Modelling and simulating three phases in steel: austenite, ferrite and cementite

Steel is an important material used in the construction of many different things. Steel is originally an alloy of iron (Fe) and a little bit of carbon (C), normally up to about 2,1% of the total weight. To improve certain properties of steel other alloying elements such as manganese, nickel, chromium, molybdenum, boron, titanium, vanadium, tungsten, cobalt, and niobium are added. The iron atoms in steel are structured in two different crystalline forms, face centered cubic (FCC) and body centered cubic (BCC). These two crystalline forms can contain a different amount of carbon, influencing its hardness, ductility and tensile strength. The FCC structured steel is called austenite (γ), BCC structured steel is called ferrite (α). In the transition from austenite to ferrite by cooling, cementite (θ) can be present. Cementite is a stoichiometric compound with formula Fe_3C, meaning 6.67% of its weight is carbon and 93.3% is iron.

Model

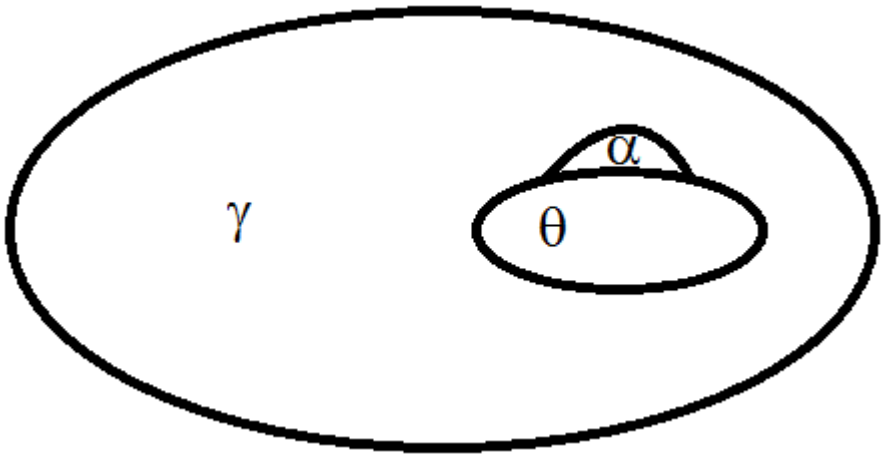

Figure 1: Sketch of the nucleation of ferrite (α) on the interface of austenite (γ) and cementite (θ).

The transition from austenite to ferrite can modelled by a so called Stefan problem. It describes the diffusion of carbon in steel over the different phases and the movement of its interfaces. When numerically solving the Stefan problem, keeping track of the interfaces can be complicated, especially when there are multiple phases connected. In this project it is modelled how ferrite starts growing just after nucleating at the interface between austenite and cementite as the steel is cooled down (see Figure 1).