Prediction of grain size during solidification

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A fine and equiaxed microstructure not only facilitates the casting process but also improves the performance of final components. Therefore, the prediction of grain size for alloys solidified under varying conditions is of both scientific and technological importance.

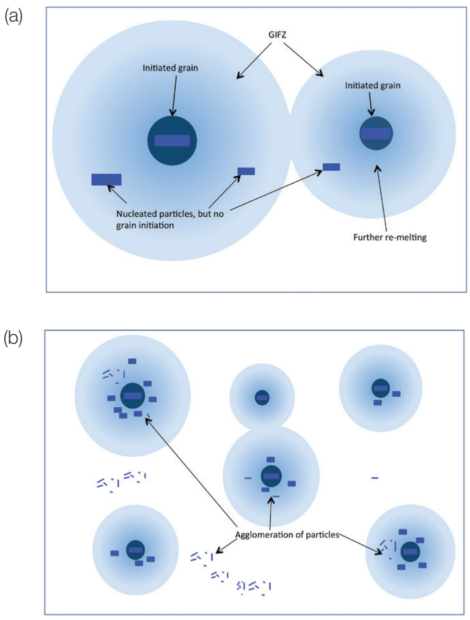

FIGURE 1. Schematic illustration of the mechanisms of grain initiation free zone (GIFZ) and re-melting, which affect microstructure formation.

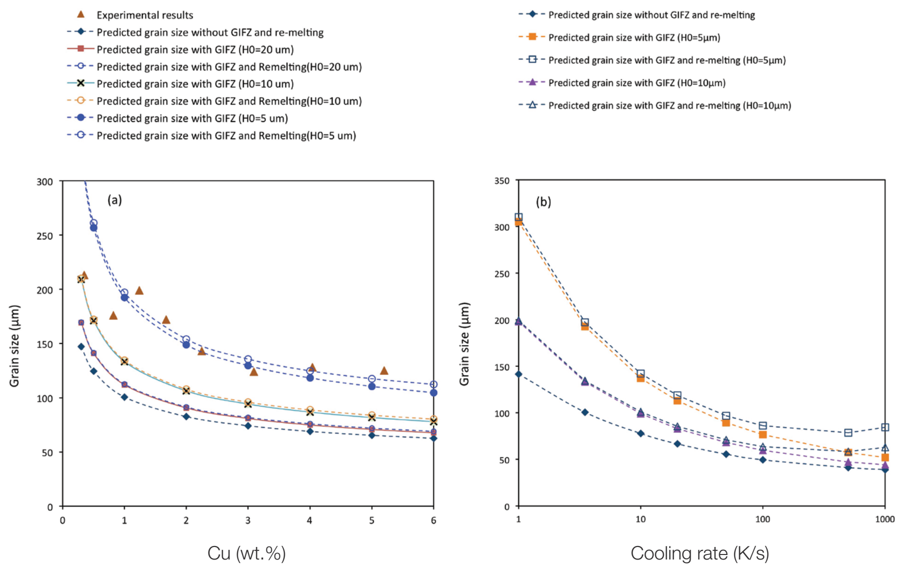

FIGURE 2. The numerically calculated grain size as a function of (a) Cu concentration and (b) cooling rate for Al-Cu alloys showing the agglomeration, from H_0=10 μm to H_0=5 μm, strongly affects the grain size.

However, current models for predicting grain size for isothermal solidification have a limitation in that their predicted grain size is much less than the experimental results. This work aims to develop a numerical model for isothermal solidification to predict grain size more accurately by incorporation of the underlining mechanisms of grain formation.

The free growth criterion [x] specifies which nuclei can initiate grains and contribute to the solidified microstructure. However, we found that not every initiated grain can survive during solidification. Theoretical analysis shows that an initiated grain according to the free growth criterion will not survive under the following two circumstances (Figure 1): (a) a nuclei located in the solute field of a growing solid particle will not initiate a grain albeit it satisfies free growth criterion, we name this solute field as grain initiation free zone (GIFZ); and (b) an initiated grain will re-melt if its solute field overlaps with the solute field of a larger grain, and this is named the re-melting mechanism. By assuming a log-normal spacing distribution for nuclei and a normal spacing distribution for initiated grains, we have developed a numerical model to predict grain size of solidified microstructure.

Based on the numerical analysis we found that the GIFZ mechanism has a strong influence on the predicted grain size depending on the extent of nucleant particle agglomeration while the re-melting mechanism has very little impact on grain size (Figure 2a), taking Al-Cu alloys for example, indicate that the agglomeration of nucleated particles strongly affects the grain size. In addition, we found that the effect of GIFZ decreases with cooling rate (Figure 2b).

The implication of this work is that for effective grain refinement it is crucial to disperse the nucleant particles. Nucleant particles, such as TiB_2 introduced by addition the Al-Ti-B grain refiner and native MgO particles in Mg-alloy melts, usually have a submicron or even nanometre size. They have a strong tendency for agglomeration, which reduces their efficiency for grain refinement. We have demonstrated in this work that appropriately dispersed nucleant particles can half the grain size.

Further work will focus on precisely predicting the grain size in practice solidification conditions.