**Stopping the corrosion of Mg**

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Corrosion is a huge waste of money (about $276 billion in the USA in 2002), as well as a nuisance. It is also complicated: there are multiple coupled processes occurring over a range of length and time scales. We will try to understand, and inhibit, the aqueous corrosion of Mg, for which computer simulation is now recognised as necessary.

Aqueous corrosion at a metal surface depends on the applied potential, surface composition, and ion concentrations in the aqueous medium. This makes corrosion rates sensitive to events in remote parts of the system, and hence they depend on both local reaction rates (atomic scale), diffusion through surface layers (nanoscale), and diffusion through the surrounding water (mesoscale). Associated with these length scales is a range of time scales. We will address the atomic and nano scales by studying key atomic processes and how they couple within a nanoscale crevice.

Initially we will study the mysterious Negative Difference Effect in which the forward reaction $H^+ + e^- \Leftrightarrow \frac{1}{2}H_2$ accelerates when the number of electrons is reduced [1]. We will use molecular dynamics (MD) simulations to study atomic scale processes: the detachment of an Mg atom, its diffusion through an oxide/hydroxide layer and subsequent hydration, and the reaction of $H^+$ with Mg and its oxide/hydroxide coating. This is challenging as electrons we need to flow freely into and out of the computational cell. Our recently discovered solution is to use tight binding MD with Hairy Probes [2]. These results will be fed into a kinetic Monte Carlo code to be built by PDRAs that are part of the group. This will enable investigation of how the processes work together in a confined space to produce the resulting corrosion.

This project is a collaboration with our industry partner Magnesium Elektron and is fully-funded for Home and EU students. Technical and scientific enquiries may be directed to Dr Andrew Horsfield (a.horsfield@imperial.ac.uk). General admissions enquiries should be directed to the TSM-CDT Senior Administrator, Ms Miranda Smith (miranda.smith@imperial.ac.uk).