Dissolution of Calcium Hydroxide Surfaces from Simulations and Experiments

MARCO MOLINARI[1,2,*], GIOVANNI L. PESCE[3,4], JAMES GRANT[2], RICHARD J. BALL[4], AND STEPHEN C. PARKER[2]

[1]Department of Chemistry, University of Huddersfield, Queensgate, Huddersfield, HD1 3DH, U.K. (*correspondence: m.molinari@hud.ac.uk)
[2]Department of Chemistry, University of Bath, Bath, BA2 7AY, U.K.
[3]Department of Architecture and Built Environment, Northumbria University, Newcastle upon Tyne, NE1 8ST, U.K.
[4]Department of Architecture and Civil Engineering, University of Bath, Bath, BA2 7AY, U.K.

Dissolution and carbonation of hydrous minerals such as Portlandite, $Ca(OH)_2$, are important processes for a number of environmental and technological applications. These include carbon capture and storage, geological disposal repositories for nuclear waste, and emerging low carbon technologies for construction.

Lime putty (a mixture of hydrated calcium hydroxide $Ca(OH)_2$ with excess water) is of particular interest and used extensively in heritage conservation. Ageing over months or years is an important stage in its production, and it is associated with a reduction in the size of $Ca(OH)_2$ platelets. This results in improved properties in the form of greater plasticity, workability and water retention. Although lime putty has been used for thousands of years, the mechanism for particle size is still not fully understood.

Here, we combine computational and experimental techniques to investigate the $Ca(OH)_2$–H_2O system to elucidate morphological and dimensional changes during dissolution of the mineral Portlandite, one of the major process occuring during aging and at the beginning of carbonation. We found that there is an enhanced dissolution at the edge surfaces of portlandite compared to the perfect cleavage {001} surface. We provide experimental evidence following the dissolution of single nano-crystals of $Ca(OH)_2$ using AFM under controlled conditions, and ab initio computational data for the adsorption of H_2O at $Ca(OH)_2$ surfaces and the ease of removal of calcium surface ions.

ORCID
Marco Molinari: 0000-0001-7144-6075
Giovanni L. Pesce: 0000-0001-6677-8622
Richard J. Ball: 0000-0002-7413-3944
Stephen C. Parker: 0000-0003-3804-0975