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Structure of jadeite-diopside melts at high pressure by in situ x-ray diffraction

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Properties of silicate melts control magma-related processes such as volcanic activity and evolution of the Earth. Since these processes take place in Earth's deep interior, there is considerable interest in documenting experimentally how pressure affects properties of silicate melts. Macroscopic physical properties are largely determined by the microscopic structure. The bond length and strength between tetrahedrally coordinated cation (T=Si⁴⁺, Al³⁺) and oxygen (T-O length) are especially important in the relationship between structure and physical properties of silicate melts. For silicates, T-O lengths are the shortest among a large variety of melts, therefore we need XRD data with large Q coverage in order to obtain accurate T-O length experimentally. In this study, we tried out XRD experiments by Paris-Edinburgh press, which enables us to get XRD patterns to 2theta angles as high as 40 degree, and photon energies in excess of 100 keV. On the basis of the structural investigation at ambient pressure, the jadeite melt is a typical polymerized melt, while the diopside melt is depolymerized. Considering the structural parameters under ambient condition the ratio between non-bridging and tetrahedrally bonded oxygen (NBO/T), jadeite melt is 0 and diopside melt is 2. Therefore, these two compositions would allow us to examine the relationship between structure and composition of silicate melts.

High-pressure and high-temperature XRD experiments were carried out in the Paris-Edinburgh press, which was developed by GSECARS and installed at the HPCAT beamline 16-BM-B of APS. The compositions of starting materials were synthetic jadeite (Jd), diopside (Di), and Jd₅₀Di₅₀. The sample container was graphite. The encapsulated samples were enclosed in an hBN cylinder, which served both as an electric insulator and a pressure marker. High-temperature was generated by resistive heating of graphite heater outside the BN cylinder. Pressure medium consisted of ZrO₂, MgO and boron-epoxy. The center of the pressure medium was boron-epoxy and MgO, because of their low absorption to X-ray. The incident X-ray was collimated by a vertical slit (0.5 mm) and a horizontal slit (0.1 mm) to irradiate the sample. The diffracted X-ray was detected by a Ge solid state detector with a 4000 multi-channel analyzer, through vertical (0.5 mm) and horizontal (0.1 mm) receiving slits as well as a collimator. The diffraction patterns were collected for 12 fixed diffraction angles (2theta=3, 4, 5, 7, 9, 11, 15, 20, 25, 30, 35, 39.5 degrees).

The structure measurements of jadeite-diopside melt were carried out in the pressure range from 1 to 5 GPa and at 1600 to 2000 K. Results on structure factors S(Q) and radial distribution functions G(r) of these melts at high pressures and high temperatures will be discussed.

Keywords: melt, high pressure, high temperature, structure, X-ray diffraction