

Distribution of Ta and Nb between silicate and aluminofluoride (salt) melts

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Experiments in the model system Si-Al-Na-Li-H-F-O at $T=800^{\circ}\text{C}$ and $p=1\text{kbar}$ show possibility of equilibrium crystallization of fluorine minerals (cryolite, topaz, villiomite) or the origin of immiscible aluminofluoride melt (brine) in case of high fluorine concentration in the system. The area of coexistence of two immiscible silica and salt melts extends for both nepheline- and quartz-normative compositions of silica melts.

In case of two melts coexistence tantalum and niobium are distributed into the silicate melt. By virtue of the different values of partition coefficients the ratios of tantalum to niobium in residual aluminosilicate melt increase.

The experimentally determined phase relations are in general agreement with compositions of topaz and/or cryolite bearing granites from different regions.

In natural systems, in the final stages of crystallization high amounts of incompatible elements can lead to the separation of salt melt. Brine appears to be an effective concentrator of significant ore elements such as REE, Y, Sc, U, Th, Mo, W etc. [1]. Occurrence of salt melt can also lead to increasing of Ta/Nb ratio in the most evolved varieties of rare metal granites observed in numerous massifs [2].

[1] Gramenitskii & Shchekina (2001) *Geochem.Int.* **43**, 39-52.

[2] Syritso *et al.* (2001) *Petrology* **9/3**, 268-289

Modelling single phase bimolecular reactive transport directly on pore-scale images

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Geochemical reaction rates estimated in geological porous media are found to be significantly lower than those measured in the laboratory. Traditional advection dispersion reaction equations (ADRE) frequently cannot accurately describe reactive transport in heterogeneous porous media. Therefore, there is still a lack of understanding of the integration between coupled transport and geochemical reactions at multiple scales. We simulate the transport of fluid reactants (A and B) directly on *mm* sized images obtained using micro-CT scanning with a resolution of a few microns. We use a streamline-based particle tracking method for simulating flow and transport. For reaction to occur, both reactants must be within a diffusion distance of each other in a time step. We assign a probability of reaction (P_r), which is a function of the reaction rate constant (k_r) and the diffusion length. Firstly we validate our model for reaction only against analytical solutions of the bimolecular reaction ($A + B \rightarrow C$). Then we couple reaction and transport to perform simulation on the micro-CT images. We find that heterogeneity of the pore structure plays a significant role in altering the average reaction rates. The heterogeneous pore structure prevents contact between reacting species, thus decreasing the reaction rate. We validate the model through predicting the experiments by Gramling *et al* [1].

[1] Gramling *et al* (2002) *Environmental Science & Technology* **36**, 2508-2514