

Contrasting mobility of elements in shear zones; Examples from Sanandaj-Sirjan metamorphic-plutonic belt, Western Iran

S. ALIREZAEI

Faculty of Earth Sciences, University of Shahid Beheshti, Tehran, Iran (s-alirezei@sbu.ac.ir)

The Sanandaj-Sirjan metamorphic-plutonic belt extends in NW-SE direction for about 1500 km, with an average width of 150km, in western Iran. The belt is characterized by Phanerozoic continental sedimentary and magmatic rocks, sheared and metamorphosed at various scales and under variable P-T conditions.

Three small-scale shear zones in I-type biotite granites were sampled to investigate the mobility of element in the course of shearing. A transition from the fresh, non-sheared rocks to protomylonite, mylonite and ultramylonite occurs in <50m in the shear zones. Representative samples were analyzed for a wide range of elements at ACME labs, Vancouver.

1. Sheikh Choopan. The sheared rocks are intensely enriched in silica, from 17% in the protomylonite to 28% in the ultramylonite, and depleted in most major and trace elements. Calcium is depleted 80-95% of the original contents. Even aluminum is considerably depleted. REEs, HFSEs and ore metals are increasingly and significantly depleted toward the ultramylonite.

2. Darabi. Most major elements remained constant; Potassium is enriched; calcium variably enriched and depleted; iron depleted between 15-45% original contents. LILEs and LREEs are variably enriched.

3. Hajqara. Most major elements remained constant; K, Ba, Rb, Cs, and Pb are significantly enriched (25-75% original contents); Na moderately depleted; Si slightly enriched. LREEs are clearly enriched; HREEs remained constant. REEs display a flat pattern in the mylonites, except a distinct negative Eu anomaly, common to all rocks. The mobility of the elements in the shear zones was controlled mainly by the nature of the fluids involved rather than the host rock lithology.

Computer simulation of the interaction of water & carbonate with oxide minerals

J.P. ALLEN^{1*}, S.C. PARKER¹ AND D.W. PRICE²

¹Department of Chemistry, University of Bath, Claverton Down, Bath, BA2 7AY, United Kingdom
(*correspondence: ch1jpa@bath.ac.uk)

²AWE, Aldermaston, Reading, RG7 4PR, United Kingdom

There is now considerable interest in the interaction and sequestration of carbon. We have begun by considering the interaction and incorporation of carbon via carbonate formation at mineral surfaces, particularly the model systems of magnesium and calcium oxides.

We describe recent work using potential based atomistic simulation techniques. These simulations are quick and efficient, enabling them to be both a useful 'screening tool' to identify important structures as well as enabling the evaluation of free energies.

Carbonate addition has been modelled on the low index surfaces in the presence of water, namely the {100}, {111} and {310} surfaces, comprising of 182902 different static lattice energy minimisation calculations. Water has been considered as both associative (hydration) and dissociative (hydroxylation). The surface coverage of both carbonate and water has also been varied so that not only the lowest energy surface can be identified, but also the effect that the different concentrations have on the surface energy profile.

Key observations from this study include:

- Carbonation of the {310} surface produces more stable surfaces than the {100} surface, due to the presence of a step.
- Direct carbonation of the hydroxylated {111} surface is unfavourable, suggesting a dehydroxylation step is required prior to carbonation.
- Hydrated water is more easily displaced by carbonate than dissociatively adsorbed water.
- Calcium surfaces produce lower energy surfaces than the magnesium analogues.

These results suggest that although both materials would be suitable for aqueous carbonation, hydroxylation of the surfaces could limit the uptake of carbon dioxide. Additionally, the presence of higher energy surface features, such as steps and vacancies could be used to enhance reactivity. The results also demonstrate the viability of atomistic simulation techniques for probing surface modifications. The next stage is to consider the carbonation and reactivity of silicate minerals.