The rutile (110)-electrolyte solution interface to 250°C: A surface complexation synthesis of titration, ab initio, MD, and X-ray spectroscopic results

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We have been conducting potentiometric titrations of rutle powders dominated by the 110 crystal face to 250°C in several so-called "inert" electrolyte solutions (NaCl, NaTr (Tr⁻=trifluromethanesulfonate), RbCl) over the past dozen years. More recently (since about 2000) these bulk, macroscopic measurements have been augmented by ab initio and molecular dynamics (MD) simulations, as well as synchotron-based x-ray spectroscopic measurements, in order to obtain an unambiguous understanding of the rutile 110-electrolyte interface from the micro- to macroscopic scales.

The focus of this contribution will be our most recent attempts at incorporating the molecular information afforded by our ab initio, MD, and x-ray results into Surface Complexation Models (SCM's) that accurately reflect both this microscopic reality and our bulk surface titration data. A MUSIC model description of surface protonation that utilizes actual surface Ti-O bond lengths, as well as the numbers and lengths of H-bonds from and to associated water molecules is able to adequately reproduce the experimentally determined pH_{zpc} values of our rutile powders to 250°C. Addtionally, considerable fractions of the so-called "inert" electrolyte cations (Na^+, Rb^+) are in fact observed to bind in distinct configurations (primarily bidentate and tetradentate) above the rutile 110 surface, and these binding geometries can be adequately captured by Stern-based representations of electrical double layer (EDL) structure. A principal conclusion of these efforts is that although the developed SCM's can satisfactorily represent the molecular-scale reality uncovered to date, they do not do so uniquely.

Planetary formation from icy planetesimals around 1 AU

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Formation and Evolution of Icy Planetesimals

Standard scenario of planet formation have been developed on the assumption that the primordial solar nebula is optically thin, so that H_2O ice condenses only outside 2.7 AU from the Sun. The solid material is composed of only rocks at the terrestrial planet formation region (Hayashi 1981).

However, it is widely accepted in the astronomical community that the protoplanetary disks are initially opaque owing to the floating small dust particles and become transparent at the late stage of planetary formation. In optically thick disks, the interior of the nebula is shadowed from direct exposure to sunlight, so that H_2O ice is prevented from sublimation outside about 0.7 AU (Chiang and Goldreich 1997).

As planetesimals are likely formed in such opaque protoplanetary disks, they should contain a large amount of H_2O ice. We call such planetesimals "icy planetesimals" hereafter. We perform numerical simulations of formation of protoplanets from icy planetesimals focusing on the competition between accretion and sublimation of H_2O.

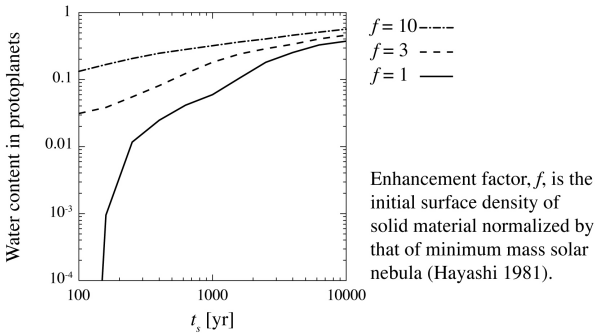

Figure 1: Water content in protoplanets.

Results and Discussion

Fig. 1 shows the water content in the system when Mars-sized objects are formed after runaway accretion. It indicates that planets with diverse water contents (i.e., from dry planet to water-ball planet) can be formed. Water content is strongly dependent on the initial surface density of solid material and the time interval, t_s, between the icy planetesimal formation and the onset of icy planetesimal sublimation. We also find that final water content is dependent on object size. Most of water in the system is contained in largest protoplanets, while most of small planetesimals have lost their initial water.

References

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