Atomic-scale structure of the orthoclase (001)-water interface measured with high-resolution x-ray reflectivity

P. Fenter[1], H. Teng[1], P. Geissbühler[1, 2], J.M. Hanchar[3], K.L. Nagy[4], and N.C. Sturchio[1]
[1]*Environmental Research Division, Argonne National Laboratory, Argonne, IL 60439-4843 USA*
[2]*Department of Physics, University of Washington, Seattle, WA 98195 USA*
[3]*Department of Geological Sciences, The George Washington University, Washington DC 20006 USA*
[4]*Department of Geological Sciences, University of Colorado, Boulder, CO 80309-0399 USA*

Introduction

Feldspars, the most common minerals in Earth's crust, are destroyed by low-temperature weathering processes. Much effort has been given to understanding the low temperature destruction of feldspar (e.g., through dissolution) because of its importance in soil formation and various geochemical cycles. A major obstacle, however, has been the lack of direct, *in situ* structural measurements of the feldspar-solution interface at the atomic scale. Only recently, with the advent of high-brilliance synchrotron radiation sources, has it become possible to make such measurements by using x-ray scattering methods. Here we describe our first efforts to understand the interfacial structure of the orthoclase-water interface [1].

Methods and Materials

X-ray scattering techniques are ideal for probing mineral-fluid interface structure because x-rays penetrate macroscopic quantities of fluids (such as water) with limited attenuation. The x-ray reflectivity (i.e., the ratio of the reflected to the incident x-ray fluxes) is directly related to the laterally averaged electron density, $\rho(z)$, near a reflecting interface [2].

The material used in this study was gem-quality orthoclase from Itrongay, Madagascar. Cleavage of the orthoclase in air was followed quickly (< 1 min) by immersing the cleavage surface in deionized water at room temperature and mounting the crystal in the x-ray reflectivity cell. Experiments were performed in a static thin-film configuration [2], with a water layer having an estimated thickness of 10–50 µm at the orthoclase surface contained by an 8 µm Kapton film.

Results and Discussion

The x-ray reflectivity data are shown in Fig. 1. The solid line corresponds to the best-fit model shown in Fig. 2. Significant features of this model are 1) the absence of a K atom in the outermost layer (shown as dashed open circles); 2) the coverage and position of a layer of an adsorbed species above the outermost Si bilayer, which we associate with oxygen atoms bound to the surface Si atoms (presumably in the form of hydroxyl groups to saturate the broken Si-O bonds created by cleaving); 3) the location of the fluid water layer above the orthoclase surface plane; and 4) the complex structural relaxation in the outermost layers to a depth of three to five unit cells.

A notable feature in the present model is the absence of the 32 Å-thick potassium depleted layer at the orthoclase-water interface that had been reported previously [3]. The expected
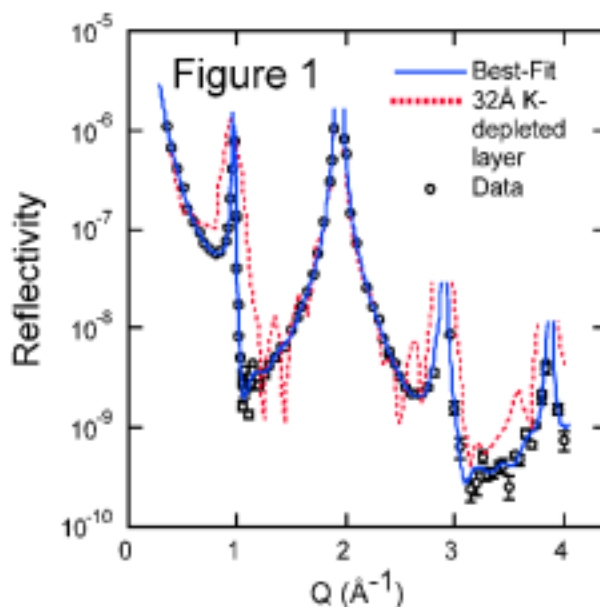

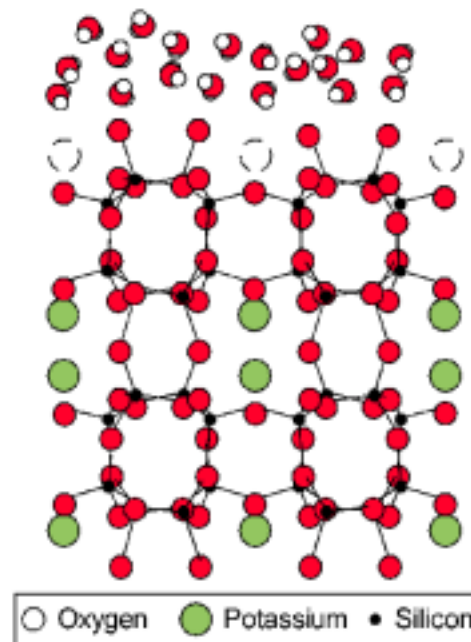Figure 1: X-ray reflectivity data.

Figure 2: The best-fit model.

reflectivity for such a layer is shown in Fig. 1, and demonstrates the high sensitivity of these measurements. Our results reveal that only top-layer potassium ions were released during the ~13 hour duration of this experiment.

Acknowledgments

References

[1] P. Fenter, H. Teng, P. Geissbühler, J.M. Hanchar, K.L. Nagy, and N.C. Sturchio, submitted to *Geochim. Cosmochim. Acta* (2000).
[2] P. Fenter and N.C. Sturchio, *Geochim. Cosmochim. Acta* **63**, 3145–3152 (1999).
[3] M. L. Farquhar, R. A. Wogelius, and C. C. Tang *Geochim. Cosmochim. Acta* **63**, 1587–1594 (1999).