Abstract template:

Title

Time Evolution Studies of the H_2O/Quartz Interface using Sum Frequency Generation (SFG), AFM, and Molecular Dynamics

Reference

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Authors

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Abstract

Many interfacial studies on solid surfaces, for example, quartz/water, assume that a standard cleaning procedure regenerates the surface reproducibly. In the reported work, the results of two surface specific techniques, sum frequency generation (SFG) spectroscopy and atomic force microscopy, show that the effects of prolonged exposure to Nanopure water and to pH10 NaOH are distinctly different. In conjunction with the experimental data, molecular mechanics is used to correlate the SFG spectral frequencies to the hydrogen stretching vibrations of the surface-bound water molecules. It is found that after 17 days of soaking in water, water molecules penetrate into the SiO2 matrix to produce a swollen and amorphous layer; it is likely that broken Si-O bonds from the polishing process serve as nucleation sites for hydration and swelling. Disorder introduced in the interfacial water layer is detected by the rising intensity of the weakly hydrogen-bonded SFG peak at 3450 cm-1. Dominance of the 3450 cm^{-1} is absent in a pH 10, NaOH-soaked quartz disk, indicating that the strong hydrogen-bonded network in water remains intact.