Popular Abstract -
Orientation dependant grain boundary diffusion in polycrystals

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When the surface of a metal is in contact with other external substances these tend to diffuse, that is to flow, into the material. The introduction of these impurities can alter the mechanical properties of the metal, which can be either beneficial or disastrous for the metals intended use case.

Firstly, lets consider a common diffusion process, which involve hydrogen, one of the building blocks of water. The diffusion of hydrogen into steel can result in severe degradation of the structural qualities of steel and can effect the expected lifetime of affected structures. Furthermore, diffusion can also be found between layers of different metals where the layering is used to utilise the strength of the different materials. However, due to diffusion, atoms from each material will diffuse into each other and change the material properties respectively. These two examples showcase the importance in understanding the diffusion processes and in extension grain boundaries, as these dictate, to a large degree, the diffusion characteristics.

This thesis is primarily focused on metals, such as iron, which is made up of multiple grains, for which the structure looks similar to that of grains of sand, or a mosaic. This type of structure is refered to as a polycrystal. The interface between grains is refered to as a grain boundary and exists because of bad structural fit between neighboring grains. Diffusion along these grain boundaries has been found to be higher than within the grains. Furthermore, the rate of diffusion along grain boundaries have also been found to depend on the geometry and relative orientations of neighbouring grains. It is this orientation dependants that has been studied in this thesis. In which a model has been derived to express this orientation dependants. The derived model was found to correlate well with experimental data. This model was used to simulate different diffusion processes in a polycrystal material. Simulations show that different orientations of the grains result in different effective diffusion rates through the polycrystal and as such the collection of orientations, also known as the texture, of the material is important and must be considered. This knowledge can be use to consciously chose a texture which give desired diffusion characteristics.