Modeling plastic deformation of minerals under mantle strain-rates

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Mantle convection involves plastic deformation of minerals and rocks under extreme conditions that are very difficult to reproduce in the laboratory. In particular, experimental strain-rates are at least 6 orders of magnitude larger than in nature. Extrapolation to natural conditions of semi-empirical constitutive flow laws parameterized on laboratory data is thus very unsafe and leads to significant discrepencies with observations (e.g. post-seismic deformation). Here we describe a physically-based model able to describe the rheology of MgO (the magnesium end-member of the second most abundant phase of the lower mantle) under very low strain-rates representative of mantle convection. Our multiscale numerical model involves : (i) dislocation core modeling based on the Peierls-Nabarro-Galerkin model, (ii) thermal activation modeling of dislcoation glide based on the kink-pair theory, (iii) critical resolved shear stress modeling based on the Orowan equation (in ther thermally-activated regime) or on Dislocation Dynamics modeling (in the athermal regime). The kink-pair theory allows to describe the mobility of dislcoations under very low stresses without extrapolations. We show that decreasing the strain-rate counteract the influence of high-pressure and emphasizes the athermal regime for MgO in lower mantle conditions.

This approach will be further applied to other phases of the Earth's mantle within the ERC-funded *RheoMan* project (wwww.rheoman.eu)

Reactive Trasnsport Modelling of Gas Formation and Mineral Precipitation in a Granular Iron Column

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The (bio)geochemical reactions resulting in the degradation of contaminants in aquifers and remediation systems are often coupled to physical processes that can affect the rate of reaction or the rate of solute transport. In granular iron permeable reactive barriers (PRBs), the precipitation of secondary minerals can lead to armoring of the iron surfaces, reducing reactivity, and also reducing permeability due to the reduction in porosity [1-3]. The generation of hydrogen gas in granular iron PRBs can lead to the production of gas bubbles that can also reduce permeability due to pore blocking [3-5].

Processed-based reactive transport modelling was used to simulate the coupling of these proceses to the treatment of trichloroethene (TCE) with granular iron in a laboratory column experiment. This was carried out with the multi-component reactive transport model MIN3P [6], which was enhanced to couple gas formation and release, secondary mineral precipitation, and the effects of these processes on hydraulic properties and iron reactivity.

The simulation reproduced the observed temporal and spatial trends in gas formation, permeability changes, and TCE degradation. The simulation showed an initial sharp decrease in permeability due to hydrogen gas production and gas bubble formation throughout the column. Over time, as the reactivity of the granular iron decreased due to armoring by secondary minerals, the degree of gas saturation throughout the column decreased, but the porosity of the column also decreased as a result of the secondary mineral formation. The result is a steady decrease in permability. The simulation demonstrated that after 704 days, armoring by carbonate mineral precipitation resulted in TCE breakthrough at 473 days followed by a steady increase in TCE concentrations in the column effluent.

The enhanced MIN3P model effectively demonstrated the coupling of geochmical and physical processes in this system. The simulation results suggest that the spatial and temporal evolution of gas formation and secondary mineral precipitation are critical factors in determing the effectiveness and longevity of granular iron PRBs.

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