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PARTITION COEFFICIENT SELECTION –
CRITICAL APPROACH IN PETROGENETIC MODELLING

Abstract: Melt composition reconstruction has been performed using geochemical data provided by bulk rock and feldspar composition. LA-ICP-MS traverses on feldspar have been used to reconstruct the petrogenetic mechanism leading to the formation of compositional zoning. Two processes have been involved into feldspar crystallization: fractional crystallization and mixing. Partition coefficient selection has been done using LA-ICP-MS data under assumption that the crystallization took place near equilibrium.

Keywords: feldspar megacryst, partition coefficient, melt reconstruction, trace elements, fractional crystallization, mixing

INTRODUCTION

Within Variscan granites of the Bohemian Massif (BM) phenocrysts of alkali feldspars are frequently found in granites *sensu stricto* as well as in hybrids. The megacrysts accompany also the porphyritic granite facies of hybridic nature (Jizera type in Czech nomenclature) in Karkonosze pluton (NW extreme of BM). They have been formed within magma mixing regime and were influenced by fractional crystallization (FC) (Słaby et al., 2002; Słaby, Götze 2004). One of the features reflecting their crystallization conditions in an open system is the trace element zoning, showing their itinerancy between magma pulses of various degree of hybridisation. Precise determination of trace element concentration in the zones provides base for modelling of their crystallization path. The modelling using geochemical tools needs reliable partition coefficients (K_d), adjusted to particular, calculated case. The arbitrary choice of their value could lead to considerable discrepancies between the constructed model and the real operating petrogenetic mechanism. We suggest using the bulk rock trace element composition and trace element composition of several alkali feldspar zones as base for determination of mutual partition relation: crystal-melt. In the present study LA ICP MS data on Karkonosze megacrysts and their host rock have been used. The data allow modelling of feldspar crystallization path and simultaneously allow a verification

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of partition coefficients used for the calculation by comparison with of whole rock composition.

PARTITION COEFFICIENTS: ALKALI FELDSPAR – MELT

Partition coefficient shows the relation between element concentration in the melt and crystal formed from the melt. Usually they are estimated using experimental work or taking data from natural systems, where crystallization proceeds in two stages (phenocrysts – matrix relation). The complexity of natural systems causes, that experimentally estimated values should be used with caution (see for instance Bennett et al. 2004). The problem arises, when we need to select the values for modelling. The database provides, even for similar environments, a wide range of values. Below we show extreme $Kd = \text{feldspar/felsic melt}$ values for three trace elements most frequently estimated in alkali feldspar: Ba, Sr, Rb (Tab. 1).

Table 1. Partition coefficients for alkali feldspar grown in felsic melts.

Element	Kd	References
Ba	24	Nash, W.P. and Crecraft, H.R. <i>Geochimica et Cosmochimica Acta</i> 49: 2,309-2,322: 1985
	1	Stix, J. and Gorton, M.P. <i>Geochimica et Cosmochimica Acta</i> 54: 2,697-2,708: 1990
Sr	22.1	Ewart, A. and Griffin, W.L. <i>Chemical Geology</i> 117: 251-284: 1994
	0.65	after Rollinson, H., <i>Using Geochemical Data</i> , Longman, 1993
Rb	2.4	Nash, W.P. and Crecraft, H.R. <i>Geochimica et Cosmochimica Acta</i> 49: 2,309-2,322: 1985
	0.11	Ewart, A. and Griffin, W.L. <i>Chemical Geology</i> 117: 251-284: 1994

TRACE ELEMENT DATA ON MEGACRYST ZONING

Trace element concentrations have been estimated for megacrysts collected from hybrids and evolved granites: Fojtka granodiorites (Czech part of the pluton), Rudolfov granodiorite (Czech part of the pluton), Szklarska Poręba Huta granite (Polish part of the pluton) by means of EMPA and LA ICP MS (at NHM London).

Table 2. Geochemical data on rocks and megacrysts (ppm).

Element	Rock			Megacrysts					
	F	R	SPH	F Ba-rz	F Ba-pz	R Ba-rz	R Ba-pz	SPH Ba-rz	SPH Ba-pz
Ba	426	485	9	3515	143	4066	245	1727	101
Sr	273	253	17	375	69	140	126	215	183
Rb	188	142	190	344	262	421	273	509	281

Explanation: F – Fojtka, R – Rudolfov, SPH – Szklarska Poręba Huta, Ba-rz – barium-rich zone, Ba-pz – barium-poor zone

All the megacrysts display explicit chemical zoning, which might be related to crystallization in mafic-like melt and felsic-like melt. Although many elements seem to be good determinants of the environment condition, within them barium concentration shows the most explicitly character. The concentration is much

higher in the more mafic hybrids. Feldspar zones formed in these hybrids are also barium-rich (Słaby et al., 2002; Słaby, Götze 2004). Barium-poor zones in feldspars correspond to crystallization in felsic-like melt. The bulk composition of evolved granites is impoverished in barium too. Feldspars show itinerancy between both environments during their growth. The data on whole rock composition and feldspar zones is presented in Table 2.

RECONSTRUCTION OF MELT COMPOSITION

Melt composition has been reconstructed using mineral zones composition and various Kd . The obtained values (element concentrations in the melt) for Ba-rich zones have been compared with element concentration in the granodiorites, the ones for Ba-poor zones respectively with element concentration in granite. Throughout the comparison the most suitable for the investigated system Kd has been chosen.

Table 3. Reconstructed melt composition:

Melt	K_{Ba}	K_{Ba}	K_{Ba}	K_{Sr}	K_{Sr}	K_{Sr}	K_{Rb}	K_{Rb}	K_{Rb}
	max	min	ch- 11.4	max	min	ch- 0.65	max	min	ch- 2.4
F (m)	146	3515	308	17	577	577	143	3127	143
R (m)	169	4066	357	11	215	215	175	3827	175
SPH (m)	72	1727	151	10	331	331	212	4627	212
F (f)	6	143	13	3	106	12	109	2382	146
R (f)	10	245	21	6	194	21	114	2482	152
SPH (f)	4	101	9	8	282	31	117	2555	156

Explanations: (m) mafic-like melt, (f) felsic-like melt), ch- value of finally chosen partition coefficient

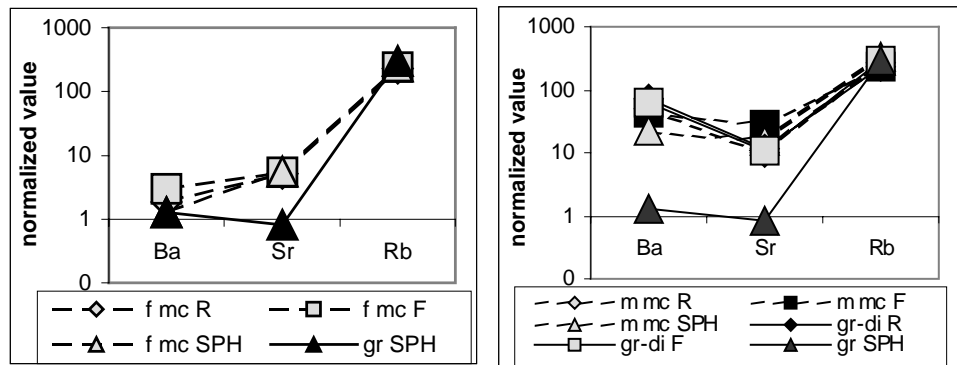


Fig. 1. Reconstructed mafic-like (m) and felsic-like (f) melt in comparison to whole rock composition (values normalized to primordial mantle). See Table 2 for samples explanation.

The choice has been verified by feldspar crystallization path model done for open system (mixing model – not shown in the paper). Table 3 (a, b) includes calculated melt composition for extreme Kd values (max and min) and for the one recognised (ch- chosen) as the most approximate for the system. Figure 1 presents the results of calculations.

CONCLUSIONS

The compositional zoning formed in alkali feldspar reflects geochemical composition of the melt. In turn, due to megacrysts itinerancy the rock sample hosting them finally, mostly points to the relation: last zone composition – melt. Feldspar zoning gives information about all hybridised environments, they passed through during their itinerancy, even those, which are not presently exposed on the surface. Especially the information about early magma evolution preserved in feldspar composition might be valuable. The reconstructed mafic-like melt composition varies significantly comparing with bulk composition of hybridised rocks whereas the felsic-like melt composition seems to be immutable and similar to evolved granite composition. During magma evolution, the incorporation of trace elements into feldspar was not constant and depended on other minerals competition. The variation of strontium reflects very well this competition. The partition coefficient K_{Sr} changes increasing in more felsic melt. Similarly, rubidium shows alterability in incorporation into growing crystal phase during progressively undergoing hybridisation. Its partition coefficient usually chosen for geochemical modelling of granite magma evolution is low. In Karkonosze granitic rocks rubidium behaves clearly as incompatible. But it is strongly fractionated into feldspars. Feldspars in turn are not extracted from melt during granite crystallization. Rubidium shows also almost no imprint of mixing. Its activity in the melt is influenced by fractional crystallization. For modelling of FC the choice of proper K_{Rb} is of crucial importance. Rubidium concentration in feldspar zones points to high K_{Rb} value. Simultaneous crystallization of biotite and feldspar testifies equilibrium (not kinetically driven) element partition between melt and crystallizing phases. The least variability is observed in K_{Ba} chosen for feldspars. We might assume the same value for feldspars crystallizing in both mafic and felsic melt. This is because barium behaviour is strongly influenced by mixing and almost not sensitive to FC. The simple calculation presented in the paper proves, that precise data on mineral zoning are imperative during Kd data preparation for geochemical modelling.

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