Contrasting fracture patterns induced by volume-increasing and -decreasing reactions: Implications for the progress of metamorphic reactions

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A B S T R A C T

Hydration and dehydration reactions during metamorphism cause drastic changes in porosity and fluid pressure in a rock, and some of these reactions proceed with fracturing. For this paper we have developed a model for coupled hydraulic–chemical–mechanical processes, using the distinct element method, in order to understand the relationships among chemical reactions, fluid flow, and fracturing during metamorphism. The model considers fluid advection along fractures and the dependence of reaction rates on fluid pressure. With the help of the model, volume-decreasing dehydration reactions and volume-increasing hydration reactions are investigated in detail as analogs of prograde and retrograde reactions, respectively. Both types of reaction proceed inwards from drained boundaries or fractures, but they show contrasting fracture patterns. A volume-decreasing dehydration reaction produces tree-type fractures, with the new fractures generated as branches of a pre-existing fracture. A volume-increasing hydration reaction produces a polygonal network of fractures, where new fractures nucleate at sites far from the pre-existing fracture, and extend to form T-junctions. These contrasting fracture patterns are essentially controlled by solid volume changes during reaction rather than by the fluid pressure gradient. In the case of the tree-type fractures, the fractures are continuously generated at the reaction front, and the reaction proceeds smoothly by positive feedbacks between reaction, fracturing, and fluid flow. In contrast, in a volume-increasing hydration reaction, fracturing initially occurs in response to the irregular boundary shape, but as the reaction progresses, a compressive stress field is generated, which inhibits further fracture generation. The compressive stress field also prevents fluid flow by closing the pre-existing fractures, which slows down the reaction. These contrasting feedback systems between volume-decreasing dehydration and volume-increasing hydration reactions help to explain why prograde metamorphic reactions proceed pervasively, and why the progress of a retrograde hydration reaction tends to be localized along fractures so that relics of peak metamorphism are commonly preserved.

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1. Introduction

Hydrous minerals play an essential role as carriers of H_2O from the surface of the Earth to its deep interior. Dehydration and hydration reactions during metamorphism cause drastic changes in fluid pressure and porosity as well as the mineralogy of a rock, and they are therefore thought to be one of the controls on the generation of earthquakes in subduction zones (e.g., Kirby, 1995; Miller and Nur, 2000; Nakajima et al., 2013). The spatial distribution of H_2O within the earth is usually evaluated from the amounts of hydrous minerals, based on thermodynamic equilibria among minerals in mantle and crustal rocks (e.g., Poli and Schmidt, 1997; Hacker et al., 2003). However, it is not clear whether thermodynamic equilibria and H_2O saturation are always attained in such rocks in the Earth's interior. According to geophysical and petrological observations, metamorphic reactions are not always completed at any particular temperature and pressure (e.g., Skelton et al., 2005; Clarke et al., 2006), and it is therefore important to know the effective reaction rate and the progress of the reaction if we are to understand global water circulation and related dynamic processes.

Dehydration reactions commonly occur during prograde metamorphism, and they result in a decrease in solid-volume; in contrast, hydration reactions commonly occur during retrograde metamorphism, and they result in an increase in solid-volume (Yardley, 1997). Because both types of reaction involve fluid H_2O, the transport of the fluid is thought to be a key control on the progress of

the reactions (e.g., Macdonald and Fyfe, 1985). Fractures act as the dominant fluid pathways and are the sites of reactions, especially at crustal depths. In metamorphic rocks, reactions are commonly accompanied by fracturing, as shown, for example, by the mesh textures in partially serpentinized peridotites (e.g., Iyer et al., 2008; Jamtveit et al., 2009; Okamoto et al., 2011), by the veins associated with hydrofracturing (Nishiyama, 1989), and by the replacement during retrograde metamorphism (e.g., Okamoto and Toriumi, 2005).

Reaction-induced fracturing has been examined in numerical simulations using the distinct element method (DEM) (Jamtveit et al., 2000, 2008, 2009; Malthe-Sørenssen et al., 2006; Røyne et al., 2008; Jamtveit and Austrheim, 2010). In these numerical simulations, the reaction rate is defined as a function of the concentration of volatiles which diffuse from the fractures (e.g., Malthe-Sørenssen et al., 2006). Jamtveit et al. (2000) and Malthe-Sørenssen et al. (2006) revealed that a volume-decreasing reaction produces a fracture network that is like a fractal tree, and that the migration of the reaction front during such fracturing is faster than when it is solely controlled by diffusion. Røyne et al. (2008) showed that a volume-increasing reaction causes hierarchical fracturing which produces a polygonal network of fractures. The structures in natural fracture systems are similar to those produced by these numerical simulations, which suggests that the modeling can represent the essential processes of chemical reaction and fracturing in nature. Nevertheless, the following questions remain:

1) In previous model studies (e.g., Malthe-Sørenssen et al., 2006), diffusion of volatile species from fractures was considered, but the effects of fluid flow and local variations in fluid pressure on the progress of hydration/dehydration reactions are unclear.
2) The previous studies showed that positive or negative solid-volume changes during reaction produced characteristic fracture patterns, but the ways in which these different fracturing processes controlled the overall reaction rate were not clarified.

In this paper we present a new model that uses the DEM and involves coupled hydraulic–chemical–mechanical processes. Fluid advection along fractures is introduced, and the reaction rate is taken to be a function of fluid pressure. We then use this model to examine the progress of volume-decreasing dehydration reactions and volume-increasing hydration reactions as analogs of prograde and retrograde metamorphism, respectively. In common with previous studies (e.g., Jamtveit et al., 2000; Malthe-Sørenssen et al., 2006; Røyne et al., 2008; Jamtveit and Austrheim, 2010; Ulven et al., 2014), tree-like and polygonal fracture patterns are produced in our model. We reveal how the feedback system operates between chemical reactions, fluid flow, and fracturing, and how it controls the overall reaction rate. Finally, we discuss the implications of these findings for the progress of prograde and retrograde metamorphism.

2. Simulation methodology

2.1. Formulation of the mechanics of bonded particles

We employed 2D DEM (two-dimensional distinct element method) during our modeling, and revised the original DEM code to simulate coupled hydraulic–chemical–mechanical processes deep below the surface. The DEM can directly represent grain-scale microstructural features of a rock, such as pre-existing flaws, pores, microcracks, and grain boundaries. In the DEM model, these grain-scale discontinuities induce complex macroscopic behaviors without complicated constitutive laws, and this suggests that the model may be more appropriate for the analysis of

rock fracturing than other numerical techniques. Since details of the fundamental DEM algorithm can be seen in the literature (Potyondy and Cundall, 2004; Shimizu et al., 2011), only a summary of the formulation for our research will be given.

In 2D DEM, the intact rock is modeled as a dense packing of small rigid circular particles. Neighboring particles are bonded together at their contact points with a set of three kinds of springs (normal, shear, and rotational springs). The interparticle forces are calculated according to the relative motion between the bonded particles.

In this study, the bond break occurs when the normal tensile stress, σ, exceeds the tensile strength of the normal spring, S_t. Upon breakage of the spring, no tensile force acts between the particles. The normal stress, σ, is calculated as $\sigma = f_n/A_c$, where f_n and A_c are the normal force and the cross sectional area of the bond, respectively. The increment of the normal force, f_n, is given as

$$f_n = k_n \cdot d_n, \tag{1}$$

where k_n and d_n are the stiffness of the normal spring and the relative normal displacements between bonded particles, respectively. The stiffness of the normal spring is given by the equation

$$k_n = \frac{E_p A_c}{l}, \tag{2}$$

where l is the bond length and E_p is Young's modulus of particles and bonds. In this study, a negative stress value represents tension.

When the unbonded particles or particles with bond breakage are in contact with each other, springs and dashpots are introduced into the contact points in both the normal and tangential directions, and the compressive normal force and the tangential (frictional) force act at the contact points. The details of this contact behavior follow the work of Cundall and Strack (1979).

2.2. Fluid flow

The fluid flow algorithm, which considers the fluid viscosity and permeability, is introduced into the DEM code to reproduce fluid flow in the rock model (Shimizu et al., 2011). In the fluid flow algorithm, the rock model is divided into a series of enclosed domains by connecting the centers of adjoining particles to calculate the change in fluid pressure (Fig. 1a).

In our model, fluid flow does not occur between bonded particles, and the apertures between adjoining unbonded particles or the generated microcracks are assumed to be the flow channels. The fluid flow in a channel is assumed to be laminar flow between two parallel plates with a certain aperture, and it can be expressed by the Poiseuille equation so that the volumetric laminar flow rate, Q, is given by the equation

$$Q = \frac{w^3}{12\mu} \frac{\Delta P}{L_P} \tag{3}$$

where w and L_P are the aperture and the length of a flow channel (a microcrack), respectively. L_P is obtained from the harmonic mean of the radius of two particles. ΔP is the difference in pressure across the channel, and μ is the viscosity of the fluid. The plane thickness is assumed as a unit. In this study, the aperture of the flow channel, w, varies with the stress field around the particle, and a minimum aperture, w_{min}, is assumed to control the fluid flow in the microcracks. As a measure of fracturing, the normalized crack density is measured, which is the percentage of the total length of microcracks per total bond length (length of potential cracks).

The fluid pressure acting on the surface of surrounding particles accumulates in each domain, and the fluid pressure is updated