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Recalculation of the volumes of BO_3 and BO_4 units in alkali borate glasses

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In a previous work [1] the density of alkali borate glasses was treated from a specific point of view which was, at that time, a new one. It is assumed that up to about 33 mol% R_2O (alkali oxide) these glasses are composed of symmetric BO_3 units and BO_4 tetrahedra. The density data of glasses having up to 33 mol% R_2O were analyzed manually to calculate the volumes of the BO_3 units and BO_4 units. The analysis is based on the relation

$$D = [N_3M_3 + N_4M_4]/[V_3M_3 + V_4M_4]. \quad (1)$$

Here D is the density, N_3 is the number of BO_3 units per mole of glass, M_3 is the mass of BO_3 unit and V_3 is its volume. N_4, M_4 and V_4 represent the corresponding parameters for the BO_4 units. Equation 1 can be solved to calculate V_4 and V_4 as a function of glass composition. Details for calculations are given in reference [1].

On the basis of former studies on silicate glasses [2] we came to a common conclusion that in the mixed and multiple modifier glasses the volume of any structural unit remains the same as in the corresponding binary silicate glass. Recently we treated the density of mixed alkali borate glasses [3]. A trial has been done to calculate the density of such glasses by using V_3 and V_4 of binary alkali borate glasses. There was a marked difference between the determined and calculated densities. To get V_3 and V_4 of binary alkali borate glasses [1], the calculations were carried out using the density data presented in Fig. 1. For this reason we thought it may be useful to recompute V_3 and V_4 from the equation of the fitting plot of the density data. This allows us to follow the change in these volumes through smaller increments of alkali oxide.

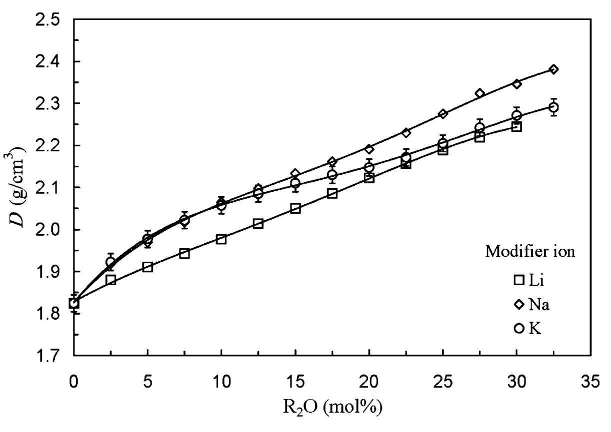

Figure 1 Density of Li_2O-B_2O_3, Na_2O-B_2O_3 and K_2O-B_2O_3 glasses as a function of the alkali oxide (R_2O) content. The data are taken from Ref. 1. The lines are fitting plots of the experimental data.

The equations of the density plots (Fig. 1) for Li_2O-B_2O_3, Na_2O-B_2O_3 and K_2O-B_2O_3 glasses are, respectively

$$D = -6.728 \times 10^{-7}C^4 + 3.915 \times 10^{-5}C^3 - 7.591 \times 10^{-4}C^2 + 1.955 \times 10^{-2}C + 1.828, \quad (2)$$

$$D = -1.143 \times 10^{-6}C^4 + 8.857 \times 10^{-5}C^3 - 2.358 \times 10^{-3}C^2 + 3.938 \times 10^{-2}C + 1.826 \quad (3)$$

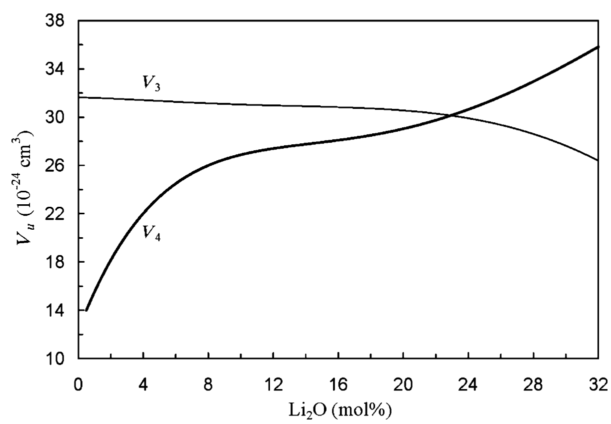

Figure 2 V_3 and V_4 as a function of the alkali oxide content in Li_2O-B_2O_3 glasses.

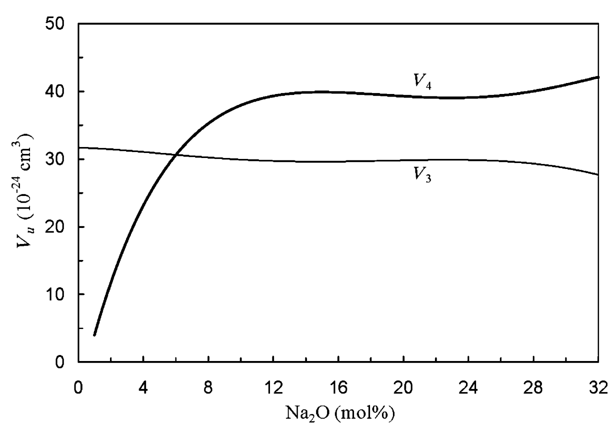

Figure 3 V_3 and V_4 in dependence of the alkali oxide content in Na_2O-B_2O_3 glasses.

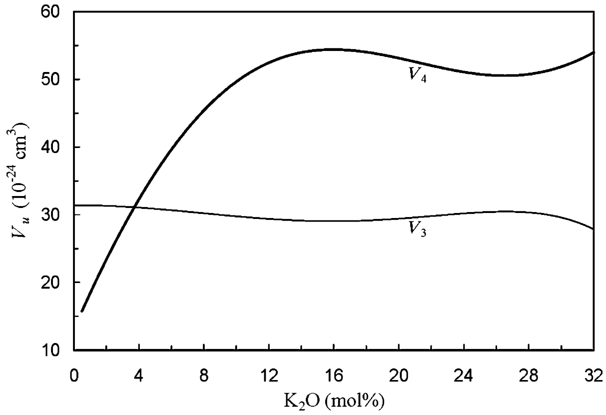

Figure 4 Correlation between V_3 and V_4 and the alkali oxide content in K_2O-B_2O_3 glasses.

and

$$D = -1.174 \times 10^{-6}C^4 + 9.777 \times 10^{-5}C^3 - 2.810 \times 10^{-3}C^2 + 4.271 \times 10^{-2}C + 1.826. \quad (4)$$

Here C is the concentration of alkali oxide in mol%. The volumes obtained from these relations are presented in Figs 2–4, as a function of the alkali oxide content. The trends observed in Figs 2–4 do not differ, in general, from those reported in reference [1]. There are however certain differences in the values of V_3 and V_4. The densities calculated from the newly obtained volumes agree well with the experimental densities of mixed and multiple alkali borate glasses [3]. These results reveal that in complex borate glasses the volumes of structural units are the same as in binary glasses.

References

1. H. DOWEIDAR, *J. Mater. Sci.* **25** (1990) 253.
2. *Idem.*, *Phys. Chem. Glasses* **40**(2) (1999) 85.
3. H. DOWEIDAR, Y. M. MOUSTAFA, G. M. EL-DAMRAWI and R. M. RAMADAN, "Structural Analysis of the Density of Mixed Alkali Borate Glasses" (to be published).

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