

On the arrangement of sodium atoms around structural units and vibrational properties of a sodium borosilicate glass

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We have used first principles simulations in order to investigate the properties of a sodium borosilicate glass of composition $3\text{Na}_2\text{O}-\text{B}_2\text{O}_3-6\text{SiO}_2$ (NBS). This composition is similar to that of the glass wool used in our daily life. The study was carried up using first principles molecular dynamics within the density functional theory framework as implemented in the VASP code [1].

In this talk, we will present the analysis of the local environments of the three building structural units of the glass network, namely silicon atoms in 4-fold coordination, and boron atoms with 3- or 4-fold coordination. We will also discuss the local distribution of the Na atoms around the basic structural units. Indeed we have identified their preferential neighborhoods and how the nature of network former and its coordination infer on the shape of these preferential regions of Na atoms.

The vibrational properties have been equally studied, and the contributions of the various species have been identified. We have found that 3- and 4-fold coordinated boron atoms give rise to distinguished spectral features. Moreover, the partial vibrational density of the 3-fold coordinated B atoms has been found to be a weighted sum of 2 specific contributions so-called 3-fold symmetric coordinated B atoms and asymmetric coordinated B atoms.

[1] Kresse & Hafner (1993) *PRB* **47**, 558; Kresse & Furthmüller (1996) *Comp.Mater. Sci.* **6**, 15; Kresse & Furthmüller (1996) *PRB* **54**, 1116

Different diagenetic behaviors of As, Mo and Sb in Lake Biwa, Japan

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Lake Biwa, the biggest lake in Japan, is suitable field to study diagenetic behavior of redox sensitive oxyanions, since clear diagenetic accumulation of Mn and As in surface sediment have been observed from entire lake. Redox conditions, evaluated by the depth profiles of solid phase speciation of Mn and As determined by XANES, were significantly varied depending on the sampling location within the lake. Here we show the comparison of depth profile of As, Sb, and Mo in both solid phase and porewater among various redox conditions. Of the seven stations studied, As profiles in porewater showed clear concentration peak in six. The depth of these peaks ranged from 3 to 1 cm below sediment-water interface, and arsenite was the dominant species around the areas where the peaks appeared. The peak values of As in solid phase always appeared 1-2.5 cm above the places where the peaks of porewaters were found. Predominance of arsenate in surface sediments suggested diagenetic accumulation of As, whereas As-S species becomes predominant below As peak areas in porewater. Both Mo and Sb showed cocentration peak in 5 stations. Two stations in which the peaks were not observed are in areas with most reducing conditions where no MnO_2 enrichment was observed even in the top layer (0-5 mm). In the other 5 stations, depth of the peaks in porewater were always in the following order: As>Sb>Mo. Difference in peak depth between As and other 2 elements were 0.75-1.5 cm, whereas difference between Sb and Mo were <0.75 cm. It is well known that these oxyanions have high affinity to Fe (oxy)hydroxides. However, if the dissolution of this phase predominantly controls the solid-water partitioning of these oxyanions, the porewater profile should be similar. Distinctly higher depth of As peak is likely attributed to arsenate reduction to arsenite which enhances the mobility of As. Slight differences in Mo and Sb is possibly due to high affinity of Mo to MnO_2 that reduces more easily than Fe (oxy)hydroxides. Although these relative mobility should change in more sulfidic setting like seawater, such a comparison is rather limited in freshwater system so far, thereby the finding of this study can contribute for better understanding of diagenetic behavior of these elements.