STRUCTURAL, ELECTRONIC, AND VIBRATIONAL PROPERTIES OF A SODIUM BOROSILICATE GLASS FROM FIRST PRINCIPLES STUDIES

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We have carried out first-principles molecular dynamics simulations of a sodium borosilicate (NBS) glass within the framework of DFT. The composition is $6SiO_2$-$3Na_2O$-B_2O_3 and the density was fixed to 2.51g.cm^{-3}. The system size is 320 atoms (*i.e.* 60 silicon, 180 oxygen, 60 sodium and 20 boron atoms) which is rather demanding for *ab-initio* simulations and has been chosen to obtain a good statistics, in particular for quantities associated to the lowest concentrated element (boron).

The simulations have been started at 4500K in the canonical ensemble (NVT) and followed by a simulation in the microcanonical ensemble (NVE). Subsequently, the system is progressively cooled to 300K within 60ps. In order to characterized the structure of the system we have calculated the pair correlation functions, the angular distributions, the Q_n distributions, the non bridging oxygen's concentration as well as the partial structure factors. Moreover, we have studied the environment of 3- and 4-fold (B^{III} and B^{IV}) coordinated boron atoms. Furthermore, the vibrational density of states has been studied in details. Indeed, both B^{III} and B^{IV} atoms have specific frequencies, and the partial vibrational density of the 3-fold coordinated B atoms has been found to be a weighted sum of two specific contributions: 3-fold symmetric coordinated B (B^{III}_{s}) atoms and asymmetric coordinated B (B^{III}_{a}) atoms. Identically, the partial vibrational density of the 4-fold coordinated B atoms has been found to depend on the nature of their second neighbor namely so-called B^{IV}_{Si4-B0}, B^{IV}_{Si3-B1}, B^{IV}_{Si2-B2}, B^{IV}_{Si1-B3}, and B^{IV}_{Si0-B4} respectively with 4 Si and 0 B atoms as second neighbor and so on. The infrared spectra of our glassy models is also presented.

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