

Structural study of phase transformation in B₂O₃ liquid under high pressure

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A new assembly with thick thermo-insulations and X-ray windows was developed for structural studies on liquid at 10 GPa and 1300-1500C. Diffraction data on P₂O₅ in polymeric liquid phase were successfully obtained.

キーワード : B₂O₃, P₂O₅, 液体、構造、放射光

1. 目的

The purpose of the study was to investigate the structural aspects of the hypothetical coordination phase transformation in B₂O₃ and P₂O₅ liquids by in-situ high-pressure x-ray diffraction experiments at high pressures 6-11 GPa. Before we have studied the structure of B₂O₃ and P₂O₅ liquids up to 5 GPa [1]. There no strong structural changes were observed. B₂O₃ undergoes coordination structural changes under pressure both in crystalline (around 4 GPa) and glassy (6-16) GPa states. P₂O₅ crystal and glass previously were not studied. Since boron, phosphorus and oxygen are low-z elements the large volume high-pressure cell as well as high intensity x-ray source were needed to execute the structural study.

2. 方法

In 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. The standard high pressure cell design with boron-epoxy cubes enables us to reach temperatures around 1000C at 10 GPa region. The melting temperature of both substances under investigation at very high pressures around 10 GPa reaches 1300-2000C. To get such temperatures in small cubic press (4mm anvils) we elaborated new assembly with thick thermo-insulations and X-ray windows.

3. 研究成果

The present experiments showed, at very high temperature the conductivity and thermal conductivity of the insulator parts increases and working temperatures of the new cell at 10 GPa is 1300-1500C. It is much better than that of standard one but it is not enough to study B₂O₃ liquid (melting temperature is 1500-1800C in 6-10 GPa pressure interval). As a result we studied only P₂O₅ liquid. The P₂O₅ samples and assemblies were prepared in Ar box then they were rapidly installed into the press. At first we have obtained for the first time the structural data of P₂O₅ molecular crystal at room T up to 11GPa. At heating at 600-800C region the molecular phase transformed to the polymeric phase. The structure of this polymeric phase is different from that of polymeric phase obtained at 0-6 GPa pressure interval implying the existence of phase transformation between 6 and 10 GPa in crystalline state. The melting temperature of P₂O₅ at 10-11 GPa is 1400+-100C.

4. 結論・考察

The structure of the P₂O₅ melt was investigated at 6 scattering angles 4,6,8,10,14,18. The quality of the structural data is high enough to get reliable structure factor and total correlation function. The structural analysis of both melt and crystalline phase of P₂O₅ is in progress now. The authors believe that the new high-pressure assembly can be improved by the partial change of insulator material (ZrO₂ instead of LaCrO₃). Thus, the study of B₂O₃ melt under pressures 6-10 GPa will be continued in future using updated assemblies.

5. 引用(参照)文献等

[1] V.Brazhkin, Y. Katayama et al " Structural transformations in liquid , crystalline and glassy B₂O₃ under high pressure" ZHETP Lett. 78 (2003) 393