Effect of CO₂ on the Mechanical Properties of Minerals in Caprock: A Microscopic Perspective on Caprock Sealing Capacity for CCUS

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Caprock sealing capacity is a key factor in the evaluation of carbon capture, utilization, and storage (CCUS) projects. Hydromechanically induced fractures in caprocks can cause severe leakage. The mechanical properties of caprock are crucial in risk assessment, which can be affected by the minerals or constituents. In this study, we investigate the effect of CO₂ on the mechanical properties of typical minerals in caprock through experiments and simulations. The experimental method for nanomechanical tests was improved to characterize the evolution of modulus in the presence of fluids. Molecular dynamics simulations were carried out to estimate the changes in strength and fracture toughness. Our results indicate that the mechanical properties of minerals may change after exposure to CO2 due to the physical CO₂-mineral interactions, which is different from geochemically induced fracture. The changes in elastic modulus can lead to complex stress conditions due to swelling/shrinkage, and the presence of oil phase may further complicate the behavior. The strength and fracture toughness can be reduced by CO2 significantly, especially in CO2-philic constituents such as organic matters. Our findings imply that CO2 can decrease the strength and fracture toughness of organic-rich layers, and microfractures may propagate through CO₂-philic constituents. This study provides a microscopic perspective on evaluating the caprock sealing capacity for CCUS, which has important implications for risk assessment.