

Effect of Al/B substitution on structure and properties of silicate glasses and melts

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The relationship between physical properties and structure of glasses and melts in the system $MO-T_2O_3-SiO_2$ (with $M=Na_2, Ca$ and $T=Al, B$) are technologically and geologically important, in particular to understand the microscopic origin of the configurational thermodynamic properties. The connection of these network former is fundamental to understand the physical properties of magmatic liquids.

The configurational properties of melts and glasses provide fundamental information needed to characterize magmatic processes. A principal difficulty, however is to link the "macroscopic" configurational entropy with the structure of melts. This has been done by combining viscometry with Raman and NMR spectroscopy studies. From the viscosity measurements at low and high temperatures, we have obtained the configurational entropy, S_{conf} ($\log \eta = Ae + Be/TS_{conf}$, where η is the viscosity, T the temperature and Ae, Be two constants).

Silicon, aluminum, and boron are 3 network formers playing different role on the silicate network, whereas Si is the strongest network former in coordination 4, 5 or 6 as a function of T, P ; Al can play different function as a network former in 4- or 5-fold coordination and probably as a network modifier in 6 fold coordination. Boron observed in 3 or 4 fold coordination is always a network former but for very "fragile" glasses.

For the glass the Al/B substitution produce a small decrease of the molar volume while this substitution produced a strong decrease of viscosity and glass transition temperature while the fragility of the network is less affected by this chemical change. Raman spectra show significant change in the D1 and D2 bands. NMR spectroscopies show also significant change as a function of chemical change and temperature. All this observations will be discussed and interpreted in order to link microscopic versus macroscopic changes.

Historical deposition of Polycyclic Aromatic Hydrocarbons in an Amazon estuary

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Polycyclic aromatic hydrocarbons (PAHs) are ubiquitously distributed in the aquatic environments, coming from natural and anthropogenic sources. PAHs can accumulate in sediments and their historical deposition can show source alterations throughout time. The study area, Guajará Bay, is located in northeastern Amazon and Belém (one of Amazon's biggest cities) is located in its margins. To evaluate the temporal changes of PAHs in Guajará Bay a sediment core was collected in 2010. Total PAH concentration (ΣPAH) ranged from 46.9 to 595 $ng\ g^{-1}$ (dry weight) along the core. The core can be divided in two periods regarding PAHs sources to the area. In the first period, corresponding from 1900's to the early 1960's, ΣPAH remained constant, with an average of 79 $ng\ g^{-1}$ (d.w.), possibly characterizing base levels of PAHs for this region. Composition of individual PAH showed a predominance of alkyl-PAH over its parental compound such as methylphenanthrene over phenanthrene. Usually, these PAHs are associated with petrogenic inputs, however, there is no evidence of oil during this period in the region. Thus, the higher proportions of alkyl-PAHs could be related to natural sources, such as organic matter diagenetic transformation or biogenic synthesis. During the second period, which starts in the late 1960's, ΣPAH increases, reaching its maximum value at the top of the core. Diagnostic ratios showed a predominance of pirolitic PAH in the area, suggesting that this input is probably related to the intensification of the urban and industrial development, encouraged by the government since 1950's. The variation of PAH contents was closely related to the changes in the environment of the Amazon area evaluated.