弾性波速度および放射光X線回折測定と分子動力学シミュレーションによる$CaAl_2O_4$ガラスの圧力誘起ポリアモルフィック転移の解明

Pressure-induced polyamorphic transition in $CaAl_2O_4$ glass revealed by elastic wave velocity and X-ray diffraction measurements and molecular dynamics simulations

*大平 格[1]、河野 義生[2,3]、Gréaux Steeve[3]、Drewitt James W E[4]、Jahn Sandro[5]、則竹 史哉[6]、尾原 幸浩[7,8]、廣井 慧[7,8]、近藤 望[9]、Hrubiak Rostislav[10]、肥後 祐司[8]、辻野 典秀[8]、柿澤 翔[8]、新田 清文[8]、関澤 央輝[8]
*Itaru Ohira[1], Yoshio Kono[2,3], Steeve Gréaux[3], James W E Drewitt[4], Sandro Jahn[5], Fumiya Noritake[6], Koji Ohara[7,8], Satoshi Hiroi[7,8], Nozomi M Kondo[9], Rostislav Hrubiak[10], Yuji Higo[8], Noriyoshi Tsujino[8], Sho Kakizawa[8], Kiyofumi Nitta[8], Oki Sekizawa[8]

1. 学習院大・理、2. 関西学院大・理、3. 愛媛大・GRC、4. ブリストル大・物理、5. ケルン大・IGM、6. 山梨大・総合研究、7. 島根大・材料エネルギー、8. 高輝度光科学研究センター、9. 岡山大・IPM、10. アルゴンヌ国立研究所・HPCAT
1. Gakushuin Univ. Sci., 2. Kwansei Gakuin Univ. Sci., 3. Ehime Univ. GRC, 4. U. Bristol Phys., 5. U. Cologne IGM, 6. U. Yamanashi Interdisciplinary Research, 7. Shimane Univ. Materials for Energy, 8. JASRI, 9. Okayama Univ. IPM, 10. ANL HPCAT

In recent years, there has been increasing emphasis on the fabrication and characterization of non-conventional network glass formers such as $CaO–Al_2O_3$, $BaO–Al_2O_3$, and $BaO–TiO_2$ in material science [e.g., 1]. Although these systems are different from those of magmas traditionally studied in geoscience field, recent experiments have confirmed the formation of network-modifiers- and Al-rich partial melts at the conditions of the transition zone and the lower mantle [2,3]. Therefore, the high-pressure studies of non-conventional network glass formers, as well as typical network-forming oxide glasses such as SiO_2 glass, are also important in understanding the pressure-induced changes of structure and physical properties of the magmas in the deep earth.

In this study, we conducted elastic wave velocity and XRD measurements and molecular dynamics (MD) simulations on $CaAl_2O_4$ glass. Ultrasonic velocity measurements up to 24 GPa at BL04B1 at SPring-8 reveal abrupt and irreversible increases in the v_P and v_S at ~8–10 GPa. Total structure factor and pair distribution functions measured by synchrotron XRD at 16-BM-B at APS and BL37XU at SPring-8 show a rapid change in the intermediate range structure, which is likely attributed to a rearrangement of Ca ions over this narrow pressure condition. Structure models obtained from MD simulations reveal that this intermediate range structure is explained by a transition of Ca–O void radius distribution from a bimodal distribution with peaks at ~2.1 Åand ~2.4 Åto a single distribution centered at ~2.1 Å. The abrupt structural changes involving the rapid increase in elastic wave velocity in $CaAl_2O_4$ glass are markedly different to the continuous transformations reported in SiO_2 glass. The polyamorphic transition observed in this study may be one of the key mechanisms in the densification and the changes in seismic wave velocity of the magma just above the 410 km discontinuity.

References

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