Geophysical Research Abstracts,
Vol. 11, EGU2009-11861, 2009
EGU General Assembly 2009

Thermodynamic modeling of phase relations and metasomatism in shear zones

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Ductile shear zones have been recognized for a long time as privileged sites of intense fluid-rock interactions in the crust. In most cases they induce focused changes in mineralogy and bulk chemical composition (metasomatism) which in turn may control the deformation and fluid-migration processes. Therefore understanding these processes requires in a first step to be able to model phase relations in such open system.

In this contribution, emphasizes in placed on metasomatic aspects of the problem. Indeed , in many ductile shear zones reported in metagranites, deformation and fluid-rock interactions are associated with gain in MgO and losses of CaO and Na2O (K2O is also a mobile component but it can be either gained or lost). Although the mineralogical consequences of this so-called Mg-metasomatism are well-documented (replacement of K-feldspar into phengite, breakdown of plagioclase into ab + ep, crystallization of chlorite), the origin of this coupled mass-transfer is still unknown.

We have performed a forward modeling of phase relationships using petrogenetic grids and pseudosections that consider variations in chemical potential (μ) of the mobile elements (MgO, CaO, Na2O). Chemical potential gradients being the driving force of mass transfer, μ-μ diagrams are the most appropriate diagrams to model open systems where fluid-rock interactions are prominent. Chemical potential diagrams are equivalent to activity diagrams but our approach differs from previous work because (1) solid solutions are taken into account (2) phase relations are modeled in a more realistic chemical system (Na2O-CaO-K2O-FeO-MgO-Al2O3-SiO2-H2O) and (3) the use of pseudosections allows to predict changes of the mineralogy (modes, composition) for the specific bulk composition studied. A particular attention is paid to the relationships between component concentrations and chemical potentials, which is not obvious in multi-component system.

The studied shear zone is located in the Grimsel granodiorite (Swiss Alps). Fourteen samples have been taken along a 80 meter-wide strain gradient from the undeformed granodiorite protolith to the ultramylonitic zone. The metastable magmatic assemblage consists of oligoclase (50 vol%), quartz (20 vol%), K-feldspar (17 vol%), and biotite (13 %). With increasing strain, K-feldspar and oligoclase rapidly disappear to produce albite and epidote porphyroblast (up to 45 and 5 vol% respectively) with phengite in shear planes (15 vol%). In the mylonite and ultramylonite, magmatic phases have been completely recrystallized and the metamorphic albite volume decreases down to 25 vol% whereas phengite constitutes up to 30 vol% of the rock. Epidote is absent in the ultramylonite. In localized shear bands, the metamorphic assemblage consists of phengite, chlorite, biotite and quartz. Mass balance calculations show that the ultramylonite is enriched in MgO (up to 130%) while CaO and Na2O are remove (80% and 45% respectively). However, mass transfer is even stronger in the chlorite-bearing shear bands, where CaO and Na2O have been completely leached out.

Chemical potential pseudosections are constructed using the bulk composition of the unaltered granodiorite, with K2O, FeO, Al2O3 and SiO2 content remaining constant. Deformation occurred under water-saturated conditions at 6 kbar and 450°C. MgO, CaO and Na2O are considered as “perfectly mobile” components and therefore their chemical potentials, which is fixed by the externally-derived fluid, control the stability of the phases. μMgO vs μCaO and μMgO vs μNa2O diagrams, show that the breakdown of a Kf-ab-ep assemblage into phengite and the subsequent crystallization of chlorite require the introduction of a fluid with a μCaO and μNa2O significantly lower than in the unaltered metamorphic assemblage (Kf-ab-ep-Kf-Bio-q). Equalizing the chemical potential gradient of CaO and Na2O, established between the fluid and the metamorphic assemblage, is achieved by the complete removal of CaO and Na2O. The most striking result is that chemical potential diagram predicts that the loss of CaO and Na2O and the crystallization of chlorite-bearing assemblage at the expense of Kf-ep-ab imply a gain of MgO to reach equilibrium: “Mg-metasomatism” is therefore controlled and induced by the metamorphic assemblage. Finally fluid-rock interactions and mass transfer result in an increase in phyllosilicates in the shear zone from 13 to 32 vol%, which should strongly enhance the strain localization process.

To conclude, our approach allows to predict and to quantify the mineralogical changes induced by fluid-rock interactions in a shear zone for any bulk composition or P-T composition.