Glass properties: compilation, evaluation, and prediction

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Abstract

To test the validity of glass structural models and predictive potential of these models it is necessary to have reliable composition dependencies of glass properties. Usually, the most reliable dependencies can be obtained only on the basis of statistical processing of all available information on a selected property and glass-forming system. For this purpose the use of a state-of-the-art glass property database is highly advisable. In the paper several examples of the analysis of property-composition dependencies for binary glasses are described.

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1. Introduction

It is well known that new ideas, hypotheses, or theories of a glass structure are generally based on the results of direct structural studies of glasses. At the same time in order to test a developed structural model it is important to compare predictions of composition and temperature dependencies of certain glass properties based on this model with experimental data. Sometimes information on glass properties could also be used for refinement of a structural model.

However, these experimental data should be highly reliable. We know that the quality of published data differ from each other greatly. How can we determine the most accurate dependence? It is well known that there are some results that were obtained by such a blameless experimental technique that they do not need any additional testing or parallel measurements. Probably, one of the most impressive examples of this is the study of the influence of minor additions of second alkali ion on electrical conductivity of a binary alkali silicate glass [1]. The results of these measurements are completely reliable and they should be taken into account when

developing any model of a mixed-alkali effect. Nobody has tried to repeat such kind of measurements so far because to conduct the studies at the same quality level is very difficult and otherwise there is no sense in repeating these measurements. Unfortunately, this is a rather rare exception from the general rule: the reliability of nearly any single set of experimental data is not high enough and any conclusions concerning structural modeling based on these results should be drawn with great enough caution. According to my experience, there is only one general way of solving this problem. It is necessary to collect all the data published so far and, if they are numerous enough, to process them statistically. It was a challenging task some time ago. Not any more now. In this paper several examples of such present-day solutions of some problems related to the study of glass structure will be demonstrated.

Two glass property databases are available at present, they are the Japanese INTERGLAD [2] and American SciGlass Information System [3]. The INTERGLAD software was developed mainly to satisfy the requirements of scientists dealing with applied glass science. The SciGlass is more universal and can efficiently meet the demands of the basic science as well. Thus the SciGlass program product is used in this paper. The latest version of the SciGlass database contains property data for more than 230000 glasses and covers

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more than 80% of the existing information on glass properties.

2. General way of determination of the most reliable dependencies

The simplest way to demonstrate the use of the Sci-Glass database is to analyze data for binary glasses. Let us select, for example, density of lithium borate glasses. In the composition range from 0 to 40 mol% of Li_2O 313 points taken from more than 100 publications were found. On the base of all these points an approximating cubic polynomial equation was obtained by the method of least squares. Then 11 defective data were found and removed. All points were considered as defective data, when the point deviations from the approximating curve exceeded 2σ. Here σ is the root-mean-square difference between the experimental points and approximating curve. After that a new approximating curve was drawn (see Fig. 1). Unfortunately, it is impossible to give here the references to all publications from which the data used for drawing this and the next graphs were taken. Otherwise a list of references would be too long. Whereas all references can be found in the SciGlass Information System.

It is worth noting that for this particular set of data about half of all points have been taken from papers published before 1983 and the other half belongs to more recent publications. At the same time among nine found defective data eight have been taken from papers published in 1983 or later. Unfortunately it is only one example of the general trend: recent publications contain much more questionable glass property data than
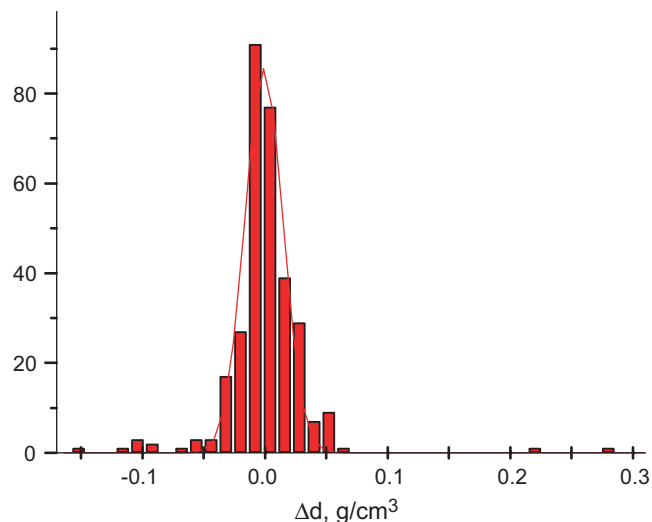
Fig. 2. A histogram of the differences between the values calculated by the equation describing the approximating curve in Fig. 1 and experimental values of density of sodium borate glasses. The solid line is the Gaussian approximation of the presented data.

the earlier ones. This problem is discussed in some details in Ref. [4].

The equation describing the approximating curve in Fig. 1 can be considered as the most reliable description of the studied dependence. It can be proved by the analysis of distribution of deviations of all points (including defective data) from the calculated property values for similar compositions by the approximating equation. The result is shown in Fig. 2. It is seen that all values can be divided into two groups. The distribution of the main group of these deviations can be described reasonably well by a Gaussian curve. The positions of the points belonging to the second group (usually containing from 4% to 8% of all data) are well outside the Gaussian curve and are absolutely irregular. These points are defective data and their removal is actually the necessary step of the described procedure.

Thus, the main steps of the recommended procedure are as follows: (1) selection of all the existing data; (2) statistical processing of all data and removal of found defective data (if the number of the sources used is not less than 8 or 10); (3) approximation of the remained points by a polynomial.

Several examples of the use of the described approach are presented below.

3. Study of boron anomaly

The term 'boron anomaly' was introduced in the glass science in the 30s of the last century and was related to a specific shape of the dependence of a thermal expansion coefficient (TEC) on the composition of a binary sodium borate system (see Fig. 3). A minimum of TEC was
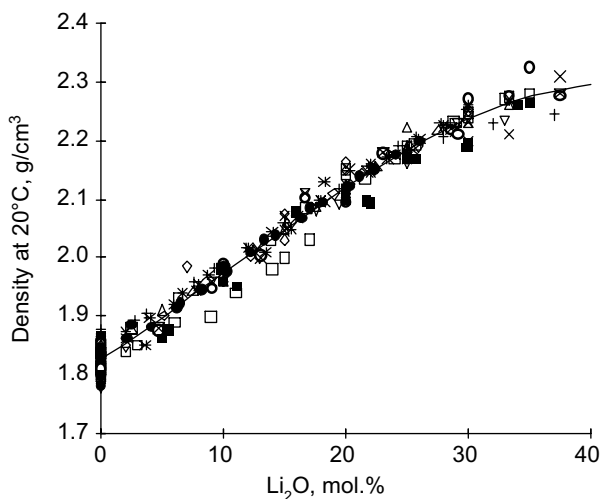

Fig. 1. Density of lithium silicate binary glasses. The graph is drawn after deletion of defective data. For compilation of data and graph drawing the MDL SciGlass Information System [3] was used. Points taken from different publications are shown by different signs.

clearly positioned somewhere between 16% and 17% of Na_2O. It is to be noted that a great scatter of data in this figure is mainly due to the difference in the temperature ranges of TEC measurements published by different authors. Therefore, no statistical processing of the presented data including the removal of defective data was performed in this case.

The structural interpretation of this dependence was proposed by Biscoe and Warren [5]. By a study of X-ray diffraction of sodium borate glasses these scientists found that addition of Na_2O to B_2O_3 glasses transformed B_3 units (three boron–oxygen bonds) to B_4 units (four boron–oxygen bonds) and that such transformation could take place only in a limited range of Na_2O concentration. At the same time the accuracy of the studies of radial distribution curves was not enough to determine this limit.

Thus, they assumed that the minimum of TEC in this curve corresponds to the limiting concentration of sodium oxide transforming B_3 to B_4. Clearly, the number of studies of this dependence was at that time considerably lower than it is now (see Fig. 3), but the found dependence was practically the same. Biscoe and Warren assumed that further additions of Na_2O would lead to breaks in B–O–B bonds and accordingly to an increase in TEC. Nearly all glass scientists at that time were fully convinced of this interpretation.

However, in 1963 Bray and O'Keefe [6] showed by NMR studies that B_4 groupings were formed up to the concentration of alkali oxides equal to about 30–32%. Accordingly, correlation of property data with a structural model for alkali borate glasses proved to be much more difficult.

Since then a number of authors have discussed the structural aspects of the boron anomaly. Description of these discussions is out of the scope of this paper. Here I will concentrate on the problem of property-composition dependencies in alkali borate glasses. To demonstrate experimental data I have selected the dependencies for a lithium borate system because in this system the glass-formation range is the broadest one.

Fig. 4 shows the main results of the famous publication by Bray and O'Keefe. It is seen that in the concentration range from 31% to 35% of Li_2O not only an increase in B_4 with increasing concentration of lithium oxide stops but also the beginning of a rather rapid disintegration of the already formed boron oxide tetrahedrons takes place.

I believe that, if we want to compare a certain structural model with composition dependencies of glass properties, we should bear in mind the composition dependencies of all properties that have been studied for a selected system in a more or less wide composition range. Fig. 5 shows such dependencies for six various properties of lithium borate glasses. It is remarkable that shapes of nearly all these dependencies differ greatly from each other. It is to be noted that while the dependence of a B_4 content on the concentration of Li_2O has a well developed maximum in the range 37–42% of Li_2O (see Fig. 4), the dependencies of most properties change in this range quite smoothly, if they change at all. This should be definitely taken into account when developing any structural model.

Probably, the best base for structural interpretation of all property dependencies is the scheme, given by Shelby [7] (Fig. 6). To draw the scheme he used the information presented in the review paper by Griscom [8]. Comparison of dependencies presented in Fig. 5 with the information given in Figs. 4 and 6 shows that only a part of composition-property dependencies correlate
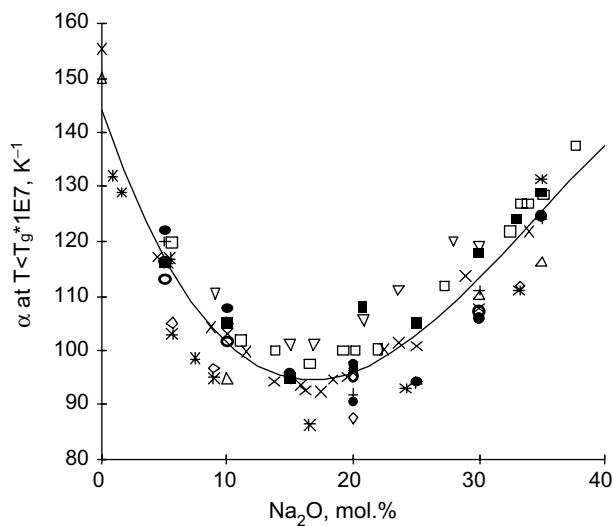

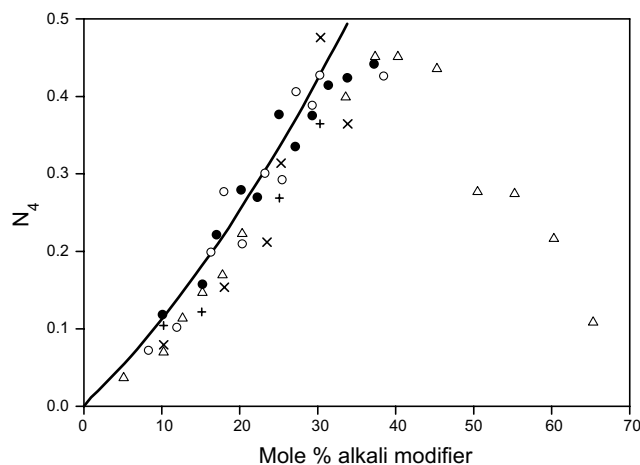Fig. 3. Concentration dependence of thermal expansion of sodium borate glasses.

Fig. 4. The fraction of B_4 of boron atoms in the four co-ordination in alkali borate glasses. (●): Na_2O; (○): K_2O; (△): Li_2O; (+): Rb_2O; (×): Cs_2O [6].
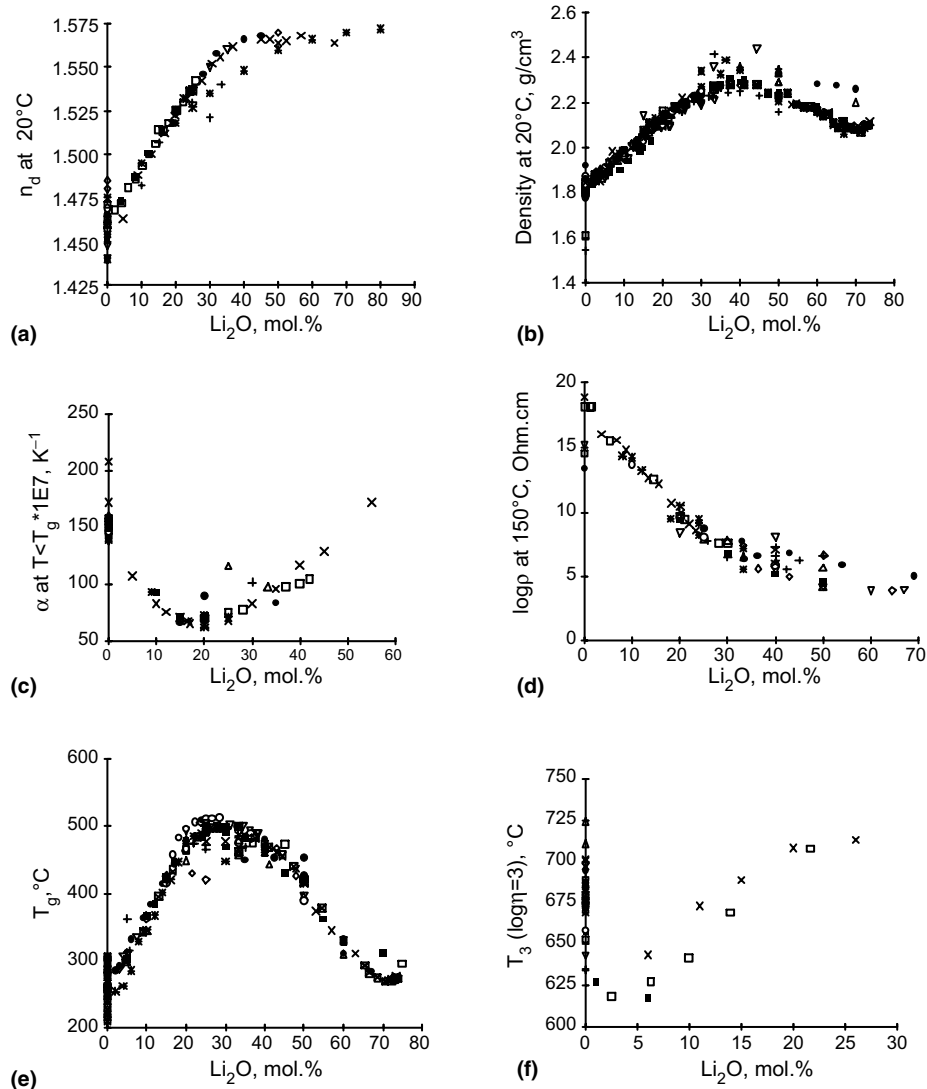
Fig. 5. Concentration dependencies of several properties of binary lithium borate glasses.
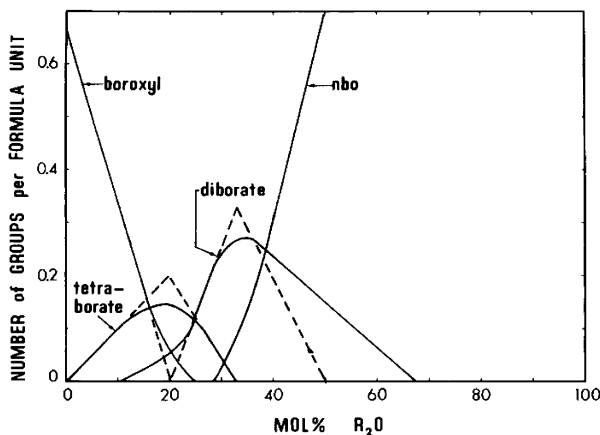

Fig. 6. Simple structural model for alkali borate glasses [7].

reasonably well with changes in concentration of B_4 groups. Some other properties demonstrate connection

of the changes in their values with changes in concentration of various types of structural units.

Prior to make a serious analysis of correlation between a structure and properties, one should study every graph of Fig. 5 in all possible details. I will give here only one example of this procedure.

As far as I know, the latest paper where correlation between properties and a structure of lithium borate glasses was discussed, was published by Conzone et al. [9] in 2001. The data presented in this paper included the dependence of a refractive index on concentration of Li_2O in lithium borate glasses (see Fig. 7). It is seen from the figure that the maximum refractive index was reached at 25% of Li_2O. If this result proves to be a reliable one, it should be used for testing any corresponding structural model. Before doing that, however, one has to compare these data with those published earlier. Fig. 8 shows the results of such comparison. Here we have 67 points for Li_2O–B_2O_3 glasses. The points for binary
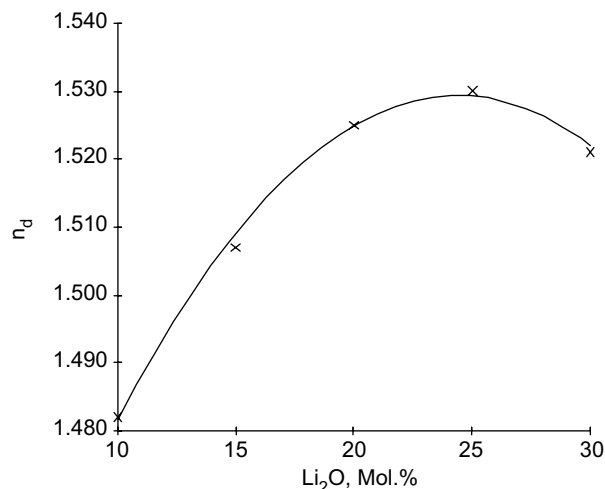
Fig. 7. Dependence of n_d on the concentration of Li_2O in binary lithium borate glasses according to the data by Conzone et al. [9].
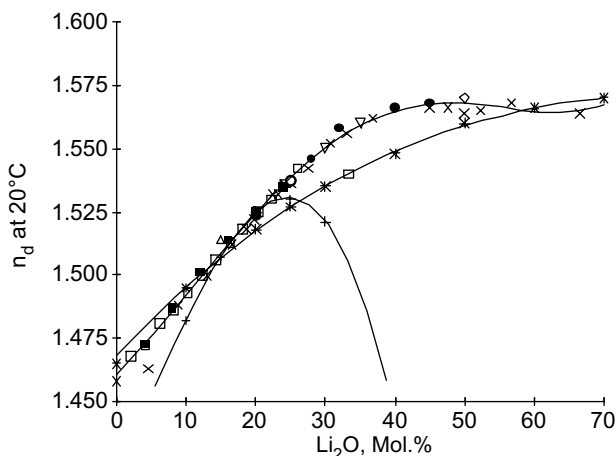

Fig. 8. Comparison of the curves approximating the composition dependencies of the refractive index for binary lithium borate glasses according to the data published by Conzone et al. [9] and Lorosch et al. [14] with the curve approximating the results for sets of data taken from papers published earlier [10–13]. (+): data by Conzone; (∗): data by Lorosch.

glasses were taken from 12 publications. It is a good enough basis to analyze the results.

We can see that besides several points taken from the papers presenting measurements for only one composition, there are four sets of data (taken from Refs. [10–13]) where the points form a common composition dependence of a refractive index. Note that these four sets include also the only set of data (for this particular graph) that was obtained for chemically analyzed glasses [10]. Let us ignore two single points that are obviously defective data and concentrate on the two remaining sets of data that deviate markedly from the general dependence. One set belongs to the already mentioned work by Conzone et al. The other set was taken from the

paper by Lorosch et al. [14]. The conclusion seems to be obvious. At present this common dependence should be considered as the only base for any attempt of interpretation of property data based on any structural model.

At the same time it is necessary to stress that it is too premature to consider the data by Lorosh et al. and Conzone et al. as definitely erroneous ones. It is possible that these data deviate from the data of other scientists due to some specific features of the experimental technique. However, only the authors themselves are able to find the reasons of such deviations. To avoid such problems one can recommend the following. When a scientist selects a new object for an investigation, he/she should find all data that have been published so far and start comparing his/her first results with these data. If these results do not match most of the results published before, a scientist should pay maximum attention to this fact and try to analyze possible reasons for the discrepancy. A scientist may find some defects in the applied technique and correct them. It will make results of all other measurements more reliable. Or he/she may find some objective factors influencing the results obtained. In any case all this should be stated in a paper. All these measures will decrease the so-called information noise in glass property data, the recent growth of which has become really alarming.

4. Notes on the possible role of deviations of actual compositions of studied glasses from those reported in the papers

The factor of incorrect determination of actual glass compositions is one of the most important ones among various factors leading to errors in glass property measurements. There are two main aspects of this factor. The first one is the change in component concentrations of a batch in the course of melting due to different volatilities of various components of a batch. The second aspect is the influence of impurities that were introduced into a glass unintentionally. The properties of boron oxide and borate glasses are to be influenced quite strongly by the two mentioned reasons. Thus I will use some examples presented in the previous section as a base for discussing the effect mentioned above. Note that in general the problem of the analysis of the influence of composition errors on property errors is many-sided and complicated. Therefore, in this paper only a very short description of the problem with minimum specific examples is presented.

Let us begin with the influence of impurities. Fig. 5 shows that practically for all properties of B_2O_3 glasses and melts the ranges of property values obtained by various authors are particularly wide. One can assume that this scatter of data is partially connected with the

difference in water content. At the same time it is impossible to explain the differences in the reported properties of boron oxide only by this factor. Only one example of this is given here (and similar ones can be found in great number). It is obvious that an increase in concentration of water should lead to a decrease in a T_g value. For example, according to Poch [15], T_g of dry vitreous boron oxide is equal to 305 °C, while T_g of the same glass containing 1.07 mol% H_2O is equal to 240 °C. At the same time, according to Ramos et al. [16], $T_g = 295$ °C for boron oxide glass containing 0.4 mol% H_2O, and $T_g = 282$ °C for glass containing 3.4 mol% H_2O! The difference in T_g presented in these two papers for water-containing glasses is rather impressive. Certainly, one can take into account the probability of the difference in heating rates used in the studies in question. Poch measured T_g by the dilatometric method and thus possibly he applied a standard heating rate equal to 3 K/min (there was no information on this in the paper). At the same time, Ramos et al. used the DSC method with a heating rate of 10 K/min. An increase in a heating rate should lead to an increase in T_g. It is well known that one can calculate this increase from the temperature dependence of glass viscosity [17]. By using the SciGlass Information System [3] one can find that within the glass transition range the viscosity of boron oxide changes by one order of magnitude when the temperature changes by 14 K. It means that when a heating rate increases by half an order of magnitude an increase in T_g by 7 K will result. Accordingly, a great difference in the data obtained by Poch and Rames et al. is impossible to relate to the supposed difference in heating rates of samples and hence is impossible to understand. The puzzling result reported by Seddon and Turner [18] is also worth mentioning. For T_g measurements they used the dilatometric method with a heating rate of 10 K/min. Before these measurements the authors melted B_2O_3 at 1400 °C 'for a long time', which means that only traces of water could remain in the studied samples. According to them, a T_g value for B_2O_3 glass was found to be 211 °C. It is to be noted that in the SciGlass System one can finds references to several other papers describing the properties of presumably dry B_2O_3 with T_g equal to or less than 220 °C.

Thus, even for such glass as B_2O_3, that is particularly hygroscopic, the scatter of data could be attributed to the difference in water content only partially. One can only hope that in the near future some inquisitive experimenters will try to compare their data with those compiled in the SciGlass System and find at least some of the reasons for the data scatters described.

So far, there is no systematic study of the dependence of properties of alkali borate glasses on alkali content, where water impurities have been determined for the studied glasses. One can suppose that in such situation the best way to find the most reliable composition

dependence for a property is not to use the statistical approach but to consider results for a series of data obtained in one study. It may be the case, if three conditions are met. First, all glasses should be melted in exactly the same time–temperature regimes. Second, the hygroscopicity of all glasses of the series (including pure B_2O_3) should be the same. Third, we should be sure that the influence of water on a studied property is the same for all studied compositions. Neither of these conditions could be considered as a correct one. It seems obvious enough and it is not reasonable to discuss it at length in this paper.

Now let us consider the factor of changes in the contents of the main components of alkali–borate glasses in the course of their melting. Clearly, the only way of guaranteed minimization of the error related to this factor is the chemical analysis. Unfortunately, the number of publications on properties of alkali–borate glasses where compositions are given by analysis, is rather small. At the same time the difference between compositions by batch and actual compositions of glass may vary quite considerably. There are many ways to decrease volatility. It is also possible to try to compensate volatility by special addition of the most volatile component to a batch. Usually, the authors do not mention these details in their papers. It is worth noting that I have compared the approximated composition dependencies of densities of sodium silicate glasses (they were selected for reasons of being of the greatest number in the published data) separately for the analyzed glasses and glasses with batch compositions. As one may expect, the scatter of data for the first series of glasses was much smaller than for the second series. However, to my surprise, the approximated values of density for the selected compositions were practically the same!

The same conclusion can be made from the discussion presented in the previous section in connection with the composition dependencies of a refractive index for lithium–borate glasses. As is clear from Fig. 7, the point positions for compositions by batch taken from Refs. [11–13] nearly ideally agree with the point positions taken from the paper containing compositions by analysis [10]. Note, that the latter paper was published in Russian (at that time Russian journals were not translated into English) and there were no chances for other authors to know about this publication.

It is worth comparing the information on the errors presented in the papers with the differences between the property values reported by different authors. As an example, I have selected the papers containing data on a refractive index of lithium borate glasses. Among 12 papers containing these data (some of them present only one value) only 3 papers included information on measurement errors. The reported errors were as follows: ±0.0001 [10] and ±0.002 [9,13]. Due to a great number of points (14) within a comparatively narrow

composition range (from 0% to 25% of Li_2O) the paper by Bresker and Evstropiev [10] makes it possible to determine the actual scatter of the experimental data in relation to the experimental curve. Using the approximation by a cubic polynomial, one can obtain the value of a root-mean-square error equal to ±0.0008. It is far from being high, but nevertheless it is much higher than the error values given in the paper. It follows from this comparison that Bresker and Evstopiev presented in their paper the error of the used device (interferometer), but not the error of the actual results. Using the mentioned approximating curve it is easy to determine to what change in composition the above-mentioned error corresponds. The influence of the measurement errors in this case can be neglected (it is too small in comparison with the total error). The change in 0.0008 of a refractive index corresponds to the change in 0.25% Li_2O. Thus the root-mean-square error of determination of composition of these binary glasses was ±0.25 mol% of Li_2O. In the discussed paper, as it was already mentioned, the glasses were analyzed. The determined composition error characterizes the quite reasonable accuracy of the chemical analysis. As to Refs. [9,13], the authors seemed to describe the errors of the Becke line method that was used for their measurements. It is remarkable, however, that if one approximates all data from Refs. [10–13] by a cubic polynomial curve, the root-mean-square error for the points from Ref. [13] will also be equal to ±0.002. At the same time, the refractive indexes for two glasses with minimum and maximum concentrations of Li_2O presented in Ref. [9] (cf. Fig. 8) deviate from the approximating curve mentioned above by 0.01 and 0.03, correspondingly.

Let us draw a general conclusion from the text of this particular section. As follows from Fig. 5, the scatter of properties for pure B_2O_3 is considerably wider than the similar scatter for binary glasses. At present it is difficult to understand why this is the case. It is just a fact that should be taken into account. It means that neither the physicochemical nor the statistical approaches can be used for reliable determination of the property changes of boron oxide with minor additions of alkali oxides (say, from 0.5 to 2 mol%). At the same time, the scatter of the data for alkali–borate glasses containing more than 2 mol% R_2O seems reasonable enough for the use of the statistical approach. In principle, the best results can be obtained in the cases when, in addition to the statistical approach, a special analysis of some specific results is used. This was demonstrated in the previous section for the concentration dependence of a refractive index. However, the general trends of most dependencies can be clearly seen just on the base of the statistical approach, as was demonstrated by Fig. 5. Hopefully, the presented data and their discussion has shown clearly enough that the revealed trends of composition dependencies are much more reliable than

any dependence obtained on the base of a randomly selected series of measurements.

5. Breaks in property-composition dependencies in alkali–silicate glasses

Let us consider the problem of breaks in the property-composition dependencies in the vicinity of some specific (usually stoichiometric) compositions. If the existence of such breaks is unambiguously proved, this information should be taken into account in any structural model of the corresponding glasses.

Probably, the last paper concerning this problem was published by Doweidar [19]. The author studied density of binary sodium–silicate glasses and found that in the composition range from 0 to 33.3 mol% of Na_2O (i.e. sodium disilicate) the dependence of density on composition is practically a linear one, however with 33.3% of Na_2O the dependence has an obvious break. These results support the following structural model. Addition of Na_2O to SiO_2 leads to formation of non-bridging oxygen. At first, silicon–oxygen tetrahedrons with four bridging oxygen atoms (Q_4) transform into tetrahedrons having one non-bridging oxygen atom (Q_3). In a glass corresponding to sodium disilicate all silicon–oxygen tetrahedrons are of the Q_3 type and only in the course of further increase in Na_2O concentration the tetrahedrons with two non-bridging oxygen atoms (Q_2) appear.

It is now desirable to find, if this break is real or not. Inspect the data by Doweidar, as the first step. Let us draw approximating curves through the points belonging to wide enough composition ranges below and above sodium disilicate composition and then extrapolate these dependences to all studied concentrations of
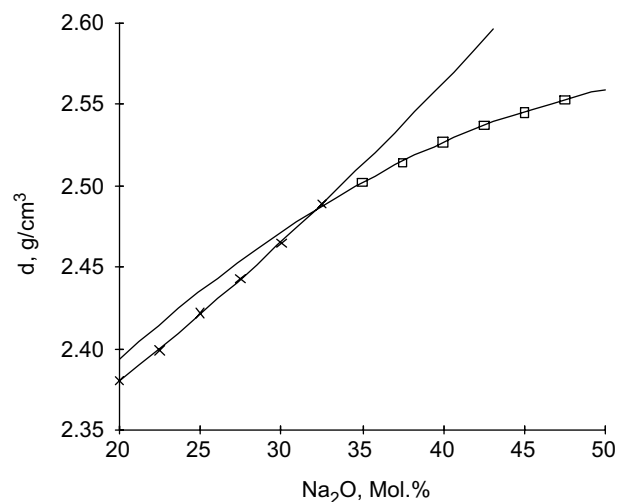

Fig. 9. Illustration of the way of finding a break in the composition dependence of density in sodium silicate glasses by using the data of Ref. [19]. See details in the text.

sodium oxide. If at a crossing point the angle between two curves differs considerably from 180°, it may be considered as an evidence of the existence of a break.

Fig. 9 shows the described processing of Doweidar's data. Here the existence of a break is quite obvious. However, one should find how reliable these measurements were. Bearing this objective in mind it is necessary to collect the results of all density measurements of sodium silicate glasses performed so far. Let us draw approximating curves in the ranges 20–33.3% and 33.3–50% of Na_2O and compare the extrapolations of these curves with the experimental data. The results are shown in Fig. 10. Both extrapolated curves practically coincide with each other.

It is worth mentioning that the same kind of data processing for density of lithium silicate glasses leads to an absolutely different result. Fig. 11 shows that in this case the break of the dependence in a narrow composition range in the vicinity of lithium disilicate is evident.

Note, that the absence of a break in the case of sodium silicate system is not an evidence of the absence of the change in transformation from Q_4 to Q_3 to transformation from Q_3 to Q_2 in the vicinity of a sodium disilicate composition. We have a direct evidence of such a change (see Ref. [20]). Therefore the only conclusion that can be made from Fig. 10 is that both types of tetrahedron transformations affect the density in nearly the same way.
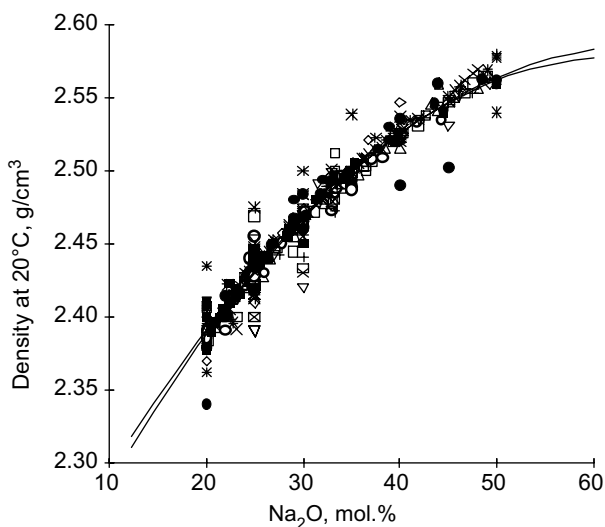

Fig. 10. The same as in Fig. 9 after processing of 461 results taken from 155 publications. Twenty-five points were removed as defective data.
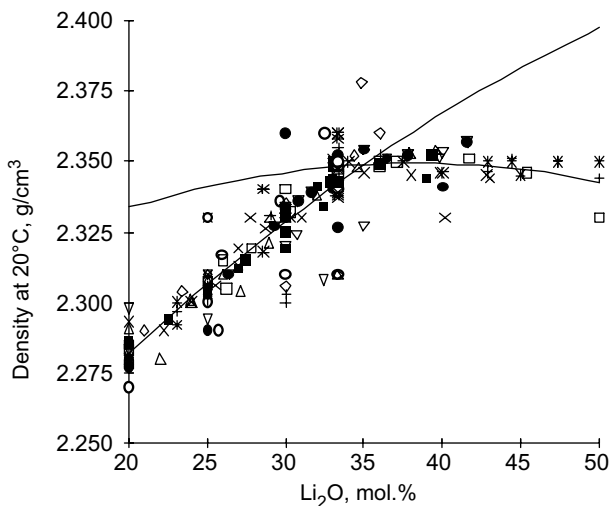

Fig. 11. The same as in Fig. 10 for lithium silicate glasses after processing of 198 results taken from 81 publications. Sixteen points were removed as defective data.

6. On prediction of property-composition dependencies

Finally, an example of an attempt of a direct use of the theory to predict glass property data will be considered. In the last decade Kerner developed a new theory of glass formation and glass transition. In one of his last publications [21] he wrote: 'The most important result of the suggested model is a comparatively precise prediction of the dependence of glass transition temperature on the concentration of a modifying oxide'. According to Kerner [21], one of the few examples of this prediction is the dependence of T_g on composition of sodium silicate glasses for concentrations of Na_2O from 0% to 15%.

Let us start with T_g of silica glass. It is known that the difference between T_g and T_{13} (temperature corresponding to viscosity equal to 10^{13} P) is a minor one. In the SciGlass database there are 52 values for T_g and T_{13} of this glass. It is well known that viscosity (and correspondingly T_g) of silica glass depends particularly strongly on minor impurities including water. Therefore, the scatter of the data is high enough here. Fifty-one points are positioned between 1250 and 1004 °C (mean value is 1156 °C). However only one point is outside the range stated above. T_g for this point is equal to 1460 °C (see Ref. [22]).

Some of readers of the present paper can point out that viscosity of silica glass depends strongly on minor impurities and suppose that only the authors of Ref. [22] managed to remove all impurities from silica glass and thus to obtain a true values of its viscosity. Although it is difficult to expect that nobody of the authors of more than 20 other papers could prepare a pure enough silica glass, some doubts could remain. Fortunately, Leko et al. [23] published results of a detailed study of the influence of impurities on viscosity of silica glass. By the way, it was found that the influ-

ence of alkali impurities in this case is about two orders of magnitude stronger than the influence of water. The authors determined levels of main impurities below which changes of their compositions do not affect the viscosity and accordingly determined the value of T_{13} which are connected solely with viscous flow of pure SiO_2 network. This value appeared to be equal to 1220 °C. Afterwards these findings were confirmed in the paper by Bihuniak [24]. Thus, the results presented in Ref. [22] are obviously incorrect. As usual, it is rather difficult to be sure about the reasons of such great error. One of the possibility is the fact that glasses studied in Ref. [22] were initially held at 1400 °C during 3 days in nitrogen atmosphere.

To check the validity of his theory Kerner used the value of T_g that was equal to 1430 °C without providing any references.

Fig. 12 demonstrates the comparison of Kerner's prediction with the experimental data. It should be taken in mind that in the composition range between 2% and 20% of Na_2O sodium silicate melts have a tendency to phase separation (note that Kerner did not mention this fact). The composition dependence of T_g for imaginary homogeneous glasses should be somewhat different. However, it would only slightly influence the discrepancy between the predicted and experimental dependencies of T_g. This assertion is supported by the corresponding dependence in a potassium silicate system, where there is no tendency to phase separation (Fig. 13).

The conclusion made from the last example is rather obvious. The desire of scientists to use their theories to predict glass properties should be definitely welcomed. However, one can advise these scientists, when selecting data on glass properties for testing the validity of theoretical predictions, to do this by using all the existing information and not taking randomly the first results that happen to come into a scientist's view.
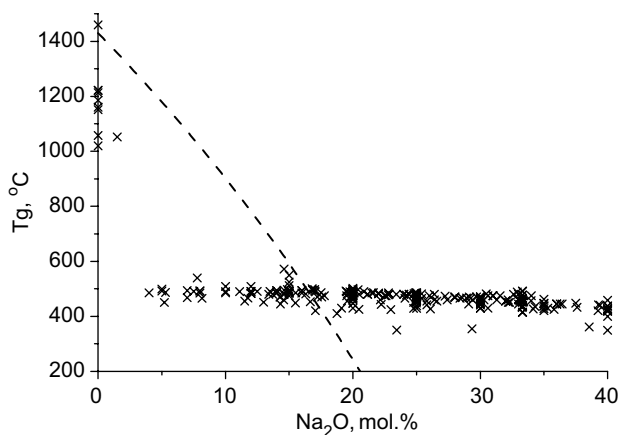

Fig. 12. Comparison of experimental data for dependence of T_g on composition of binary sodium silicate glasses with the prediction of such dependence made by Kerner [21]. Crosses: experimental data; the dashed line: prediction by the Kerner's model.
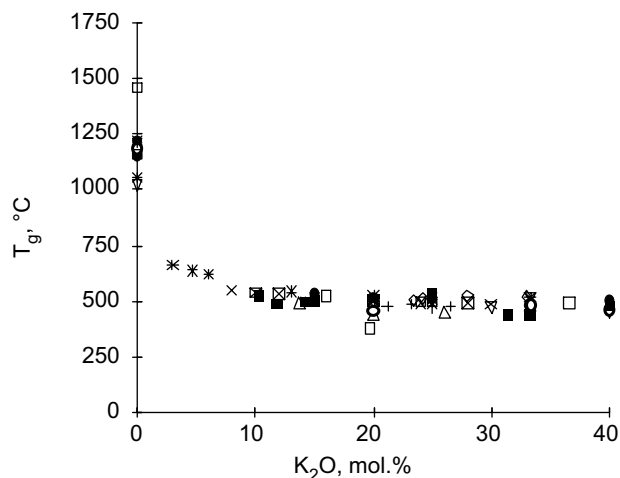

Fig. 13. Concentration dependence of T_g for binary potassium silicate glasses.

It is to be mentioned that at present the only general enough way of prediction of glass properties is the use of numerous methods of calculations of these properties by composition and temperature of glasses of interest. Some of these methods appear to be quite reliable ones. It is reasonable to stress, however, that it is impossible to find the most reliable method for any selected property and recommend this method for universal use. It was found (see, for example, Ref. [25]) that for every selected composition area one should perform a comparison of quite a few methods with the existing experimental data. If these data are taken from numerous enough publications, such comparison will make it possible to select the best method (or sometimes two or three methods of a similar quality) for this particular composition area. A different calculation method may prove to be the best one for another composition area. The corresponding procedure can be performed easily and quickly with the help of the SciGlass Information System [3]. Such comparison also permits determining the value of a systematic error in calculations by a selected method in a selected composition area. Correction for this error makes the calculation results even more accurate.

Such approach makes it possible to determine composition dependencies of a selected property for a series of multi-component glasses that could be specially designed for testing the predictive quality of a structural model.

7. Conclusion

The main conclusion of the information presented in this paper is as follows. Both when studying and applying the property-composition dependencies in comparatively simple glass-forming systems it is necessary to

analyze the whole set of the so far published experimental data belonging to a selected property and system. Certainly, every scientist can do this by his/her own means, just like any highly qualified scientist used to do it in the middle of the last century. However, it is much more reasonable to collect the necessary data by using one of the two existing glass property databases. It will simplify the work by many orders of magnitude. There are reasons to state that at present the SciGlass Information System is the most convenient instrument for reaching such an objective.

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