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High pressure form of $AlPO_4$ with moganite structure

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We recently found three high-pressure phases of $AlPO_4$, and structural and NMR spectroscopic study of two phases (P-1, P21/c phases) are reported (Kanzaki et al., Acta Cryst. B, 2011). Third phase (synthesized at 5 GPa and 1500 ^oC) is later found to have moganite-type structure. Although moganite-type phase is reported for "PON" at high pressure, this is first moganite phase found in ABO_4 system.

$AlPO_4$ moganite was fuond in the sample recovered from 5 GPa and 1500 ^oC synthesized at SPring-8 using SPEED 1500 press. Micro-Raman spectroscopic inspection of the sample revealed the phase is previously unknown phase. ^{31}P MAS NMR and ^{27}Al 3Q MAS NMR indicate two tetrahedral sites for both Al and P, with intensity ratio 2:1. Powder X-ray diffraction of the sample is obtained by Rigaku's SmartLab. Since originally the structure was unknown to us, the structure was solved by FOX using XRD pattern with help of NMR information, and refined by Rietveld method (RIETAN-FP). The structure can be regarded as an ordered replacement of Si in moganite with Al and P, like berlinite. As a result, the space group of the phase is P2/c (moganite SiO_2 and PON are I2/a). First-principles calculation of the phase confirmed its structual stability. First-principles NMR properties calculations using GIPAW method were conducted, and the calculated parameters for moganite phase are consistent with those observed ^{31}P and ^{27}Al NMR.

The phase was also observed in in-situ high T-P powder X-ray diffraction measurements at BL04B1, SPring-8. Moganite phase stablizes at 4 GPa from berlinite. Moganite phase transforms to $AlVO_4$ (P-1) phase at 6 GPa and below 1250 ^oC, but at 6 GPa and above 1250 ^oC transforms to P21/c phase. Contrast to this, no moganite stability field was known for SiO_2 to date. Moganite phase was also reported in PON from high-pressure runs, but moganite phase was low pressure form of quartz phase (Chateau et al., Am. Mineral., 1999). Therefore, pressure-induced phase transformation sequence is opposite between $AlPO_4$ and PON. Differencies of enthalpy and volume of quartz and moganite is small, thus these properties might be reversed with chemistry.

Temperature-induced displacive phase transformation for SiO_2 moganite was reported (Heaney & Post, Am. Mineral., 2001), similar to those of quartz and cristobalite. Thus, such transition might be expected for $AlPO_4$ moganite. We are planning high-T Raman study to confirm this transition, and will report at the meeting.

To date, no synthesis condition for SiO_2 moganite is known, and only natural samples with low cristallinity and coexsiting other phases have been used for research. $AlPO_4$ moganite can be synthesized, and thus can be used for study to understand behavior of moganite structure.

Keywords: moganite, AlPO4, high pressure, phase transformation, crystal structure