mez-Starck, N Vogt, W Hutter *J. Mol. Struct.* **485**–**486** 249 (1999)
111. L Xu, G Li, S Wang, H Lu, H Wang, C Hu, X Jiang, Y Xiao, Y Xiao, X Lu *J. Chem. Inf. Comput. Sci.* **31** 375 (1991)
112. T Nakanomyo, Y Akiyama, T Itoh, S Wada, N Mori, A P Tsai, Y Kawazoe *Sci. Repts. Res. Inst. Tohoku Univ.* **37** 228 (1992)
113. S Talbot-Besnard, M Rubinstein, C Droniou *Ann. Chim. (France)* **13** 611 (1988)
114. A I Priven, O V Mazurin *Adv. Mater. Res.* **39**–**40** 147 (2008)
115. O V Mazurin *J. Non-Cryst. Solids* **351** 1103 (2005)
116. O V Mazurin, Yu Gankin *J. Non-Cryst. Solids* **342** 166 (2004)
117. O V Mazurin, V V Gusarov *Fiz. Khim. Stekla* **28** 74 (2002) [f]
118. T Saitou, H Oguro, T Fukami, T Iseda, in *Proceedings of the Japan Society of Information and Knowledge, 1999* p. 63
119. M Nagy, H H Over, E Wollfart *Data Sci. J.* **4** 151 (2005)
120. H H Over, E Wolfart, W Dietz, L Toth *Adv. Eng. Mater.* **7** 766 (2005)
121. V Janovec, P E Tomaszewski, L Richterova, J Fabry, Z Kluiber *Ferroelectrics* **301** 169 (2004)
122. R Caracas *J. Appl. Crystallogr.* **35** 120 (2002)
123. H Tsuji, N Yokoyama, M Fujita, Y Kurihara, S Kano, Y Tachi, K Shimura, R Nakajima, S Iwata *J. Nucl. Mater.* **271**–**272** 486 (1999)
124. Y Kaji, Y Miwa, T Tsukada, H Tsuji, H Nakajima *J. Nucl. Sci. Techn.* **37** 949 (2000)
125. Y Kaji, H Tsuji, M Fujita, Y Xu, K Yoshida, S Mashiko, K Shimura, S Miyakawa, T Ashino *Data Sci. J.* **3** 88 (2004)
126. E Vasilenko, T Meshcheryakova, F Batsylev, E Poryseva *Inform. Res. Rossii* (4) 5 (2009)

[a] — *Inorg. Mater. (Engl. Transl.)*
[b] — *Dokl. Phys. (Engl. Transl.)*
[c] — *Crystallogr. Rep. (Engl. Transl.)*
[d] — *Herald Russ. Acad. Sci. (Engl. Transl.)*
[e] — *J. Struct. Chem. (Engl. Transl.)*
[f] — *Glass Phys. Chem. (Engl. Transl.)*