Structural study of P_2O_5 and B_2O_3 liquids under high pressure

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The structure of B_2O_3 and P_2O_5 oxide melts was studied for the first time in 5-8.5 GPa, 1100- 1600°C pressure, temperature –region using an in-situ x-ray diffraction technique.

キーワード：B_2O_3, P_2O_5, liquid, structure, synchrotron radiation

１．目的

The problem of phase transformations in disordered substances - liquids and glasses under pressure is one of the hottest topics of condensed matter physics.　Among simple oxide substances liquid P_2O_5 and B_2O_3 is attractive candidates for the search of the structural coordination changes under high pressure The purpose of the study was to investigate the structure of B_2O_3 liquid and P_2O_5 liquid and under high pressure. At room pressure P_2O_5 liquid is molecular- based (P_4O_{10}) polymeric liquid with high viscosity and nice glass-forming properties. This substance almost has not been studied under pressure up to date both in solid and liquid phase. In 2004-2006 years P_2O_5 liquid and solid were investigated up to 5 GPa and 1000°C. During executing the project 2007B3608 we have managed to get molten state of P_2O_5 at 10 GPa (melting temperature is around 1200-1300°C) and have recorded high quality diffraction spectra of the melt.　B_2O_3 liquid at normal pressure has coordination number (B-O) in the first sphere equal 3 similar to normal pressure glassy and crystalline phases. It was supposed that B_2O_3 liquid under pressure should transform to the denser phase with higher boron coordination similar to crystalline phase that undergoes a phase transition to 4-coordinated phase at 4 GPa. In 2003-2004 we have tried to study the structure of B_2O_3 liquid under pressure by in situ x-ray diffraction method (energy dispersive technique) using BL14B1 station of SPring-8. No significant changes of the liquid structure were observed at pressures up to 4.5 GPa. . The aim of present project was to make in situ x-ray diffraction study of B_2O_3 liquid in 6-9 GPa pressure region and to get more diffraction spectra of P_2O_5 liquid in 5-10 GPa region..

２．方法

Large-volume presses are the most suitable pressure apparatus for structural studies on disordered materials under high-pressure and high-temperature. In the present study we use cubic large-volume press installed at BL14B1 beam-line. We used energy dispersive technique and have got spectra at 2θ ranged from 3 to 18 degrees.

３．研究成果

During this project we significantly improved the assemblies design using new combination of special shields and cups made from thermal insulating materials. As a result we succeed to reach record temperatures 1500-1600 °C at pressures 5-10 GPa using small 4 mm- ends -hard alloy anvils and boron epoxy cubes. The assemblies were enough stable to sustain necessary parameters during several hours. B_2O_3 liquid structure was successfully studied for the first time in the 4.5- 8.5 GPa region. We have got structural information at 5 pressure points (4.7, 5.6, 6.0, 6.9 and 8.2 GPa) for B_2O_3. Besides B_2O_3 melt study we have got one set of high quality structural data for P_2O_5 melt at 7.3 GPa and 1100°C. Thus now P_2O_5 liquid and solid are studied in details as for their structure in whole pressure range from 0 to 10 GPa.

４．結論・考察

Significant structural modification of the B_2O_3 melt at compression was found. The position of the 1st maximum of the structural factor is shifted to higher wave-vectors as the relative intensity of the 2d maximum increases. These structural changes sharply start at 5-5.5 GPa and continue at further compression. One may propose that there is a significant coordination change in B_2O_3 melt at 5-8 GPa region. To prove it we are going to calculate total correlation function to define average coordination numbers. The analysis of structural data for P_2O_5 is also in progress.

５．引用(参照)文献等

[1] V.Brazhkin, Y. Katayama et al " Structural transformations in liquid , crystalline and glassy B_2O_3 under high pressure" ZHETP Lett. 78 (2003) 393