New stable members at the phase diagram of $CaCO_3$ at pressures to 35 GPa

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We determined phase transitions in $CaCO_3$ at pressures up to 35 GPa and high-temperatures using in situ X-ray diffraction and synchrotron radiation combined with multianvil technique or diamond anvil cell. In addition to geological importance, this investigation has crystal-chemical and fundamental aspect as in this region enigmatic phase transitions from aragonite to disordered calcite or other phases takes place (Suito et al., 2001; Ishizawa et al., 2013). In present experiments we observed transition of aragonite to presumably disordered calcite phase at 1 to 5 GPa and 1273-1473 K, however at 8 GPa and higher temperature we observed transition to new phase, which we tentatively named disordered aragonite. At 14 GPa and 19 GPa we observed aragonite transition into two new different phases at 1773 K. At 30 GPa transition to new structure occurred at 1773-1873 K. An intermediate stable/metastable phase was also observed at 1373-1773 K and 30 GPa. The structures of the new phases were not refined at present, however, they were characterized using orthorhombic symmetry. At 30 GPa new phase may be similar with $P2_1c$-I phase, predicted by *ab initio* computations (Pickard and Needs, 2015). In addition, we determined melting line of phases in the $CaCO_3$ system, which is flat above 6-7 GPa and at 30 GPa it was 200 K lower than previously reported. In this study we significantly improved knowledge of $CaCO_3$ phase diagram, which may be important for thermodynamic calculations of chemical reactions involving carbonate phases relevant to the deep mantle. Indeed, additional refinement of new phases may be needed because it was not possible to quench them to ambient conditions.

Keywords: carbonate, high pressure, mantle, phase diagram

