

## Hydrogen isotope geochemistry of basalts from Samoa

J.A. O'LEARY<sup>1</sup>, E.H. HAURI<sup>1</sup>, S.R. HART<sup>2</sup> AND H. STAUDIGEL<sup>3</sup>

<sup>1</sup>Department of Terrestrial Magnetism, Carnegie Institution of Washington, Washington DC, 20015 U.S.A.

<sup>2</sup>Department of Geology & Geophysics, Woods Hole Oceanographic Institution, Woods Hole MA 02543 USA

<sup>3</sup>Scripps Institution of Oceanography, University of California-San Diego, La Jolla CA 92093 USA

Hydrogen is present at low concentrations (tens to hundreds of ppm H<sub>2</sub>O) throughout the upper mantle but exerts a strong influence on the melting behavior and rheologic properties of peridotite. The distribution of hydrogen in the entire mantle is a key constraint on mantle convection that remains unquantified. The D/H ratio of hydrogen in fluids and in silicate materials can be fractionated by tens of per mil under mantle conditions and offer an opportunity to identify and describe hydrogen storage and transport processes within the mantle. To pursue this goal we examined the hydrogen isotope composition of submarine ocean island basalt glasses collected from Malumalu, Vailu'lu, and Ta'u in the Samoan island chain. Lavas from the Samoan islands contain extreme trace element and radiogenic isotope enrichments that define the EM 2 (enriched mantle 2) mantle endmember [1]. The D/H composition of Samoan lavas vary between -79 and -37 per mil, a similar range to what is found in other ocean island basalt localities and in back-arc basin basalts that are influenced by fluids released from subducting ocean crust. The lowest  $\delta D$  values of Samoan glasses (-79 per mil) are close to the mode of values for mid-ocean ridge basalts (-75 per mil) while the highest value is similar to the isotopic composition of serpentine in equilibrium with seawater. This range in hydrogen isotope composition suggests that the mantle source region of Samoan lavas may contain fluid derived from ancient subducted ocean crust that has retained a distinct hydrogen isotopic composition over the timescale of mantle mixing.

Correlations between La, <sup>87</sup>Sr/<sup>86</sup>Sr, and water content in Samoan lavas are attributed to equilibration of initially water rich subducted materials with the ambient mantle water content [2]. Equilibration is possible due to rapid diffusion of hydrogen in mantle minerals [3]. The preservation of D-rich compositions in the source of Samoan basalts suggests that hydrogen isotope anomalies are not diffusively lost, possibly due to high concentrations of D-rich hydrogen in subducted materials that result in large regions of the mantle with high D/H ratio.

### References

- [1] Workman, R.K. *et al.* (2004) *G-cubed* **5**, doi: 10.1029/2003GC000623.
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## The model structure of kaolinite in relation to surface complexation

M. OLIN, E. PUHAKKA AND J. LEHIKONEN

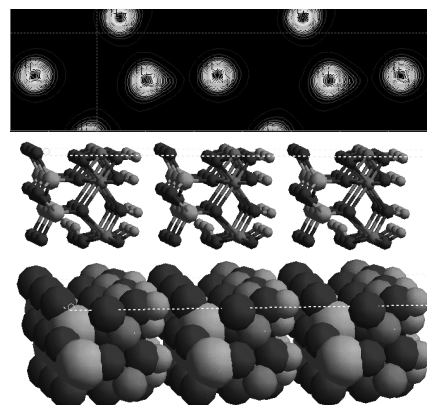
VTT Technical Research Centre of Finland, P.O. Box 1000, FI-02044, Finland (markus.olin@vtt.fi)

### Methods

Surface complexation modelling using the FITEQL software was applied to explain the surface acidity of kaolinite. In this context, a number of different models and modelling approaches were tested. Further, a density functional method, CASTEP (Accelrys, 2001), was used to investigate the crystal and surface structures of kaolinite, and to calculate surface charge densities.

### Results and discussion

To enable the interpretation of adsorption results with surface complexation modelling, an adequate characterization of the surface charging of the adsorbent is needed. In general, titration experiments are capable of providing this information for ionisable interfaces. However, results based on experimental data give only average values of surface charge densities. Therefore, in this study, molecular modelling was used to calculate surface charge densities of likely the most reactive kaolinite crystal faces separately (see Figure 1 for the (010) surface). Based on this information, an attempt will be made to constrain the number of surface sites and magnitude of surface hydrolysis constants, often considered as adjustable parameters devoid of deeper understanding, in surface complexation models.



**Figure 1:** Model (010) surface of kaolinite and its surface charge density.

### Conclusions

The molecular-level modelling produced invaluable background information of the kaolinite surface for further development of surface complexation models in terms of the surface charging and the adsorption of metal cations.

### References

- Accelrys. 2001. *Cerius<sup>2</sup>*. Release 4.6. San Diego: Accelrys Software Inc.