Grain initiation is a crucial step towards microstructure formation during solidification. A better understanding of grain initiation can help us to control the solidification processes for grain refinement and property enhancement.

This work aims to understand the grain initiation behaviour during isothermal solidification of single phase alloys with an emphasis on the interplay between heterogeneous nucleation and free growth. We used a numerical approach to investigate the grain initiation process during isothermal solidification of single phase alloys. We have identified two distinctive grain initiation modes: progressive grain initiation and explosive grain initiation. Progressive grain initiation starts with the largest particle(s), continues with the progressively smaller ones and finishes at recalescence. In contrast, explosive grain initiation is a process in which solid particles initiate grains almost simultaneously and the latent heat released by both heterogeneous nucleation and the initial free growth can cause immediately recalescence (Figure 1). It occurs during solidification of engineering alloys which contain very impotent nucleant particles (either in-situ or ex-situ), and have no other more potent nucleant particles of significance in the melt (Figure 2).

Such grain initiation behaviour is best presented by a grain initiation map (Figure 2c), which is a plot of cooling rate against the nucleation undercooling showing the conditions for progressive, explosive and transition zones for grain initiation. Further theoretical analysis has shown that explosive grain initiation is favoured by solidification of dilute alloys containing only impotent nucleant particles of a large number density and small particle size under high cooling rate.

Effective grain refinement requires appropriate manipulation of the interplay between heterogeneous nucleation and grain initiation. The traditional wisdom is to enhance heterogeneous nucleation by addition of potent nucleant particles. In this work we have shown both theoretically and experimentally that the most effective grain refinement can be achieved by impeding heterogeneous nucleation with the least potent nucleant particles assuming that no other more potent particles of significance exist in the alloy melt. In addition, we have demonstrated that it is more advantageous to make the best use of native solid particles for effective grain refinement rather than to develop grain refiners for chemical inoculation.

As part of the future work, we will develop this numerical model further to analyse the competition for nucleation between different types of nucleant particles that co-exist in the melt.