Atomic-resolution imaging at mineral-water interfaces

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Mineral-water interfaces are ubiquitous both in nature and technology. This is why mineral-water interfaces are decisive in many fields, including, *e.g.*, biomineralization, ice nucleation, catalysis and sensing, to name but a few. Understanding the interaction of minerals with their surroundings requires the knowledge of the interfacial structure at the atomic level. Such an atomic-level information can be gained by three-dimensional atomic force microscopy, which provides real-space structural information of the mineral surface and the interfacial hydration structure.

In this talk, silver iodide (AgI) will be discussed as a prototypical ice nucleating mineral. The high ice nucleating ability of AgI is typically explained by the close lattice match of the silver iodide cleavage plane and the basal plane of ice I_h. However, the relevant AgI surfaces are polar, *i.e.*, thermodynamically instable. This fact implies the existence of a stabilization mechanism, which is, however, unknown at present. Possible stabilization mechanisms for polar surfaces include (i) surface reconstruction, (ii) ion adsorption and (iii) internal charge transfer. Our atomic-resolution images of the AgI-water interface closely resemble the bulk-truncated geometry, regardless of the termination. These measurements thus reveal no indication for a reconstruction of the AgI cleavage planes at the atomic scale. The same is true upon cleavage in ethanol, which greatly reduces the possibility for ion adsorption as an explanation for the stability. Therefore, another stabilization mechanism seems to be at play, which might be linked to the larger-scale facetted structure seen in the images. Unravelling the relevant stabilization mechanism is a prerequisite for understanding the ice nucleation ability of AgI.

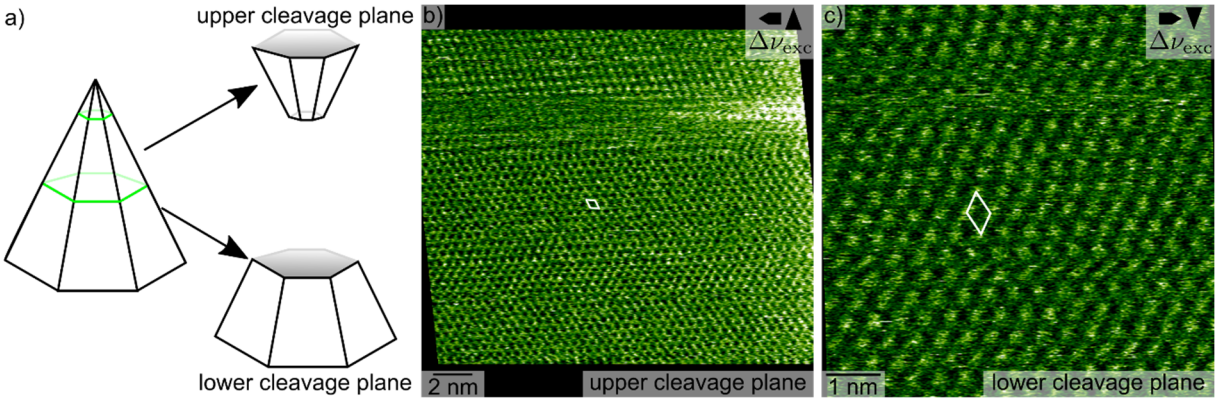

Fig. 1. Atomically resolved AFM images of the β-AgI (0001) cleavage planes. a) Cleavage of silver iodide crystals, resulting in an upper and a lower cleavage plane. Atomic resolution on the b) upper and c) lower cleavage plane, one of which is terminated by silver, the other by iodide ions.

[1] F. Sabath, C. Aleff, A. Latus, R. Bechstein and A. Kühnle, Adv. Mater. Int., **9**, 2201065 (2022)