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Phase transitions of $CaCO_3$ at high P and T determined by in-situ Vibrational Spectroscopy in Diamond-Anvil-Cells

Monika Koch-Müller (1), Sandro Jahn (1), Natalie Birkholz (1,2), and Ulrich Schade (3)

(1) Deutsches GeoForschungsZentrum Potsdam, Sektion 3.3, Potsdam, Germany (mkoch@gfz-potsdam.de, +49 331 288 1402), (2) Angewandte Geowissenschaften, TU Berlin, Berlin, Germany, (3) Helmholtz Zentrum Berlin für Materialien und Energie, Berlin, Germany

Carbonates are the most abundant carbon-bearing minerals on Earth. They can be transported into the upper and lower mantle via subduction processes. Knowledge of the stability of solid carbonates adapting different structures with increasing pressure and temperature is therefore of great importance to understand the structure and dynamics of the Earth. Even for the very simple system $CaCO_3$ the phase relations of at high pressure and temperature are still not fully understood. It has been known for many years that calcite (cc) can adopt different structures with increasing pressure (e.g. Bridgman, 1939: cc-I to III; Tyburczy and Ahrens, 1986: cc-VI). But only recently Merlini et al. (2012) were able to solve the crystal structures of some of these high-pressure polymorphs namely cc-III, cc-IIIb and cc-VI. They report that cc-VI has a higher density then aragonite under the same conditions.

To study the stability of the $CaCO_3$-polymorphs, experiments were performed in conventional diamond anvil cells (DAC) at ambient temperatures as a function of pressure up to 30 GPa as well as in internally heated diamond anvil cells (DAC-HT) in the pressure range 9 to 20 GPa and temperatures up to 800 K. As probe for the structural changes we used conventional mid-infrared-, synchrotron far-infrared- and Raman-spectroscopy. Within the cc-III stability field (3 to 15 GPa at room temperature, e.g. Catalli and Williams, 2005) we observed in all types of experiments consistently two different spectral patterns: one at lower $P < 5$ GPa and another at $P > 5 < 15$ GPa independent on the starting material and the pressure- and time-path of the experiments. Whether these P-induced structural changes may be linked to the above mentioned different structures of cc-III is not yet clear. Also, in all types of experiments we confirmed the transition of cc-III to cc-VI at about 15 GPa at room temperature. Merlini et al. (2012) speculated that temperature may stabilize the structures of cc-III to lower pressure and surprisingly we found the same for the cc-III to cc-VI transition. The reaction has a negative slope of about -0.007 GPa/K. However, our density-functional theory calculations indicate that cc-VI is still metastable in respect to aragonite at least at zero K. We will prove if temperature and the incorporation of smaller cations than Ca have an influence on the stability relations.

References:

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