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Single Crystal Periclase Hydration Mechanism and Hydration-induced Fracturing

DONG YOUN CHUNG[1], SAI K R ADAPA[2], ANDREW G. STACK[2], JULIANE WEBER[2] AND LAWRENCE M ANOVITZ[2]

[1]Pennsylvania State University
[2]Oak Ridge National Laboratory
Presenting Author: dmc6486@psu.edu

Periclase (MgO) has been suggested as an economical alternative to CaO in direct air capture (DAC) of carbon dioxide based on its lower decarbonization temperature (400 °C for MgO, 650 °C for CaO). Carbonation of periclase occurs more rapidly with higher humidity, and hydration to brucite ($Mg(OH)_2$) was suggested as an intermediate step during magnesium carbonate formation. However, the carbonation reaction kinetics are significantly slowed by the generation of a passivation layer on the surface. The passivation effect may be offset by the fracturing caused by 110 % volume expansion during the hydration reaction. Therefore, understanding the mechanisms of hydration and resulting reaction-induced fracturing is important to evaluate the practicality of using periclase for DAC.

With this aim, in this study, we performed an experimental study on the reaction of single crystal periclase cleaved along (100) direction with the condensed liquid water and vapor. Scanning electron microscopy (SEM) analysis of the periclase surface reacted with the liquid water shows that brucite plates evolved mostly perpendicular to the reaction surface. The brucite particle size was approximately 5 times larger and euhedral when formed adjacent to the cleavage steps of the periclase. This indicates surface roughness and exposed crystal planes significantly affect the extent of the hydration reaction. Spontaneous fracturing occurred mostly at the edge of the crystals, along the preexisting crack. In addition, crystals exfoliated even in the middle of the surface when reacted at 150 °C for 4 hours. We suggest that volume expansion caused by periclase transformation to brucite generated the surface strain that evolves crack propagation and exfoliation, which exposes fresh surfaces of the periclase.

On the periclase surfaces reacted with vapor, brucite islands were observed mostly along cleavage step or fractures. The number of brucite islands increased with time. The result suggests that water droplets, which tend to concentrate on the steps, play a significant role in the hydration of periclase in the presence of the vapor water. To summarize, the hydration of periclase is substantially accelerated on cleavage steps, in both reactions with liquid and vapor water.