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Glass Property Databases: Their History, Present State, and Prospects for Further Development

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Abstract. Specific features of two global glass property databases, Interglad and SciGlass, are described. It is shown that the Interglad database is more convenient for specialists who use commercial glasses in practice and are to know the properties of these glasses and particular details of their usage, whereas the SciGlass database is more helpful for scientists who investigate glass properties and develop new glasses. Some prospects of further development of glass property databases are characterized.

Introduction

Being known for many thousand years, glass is a material that until now has been widely applied in numerous areas of modern life. One of the practically important characteristics of glasses is their ability to vary their properties gradually by gradual changes of chemical compositions. Glass is a unique material whose properties are mainly determined by chemical composition and temperature; therefore, relationships between composition, temperature and properties of glasses are the key knowledge for developing glasses with desired combinations of properties. The same kind of knowledge is necessary for any basic glass research as well.

The importance of compiling the existing information on glass property data is so obvious for any specialist on basic or applied glass science that there is little point in proving it in this article. The publication of the first handbook on glass properties by famous W. Eitel in 1932 [1] was met with enthusiasm by glass scientists all over the world. Note that modern glass property databases contain information about properties of more than 50 times greater number of glasses than that compiled in the mentioned handbook.

After Eitel's handbook only two glass property handbooks have been published so far: by Mazurin, Streltsina and Shvaiko-Shvaikovskaya in 1973-1998 [2] (English version was published in 1980-1990 [3]) and by Bansal and Doremus in 1986 [4]. The latter handbook contained nearly 700 pages, eight volumes of the former contained about 3,500 pages. However, even the authors of the book [2] were able to compile only part of the property data available at that time. With the advent of the era of electronic databases publications of glass property handbooks have stopped altogether.

Japanese specialists from the company "New Glass Forum" were the first who developed the electronic glass property database, Interglad [5]. Its first version was released in 1991. In 1996, another database, SciGlass, appeared in the market under the SciVision copyright. Today the SciGlass database is developed and supported by the American company "Institute of Theoretical Chemistry" (ITC, Inc.) [6]. At present each of the mentioned databases contains composition and property data on several hundred thousand glasses and glass-forming melts.

It is necessary to note that now there are a considerable number of databases containing among other information a certain amount of glass property data. However, the total amount of this kind of data in any of these databases is very small in comparison with the data compiled in the Interglad and SciGlass databases. Thus it is reasonable here to discuss only these two databases that can be called global glass property databases.

We have to point out that being the authors of the SciGlass system we cannot be completely unbiased in our consideration, although we tried to be as much objective as possible. Nonetheless, we hope that this paper might be helpful for specialists interested in the usage of glass property data.

Concepts of the Interglad and SciGlass databases

Although the first version of the Interglad database was released five years earlier than SciGlass the latter database has much older history. Actually, the history of SciGlass dates back to 1960 when a team of scientists working at the Institute of Silicate Chemistry (Leningrad, USSR) began compiling glass property data. In due course this led to the publication of a series of volumes of the handbooks mentioned above [2, 3] their authors getting extensive feedback from the readers. Thus, when starting the development of the electronic glass property database this team had not only a large enough systematic collection of the published data but also a clear enough understanding of the needs of glass scientists. The Interglad team started its work on the database content in 1989 [7]. The main supporters of this work were the leading Japanese glass-making companies. Naturally, both the knowledge and requirements of specialists working in glass industry greatly influenced the content and structure of this database.

As a result, the basic concepts of the Interglad and SciGlass databases were considerably different. The Interglad was initially developed as a database for producers and users of glass articles, whereas SciGlass was compiled from the very beginning as a system for scientists of both the basic and applied glass science. Later, these databases became much closer to each other in both the content and functionality. However, the difference in the mentioned concepts caused multiple particular differences between these systems that should be taken into consideration when using each of them in practice. We think that this situation is very beneficial for users of the glass property databases. A user can select the database that meets his/her main interests in the area of glass properties. As to the needs of big glass companies that are not only producing glasses but are also interested in modifications of the existing commercial glasses and development of new ones, they have every reasons to use both databases that are from our point of view mutually complementary.

Data amount

The latest release of SciGlass [6] contains property data of slightly more than 300,000 glasses. The Interglad database contains data on somewhat less than 300,000 glasses and other materials. The difference in the mentioned numbers is not great. However, the selection of objects differs appreciably. From the very beginning the authors of SciGlass compiled only the data on properties of glasses and glass-forming melts and only of those materials for which their exact compositions were known. Thus the data on properties of enamels, glazes, glass-ceramics etc. are not included into the SciGlass database. Properties of any commercial glasses can be found in SciGlass only in the cases when the authors could find information about their compositions. Definitely, for some users such restrictions are inconvenient. Thus it is fortunate that in Interglad one can find properties of not only glasses but also of a considerable number of materials containing crystalline phases. For some specialists it is also quite important to find information about properties of a great variety of commercial glasses even in the cases when the compositions of these glasses are not disclosed by their producers.

This may raise the following question. If the number of objects in SciGlass is even somewhat greater than in Interglad and at the same time the Interglad covers a much wider variety of materials than SciGlass does, what compensates this difference in SciGlass? The main factor is as follows.

It is well known that in scientific papers a considerable part of experimental data is published in a graphic form. Specialists' opinions differ as to the compilation of data presented in graphs. For example, Bansal and Doremus [4] included in their handbook only the data taken from tables. We can see certain reasons for this. It seems clear that in general, table values should be somewhat more precise than values presented as points in figures. Probably, this particular reason led the authors of Interglad to the decision not to use graphic data in their database. On the other hand, it is easy to show that experimental errors in many publications can be much greater than the errors connected with graph formations. Thus there are no reasons to ignore such an important source of information as graphs. The authors of SciGlass have used sophisticated digitizing software that makes it possible to transform graphs into a numerical form with high accuracy. The graphs are especially often used for description of properties of binary, ternary, and quaternary glasses. As a result, in SciGlass there are about twice as many property data on these groups of glasses as in Interglad.

The digitizing procedure also helps in collecting a great number of absorption spectra in SciGlass and enabling users to transform the spectra in about a hundred versions of pairs of axes.

Data presentation

When a user finds information about a commercial glass in Interglad he/she sees not only the available data on the properties of this glass, but also the information about the form of articles produced from this glass. In SciGlass the latter type of information is absent. At the same time in the SciGlass database a user can find a concise description of the whole procedure of glass synthesis and property measurements (if available) for a presented set of data. For a scientist such information can be quite important; for a businessman it can be considered as irrelevant.

Similar difference is specific for references. The authors of Interglad extracted a great amount of information from the two mentioned above handbooks [3, 4] and referred to these handbooks and not to originals. It is more than enough for a technologist or businessman, whereas a scientist is usually interested in references to original publications. In SciGlass only original references are presented. If authors have published their data in several different sources, the references are given to all these sources. In the latest version of SciGlass [6] full references including paper titles are given.

Data search

An important common feature of both databases is a search for "standardized" property values. For most properties, these values correspond to fixed temperatures. For viscosity, it is also possible to search for temperatures corresponding to fixed viscosity values (10, 100, …, 10^{13} dPa·s). Thus, a user of a database could not only *get* the data taken from multiple sources, but also *compare* them with each other. Interglad allows a more extended search for data on commercial glasses. SciGlass presents much more options when searching for data taken from scientific publications.

Property prediction

It seems obvious that every good material property database should include the ways of predicting properties of materials that have not yet been studied. Both databases in question enable their users to make such predictions. However, the basic approaches to property predictions in these databases are cardinally different. This difference seems worth considering it in more detail.

For many years all prediction tools in SciGlass have been based on the use of popular methods of property calculations, as well as the universal method of Priven2000 [8] that was specifically developed for the use in SciGlass. The specific routine providing a possibility to compare results of property calculations by several methods with the experimental data for a given area of glass composition was included into SciGlass. It allows a user to select the most reliable prediction method for the case of interest and to estimate a confidence interval for a calculated property value.

The Interglad team chose another way of property prediction: after finding the values of a glass property in a given concentration range, the Interglad program could build a linear regression model that describes the concentration dependence of the given property in the selected composition range. In some cases, such predictions can be more reliable than those made by using the models presented in SciGlass; namely, in composition areas where the linear regression approach can describe property-composition dependencies rather accurately and enough data exist. Wide use of the so called additive formulas in various methods of glass property predictions (see many examples in Ref. [9]) confirms this possibility. At the same time very complicated dependencies of glass properties on chemical compositions are not uncommon. In such composition areas the use of linear regression can lead to very great errors. Some examples are considered in our web-paper [10]. Thus, safe use of this procedure is possible only in the case if the calculation results are provided with the reliable estimation of their confidence intervals.

Recently the SciGlass team proposed a method of determination of the confidence intervals for property values calculated from chemical compositions. This method is based on using the combination of the existing models of property calculations with application of elements of the statistical analysis [11]. Numerous checks of such determinations based on the analysis of the experimental data-points surrounding a given composition showed a high reliability of the obtained results.

Search for glass compositions with prescribed combination of properties

Both property prediction instruments described above can be used when solving one of the most important and difficult problems in the applied glass science: finding a new glass composition with desirable combination of properties. Some helpful tools to solve this problem are presented in both Interglad and SciGlass databases. However, these tools are very different.

The developers of Interglad tried to solve the mentioned problem by using the above-considered regression models describing the concentration dependence of selected properties in a given concentration range. The Interglad program enumerates possible glass compositions step by step and tries to fit users' requirements. Such approach could be satisfactory, if the models predict accurately enough not only the absolute values of the number of properties for particular glass compositions, but also property *changes* after *small changes* in glass compositions. Unfortunately, practice shows that the linear regression models rarely solve the latter task properly. Thus, a particular composition found by using this procedure could rarely be optimal. However, in some cases this procedure can help finding the *general direction* of search, which is also useful.

A completely different concept has been realized in SciGlass. Using the model described in [8], several dozens of various properties are pre-calculated for more than 200,000 compositions reported in the publications covered by SciGlass. The calculated values are stored in the database and are available for search. It is worth noting that each glass composition found by using this search *has been really synthesized* and a user can see the details of the experimental investigation of this glass by inspecting the corresponding information stored in the database. However, this approach has also its drawbacks. The most serious of them is the fact that when searching for unusual combinations of properties a user often finds glasses belonging to rather specific composition areas where the accuracy of the model [8] can be many times less than in well-investigated concentration ranges. Thus, it is hardly possible to get an *exact* glass composition with a *given combination* of property values. Usually it is only possible to determine a *prospective area of compositions* where a given combination of properties can be found. Further search requires experimental investigations.

As is evident from the foregoing, in both databases considerable improvements in the search for practically applicable glasses with desirable combinations of properties are needed. However, there are reasons to state that even now both glass property databases can provide a considerable help in a successful achievement of this objective. We think that the most efficient way of doing this it is the use of the approaches suggested by both of these databases.

Challenges of today and possible ways of their solution

As more and more data are compiled in the global glass property databases, the major problems concerning further development of these databases become more and more clear.

Quality of experimental data. Even with a great progress in the development of property measurement equipment, the quality of published experimental data has been steadily decreasing during the last few decades (see, for example, [10, 12, 13, 14]). It is an alarming phenomenon that should be taken into consideration by everybody who wants to use reliable glass property data.

We are sure that the only realistic way of counteracting to this deadly (for the future of glass science) tendency is an active use of global glass property databases by editors and referees of scientific journals, as well as by glass community in the whole. Comparison of experimental data found in new publications with all the data published earlier within the same composition areas helps evaluating the real quality of new data. In principle this makes it possible to find out reliable groups of authors and reliable scientific institutions and accordingly to select publications containing reliable data for composition areas that have not yet been studied by sufficient number of authors.

In 2007 the first steps in this direction were made [14, 15]. However, from our point of view much more attention should be given to this problem by the international glass community. As to the developers of the global glass property databases, they should include into their databases special options that will allow a comparison of new data sets with the already existing data and, if possible, an automatic estimation of reliability of new data. We think than in in the not too distant future a user of a glass property database has to be able to select one of the two data sets: all data compiled in a database, or only the data of a high enough level of reliability.

Prediction of chemical durability and liquidus temperature. One more challenge is a simulation of properties, such as chemical durability to various media and liquidus temperature. These properties are extremely important for any practical glass. However, up to now these properties cannot be predicted in more or less wide concentration areas of practical importance.

In the case of chemical durability, the difficulties are mainly caused by the number of factors affecting the results of measurements: the type of aggressive medium, temperature, time, size and shape of glass samples, etc. It is obvious that composition dependencies of chemical durability in various acids, water, or alkali solutions can be absolutely different. At the same time, it is a reasonable possibility that within most of the experimental methods used for studies of glass durability in a certain group of media, certain standardized descriptions of glass durability can be found. Probably, the best solution here can be establishment of certain levels of durability similar to well-known hydrolytic classes. Even such approximate characteristics of the influence of compositions on chemical durability in certain groups of solutions can be quite useful in searching optimal glass compositions.

As to the prediction of liquidus temperatures, one of the problems is a very complicated form of their concentration dependences, mostly containing sharp breaks and other specific points. However, the main difficulty here is the fact that liquidus temperatures depend not only on thermodynamic characteristics of melts but also on thermodynamic characteristics of primary crystalline phases. Accordingly, in a foreseeable future it seems unrealistic to expect of the development of a more or less universal method of predictions of liquidus temperatures covering dozens of components in wide concentration ranges. At the same time for narrow composition areas it seems realistic and quite helpful to develop empirical models like [15] on the base of available experimental liquidus data.

Lack of available data. Today the global databases [5, 6] seem to contain the majority of experimental data about glass and melt properties published worldwide. Considering some decrease of financial support of glass property studies during the last decades we can assume that in the near future the content of both databases would not be increased as quickly as it was in the past. At the same time, in many cases the number of available data is insufficient for solving practical problems.

One of the possible ways of improvements of this situation can be the implementation of unpublished experimental data to the databases. It is no secret that a great number of experimental data remain unpublished for various reasons. In many universities and research centers, thousands and thousands of unclassified data collect dust for years. It is in the interest of the whole glass community to find ways of supplying global glass property databases with this kind of data.

Lack of steady cooperation with glass societies. The considered glass property databases are very powerful tools which can help a great deal in solving various problems of fundamental and applied glass science and technology. We are sure that the international glass community should be very interested not only in further development of these databases but also in encouraging copyright owners of the databases to develop them in the directions which are the most important for further progress of glass science and technology. It seems rather strange and disappointing that when we ask the authors of publications to supply us with some important details of an experimental procedure that were omitted in their papers, we receive replies only in about a quarter of cases. Surprisingly small is also the number of references to both global databases in scientific papers.
We ask the leaders of ESG to consider the possibilities of establishing a certain system of cooperation between ESG and representatives of copyright owners of the SciGlass database as the first step in selecting optimal directions of further development of global glass property databases.

Conclusion

The existing two global glass property databases meet various needs of glass specialists in information on glass properties accumulated by several generations of scientists throughout the world. These databases have much in common but at the same time they have considerable differences resulted from their initial orientations to different groups of specialists.

Due to the increasing number of publications containing suspicious property data the role of glass property databases becomes more and more important for further progress of both glass science and technology. Accordingly, the development of sophisticated statistical methods of evaluation of the quality of the existing data and reliable prediction of properties of glasses that have not yet been studied can be of great interest to specialists interested in the study, development and manufacture of any kinds of glasses. Thus the active involvement of international glass community in encouraging and supervising such activity is highly desirable.

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