

## Atomic-scale structure of the quartz (10 $\bar{1}0$ )- and (10 $\bar{1}1$ )-water interfaces

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### Introduction

Quartz is ubiquitous in the continental crust, and plays a key role in controlling the dissolved silica concentration in aqueous systems. To better understand and model the kinetics of quartz dissolution and precipitation, an extensive knowledge of the quartz-water interface structure is desirable. In this study, we probed the structure of prismatic (10 $\bar{1}0$ ) and pyramidal (10 $\bar{1}1$ ) growth faces of natural quartz crystals by atomic force microscopy (AFM) and in water by high-resolution X-ray reflectivity. Quartz slabs were sonicated in acetone, methanol, and deionised water to remove surface impurities. TappingMode AFM images were collected with a silicon tip. Reflectivity measurements were recorded on the wet surfaces at the 12-ID station (BESSRC-CAT, Advanced Photon Source, Argonne National Laboratory).

### Results and interpretation

AFM images revealed the presence of ~ 0.1 to 1  $\mu\text{m}$ -wide flat terraces delimited by steps of one to several unit cells in height. These steps essentially follow directions given by the intersection of growth faces. Modeling of X-ray reflectivity data indicates that the atomic structure near the quartz surface is obtained from the quartz bulk structure, assuming slight relaxation of atomic positions (< 0.4 Å for terminal oxygens and < 0.2 Å for silicon and oxygen atoms fully coordinated to structural tetrahedra). Vertical relaxation of atomic positions is limited to a depth of 14 Å. Surface silica groups on flat terraces have only one free Si-O bond each (presumably hydroxylated), except for some having two free Si-O bonds observed on a single (10 $\bar{1}0$ ) surface. Electron density profiles for the probed interfaces are consistent with a single layer of water adsorbed in an amount equivalent to the number of surface silanol groups, but no additional organization of water was detected into the bulk solution. We found no evidence for the presence of a layer of disordered or amorphous silica, even for a (10 $\bar{1}1$ ) quartz slab kept in deionised water for 10 months prior to reflectivity measurements. These results provide strong constraints on the nature of surface functional groups exposed at the (10 $\bar{1}0$ ) and (10 $\bar{1}1$ ) faces of quartz.

## Progress in tritium/<sup>3</sup>He dating of shallow groundwater

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During the past decade, the transient tracers tritium and its radioactive decay product, <sup>3</sup>He, have been developed as age tracers for dating of shallow groundwater. Starting from systematic exploration of the method in relatively simple, typically sandy, aquifers, the method has been applied to increasingly complex hydrogeological settings including fractured aquifers or karstic formations.

It has been shown that the tritium/<sup>3</sup>He method yields valuable insight into flow patterns, age gradients, or mean residence times of young groundwater, especially if combined with other transient tracers such as CFCs. Modelling studies usually enhance the information that can be derived from qualitative interpretation of the tracer data.

We briefly summarize the main methodological aspects of tritium/<sup>3</sup>He dating of groundwater and demonstrate its effective use on the basis of case studies. The case studies include simple flow systems, as well as complex hydrogeological settings. Tritium/<sup>3</sup>He data are compared to CFC data and groundwater flow models. Under favourable conditions, waters recharged before the occurrence of the tritium 'bomb' peak in the early 1960s can be dated by this method.