Different paths of chemical alteration during grusification of granites from S Poland

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Four type of grusified granites were taken under consideration. Three of the investigated gruses were developed on the Variscan granites from Karkonosze Mts. (Kowary Średnie [KS] and Głębock [GL]) and Tatra Mts. (Skrajna Turnia Mt. [ST]), one on the Early Paleozoic (ca. 500 Ma) Izera Granite (Siedlęcin [SI]).

Each of studied gruses shows significant variation in the LOI (loss of ignition) value, what can be connected with degree of alteration of parent granite. Changes in contents of major elements differ for each grus localization. ST grus shows significant changes of amount of major elements in relation to degree of alteration of rock (decreasing trends in SiO_2, Na_2O, and CaO, and increasing trends in Al_2O_3, K_2O, MgO and Fe_2O_3 contents versus LOI); SI grus shows increasing trend for Fe_2O_3 and MgO and decreasing trend for SiO_2 (vs. LOI); in KS grus increasing trends occur for Fe_2O_3 and MgO, and decreasing trends for Na_2O and CaO, whereas SiO_2, Al_2O_3 and K_2O content variation is non-systematic in relation to LOI. In GL grus the only slightly increasing content of Fe_2O_3 is visible (vs. LOI).

Using several indices of alteration [1, 2] we were able to notice differences in the paths of chemical alteration during grusification. Because the main alteration process during grusification is connected with decomposition of plagioclase, chemical alterations can be observed on plots based on changes of alkali and Al_2O_3 content (e.g. CIA and PIA; [1, 2]). CIA and PIA plots for ST are steeper, for SI more flattened, and for KS and GL trends are less uniform (vs. LOI). The WPI [3], which use all major elements, shows most uniform plots for each of the investigated gruses, but PI [3] shows trends only for Tatra and Izera granites, what indicate, that silica was immobile during grusification of Karkonosze granite.

The Alteration Box Plot [4] used for hydrothermal and diagenetic alteration of rocks reveals sericitization and chloritization trends in ST, KS and GL and carbonatization trend in SI.

[1] Gupta & Rao (2001) *Bull Eng Geol Env* **60**, 201-221. [2] Price & Velbel (2001) *Chemgeo* **202**, 397-416. [3] Reiche (1943) *J Sediment Petrol* **13**, 58-68. [4] Large *et al.* (2001) *Econ. Geol* **96**, 957–972.

Fluid-fluid phase separation under metamorphic conditions: MD simulations of a generalized composition H_2O-CO_2-NaCl

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Water and carbon dioxide are two most abundant volatile species in the Earth's crust and mantle. They represent the common solvents which, under high-temperature, high-pressure thermodynamic conditions, dissolve various amounts of other volatiles to form complex hydrothermal and metamorphic fluids. Thus, aqueous mixtures in the system H_2O-CO_2-NaCl can be considered a good approximation for most crustal and mantle fluids. Although there are many experimental thermodynamic data for this generalized system, the molecular-level understanding of their thermodynamic, transport, and phase equilibria properties is still inadequate in many respects. We performed molecular dynamics (MD) computer simulations of the H_2O-CO_2-NaCl fluids along three high-density isochores (1.0, 1.1, and 1.2 g/cm3) to systematically study their thermodynamic, structural, and transport properties in the range of temperatures from 400 to 1000ºC and pressures from 3 to 18 kbar.

The composition of $H_2O/CO_2/NaCl = 60/28/12$ mol%) was chosen to probe both homogeneous and heterogeneous regions of the phase diagram. It has been predicted from experimental data [1-3] and model calculations [4-5] that such fluid would undergo phase separation at approximately 700ºC by forming a CO_2-rich phase of low-salinity ($H_2O/CO_2/NaCl \sim 50/48/2$ mol%) and a concentrated brine ($H_2O/CO_2/NaCl \sim 66/20/14$ mol%). We try to uncover the molecular-level mechanisms driving this heterogenization process and to rationalize the properties of decompressing H_2O-CO_2-NaCl fluids under metamorphic conditions in terms of the effects of temperature and density on the molecular clusterization and ion pairing in the system controlled by the electrostatic and hydrogen-bonding interactions among the fluid species.

[1] Aranovich, L.Y. Newton, R.C. (1999) *Am. Mineral.* **84**, 1319–1332. [2] Shmulovich, K.I. Graham, C.M. (1999) *Contrib. Mineral. Petrol.* **136**, 247–257. [3] Shmulovich, K.I, Graham, C.M (2004) *Contrib. Mineral. Petrol.* **146**, 450–462. [4] Duan, Z.H. *et al.* (1995) *Geochim. Cosmochim. Acta*, **59**, 2869–2882. [5] Gerya, T.V. *et al.* (2000) *J. Geodynamics*, **29**, 17–35.