DISTRIBUTION OF RINGS AND INTERMEDIATE RANGE CORRELATIONS IN SILICA GLASS UNDER PRESSURE - A MOLECULAR DYNAMICS STUDY

José Pedro Rino
Universidade Federal de São Carlos, Via Washington Luiz Km 235-13565-905, São Carlos, S.P. Brazil

Gonzalo Gutiérrez
Facultad de Física, P. Universidad Católica de Chile, Casilla 306, Santiago 22, Chile

Ingvar Ebbsjö
The Studsvik Neutron Research Laboratory, S-611 82 Nyköping, Sweden

Rajiv K. Kalia and Priya Vashishta
Concurrent Computer Laboratory for Materials Simulations
Department of Physics & Astronomy and Department of Computer Science
Louisiana State University, LA 70803-4001
E-Mail: djpr@power.ufscar.br Web: http://www.cclms.lsu.edu/

ABSTRACT

Using the molecular dynamics (MD) method, we have studied the effect of pressure on the distribution of rings and their relationship to intermediate range correlations manifested as the first sharp diffraction peak (FSDP) for SiO_2 glass. A systematic analysis of the modifications observed in the FSDP for densities ranging from 2.0 to 3.2 g/cm^3 and temperatures from 0 to 1500 K is reported. The decrease in the height of the FSDP with increasing density is found to be proportional to the decrease in the number of 6-fold rings. For the density and temperature ranges studied in SiO_2 glass, the full width at half maximum (FWHM) of the FSDP remains unchanged.

INTRODUCTION

Structural order in silica glass can be divided into short-range order (SRO) and intermediate range order (IRO) [1-5]. X-ray [2], neutron [3] and nuclear magnetic resonance (NMR) [4] experiments reveal the presence of corner-sharing $Si(O_{1/2})_4$ tetrahedra in silica glass at normal density (2.2 g/cm^3). The IRO is manifested as the first sharp diffraction peak (FSDP) in the static structure factor, S(q) in neutron and x-ray diffraction experiments [1-3].

One of the anomalous features of the FSDP in many network glasses, especially chalcogenide glasses such as $GeSe_2$ and $SiSe_2$, is that the height of the FSDP increases with increasing temperature [1,5,6]. This is contrary to the normal behavior where the height peaks in S(q) decrease with increasing temperature. The FSDP in $GeSe_2$ and $SiSe_2$ have been shown to arise mainly from Ge-Ge and Ge-Se (Si-Si and Si-Se) correlations between 4 and 10 Å. The temperature dependence of the FSDP is found to be a balance between two competing effects: the disorder due to thermal vibrations and thermal expansion [5]. Thermal vibrations broaden the peaks in the pair distribution functions and hence reduce the amplitude of peaks in its Fourier transform, *i.e.*, the static structure factor. On the other hand, the thermal expansion decreases the frustration associated with the disordered arrangement of $GeSe_2$ tetrahedral units, thereby increasing the height of the FSDP. Neutron diffraction study by Susman et al. [7] has revealed that in SiO_2 glass the height of the FSDP decreases with increased temperature contrary to other glasses. Normal behavior of the FSDP in SiO_2 glass is a consequence of an essentially zero thermal-expansion coefficient so that the effect due to thermal vibration dominates. Using neutron diffraction, Susman et al. [8] have studied the changes in the intermediate range order up to 20%

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