https://doi.org/10.46427/gold2026.34270

Structural characterization of $MgCO_3$ H_2O and β-$MgCO_3$

RYO YAMANE[1], SHIGERU SUEHARA[1], YOSHIKI KIYOTA[2] AND HIROSHI SAKUMA[1]

[1]Environmental Circulation Composite Materials Group, National Institute for Materials Science (NIMS)
[2]Rigaku Corporation

Magnesium carbonates are key minerals in carbon mineralization. They exhibit a wide variety of hydrated phases (HMCs, hydrated magnesium carbonates). These phases—including barringtonite, nesquehonite, and lansfordite ($MgCO_3 \cdot nH_2O$; n = 2, 3, 5), as well as partially decarboxylated hydromagnesite ($Mg_5(CO_3)_4(OH)_2$ $4H_2O$) and dypingite ($Mg_5(CO_3)_4(OH)_2$ $5H_2O$)—possess anisotropic crystal structures because water molecules disrupt the three-dimensional linkage between Mg^{2+} and CO_3^{2-} in the HMC structures. Since their needle- or sheet-like morphologies can be retained during dehydration of HMCs, the morphological control of magnesium carbonates using various HMC phases has been an intriguing research topic.

Santamaria-Perez et al. recently reported a new HMC formed by compressing and heating nesquehonite at 700 MPa and 115°C in a diamond anvil cell (DAC) [1].

In this study, we successfully synthesized the new phase using a piston-cylinder high-pressure apparatus with a relatively larger sample volume than that of DAC. Thermogravimetry/differential thermal analysis (DTG-60H, Shimadzu) revealed that its chemical composition is $MgCO_3 \cdot H_2O$, hereafter referred to as MHMC (monohydrated magnesium carbonate). Structural analysis combining 3D electron diffraction (XtaLAB Synergy-ED, JEOL and Rigaku) and powder X-ray diffraction (PXRD, ULTIMA-IV, Rigaku) elucidated the crystal structure of MHMC, which consists of polymerized $MgCO_3$ rod derived from the nesquehonite structure, forming a novel tunnel-type $MgCO_3$ framework that hosts water molecules in its cavities.

Additionally, heat treatment (200-300°C) of MHMC produced a hitherto unknown $MgCO_3$ phase, hereafter referred to as β-$MgCO_3$. Structural characterization of β-$MgCO_3$ was performed by PXRD. In the Rietveld refinement of β-$MgCO_3$, a DFT-optimized dehydrated MHMC structure was used as the initial model (the Vienna Ab initio Simulation Package was employed). The results indicate that β-$MgCO_3$ forms through a topotactic transformation from MHMC, during which the tunnel-type framework is retained.

In this presentation, we will discuss the detailed structural characterization and morphological features of MHMC and β-$MgCO_3$.

[1] Santamaría-Pérez, D., Chuliá-Jordán, R., Gonzalez-Platas, J., Otero-De-La-Roza, A., Ruiz-Fuertes, J., Pellicer-Porres, J., Oliva, R., Popescu, C. Polymorphism and phase stability of hydrated magnesium carbonate nesquehonite $MgCO_3 \cdot 3H_2O$: negative axial compressibility and thermal expansion in a cementitious material (2024), *Cryst. Growth Des.* 24(3), 1159–