Hydride ion diffusion in sub-stoichiometric titanium nitrides (MENA – MSc/BSc)

Fast diffusion of hydride ions in titanium nitrides (TiN_x) have been reported, but the mechanism is not yet understood. The project will address dissolution and transport of hydride ions in TiN_x as a function of composition, and grain boundaries will be considered as potential fast diffusion paths. The project can be combined experimental and computational. The computational part includes density functional theory (DFT) studies of the solubility and diffusion of hydride ions in bulk as well as at grain boundaries as a function of composition. The role nitrogen sub-stoichiometry and its impact on the electronic structure of the materials will be and important aspect. The experimental part has potential for many types of fabrication and characterization methods. For instance, instance isotope exchange of hydrogen in thin films deposited by pulsed laser deposition (PLD).

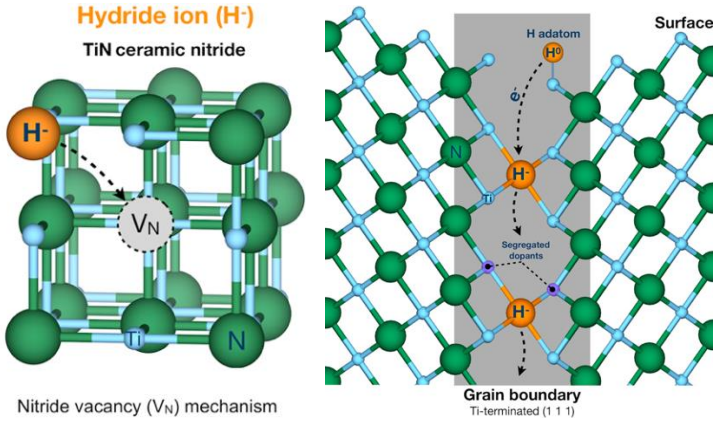

Figure 1: Hydride ions in TiN and hydrogen migration mechanisms along a grain boundary.