

Structure of MgSiO₃ high temperature C2/c clinoenstatite quenched rapidly from high temperature and high pressure

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Introduction

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.

Experimental

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. Compositions of the single crystals were determined by EPMA. The space group of C2/c is strictly determined by Weissenberg photographs and synchrotron radiation. Single-crystal X-ray diffraction measurements were carried out with a four-circle diffractometer at the BL-10A beam line of the Photon Factory, Tsukuba, Japan, using monochromatized synchrotron X-ray ($\lambda = 0.70006 \text{ \AA}$) radiation. Structure refinements were performed using full matrix least squares program RFIN2. 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 $R = 0.029$.

Results and Discussion

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.

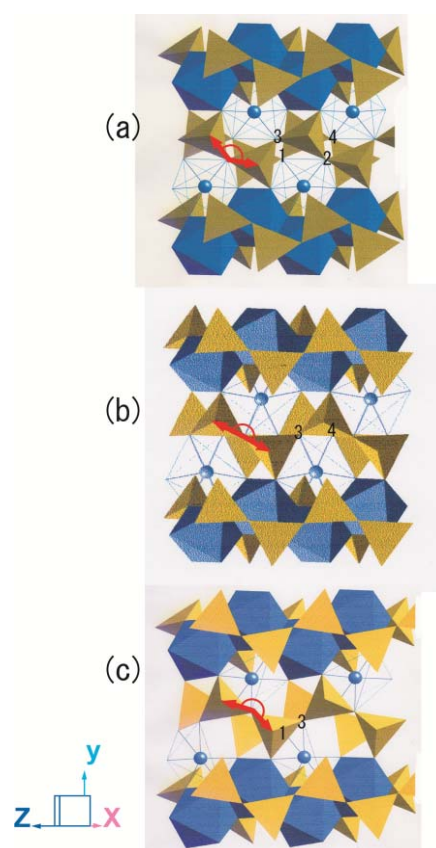


Figure 1. A comparison of the crystal structures among (a) HT-CEn, (b) HP-CEn and (c) L-CEn. Mg1O6 and SiO4 sites are shown by tetrahedral and octahedral descriptions, respectively. The spheres represent the Mg₂ ions. Each coordination environment around the Mg₂ site can be distinguished by the bonding to the O3 atoms labeled in No.1-4 [1].

References

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

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