Poster Presentation

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Crystal structure refinement of MgSiO3 high temperature C2/c clinoenstatite

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The high-temperature clinoenstatite (HT-CEn) is one of the important MgSiO3 pyroxene polymorph. The single-crystal of C2/c HT-CEn endmember is firstly synthesized by rapid pressure-temperature quenching from 15-16 GPa and 900-1900 °C [1]. No report that it is produced as single crystal or large domain has been made on the MgSiO3 endmember. The HT-CEn-type modifications are observed in Ca-poor Mg-Fe clinoenstatite and pigeonite and are always found to be unquenchable in rapid cooling. The high pressure and high temperature experiments of MgSiO3 composition were carried out with a Kawai-type multi-anvil apparatus. The samples were quenched by rapidly releasing the oil pressure load and/or by blow out of anvil cell gasket. The space group of C2/c is strictly determined by Rigaku RAPID Weissenberg photographs and synchrotron radiation. Single-crystal X-ray diffraction experiments were performed at ambient conditions using a Rigaku AFC-5 four circle diffractometer. A total of 9383 reflections was measured and averaged in Laue symmetry 2/m to give 766 independent reflections used for the structure refinements. Final reliability factors converged smoothly to R = 0.029. The single-crystal diffraction analysis shows that the unusual bonding distances frozen in this metastable structure. The degree of kinking of the silicate tetrahedral chains is 175° for HT-CEn. The chain angle for HP-CEn is substantially smaller (135°) and the angle for L-CEn turned to the opposite direction at -160° (=200°). The degree of kinking increases by being curved in more than 180° in the transition from HT-CEn to L-CEn. As for the reverse change from the expansion to the stretch, a potential barrier exists in the point of the continuity. It is suggested that the reason which can quench structure under ambient conditions is the present HT-CEn single crystal was formed by the isosymmetric phase transition from HP-CEn. HT-CEn type single-crystals cannot be frozen without pressure.

[1] *A. Yoshiasa, A. Nakatsuka, M. Okube and T. Katsura, Acta Crystallographica Section B, 2013, 69, 541-546*

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