Origin of secondary REE minerals in grusified Karkonosze granites, SW Poland

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Primary monazite-(Ce), which is one of the most common accesory mineral in Karkonosze granites, is absent in grusified granites from Głębock, Kowary Średnie and Miłków. In the grusified granites muscovite–thorite or cheralite–xenotime-(Y) pseudomorphs after primary monazite-(Ce) are present. Instead of monazite-(Ce) in grusified granites secondary rhabdophane-(Ce), florencite-(Ce), cerianite-(Ce), rhabdophane-(La) and rhabdophane-(Nd) are present.

Small (about 5 μm) automorphic crystals of rhabdophane-(Ce) and florencite-(Ce) occur inside sericitised plagioclases often along clevage planes of primary feldspar. Cerianite-(Ce) occurs as thin veins or as clusters of crystals impregnating rims of the grains of grus. Rhabdophane-(La) and rhabdophane-(Nd) crystals are usually small, xenomorphic and fill large cracks inside the grains of granitic grus.

Decomposition of primary monazite-(Ce) might be the result of the activity of hydrothermal fluids [1], which could be also the main factor of the development of microcracks in granite that led to the development of grus. REE released from the decomposed monazite-(Ce) crystalized as secondary rhabdophane-(Ce) and florencite-(Ce). Chemical analysis of primary monazite-(Ce) from Karkonosze granite and secondary rhabdophane-(Ce) and florencite-(Ce) shows, that ratios of REE in primary and secondary REE phosphates are very similar.

Secondary cerianite-(Ce), rhabdophane-(La) and rhabdophane-(Nd) crystallisation could be caused by low temperature weathering, oxidizing fluids [2].

Decomposition of primary REE minerals and multistage crystalisation of secondary REE minerals in grusified granites indicates that process of grusification *sensu stricto* was proceded by activity of hydrothermal fluids, which developed microcracks in the rock and caused brakedown of primary minerals including REE phosphates. Similar observations were obtained in grusified Tatra granites [3].

[1] Berger *et al.* (2008) *Chem. Geol.* **254**, 238-248. [2] Aubert *et al.* (2001) *Geochim. Cosmochim. Acta* **6(3)**, 387-406. [3] Kajdas B & Michalik M (2011) *Min. Mag.* **75(3)**, 1135.

Addressing the nanoscale complexity of mineral-water interfaces in MD simulations: Effects of the substrate compositional disorder on the properties of surface species

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Thermodynamic, structural and transport properties of hydrated clays and clay-related materials for many geochemical, environmental, and technological applications are routinely studied by computational molecular modeling techniques. However, simulated system size limitations often impose a considerable quasi-periodicity on the distribution of the tetrahedral and octahedral site substitutions in the T-O-T clay layers. Such quasi-periodicity is then typically propagated further even if larger models are later constructed by simply multiplying the smaller ones, and the effects of this imposed structural ordering on the calculated properties of the interfaces is not obvious.

Here we report the results of molecular dynamics simulations with a new set of larger-scale muscovite and montmorillonite models which were systematically constructed to introduce as much structural disorder in the distributions of the Al/Si and Mg/Al substitutions as possible. The effects of such disorder on the local structural and dynamic properties of the interfacial and interlayer water and hydrated ions are then carefully quantified and analyzed for a number of typical monovalent and divalent cations.

The time- and space- averaged properties of the hydrated interfaces and interlayers, such as atomic density profiles, radial distribution functions, and surface diffusion coefficients, are observed to be not particualrly sensitive to the specific details of the substrate disorder. However, local effects of the disordered distribution of charge-substituted sites in clay layers can be substantial and can influence the strength of the ionic and molecular adsorption at a specific surface site, the structure and dynamics of the interfacial hydrogen bonding network around it, and the molecular mechanisms of its local rearrangement.

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