GRAIN BOUNDARY NETWORKS AS A FUNDAMENTAL FEATURE TO DESIGN MATERIALS TO MANAGE DIFFUSION OF HYDROGEN

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Hydrogen embrittlement (HE) impacts the mechanical properties of the materials as a consequence of the mobility of hydrogen through the metal. This phenomenon is highly governed by the hydrogen – microstructure defects interactions. Thus, the spatial distribution of the microstructure heterogeneities in the volume will dictate the repercussion of the hydrogen on the material.

In this work, we focus on the effects of grain boundaries (GB) and triple junctions (TJ) and their connectivity on the diffusion and trapping of hydrogen using the percolation theory (network topology and connectivity). Here we question the role of the statistical distributions of two types of GB (random and special) numerically and experimentally in pure nickel. Four types of Triple Junctions (TJs) along with their distributions have been considered. We developed numerically several algorithms to control the distribution of the fractions of TJs based on a given fraction of Random and Special grain boundaries in 2 and 3D.

Nowadays, it is critical to design new processes and / or highly improved existing materials capable of reducing the risks of failure associated with HE. In this framework, our approach aims at acquiring knowledge at the heterogeneity scale (grain boundaries and triple junction) to properly classify their action in order to design new architectural network of grain boundaries experiments and atomistic calculations at the grain boundary scale have been performed to evaluate the distinction between the grain boundaries and review the grain boundary engineering distinction between random and special.