Computational Thermodynamics Coupled Macro-Microscale Modelling of Industrial Castings

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ABSTRACT

Industrial casting simulations demand for thermophysical properties and latent heat release data regarding multicomponent metal alloys. Latent heat in particular has been typically considered. Independent of cooling rate and proportional to the solid fraction evolution, but heat release is function of alloy chemistry and solidification velocity [1-2]. Since computation capacity increased in the last decade, computational thermodynamics coupled microstructure modelling is becoming an opportunity for solving such requirements in industrial environments.

To increase the knowledge in this field, the gravity die casting of a stepped geometry of AZ91E Mg alloy has been modelled.

An equiaxed grain growth model has been coupled to the commercial thermodynamic programmers library ChemApp using appropriate databases from FactSage and macroscale heat transfer software WinCast. Thermal histories of castings have been experimentally investigated and compared to calculations. The latent heat release dependency on cooling rate has been analysed and proved the non-proportionality with created solid fraction. Additionally, the non-equilibrium phase distribution has been also computed. The importance of accurate heat balances to link the macro- and microscales is also discussed.

References

[1]M.B Djurjevic et al., Material Science Forum 539-543, 299-304 (2007).

[2] T. Antonsson and H. Fredriksson, Metallurgical and materials transactions. B 36, 85-96(2005).