

Electrokinetic properties of the rutile/water interface: Zeta-potential prediction from computer simulations

MILAN PŘEDOTA¹, MICHAEL L. MACHESKY²,
D.J. WESOLOWSKI³ AND P.T. CUMMINGS⁴

¹Faculty of Science, University of South Bohemia, Ceske Budejovice, Czech Republic (predota@prf.jcu.cz)

²Illinois State Water Survey, Champaign, Illinois 61820-7495, USA

³Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6110, USA

⁴Department of Chemical Engineering, Vanderbilt University, Nashville, Tennessee 37235, USA

In the last 10 years we have been studying by molecular dynamics (MD) the structural and dynamic properties of aqueous solutions in contact with metal-oxide surfaces, mainly rutile [1-3]. We will present the results of our non-equilibrium MD simulations focusing on the molecular level origin of electrokinetic phenomena - electroosmosis and electrophoresis. We will comment on the asymmetry of the density profiles of cations and anions at positive and negative surfaces, discuss the properties of the diffuse and shear layers, if definable at all on the molecular scale, and present our zeta potential predictions from molecular simulations. Our results of zeta potential are in qualitative agreement with experimental data [5]. However, our molecular explanation is rather contradictory to at least some of the commonly used theories of the solid-liquid interface including the common double- or triple- layer models. We observe that the composition and structure at the interface, influenced by the surface charge, are the key factors, while the electrostatics of the aqueous solution is rather independent of the surface charge.

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Recycling plus: A new recipe for making orogenic mantle

D. PRELEVIC

University of Mainz, Germany, (prelevic@uni-mainz.de)

Fluids and melts liberated from the subducting oceanic crust ± sediments recycle a number of chemical elements back into the mantle wedge. The recycling rate of key chemical elements is controlled by the dichotomy of subsolidus dehydration vs. melting. Thermal models based on active subduction zones suggest that the majority of arcs are able to activate fluid-related transport dominantly, while the melt-related material recycling is only possible in unusually hot arcs. Paleo-subduction zones within orogenic belts, such as these within the Cenozoic Alpine-Himalayan belt, may serve as an advanced source of information regarding recycling styles during subduction. The composition of their mantle section is poorly constrained, but may be studied using postcollisional mantle-derived ultrapotassic lavas as a proxy.

The whole rock and mineral chemistry of postcollisional lavas suggests that the orogenic mantle underwent much more intense and complex material recycling than anticipated only by fluid- or melt-dominated transport. This is based on several fundamental constraints: i) Extremely enriched Sr, Nd, Hf, Pb and Os isotopic signature, which complement exceptionally low Ce/Pb and Nb/U ratios, are recognized in all mantle-derived postcollisional lavas along the Alpine-Himalayan belt; ii) Mixed ultra-depleted+ultra-enriched character of olivine phenocrysts and xenocrysts, with high Mg and Ni contents coupled with extremely high Li concentrations. Phenocrystal olivines have more than 40 ppm Li, and xenocrystal ones up to 10 ppm Li. iii) Extremely high Th/La coupled with high Sm/La of ultrapotassic mantle-derived lavas.

The above observations suggest that neither fluids nor melts alone are able to precondition orogenic mantle using known mechanisms, thus a new model is required. In my contribution, I will use the peculiar compositions of ultrapotassic mantle-derived lavas from across the Mediterranean for fingerprinting processes within the continental lithosphere. I will present a hypothesis that orogenic mantle is produced by accretion of suprasubduction fore-arc oceanic lithosphere plus trench sediments beneath older lithosphere during collisional tectonic events. The model demands conversion of principally oceanic lithosphere into the phlogopite-bearing continental lithospheric mantle and production of ultrapotassic lavas, which is a multi-episodic process.