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Structural transition of post-spinel phases $CaMn_2O_4$, $CaFe_2O_4$, and $CaTi_2O_4$ under high pressures up to 80 GPa

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ABSTRACT

Three structures of $CaMn_2O_4$, $CaFe_2O_4$, and $CaTi_2O_4$ have been proposed as post-spinel phases. Because these structures are very similar, several ambiguities and inconsistencies appear in high-pressure studies, leading to many problems that are yet to be solved. Systematic powder diffraction studies related to these three phases were conducted under high pressure using synchrotron radiation. All three samples have further high-pressure polymorphs. $CaMn_2O_4$ transforms to the $CaTi_2O_4$-type structure at about 30 GPa. The MnO_6 octahedron in the lower-pressure structure is distorted by the Jahn-Teller effect. A new phase was observed at pressures above 50 GPa during compression of $CaFe_2O_4$. Rietveld profile fitting analysis of diffraction data at 63.3 GPa demonstrated that the high-pressure structure, with space group *Pnam*, is produced via a martensitic transformation by displacing atoms in every third layer perpendicular to the *c* axis. $CaTi_2O_4$ also has a new high-pressure polymorph above 39 GPa with space group *Bbmm*. The most probable post-spinel candidate in the mantle is the $CaTi_2O_4$-type structure. The $CaMn_2O_4$-type structure is only formed at high pressure from spinel phases with atoms susceptible to Jahn-Teller distortion.

Keywords: Post-spinel, high-pressure diffraction, structure transition, $CaMn_2O_4$, $CaFe_2O_4$, $CaTi_2O_4$