COMSOL model and Matlab fitting subroutine for the determination of the hydrogen diffusivity from isothermal TDS curves

The hydrogen diffusion coefficient, D_iso, was determined by fitting a 1-D finite element (FE) simulation of hydrogen transport to the measured ITDS profile (molH/m^3/s vs. time) for each experiment. In the paper this is given in wppm/s vs. time.

COMSOL model: isothermalTDS.mph

In COMSOL, the thickness of the sample has to be specified. Also, the output times of the simulation should be the same as the experimental times used in the optimization subroutine. The rest of parameters are controlled in the Matlab optimization subroutine.

For the current study, it is assumed that a homogeneous hydrogen concentration exists across the specimen thickness at the start of the simulation (C_0iso in [molH/m^3/s]) and that the hydrogen concentration at the free surface is zero given the use of an ultra-high vacuum environment. A FE mesh sensitivity study demonstrated that mesh- independent results were efficiently obtained for a progressive mesh composed of 200 elements decreasing in size to-wards the free surface of the specimen (this is already implemented in the model).

As all experiments were performed at ambient temperature (22ºC) and did not use the heater stage of the TDS, D_iso in [m^2/s] was determined in a single step analysis through fitting the experimentally-measured hydrogen desorption rate versus time data by iteratively changing the C_0iso and D_iso values. The LiveLink tool was employed to integrate COMSOL with Matlab, where a routine for parameter optimization was developed using the curve fit function *lsqcurvefit*, which performs a least square minimization using the Levenberg-Marquardt algorithm.

Main code for parameter optimization: main.m

Function to extract data from COMSOL: funCOMSOL.m

The code is explained in the Matlab files and easy to follow.