

Structural study of P₂O₅ glass under high pressure

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The structure of P₂O₅ glass was studied up to 10 GPa, using an x-ray diffraction technique. Large difference of the structure of “cold” compressed glasses and glasses quenched from melt under pressure was found.

キーワード : P₂O₅、液体、構造、高圧、X線回折

1. 目的

The purpose of the study was to investigate the structure of P₂O₅ glass under high pressure. P₂O₅ substance ranks third among the top network-forming oxides (behind SiO₂ and B₂O₃) in terms of its use in glass products. At room pressure P₂O₅ melt is molecular- based (P₄O₁₀) polymeric liquid with high viscosity and nice glass-forming properties. One can propose polyamorphism in the P₂O₅ liquid and glass under pressure. However the structure of P₂O₅ phases under pressure previously almost has not been studied. It is mainly due to extremely high hygroscopic nature of this substance. We have elaborated the method of the samples and assembly preparation in Ar box. We also recently designed new high-pressure assembly with several levels of thermal protection which enables us to fulfill structure study at temperatures up to 2000 K under pressures up to 10 GPa. Recently we studied the structure of P₂O₅ crystalline phases and liquid state at several pressures up to 10 GPa using SPring-8 facility [1].

2. 方法

In present study we executed 2 kinds of experiments at BL14B1 of SPring-8. In one set we fabricated P₂O₅ glass at relatively low pressures (0.5-1 GPa). These glasses have the structure similar to normal pressure glass. Then we made in situ x-ray diffraction study of these P₂O₅ glasses in 1-10 GPa region both during compression and decompression and also during heating at high pressures. The second kind of experiments consisted in the preparation of P₂O₅ glass by quenching from the melt at very high pressures (4GPa, 7 GPa and 10 GPa) and further study of their structures.

3. 研究成果

We found large difference of the structure of “cold” compressed glasses and glasses quenched from melt under pressure. During room temperature compression the structure factor of glasses does not significantly change up to 10 GPa. The position of the pre-peak slightly diminishes and shifts from 1.3 Å⁻¹ to 1.7 Å⁻¹ at 10 GPa. The next peak position shifts from 1.8 Å⁻¹ to 2 Å⁻¹. These changes are almost reversible – only several percent changes of position and intensity of the peaks are observed after decompression. At highest pressures the additional structure relaxation with significant decrease of the intensity of the 1st peak is observed during heating. The structure of the glasses prepared by quenching from melt at very high pressures is quite different: the pre-peak of the structure factor is absent and this unusual structure is conserved after decompression.

4. 結論・考察

We can conclude that there are significant structural changes in the liquid between 2 and 10 GPa and the glass inherits the structure of liquid. The structural changes are associated with the modification of the intermediate-range order structure and possible change of the short range order structure. The corresponding structure modification of the glass during “cold” compression obviously occur at pressures higher than 10 GPa, the changes are only started at 10 GPa under heating to 150-500°C. The calculation of the structure factors and radial distribution functions is in progress now.

5. 引用(参照)文献等

[1] V. Brazhkin, et al., Experimental Report, “Structural study of P₂O₅ and B₂O₃ liquids under high pressure”, 2008B-E06.