XVIII IMEKO WORLD CONGRESS
Metrology for a Sustainable Development
September, 17 – 22, 2006, Rio de Janeiro, Brazil

NUMERICAL SIMULATION OF ZINC FREEZING POINT - EFFECT OF MULTICOMPONENT AND ACCURATE DATA

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Abstract: A numerical investigation of zinc freezing point is presented. Comparison of results for the solidification of same alloy using two different sets of data shows the need to have accurate phase-equilibrium data and the necessity of considering all of elements present in an alloy. The results give an indication of what areas require more careful examination if accurate modeling of freezing point is to be accomplished.

Keywords: Temperature, fixed point of zinc, numerical simulation of freezing point of zinc.

1. INTRODUCTION

The zinc freezing point (697,277 K) has been used for many years as a fixed point on International Temperature Scale of 1990, ITS-90 [1]. In view of a lack of sufficient data on the behavior of impurities in the ITS-90 defining materials fixed point, for the assessment of the fixed point quality realizations at highest levels of accuracy, it is crucial to analyse in detail the influence of the concentrations of the material's impurities using different freezing conditions [2]. Some years ago a considerable amount of work was carried out with resistance thermometers to determine on the freezing points of metals in the range of 0 ºC to 630 ºC under a variety of cooling and heating rates [3-4. Due to high cost of experiment only recently Ancsin [5-6] made a systematic study of shifts of equilibrium melting curves of samples Al and Ag. State-of-art estimates for the uncertainty component caused by impurities has been deduced from results obtained in the CIPM Key Comparions. The influence of impurities on the transport phenomena manifests itself through three coupled effects: a) the differences in the solutal expansion coefficients of the impurities in the liquid phase; b) the differences in the partition coefficients, as well as the effects of the various impurities on the liquidus temperature; and c) the differences in the rates of mass diffussion on elements in the solid phase. Since the partition coefficients of the impurities are unequal and the mass diffusivities of the elements in solid are different, microsegregation of each impurity in the solid will not be the same. Clearly, the final distribution of an impurity in the ingot will depend not only on the properties for that impurity, but also on those for the other impurities present in the alloy.

Numerical simulation based on valid mathematical models offers opportunities to gain insights into various physical phenomenas that are difficult, if not impossible, to carry out experiments. In the present study, numerical simulation of freezing of Zn-Tl alloys is perfomed using a two-phase model for conservation of continuity, momentum, energy and species. The aim of this article is to ilustrate the use of this model to simulate the solidification of a multicomponent alloy and then to show the necessity of fully accounting for all of the elements present when simulating the solidification of fixed point. In addition, the vastly different solidifications of the same alloy using two different sets of data from literature for the partition coefficient, thermophysical properties and the effect of each species on the liquidus temperature are compared.

2. METHOD

In all simulations presented here the initial temperature were 5 K higher than the liquidus temperature. The melt is initially isothermal and chemically homogeneous. The simulated geometry is shown in Figure 1.

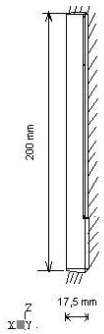

Fig. 1. Geometry of cylindrical graphite crucible

The cell's symmetry allows ¼ section of the geometry to be modeled. The top, bottom and the right wall of cell's geometry are insulated. The left wall is initially at zinc

freezing point temperature after that the wall temperature is slowly cooled (~0,01 K/s). All walls are treated with no-slip condition and are impermeable to mass and species transport.

2.2. Mathematical formulation

Numerous models have been developed for the solidification alloys, and comprehensive reviews have recently been published [7].In this stydy, the physical behavior of the solidification process is modeled through the use of a two-phase system of equations [8]. Two sets of conservation equations are derived, one based on the liquid phase and one based on the solid phase. In establishing the mathematical model for this process, the following assumptions and simplifications were used: the flow is laminar and the solid phase is stationary and rigid. This assumption is valid for columnar growth; the dissipative interfacial stress is modeled using the mushy zone permeability in analogy with Darcy's law; in the phase diagram the liquid solpe and the partition coefficient are assumed to be constants; the equilibrium conditions exist at the solid-liquid interface, homogeneous and isotropic properties in the phases; the liquid within an averaging volume is well mixed so that the interfacial average and volume average concentrations are equal.

2.2. Numerical procedure

The conservation equations were derived to be valid in all regions which allow the computational space to be described on a fixed grid. The CFD code CFX-5.7 was used in the current study. A uniform time step of 1 s was used for sets of simulations. Each time step was converged when the normalized residuals fell below 10^{-5}.The mesh contains 48994 tetrahedrons elements. The bulk of the geometry contains total number of 9990 nodes was tested and showed greater refinement.

3. RESULTS AND DISCUSSION

In order to illustrate the effects of multicomponent during the solidification of zinc alloys, four cases have been investigated.

- Case 1 simulates the solidification of a binary Zn-Tl alloy containing 8ppm of solute.
- Case 2 simulates the solidification of the same alloy with solute additions of Cd, Fe and Cu.
- Case 3 is the same as case 1, but the data of thermophysical properties (specific heat, thermal conductivity and viscosity) is taken from reference 9
- Case 4 is the same as case 1, but the data of distribution coefficient is taken from reference 10.

Comparing cases 1 and 2 will show the necessity of considering all of the elements present in an alloy when modeling the freezing point. The cases 1 and 3 are similar in some respects and the differences in the predictions of temperature are at about < 1 mK. Comparison of case 1 and 4 show the importance of accurately specifying the phase-diagram parameters.

4. CONCLUSION

A macroscopic model to study the transport of mass, momentum, heat and solute (impurity) during solidification of zinc fixed point has been used to examine the effects of multicomponent. In the results, flow driven by solidification shrinkage was not included. Results of different simulations were compared to assess the sensitivity of the model with respect to the effect of including additional elements in the calculation and with respect to the choice of phase equilibrium parameters and of thermophysical properties. In examining the solidification of a zinc alloy, the global extent of macrosegregation of an element is found to be dependent on its partition coefficient. Then, the model predictions indicated that the model is extremely sensitive to the specification of these thermodynamic parameters.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge the valuable contribution of Mr. George Bonnier (BNM-INM) who suggested this subject. This work has been made possible by the CDTN (Centro de Desenvolvimento e Tecnologia Nuclear) for which the authors are grateful.

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