Thermodynamic modeling of phase relations and metasomatism in shear zones: an example from a metagranodiorite in the Aar massif (Central Alps)

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Summary

The progressive development of ductile shear zones is promoted by intense fluid-rock interactions that drives changes in mineralogy and whole-rock chemistry (i.e. metasomatism) along the strain gradient. In diffusion metasomatism mass transfer is driven by chemical potential gradients established between the flowing externally-derived fluid and the host assemblage. Therefore modeling phase relations in metasomatised systems requires to take into account the chemistry of the reactive fluid, the whole-rock composition and pressure – temperature conditions. The most appropriate phase diagram to model metasomatism is thus isobaric, isothermal pseudosection that uses chemical potential of mobile components as variables. Such quantitative modeling approach is applied to an Alpine greenschist-facies shear zone in the Grimsel granodiorite (Aar massif, Central Alps).

Chemical potential pseudosections (μMgO-μCaO and μMgO-μNa2O) are used to estimate the chemistry of the externally-derived fluid, quantify the amount of material transferred in and out the system (shear zone) by contouring the pseudosections for amounts of mobile components. This modeling shows that the process of equilibration induces the breakdown of K-feldspar, epidote and albite to produce white mica and ultimately chlorite. To proceed, such reactions induce a loss of CaO and Na2O and require a gain of MgO. We show that in deformed granites under greenschist facies conditions, the stability or breakdown of epidote must play a first order role on the nature of mass transfer and the maintenance of shear zones open to fluid flow by producing large amounts of phyllosilicates. More generally, we conclude that metasomatism is, as expected, controlled by the composition of the externally-derived fluid but also by the sequence of metamorphic reactions involved during the process of equilibration.

Our thermodynamic quantitative approach can be applied to any metamorphic conditions and protoliths, and thus give valuable insights into metasomatism and strain localization processes.

Introduction

Ductile shear zones are considered as open-systems where metasomatism can be significant due to the intense fluid-rock interactions involved during deformation. Many authors have shown that the development of the shear zone is coeval and promoted by dramatic mineral transformations due to syn-kinematic metamorphic reactions governed by changes in P-T

conditions, fluid-rock interactions and mass-transfer (Wintsch et al., 1995; Yonkee et al., 2003; Barnes et al., 2004; Sassier et al., 2006). One of the most familiar syn-kinematic reaction observed in fault zones and shear zones of the upper crust is the feldspar to muscovite reaction (Marquer et al., 1985; Marquer & Burkhard, 1992; Fitz Gerald & Stünitz, 1993; Wibberley, 1999; Yonkee et al., 2003). This reaction, which requires an externally-derived fluid with a low K activity, induces K_2O loss and is seen as a softening process responsible for the strain localization (e.g. Gueydan et al., 2003).

The feedback effect between fluid flow, metamorphic reaction and strain localization reported above is a well accepted and documented concept (e.g. Oliver et al., 1990, Wibberley, 1999). Therefore the ability of predicting the mineralogical and geochemical evolution during syn-deformation fluid-rock interactions is critical to either estimate PT conditions of deformation or better understand the rheological behavior of shear zones. However what drives mass transfer and more particularly what controls the amount of mass transfer during deformation remains a matter of debate.

To get a more general sense of the nature of syn-deformation metasomatism in metagranites, a non-exhaustive compilation of the past-decade literature dealing with mass transfer in shear zone has been attempted. Although the nature and mass transfer must largely depend upon the composition and amount of infiltrating fluid, it appears that gain of MgO coupled with losses of CaO and Na_2O are common features for metasomatised quartzo-feldspathic rocks in ductile shear zones, independently of metamorphic conditions. This compilation, showing the quite homogeneous nature of mass transfer, raises several questions related to metasomatism in shear zones: what controls the nature of mass transfer in shear zones? Is fluid composition the most critical variable? Do metamorphic reactions play a significant role in the nature and quantity of mass transfer? Why CaO/Na_2O losses are commonly coupled with MgO gain?

Theory and/or Method

To evaluate the influence of syn-deformation mass transfer during strain localization in meta-granites, phase relations has be mapped as a function of variation in chemical potential of mobile elements (CaO, Na_2O, H_2O, MgO). Based on observed mass transfer along a strain gradient, from the precursor to the most deformed rock, μ-μ phase diagrams are used to highlight the critical effect of mass transfer on the modal and chemical evolution of phases. A particular attention is paid to phases with a strong rheological impact, like micas and chlorite known to induce strain softening.

The forward petrologic modeling is performed in the Na_2O-CaO-K_2O-FeO-MgO-Al_2O_3-SiO_2-H_2O system using a suite of phase diagrams, P-T, P-MH_2O and chemical potential (μ-μ) projections and pseudosections to investigate the influence of environmental (P and T) and compositional variables.

Phase relations modeling in open-system is applied on a well-characterized decameter-sized Alpine shear zones developed in the Variscan Grimsel granodiorite (Central Alps, Switzerland) located between the Räterishsbodensee and Grimselsee lakes.

Examples

The main chemical and mineralogical features observed in the shear zone of the Grimsel granodiorite are:
(1) loss of CaO and Na_2O coupled with a gain in MgO and H_2O
(2) crystallization of large amounts of phengite and albite with epidote at the expense of K-feldspar and plagioclase in the orthogneiss, mylonite and ultramylonite.
(3) in the highest strained sample (ultramylonite and shear bands in the orthogneiss and mylonite), the system becomes Ca-free and chlorite crystallizes in equilibrium with phengite, biotite and albite. Epidote is no more present.

(4) phengite produced by the breakdown of K-feldspar has a limited range in Si-content from 3.25 to 3.3 p.f.u. In contrast, in the chlorite-bearing ultramylonite, the amount of Tschermak substitution in phengite decreases continuously from 3.25 to a minimum value of 3.15 Si p.f.u.

A pseudosection µMgO-µCaO (Fig. 1) have been calculated at the estimated P-T conditions of the deformation (450°C and 6 kbar) with the unaltered granodiorite composition. The pseudosection is characterized by the occurrence of two portions of univariant equilibria

$$Kf + cz + Bio + H2O + MgO = Mu + q + ab + CaO \quad (i)$$
$$cz + Bio + ab + H2O + MgO = Chl + Mu + q + CaO \quad (ii)$$
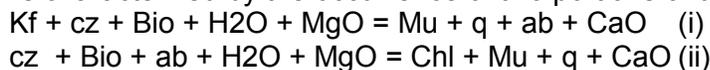
that implies a decrease a loss of CaO and gain of MgO. To estimate the amount of CaO and MgO transported in and out the system by these reactions, the µ-µ pseudosection is contoured for the variation in amount in wt% of the two mobile components, which are also converted into relative gain or loss with respect to the unaltered granodiorite composition (Fig. 1).
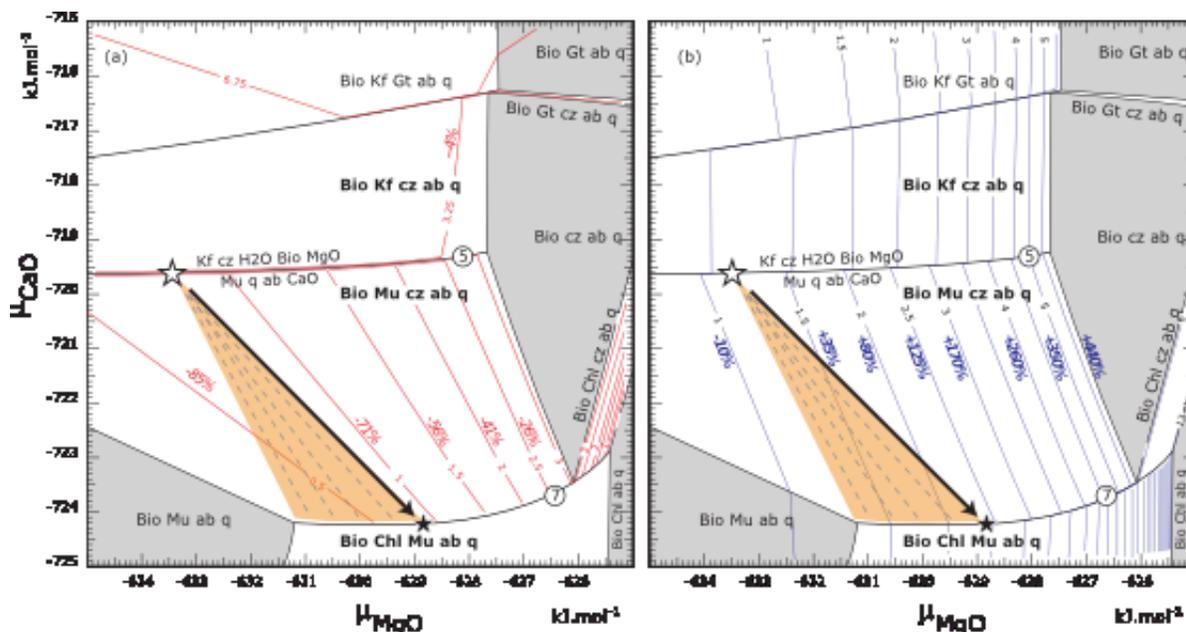

Figure 1: Quantitative µCaO-µMgO pseudosection calculated at 450°C and 6 kbar for the unaltered granodiorite composition at water-saturated conditions contoured for (a) CaO content of the system, (b) MgO content of the system. Numbers on the isopleth are expressed in wt% while those located on the side of the isopleths correspond to the relative mass change expressed in wt% with respect to the initial content of CaO (3.39 wt%) and MgO (1.13 wt%).

Modeling predicts that the complete breakdown of the metastable magmatic assemblage into a chl-phengite assemblages requires a complete loss of CaO coupled with a gain in MgO up to 125% in good agreement with the mass balance estimation. Such metasomatism is driven by the infiltration of an externally-derived fluid with a low µCaO and high µMgO with respect to the host assemblage and by the sequence of reactions and assemblages produced during the process of equilibration of the host-rock with the fluid.

The chemical potential gradient responsible for the change in bulk composition has also a strong influence on mineral composition. The µMgO-µCaO pseudosection has been contoured for the Si content of white mica per formula unit (p.f.u.). This phase diagram shows that the process of equilibration of the rock with the syn-deformation infiltrating fluid induces a decrease of Si-content of phengite from 3.26, when in equilibrium with K-feldspar + epidote + albite down to 3.12 p.f.u when white mica is in equilibrium with the chlorite-bearing assemblage of the ultramylonite at the same P-T conditions in good aggrement with measured compositions. In

this case, the observation of slightly substituted phengite in equilibrium with chlorite in the ultramylonite may be incorrectly interpreted in terms of a low pressure retrograde deformation event, while it is due to syn-deformation metasomatism at peak metamorphic conditions.

Conclusions

This contribution highlights how the infiltration of a chemically reactive fluid in a shear zone may promote metamorphic reactions and mass transfer to reach equilibrium. In this case, the driving force of metasomatism is the establishment of a chemical potential gradient between the externally-derived fluid and the host-rock assemblage under isobaric and isothermal conditions. The type and amount of mass transfer is controlled by the composition of the externally-derived fluid and the sequence of reactions and assemblages produced during the process of equilibration of the host-rock with the fluid. Since the metamorphic reactions play a major role, P-T conditions and initial bulk composition must also be taken into account when modeling metasomatism. Therefore, quantitative µ-µ pseudosections are the most appropriate phase diagram to model metasomatism since all four variables (fluid composition, phase relations, P-T conditions and bulk composition) are controlled.

Changes in mineralogy and chemistry induced by fluid-rock interactions, metamorphic reactions, and metasomatism control the rheological properties of the crust during orogenesis and more particularly the localization of strain from the mineral to the crustal scale. Numerical modeling of strain localization processes, first requires to know the syn-deformation changes of mineralogy induced by fluid-rock interactions for any P-T conditions, bulk and fluid compositions. Our thermodynamic quantitative approach, which is obviously not restricted to metasomatised granitoids, may give valuable insights into strain localization processes and more generally geodynamics at the scale of the continental crust.

Acknowledgements

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