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Densified silica glass study by RMC simulation using X-ray and neutron diffraction data

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In the nearest future it will be possible to complement high pressure x-ray measurements at synchrotron with neutron diffraction study at J-PARC. Analyzing both experimental data in combination may have a synergistic effect. One possible method is to use the Reverse Monte Carlo (RMC) algorithm [1] to derive structures of disordered materials from both diffraction data. In order to gain experience we analyze previously measured X-ray and neutron diffraction data on normal and densified silica glass SiO_2 [2,3].

High pressure study of this archetypal glass, formed by SiO_4 tetrahedrons with network structure, is still challenging. One of the main issues is understanding of permanent densification mechanism (at $p>10$ GPa at room temperature). It is known that densification is occurred mostly with modification in the intermediate range order rather than in short-range order. The fact that heating induces the structural change in the intermediate range order suggests that a thermally activated process such as rebonding (breaking of the original bonds and forming of new ones) should accompany the changes.

In order to verify topological changes by analyzing structures directly, we used RMC simulation to build 3D structural models of normal and densified glass. RMC derived a set of coordinates of the 6000 atoms of the configurations that are in good agreement with the experimental data.

RMC model reproduces the experimental data accurately and gives reasonable bond angle distributions. The O-Si-O angle distributions peak around 109 deg, only a slight broadening is seen in the densified glass. The intertetrahedral Si-O-Si angle distribution in the densified silica glass slightly shifts to lower values. Overall not much difference is seen in the other bond angles distributions. As for network topology study, RMC modeling should be done carefully. In usual way denser model is created by compacting of normal one. But in this case it is impossible to model rebonding process, since due to coordination number constraints RMC cannot change the connectivity pattern much. Therefore proper model of densified silica glass should be started from different (independent) initial configurations. To provide better understanding of densification mechanism further analysis (e.g. void space distribution) is in progress.

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