Pore-Scale Geochemical Processes

80 Reviews in Mineralogy and Geochemistry 80

FROM THE SERIES EDITOR

As the 80th volume of *Reviews in Mineralogy and Geochemistry*, this edition marks some historical changes in faces. It is the first volume since Jodi Rosso became the Executive Editor of *Elements* after many years in the position of Series Editor with this journal. I am very grateful to Jodi for her continuing support. It also marks the return of two other editors: it is now eighteen years since a volume on a similar topic was issued, Volume 34: *Reactive Transport in Porous Media*, for which Carl Steefel was also a Volume Editor; Lawrence Anovitz was also a Volume Editor for Volume 33: *Boron Mineralogy, Petrology, and Geochemistry*.

All supplemental materials associated with this volume can be found at the MSA website. Errata will be posted there as well.

lan P. Swainson, Series Editor Vienna, Austria June 2015

PREFACE

The pore scale is readily recognizable to geochemists, and yet in the past it has not received a great deal of attention as a distinct scale or environment that is associated with its own set of questions and challenges. Is the pore scale merely an environment in which smaller scale (molecular) processes aggregate, or are there emergent phenomena unique to this scale? Is it simply a finer-grained version of the "continuum" scale that is addressed in larger-scale models and interpretations? We would argue that the scale is important because it accounts for the pore architecture within which such diverse processes as multi-mineral reaction networks, microbial community interaction, and transport play out, giving rise to new geochemical behavior that might not be understood or predicted by considering smaller or larger scales alone.

Fortunately, the last few years have seen a marked increase in the interest in pore-scale geochemical and mineralogical topics, making a *Reviews in Mineralogy and Geochemistry* volume on the subject timely. The volume had its origins in a special theme session at the 2012 Goldschmidt meeting in Montreal where at least some of the contributors to this volume gave presentations. From the diversity of pore-scale topics in the session that spanned the range from multi-scale characterization to modeling, it became clear that the time was right for a volume that would summarize the state of the science. Based in part on the evidence in the chapters included here, we would argue that the convergence of state of the art microscopic characterization and high performance pore scale reactive transport modeling has made it possible to address a number of long-standing questions and enigmas in the Earth

and Environmental Sciences. Among these is the so-called "laboratory-field discrepancy" in geochemical reaction rates, which may be traceable in part to the failure to consider porescale geochemical issues that include chemical and physical heterogeneity, suppression of precipitation in nanopores, and transport limitations to and from reactive mineral surfaces.

This RiMG volume includes contributions that review experimental, characterization, and modeling advances in our understanding of pore-scale geochemical processes. The volume begins with chapters authored or co-authored by two of the *éminences grises* in the field of pore-scale geochemistry and mineralogy, two who have made what is perhaps the strongest case that the pore-scale is distinct and requires special consideration in geochemistry. The chapter by Andrew Putnis gives a high level overview of how the pore-scale architecture of natural porous media impacts geochemical processes, and how porosity evolves as a result of these. The chapter makes the first mention of what is an important theme in this volume, namely the modification of thermodynamics and kinetics in small pores. In a chapter authored by Røyne and Jamtveit, the authors investigate the effects of mineral precipitation on porosity and permeability modification of rock. Their principal focus is on the case where porosity reduction results in fracturing of the rock, in the absence of which the reactions will be suppressed due to the lack of pore space. The next chapter by Emmanuel, Anovitz, and Day-Stirrat addresses chemo-mechanical processes and how they affect porosity evolution in geological media. The next chapter by Anovitz and Cole provides a comprehensive review of the approaches for characterizing and analyzing porosity in porous media. Small angle neutron scattering (SANS) plays prominently as a technique in this chapter. Stack presents a review of what is known about mineral precipitation in pores and how this may differ from precipitation in bulk solution. Liu, Liu, Kerisit, and Zachara focus on porescale process coupling and the determination of effective (or upscaled) surface reaction rates in heterogeneous subsurface materials. Micro-continuum modeling approaches are investigated by Steefel, Beckingham, and Landrot, where the case is made that these may provide a useful tool where the computationally more expensive pore and pore network models are not feasible. The next chapter by Noiriel pursues the focus on characterization techniques with a review of X-ray microtomography (especially synchrotron-based) and how it can be used to investigate dynamic geochemical and physical processes in porous media. Tournassat and Steefel focus on a special class of micro-continuum models that include an explicit treatment of electrostatic effects, which are particularly important in the case of clays or clay-rich rock. Navarre-Sitchler, Brantley, and Rother present an overview of our current understanding of how porosity increases as a result of chemical weathering in silicate rocks, bringing to bear a range of characterization and modeling approaches that build toward a more quantitative description of the process. In the next chapter, Druhan, Brown, and Huber demonstrate how isotopic gradients across fluid-mineral boundaries can develop and how they provide insight into pore-scale processes. Yoon, Kang, and Valocchi provide a comprehensive review of lattice Boltzmann modeling techniques for pore-scale processes. Mehmani and Balhoff summarize mesoscale and hybrid models for flow and transport at the pore scale, including a discussion of the important class of models referred to as "pore network" that typically can operate at a larger scale than is possible with the true pore-scale models. Molins addresses the problem of how to represent interfaces (solid-fluid) at the pore scale using direct numerical simulation.

In addition to thanking the scientists who have contributed their time and effort to preparation of this volume and presentations at the short course in Prague, we would like to thank Ian Swainson for his patience and hard work in preparing the volume for publication. We

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