Glass Physics and Chemistry, Vol. 28, No. 1, 2002, pp. 50–58.

The Future of Information Technologies in Materials Science

O. V. Mazurin and V. V. Gusarov

Grebenshchikov Institute of Silicate Chemistry, Russian Academy of Sciences,.
ul. Odoevskogo 24/2, St. Petersburg, 199155, Russia

Received August 23, 2001

Abstract—Problems of the development of information technologies in materials science are considered. It is shown how promising is the creation of a single information system that describes the structure, phase state, and properties of various classes of materials: glasses, ceramics, polymers, composites, etc. A forecast is made concerning the development of information systems based on electronic information carriers in materials science.

INTRODUCTION

Many papers that appeared at the turn of the century and predict the possible development routes of science and technology (see, for example, [1–3]), for some reason, devote relatively little space to the general problem of the maximum saving of resources at humanity's disposal. Yet it is the successful solution of this very problem that is the main condition not just for further human progress but even for the very survival of the human race in the conditions of continued intensive population growth. An important point in this connection is the need to make thrifty use of renewable as well as nonrenewable resources (useful minerals). The fact is that the annual increment of all renewable resources is limited, and, sooner or later, humankind will reach the natural limit of their utilization potential.

One of the most important of the renewable resources, used extensively by human society, is new scientific and technical information. The scale on which such information is obtained undoubtedly depends greatly on technological progress. It also depends, in no smaller measure, on such extensive factors as appropriations for basic and applied science. In the middle of the 20th century, these appropriations grew rapidly in practically all the countries of the world. Now they are declining steadily, and the number of researchers is declining accordingly in all the technologically advanced countries. At the same time, the sphere of research is expanding continuously. As a result, the growth rate of the production of scientific and technical information is, on the whole, declining. In a number of industries, there are already signs of a definite slump in information activity.

Especially timely, in this situation, are steps to ensure that already accumulated knowledge is used efficiently. In the 1970s, information science experts were fond of referring to the findings of one of the leading American chemical companies. It followed from these findings that, if a company had to start manufacturing some chemical product that it had not made before and if the appropriate technology was unknown to it, then, should the development of such a technology, according to a preliminary estimate, cost less than $100 000, it would be more profitable to start the development work from scratch rather than search the literature for possibly available information about the methods of manufacturing such a product. Today the system of searching for information in the available scientific literature has somewhat (not cardinally!) improved, but the volume of available information has since then expanded greatly. So that the problem is at least just as acute.

Thus, the colossal volume of knowledge accumulated by humanity and gathered in giant libraries (for example, the largest storage of learning, the Library of Congress in the United States, has approximately 112 000 000 books and documents, which occupy shelves 857 km long) is used quite insufficiently. Accordingly, new generations of researchers at times study regularities already studied before them instead of concentrating all their efforts in new, as yet unexplored areas. Note, also, that in materials science the quality of new measurements may at times be inferior to the quality of old ones [4], whose results have been undeservedly forgotten.

Fortunately, humanity now has at its disposal means of radically altering the situation. This requires transferring all potentially useful information from paper to electronic carriers, moreover in a form that would make possible a speedy and absolutely reliable search for information, a comparison of data from different research projects, their generalization, processing, use as a basis for predictions, and utilization for the automated solution of the most diverse practical problems. Future advances in computer technology should expand these possibilities even more, but what is already available to humankind in this field is more than enough. Nevertheless, the transfer of scientific and technical information to electronic carriers (in the form described above) is so far proceeding relatively slowly.

0360-5043/02/2801-0050$27.00 © 2002 MAIK “Nauka / Interperiodica”

The reasons for this, in our view, are social and psychological rather than technical. The transfer of scientific information from paper to electronic carriers should radically alter many aspects of the work of specialists and cardinally change the mentality of the leaders of scientific and educational institutions and industrial companies. The assumption of leading posts by a new generation of specialists, accustomed to everyday contact with electronic technology, should greatly speed these processes. At present, specialists who are aware of the importance and absolute inevitability of the coming computer revolution in the information support of science and technology should, to the best of their abilities and potentialities, prepare the ideological groundwork for such a revolution. A large number of complex problems will have to be solved (solved speedily, when the time comes), and this will largely determine the efficiency of the global network that will be set up for the electronic system of scientific and technical information. In this situation, any preliminary experience of work in this area may prove highly valuable.

EXPERIENCE GAINED IN DEVELOPING MATERIALS-SCIENCE INFORMATION TECHNOLOGIES AT THE INSTITUTE OF SILICATE CHEMISTRY OF THE RUSSIAN ACADEMY OF SCIENCES

Work that paved the way to the institute's successes in applying information technologies to inorganic nonmetallic materials began about 40 years ago, when the Institute began compiling handbooks. The fact is that one of the most important conditions for the optimal formation of materials-science databases is an ability to unite information from the most diverse sources and, accordingly, presented in the most different formats in a single, rationally structured system of data storage. At this stage of the work, it is not so important whether a paper or electronic information carrier is used to present the results.

The great significance of handbooks in materials science was appreciated by N.A. Toropov, the director of the Institute of Silicate Chemistry in 1953–1968, as early as the beginning of the 1960s. He initiated the work of compiling the handbook *Diagrammy sostoyaniya silikatnykh sistem* (Phase Diagrams for Silicate Systems), whose first volume appeared in 1965 [5] and the last (so far), tenth volume in 1997 [6]. A very important (from our point of view) feature of this reference book deserves to be emphasized. In addition to phase diagrams, the handbook lists some of the most important properties of the crystalline phases of the corresponding system and the principal areas of the application of materials on the basis of the systems described; there is also information on the methods of interpreting the diagrams presented in the handbook. Despite the fact that the American Ceramic Society has likewise begun publishing a handbook of many volumes on phase diagrams [7], the handbook of the Institute of Silicate Chemistry, because of its above-mentioned presentation features, so far remains the only one of its kind in the world. The significance of this approach will be examined in the next section.

A few years after the publication of the first volume of the handbook on phase diagrams [8], the Institute of Silicate Chemistry undertook the publication of another reference work of the same type, *Spravochnik po svoistvam stekol i stekloobrazuyushchikh rasplavov* (Handbook of Properties of Glasses and Glass-Forming Melts) [8], which appeared only in 1999. It should be emphasized that the idea of publishing such a handbook was, in his day, vigorously supported by Toropov, and this unquestionably played a significant role in the decision to launch such a publication. This was followed by the publication of an English version of the handbook [9], which was completed in 1994. The main feature of this handbook was, once again, the inclusion in it of very detailed information concerning synthesis conditions and the methods of measuring the properties of corresponding compositions of glasses. Such information was absent in even the best of the subsequently published handbooks of glass properties [10].

As far as we know, no other materials-science handbook on any other materials (polymers, metals, semiconductors, etc.) contains detailed information about experiments performed (enabling the qualified reader to assess the reliability of the data cited). The Institute of Silicate Chemistry thus proved to be the only institution to produce handbooks of a new generation, which are best suited for creating high-quality electronic databases.

It is thus quite logical that the authors of the handbooks [8, 9] were among those who were ready to take part in creating prototype electronic information systems of the 21st century in materials science. However, creating a high-quality electronic information system required very substantial financial outlays. A very serious problem arose here: the market for databases on glasses and melts turned out to be very limited (unlike the markets, say, for databases on the properties of ceramic goods, polymers, or metals). Moreover, this market was already occupied by a Japanese databases on glass properties [11], which, despite fundamental shortcomings, was none the less well familiar to potential customers. As a result, not only was there no clear prospect of making a profit, but even the investments in producing an information system on glasses and melts might not have been recouped. Fortunately, the American company SciVision decided to take the financial risk of acquiring what might be called the invaluable experience of creating electronic materials-science information systems of a new generation.

As a result, there appeared the SciGlass information system [12], which combined the experience of experts at the Institute of Silicate Chemistry in materials science with that of programmers at SciVision in producing software products for scientific research. Many fundamental decisions were taken [13] in developing the SciGlass system, and this is confirmed by the high assessments of this software product by leading specialists on glass [14–16].

It is a fact that in recent decades quite a few experts have realized how promising is the development of electronic databases of the properties of substances and materials, and have taken concrete and successful steps in this area. Thus, one of the first databases in metallurgy and thermochemistry (MTDATA) was developed in Britain with the active participation of the National Physical Laboratory as far back as 1971. Several rival databases appeared later in the same area, such as CSIRO (Australia), THERDAS (Federal Republic of Germany), THERMOCALC (Sweden), THERMODATA (France), MANLABS (United States), F*A*C*T* (Canada), HSC (Finland), and IVTANTHERMO (Soviet Union) [17–20]. Such a variety of databases on thermochemistry could not survive for long. Work began to create the Integrated Base of Thermochemical Data (ITD), and the international consortium SGTE (Scientific Group Thermodata Europe) was set up for this purpose [20]. Undoubtedly, the establishment of special databases of definite groups of properties, which would encompass information on these properties with respect to the most diverse classes of substances, is highly important, and there is a fine outlook for the development of such databases. However, in our view, the key role in future belongs to databases of the properties of definite large classes of materials, which would unite, on a single basis, data on all the practically meaningful properties of a certain class of materials and/or substances.

It should be noted that, whereas in information scope and quality, the databases of the thermodynamic properties of substances proved to be of a sufficiently high standard, the databases containing information on the phase diagrams of systems were presented in a much less convenient format and covered a rather limited number of systems. For example, THERMOSALT contains data on the phase diagrams of only some salt systems; another database, CALPHAD, contains phase diagrams of a limited number of oxides and nitrides, published in the journal of the same name, and still another database, SLAG, of the THERMOCALC set of databases, contains data on phase diagrams based on seven oxides. All the above-mentioned databases use an unfortunate format for presenting data on phase diagrams (lacking extensive commentaries on methods of studying phase equilibria, on phase properties and structure, on potential application areas, etc.), have an inconvenient interface, embrace limited numbers of systems, and possess other faults. These circumstances-and the extensive experience of our institute's researchers in collecting and analyzing data on phase diagrams, accumulated in producing the above-mentioned *Handbook* [5, 6]—suggested starting work at the institute on creating our own version of a database and an information system on the phase diagrams and properties of ceramic materials. This work proceeded in the direction of converting the handbook of phase diagrams of silicate and refractory oxide systems to an electronic format. Although the work on this project is proceeding extremely slowly because of limited financial resources, it has been possible to demonstrate that it is full of promise. For example, some elements of the Information System of Phase Diagrams of Binary, Ternary, and Multicomponent Systems [21]—as is evident from the experience of their use by materials-science specialists, engineers, and students-significantly intensifies the process of designing new materials, analyzing changes in a material, etc. They also help to avoid strictly calculation errors that occur in converting component concentrations from some units to others, in conducting computations according to the lever rule, in determining temperatures on the liquidus surface in ternary systems, etc. In addition to these advantages, the electronic format of presenting data on phase status has made it possible to develop a basically new, animation, design of phase diagrams of multicomponent systems, which is impossible if information is presented by traditional methods [16]. Unfortunately, the authors were unable to produce a database that would cover the entire spectrum of the information available on phase diagrams. Such a database can be developed only if adequate funding were available.

THE GENERAL OUTLOOK FOR THE DEVELOPMENT OF MATERIALS-SCIENCE INFORMATION TECHNOLOGIES

Introductory remarks. As was noted above, the volume of scientific information in the world is constantly growing, and this process will continue. This, of course, is also true of such a major area of knowledge as materials science. However, it may be predicted with sufficient confidence that the principal areas of materials science, the areas in which the largest databases will be created, will be shaped mainly by practical needs. The fact is that the work of developing databases, which embrace enormous bodies of information with adequate scope and reliability, requires sizable investments and, hence, can be undertaken only with a view to extensive solvent demand.

The formation of databases of the properties of metals, ceramics and refractories, binders, polymers, composites, various chemical compounds, melts and glasses, biologically active and certain other substances is of obvious importance for practical needs. In addition to this, materials science will require at least two other specific databases: of the structure of crystals and of phase diagrams. Such databases are in a certain sense basic in solving problems of designing new materials and the technologies of their production. The outlook for developing databases of this type will be considered in the present section.

The formation of databases of the properties of substances and materials. Future electronic databases of the properties of materials (hereafter, DBPM) will have to contain absolutely all the accumulated information of practical interest about the influence of composition, production techniques, and structure on the properties of substances and materials. All the data on the properties of materials will have to be supplemented with sufficiently detailed descriptions of the methods of measuring these properties. The DBPM creators will face the task of ridding the overwhelming majority of users of the need to spend time on searching and familiarizing themselves with the original literature. The search for most of the literature containing information on the properties of substances and materials will also be simplified considerably in the near future. However, it is reasonable to assume that data from dissertations, reports, and many publications dating back to the first half of the 20th century and, all the more so, to the 19th century will even then not be readily available. But what is most important is that DBPM should make it possible to do without reading the literature in different languages (the problem of the exact translation of scientific and technical terms and notions, specific for every area of science and technology, will for a long time to come remain a stumbling block for electronic translators), analyzing the data cited, extracting them by scanning, comparing them with other data, etc. Besides, much less time will be needed to obtain the information needed. As a result, a specialist will in very many cases not have to work at all with the original papers. This, however, will also require that the DBPM be highly reliable. It is unrealistic to expect that the possibility of errors in transferring data from the original papers to the electronic format will be ruled out completely. But the percentage of errors can and must be reduced to a minimum. This means that the percentage of errors in the databases should be much lower than the percentage of errors in the original literature, most of which it will be the duty of the high-class specialists entrusted with developing the DBPM to detect and correct. The experience already gained shows that the achievement of this goal is quite realistic. Consequently, a comparison of the reliabilities of the DBPM and the original papers will be clearly in favor of the DBPM.

Thus, the DBPM of the 21st century will have to meet three express conditions: guarantee comprehensive searching of originals containing information on the properties of substances and materials, comprehensive extraction of information required for practical use, and the reliability of its representation. A natural question that arises is: when can we expect such databases to be developed?

The project nearest completion is that of creating an all-embracing database of inorganic nonmetallic melts and glasses. The SciGlass base (not covering data on chalcogenide glasses or salt melts) at present contains data on more than 200000 glasses and melts. The total number of compositions whose various properties have been studied, within the range of substances presently covered by SciGlass, is put at roughly 250000–280000. Given favorable circumstances, this database (with the above-mentioned limitations) may in a few years be almost complete. It should be borne in mind that the work of information searching and collecting has been conducted in this field since the end of the 1960s. The work on all the inorganic melts and glasses (i.e., including chalcogenide glasses and salt melts) could, in favorable circumstances, be completed by 2010. As for the other main classes of substances and materials listed above, it should be kept in mind that the information in the literature on each of them is at least an order of magnitude greater than on melts and glasses. Moreover, structuring the available information, correlating the data of different studies, and finding optimal forms of presenting the information on the conditions in which various materials and substances are prepared turns out to be far more complicated than in the case of melts and glasses, and there is much less experience of conducting work of this kind. Hence, it may be assumed that at the initial stages of the work in these areas, the search will be conducted in certain limited fields that are of the greatest practical interest at this time. The first software generalizations of such a kind will probably appear on sale in the next few years. As for the production of full-scale databases, the time of their appearance will be governed by psychological, sociological, and economic factors and can be estimated only very approximately: in 20 to 50 years.

The three above-mentioned requirements to DBPM should be supplemented with a fourth: in-line input of new information into any one of the bases. The aim should probably be a capability to input any new research results as soon as they have been obtained in this or that scientific organization. In other words, DBPM should be something in the nature of a depository accumulating ever new experimental data together with certain amounts of information about experimental conditions. The status of data inputting into DBPM should correspond to the status of a high-quality publication. Consequently, the requirements to the quality of the submitted material should likewise be very exacting. Note that there is already some experience of forming such databases, for example, bases of data on powder diffractograms (PDF) of substances. Naturally, the general transition to experimental data transmission by researchers directly to DBPM will be a fairly lengthy process. At first, the main source of information for DBPM will be journal publications, dissertations, patents, etc.

It should be pointed out that the described procedure should by no means do any significant damage to the traditional system of scientific journals. Quality scientific journals devote most of their column-space to interpreting research results and applying these results to probing the “nature of things.” These matters will, most probably, remain entirely outside the scope of the information that will be collected in DBPM. At the same time, the development of Internet-circulated electronic versions of journals will be accompanied by advances in the automation of DBPM replenishment. With this in view, the format of papers submitted to journals will have to undergo certain changes. For example, numerical and descriptive information, and illustrations, intended for inclusion in DBPM will have to formatted according to certain standards and grouped in a single block, as is done, say, in writing abstracts of papers. Nevertheless, complete automation of this procedure can hardly be expected. A monitoring of the changes in the quality of research data descriptions in the leading journals on glass over the past fifty years prompts the disappointing forecast that in the next few decades researchers will not process the results of their measurements any more thoroughly than they do now. Hence, a high DBPM quality can be achieved only by having highly competent specialists check every paper added to a base.

Obviously, the principal method by which users will be able to download the information they require will be via the Internet. Subscribers will have access to any DBPM of interest to them.

The most formidable problem of all in the system described above will probably be that of monopolies. The fact is that the formation of bases of data on each of the major classes of substances and materials (with each of the DBPM meeting all the requirements listed above) will call for considerable human resources. Only specialists of the highest caliber, possessing qualities such as a high sense of responsibility and an ability to concentrate continually on their work, will be able to form DBPM capable of fully replacing all the presently existing scientific information media in a given field. A single system of data representation, to which the scientific community would grow accustomed, will have to be developed for each class of substances and materials. Only then will all the potential advantages inherent in the system described be truly achieved. This, however, means that certain specific companies will have to emerge in the world, each of which will own one or even several DBPM covering definite classes of substances and materials, and this will, naturally, be fraught with quite a number of risks. It is impossible to predict today how exactly the world scientific community will find a way out of this predicament. But we are convinced that, in any case, a big role in forming the DBPM system will have to be played by international scientific bodies: the International Union of Pure and Applied Chemistry, the International Atomic Energy Agency, the International Academy of Ceramics, the International Commission on Glass, the already mentioned consortium Scientific Group Thermodata Europe, and others. Each of these organizations will have to not just choose, on a competitive basis, the company best suited to carry out a corresponding project, but conclude a contract with it that would stipulate its rights and duties. The contract will probably have to include a clause that would oblige the company, should it violate the terms of the contract, to turn over to an international organization all its rights to the further use of the accumulated DBPM (i.e., some new company would be enlisted to continue the work). We believe that there is no need to fear the refusal of some companies to undertake the work on these terms. The backing of an international organization should assure an extensive and stable demand for the corresponding software product and, consequently, guarantee the company high and steady revenues.

At the same time, it follows from the foregoing that the formation of single databases for various fields of science will give rise to a number of by far not scientific problems, legal as well as economic. The problem will arise of ownership rights to a whole complex of scientific learning rather than just the rights of authors to information published in separate papers, patents covering inventions, or monographs, as was the case in the past.

It should be said that, apart from the DBPM discussed above, which may be called global, there now exist and, probably, always will exist certain local DBPM that belong to large companies, universities, or other organizations. The bulk of them are probably closed to outsiders, since they contain confidential information. This was, is, and always will be the case, but has nothing to do with the present prediction. However, there are local bases that do not contain secret information and whose owners can put them at the disposal of any applicant for a certain fee. There are now quite a few such bases, above all, bases of the properties of industrial polymers, and also of pharmaceuticals and toxic substances. Presumably, the role and popularity of local bases will decline steadily as global DBPM develop. Their only attraction for some time will continue to be their information about the properties of substances and materials that for some reason or other (specifically, related to copyright) was not included in global DBPM.

An important social consequence of the appearance of global DBPM and of access to them via the Internet will be the gradual fadeout of the notions of a scientist's working day and workplace. Work with any scientific information will become possible at any hour of the day or night, anywhere in the world, including transport facilities. This will fundamentally alter the management and organization of scientific research.

Information systems founded on DBPM. The importance of DBPM and interest in them will increase severalfold if, along with the DBPM themselves, the corresponding software products incorporate additional programs that will enable the user to make maximum use of the experimental data collected in the DBPM. Some such options have already been tested with success in existing software products of this type, but most of them still await future development. It would be more correct to call such software products information systems rather than databases.

Apart from the databases themselves, the first quite obvious elements of information systems of the properties of materials (ISPM) are the various techniques of the processing of experimental data cited in the DBPM. These techniques include combining the results reported in various publications into generalized tables and graphs, their diverse mathematical treatment, the conversion of units, and the conversion of coordinates in graphs, not to mention others.

The second major ISPM element must be a calculator that includes programs for computing the properties of substances and materials represented in the DBPM in terms of experimental data. Naturally, all the practically valuable methods of computing properties must be included in the calculator. A very important condition of the successful use of this element of the information system must be the incorporation in the ISPM of a subprogram that would make it possible to match the calculated results with the experimental data for all of the system's computation techniques in any research area chosen by the user.

The next step in ISPM development should be the use of the DBPM information on the properties of substances and materials for practical calculations. For example, in the case of an Information System of the Properties of Melts and Glasses, these should include calculations of heat transmission and temperature distribution in a material of any geometric shape from a fiber to a tank furnace, calculations of the optimal modes of annealing and tempering glass products, calculations of the diffusion profiles that arise as a result of ion exchange between glass and a molten salt, etc. In the case of an Information System of the Properties of Refractories, these could be calculations of temperature fields, thermal stresses that arise in using refractory materials as a function of their shape and size, and prognostic estimates of the resistance of refractories to mechanical, thermal, and chemical effects of the medium. In the case of an Information System of the Properties of Ceramics, the above-listed calculation procedures should be supplemented with calculations of the strength of structures of various shape and size, and calculations of the corresponding functional characteristics, such as electrical resistance.

The databases of the Information Systems will also include information on all the patents issued in the world.

Finally, all DBPM, including ISPM, will generally serve as excellent illustrations for any textbooks or monographs devoted to or touching upon problems related to the area of learning covered by these software products. Today it is hard to visualize even tentatively when books on paper carriers will be fully replaced by books on electronic carriers. But it is certain that electronic versions of textbooks and monographs will begin to appear in the next few decades. Here we are referring not to texts and drawings from conventional paper books transferred to CDR—that is already being done on an ever growing scale—but to genuine electronic versions of monographs and textbooks. Such versions must make sufficiently effective use of the potential of modern electronics to search for required data, to represent illustrations (in animated form included), to issue training assignments and check their fulfilment, and also of systems of interactive references to papers, monographs, textbooks, or other information available on electronic carriers. In future, the best electronic versions of such monographs or textbooks should become natural ISPM components.

At some subsequent stage of ISPM development, it is inevitable that they will be united into a single supersystem of data on the properties of materials, which will enable the user to find or design the data best meeting his set of requirements, irrespective of the class to which these data belong.

The establishment of data bases and information systems on the phase diagrams, structure, and properties of crystals and materials based on them. A single system of databases on the phase diagrams of all classes of substances-metals, oxide and oxygen-free high-temperature compounds, aqueous and nonaqueous solutions of salts, and organic compounds-will give materials science and technology a new problem-solving capability. This will allow new materials to be designed on the basis of a substantially larger set of combinations of the initial components. Knowledge about the phase diagrams of substances of different classes can be integrated successfully for the purposeful designing of fundamentally new composites only if the database system on phase diagrams is accompanied by an information-and-calculation system that makes it possible to predict (calculate) the properties of materials on the basis of phase-status data. The groundwork for such an information system exists in the numerous research results reported in materials-science papers. The integration of various theoretical, empirical, and semiempirical dependences of the properties of materials on their chemical and phase composition, and microstructural parameters, in the form of an information-and-calculation system, will, along with indisputable benefits for materials scientists and technologists, raise new problems associated with the correct choice of this or that model and, consequently, with prediction reliability. An important role in solving such problems will be assigned to those who develop the information-and-calculation systems and who will actually bear full responsibility for prediction reliability. These specialists will have to be highly erudite in the theory of materials and possess sufficient expertise in experimental research. To evaluate the adequacy of the empirically obtained model expressions and the limits of their applicability, they will have to be capable of integrating model expressions differing in type and genesis into a single system for predicting the properties of materials, and have an understanding of the types of predictions needed by practical materials scientists and technologists. Training such specialists (materials systems specialists) will, evidently, very soon become a most important area of higher education in materials science. The creation of the above-listed databases and information-and-calculation systems will benefit not only practical researchers engaged in developing new materials and technologies, but also theoretical scientists, since, on the one hand, it will rid them of many routine operations and, on the other, give them a clearer understanding of the trends in basic research that are of greatest promise in the field of applications.

The data on some of the structural parameters of crystals are already a part of a number of databases. However, the fragmentary character of the structural information in such databases prevents their proper use at present. Future advances in electronic information systems is associated with the development of a unified system of databases of the structural properties of substances. Such a system would encompass all the information from the type of structure and parameters of the elementary cell to a complete description of the distribution of atoms and the electron density in space in both the digital and the image format. Information-and-calculation systems will in that case develop in two directions: systems have to be developed for predicting the possibility of replacing some atoms or entire atomic groups in the structure with others and the consequent shifting of atoms from their positions; there will also have to be systems on whose basis it will be possible to calculate and visualize the formation of various point, linear (dislocations), or two-dimensional defects. Such systems will make it easier to predict the possibility of synthesizing new chemical compounds and forming new structural states of compounds, and will provide insights into the possible real structure of crystalline bodies.

An important stage will be the integration of all the above-mentioned databases and information-and-analytical systems of the properties of materials, phase diagrams of systems, and structures of chemical compounds in a single complex. The hierarchic modular structure of such a complex holds out the possibility-using relatively independent procedures to replenish databases and refine, or even replace, individual information-and-analytical systems—to maintain a constant efficiency of the complex as a whole, attaching the highest priority to problems of the global unification of all its components.

An important result of the establishment of such a global system of information on materials will be the appearance of a large number of virtual chemical compounds, structures, substances, materials, and technologies, which will form a vast “market of ideas” for experimental scientists and engineers.

Advances in artificial intelligence will also have applications in developing the above-described materials-science complex of information-and-calculation systems and databases, since such a complex can become the medium for analytical and synthetic operations effected by algorithms based on systems of artificial intelligence, with researchers merely having to check the obtained conclusions.

CONCLUSION

Tremendous advances in the immediate future in the development of large databases in all areas of learning that are of considerable practical interest are so certain that the probability of their taking place may safely be put at one hundred percent. Forecasts of a series of features of the new databases-and of the information systems established on their basis-are likewise, most probably, “doomed to success.” Heated debates on this score are hardly likely. Only one major point in our forecast can evoke serious doubts among specialists. This is our conviction that unified and single global DBPM will inevitably be created for each class of substances and materials. We are aware how dangerous in principle are monopolies, especially monopolies (even if each operates in a relatively limited sphere) that embrace all the nations of the world without exception. A corresponding international organization may find it no simple matter to control the activities of a company that is in possession of a system supplying vitally important information (once specialists develop a firm habit of using an extremely convenient and reliable information system, any malfunction of that system will leave them feeling very uncomfortable). Nevertheless, from our point of view, such a course of events is, in effect, inevitable.

It is most likely that, at the initial stage of the development of information systems on the properties of substances and materials, several competing databases and information systems may appear on the market. But at some phase of this development, one of the systems will prove to be definitely superior to the others, will receive the backing of the international community, and will sell better. The company developing such a system will then be in a position to sharply intensify its work in that area and will outdistance its competitors even more. In many respects, this will be a boon for the industry. The formats of data representation and the standards of obtaining new research results will become universal and, hence, customary for both the manufacturers and the consumers of the product. It is only important that, in relying on a carefully framed agreement, the appropriate international organization should not lose control of the activities of the corresponding company.

Despite the natural desire of both individual countries and groups of countries to acquire political and economic independence, in organizing scientific and technical information the world is becoming increasingly integrated. English has actually become the only language of international communication in science and technology, and this is very effective economically and very convenient practically. The SI international system of units is slowly but steadily gaining ground in the world and will become absolutely universal when the present generation of scientists and technologists retire. The Internet is changing the world for the sole reason that the means of communication via the Web—which, according the latest figures, are used by 250 000 000 people—now employ compatible software throughout the world.

The development of a single database system and information-and-calculation systems, available to the entire scientific community, is having enormous social effects. First of all, the very development of such a global information system will require the involvement of a large number of specialists in diverse fields and of differing qualifications-consequently, it will create a large number of new jobs. Secondly, the establishment of powerful and readily available information systems will place small- and medium-sized businesses that design and produce new materials and technologies practically on a par with large companies, at any rate at the stage of the solution of scientific and technological problems. What with most economists expecting the individualization of work and the development of a broad network of small and medium businesses to solve many social problems, it is not hard to see that small as well as large companies-and, perhaps, to an even greater extent, state and public bodies—will be interested in the emergence of such an information structure. Therefore, in our view, an important role in organizing the development of a global information system on materials should be played by such state and public bodies as national academies of sciences and their associations, the International Academy of Ceramics, the American and the European Ceramic Society, and many other bodies of that nature.

In conclusion, we would like to make the point that humanity is not so affluent, not so comfortably off, and not facing such radiant development prospects that it can afford to dismember the vital work of providing information for the production of materials into a multitude of local systems, which would offer their own methods of data collection and representation and would engage in furious competition. But if the world community concludes that there is a need for future unified systems of information on the properties of substances and materials, it has to start seeking means of protecting users' interests against the costs of monopolism in this sphere.

ACKNOWLEDGMENTS

This work was supported in part by the Russian Foundation for Basic Research, project no. 01-07-90291.

REFERENCES

1. *Steklo i keramika-XXI: Perspektivy razvitiya* (Glass and Ceramics-XXI: Prospects for Development [The book compiled at the Institute of Silicate Chemistry of the Russian Academy of Sciences according to the concept of Academician V.Ya. Shevchenko]), St. Petersburg: Yanus, 2001.
2. Favorskii, O.N., Russia's Energy Supplies in the Next 20 Years, *Vestn. Ross. Akad. Nauk*, 2001, vol. 71, no. 1, pp. 3–12.
3. Rusanov, A.I., Colloid Chemistry at the Turn of the Century, *Zh. Ross. Khim. O–va*, 2001, vol. 46, no. 1, pp. 66–69.
4. Mazurin, O.V., Strel'tsina, M.V., and Shvaiko-Shvaikovskaya, T.P., Problems in Investigations of the Properties of Glasses and Melts: Some Results and Prospects on the Threshold of the New Century, *Fiz. Khim. Stekla* (in press) [*Glass Phys. Chem.* (Engl. transl.)] (in press).
5. Toropov, N.A., Barzakovskii, V.P., Lapin, V.V., and Kurtseva, N.N., *Diagrammy sostoyaniya silikatnykh sistem: Dvoinye sistemy. Spravochnik. Vyp. 1* (A Handbook on Phase Diagrams of Silicate Systems: Binary Systems), Moscow: Nauka, 1965, issue 1.
6. Grigor'eva, L.F., Kosulina, G.I., Petrova, M.A., and Sechnoi, A.I., *Diagrammy sostoyaniya sistem tugoplavkikh oksidov: Sistemy keramicheskikh vysokotemperaturnykh sverkhprovodnikov. Spravochnik. Vyp. 6* (A Handbook on Phase Diagrams of Refractory Oxide Systems: Ceramic High-Temperature Superconductor Systems), Grebenshchikov, R.G., Ed., St. Petersburg: Nauka, 1997, issue 6.
7. Levin, E.M., Robbins, C.R., and McMurdie, H.F., *Phase Diagrams for Ceramists*, Columbus: American Ceramic Society, 1964.
8. Mazurin, O.V., Strel'tsina, M.V., and Shvaiko-Shvaikovskaya, T.P., *Svoistva stekol i stekloobrazuyushchikh rasplavov. Spravochnik* (Properties of Glasses and Glass-Forming Melts: A Handbook), St. Petersburg: Nauka, 1973–1999, vols. 1–6.
9. Mazurin, O.V., Streltsina, M.V., and Shvaiko-Shvaikovskaya, T.P. *Handbook of Glass Data: Parts A–E*, Amsterdam: Elsevier, 1983–1994.
10. Bansal, N.P. and Doremus, R.H., *Handbook of Glass Properties*, New York: Academic, 1986.
11. *International Glass Data Base INTERGLAD, Version 1*, Tokyo: New Glass Forum, 1991.
12. *SciGlass (Glass Property Information System), Version 3.5*, Lexington: SciVision, 1998.
13. Mazurin, O.V., Information Systems for Properties of Glasses and Other Materials: Principles of Design, *Fiz. Khim. Stekla*, 1997, vol. 23, no. 3, pp. 249–266 [*Glass Phys. Chem.* (Engl. transl.), 1997, vol. 23, no. 3, pp. 176–185].
14. Parker, J.M., Reviews SciGlass, *Glass Technol.*, 1997, vol. 38, no. 2, p. 60.
15. Varshneya, A.K., Review of "SciGlass" Database, *Am. Ceram. Soc. Bull.*, 1997, vol. 76, no. 5, p. 82.
16. Müller-Simon, H., Neue Version (3,5 der Glasdatenbank) SciGlass erschienen, *Glass Sci. Technol.* (Frankfurt/Main), 1999, vol. 71, no. 6, p. 78.

17. Zhmoidin, G.I., From Databases to Bases of Knowledge in Metallurgy—The Industry of Information, *Metally*, 1981, no. 1, pp. 60–69.

18. Kaufman, L. and Bernstein, H., *Computing and Calculating of Phase Diagrams*, New York: Academic, 1970.

19. Thompson, W.T., Pelton, A.D., and Bale, Ch.W., *F*A*C*T* Facility for the Analysis of Chemical Thermodynamics: Guide to Operations*, Montreal: McGill Univ. Compt. Centre, 1985.

20. Bale, Ch.W. and Eriksson, G., Metallurgical Thermochemical Database—A Review, *Can. Metal. Quart.*, 1990, vol. 29, no. 2, pp. 105–132.

21. Gusarov, V.V., Sobakin, S.V., and Udalov, Yu.P., An Information-and-Analysis System for Phase Diagrams of Multicomponent Systems, in *Komp'yuternye metody v upravlenii elektrotekhnologicheskimi rezhimami rudnotermicheskikh pechei* (Computer Methods in Controlling Electrotechnological Regimes in Ore Thermal Furnaces), St. Petersburg: Izd. GTI, 1998, pp. 10–16.

22. Gusarov, V.V., Phase Diagrams: New Aspects of the Theory and Application, in *Abstracts of Papers of the VII International Conference "High-Temperature Chemistry of Silicates and Oxides,"* St. Petersburg, 1998, p. 8.

SPELL: fadeout, fulfilment