

Project description:
Development of a combined MD and DFT model for
mechano-chemical processes.

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Introduction

The interaction between mechanical and chemical processes is in many cases rate limiting for the mechanical failure of materials. For example, the slow advance of a fracture on a wind shield is due to the diffusion of hydrogen to the fracture front, where it replaces a strong covalent binding with a weaker hydrogen binding, leading to a local weakening of the material, which subsequently leads to further propagation of the fracture.

We use the term “mechano-chemical” process for stress corrosion, since there is a strong coupling between the chemical and mechanical processes. The mechanical stresses at the fracture tip focuses the chemical replacement process – the chemical replacement depends on the mechanical stress. In addition, a replacement has local consequences on the mechanical behavior of the material. In the case of stress corrosion the material is weakened, but in other processes the reaction can also lead to a local increase or decrease in volume, inducing stresses in the material.

Mechano-chemical processes are important since they can be rate limiting for material degradation processes, and hence determine the lifetime of materials. While this has many practical consequences from an industrial point of view, mechano-chemical processes can also be rate limiting in geological processes, for example in chemical weathering and in mineral replacement processes. They are also of fundamental interest because the coupling between mechanical and chemical effects for example during fracturing magnifies the microscopic effects on the tip of a fracture – and therefore exposes our understanding of the processes happening at fracture tips.

Research project

In this project we attempt to improve our understanding of the coupling between mechanical and chemical processes by developing a model of chemical replacement at a loaded fracture tip. This requires an atomic-scale description of the material close to the fracture tip and a precise description of the processes at the fracture tip. We will therefore develop a MD model coupled for example to a DFT model to address stress corrosion processes, and then use this model as a basis to develop our understanding of less well understood systems, such as mineral replacement reactions.

The project consists of the following subprojects:

Development of MD model for fracture propagation The student will develop a MD model for fracture propagation in a silica glass using a simplified

interatomic force model.

Calibration testing The MD model will be tested by comparison with known solutions and previous studies to test the stability and precision of the numerical methods used.

Coupling to DFT models The model will be improved by using for example DFT techniques to address the interatomic forces close to the fracture tip.

Application to stress corrosion The model will be applied to address stress corrosion type processes in small system simulations.