

Simulation of Aluminum Alloys Homogenization

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One of the objectives of homogenization is to dissolve soluble particles formed after solidification. This enables, together with a solution heat treatment, maximization of the amount of strengthening elements available in solid solution before the ageing of age hardenable alloys. In order to minimize heat treatment times necessary for the dissolution of soluble precipitates, it is advisable to heat treat the alloy at the highest possible temperature; however local melting (incipient melting) must be avoided as it may induce the apparition of pores in the alloy. During the heat treatment of an alloy, the incipient melting temperature depends on the temporal evolution of local compositions within the solidification dendrites / grains. In this paper, we review physical models that can accurately simulate the microsegregations after solidification as well as their resorption during homogenization. The incipient melting temperature can be predicted at any time as well as the differential scanning calorimetry (DSC) signal. Examples of application will be given for a 7xxx alloy.

Keywords: *Incipient melting, homogenizing, differential scanning calorimetry, casting, segregation.*

1. Introduction

When homogenizing an age hardening aluminum alloys, it is generally advisable to dissolve all soluble particles formed during solidification and homogenize associated concentration gradient of solute elements within casting grains. These phenomena are diffusion controlled and thermally activated: the higher the temperature, the faster the dissolution. The dissolution time can therefore be reduced by setting the furnace at the highest temperature compatible with no incipient melting of the alloy. Incipient melting, i.e. local formation of the liquid phase in areas rich in solute elements, should indeed be avoided because it may create hydrogen porosities. The incipient melting temperature of an alloy is not constant and increases with homogenizing advancement: it varies from the solidification end temperature to the solidus of the alloy when the later is completely homogenized.

The differential scanning calorimetric (DSC) method provides (see for example [1]) an efficient and quantitative tool to measure the current incipient melting temperature (temperature corresponding to the beginning of melting) and the homogenization advancement (corresponding to the enthalpy of the first melting peak). It has been used to characterize a 7449 alloy homogenizing kinetics. It is compared, in this paper, with prediction made by physical models briefly reviewed in the next paragraphs.

2. Simulation of the as cast structure

After solidification, it is possible to have a good simulation of concentration gradient within dendrites by using a modified Scheil approach which allows back diffusion in the solid solution during solidification. The basic assumptions of such an approach are: local equilibrium at the solid-liquid interface (i.e. equilibrium phase diagram is applied), infinite diffusion in the liquid phase and finite diffusion within the aluminum solid solution governed by Fick's diffusion law. The latter is simulated using an explicit finite difference scheme, assuming local equilibrium in each volume element,

calculating the solute concentration in solid solution, and using Fick's diffusion equation in the solid solution to compute solute exchange between adjacent volume elements. In our relatively dilute industrial aluminum alloys, the diffusion matrix is assumed to be diagonal. Depending on the cast microstructure, the diffusion geometry of the problem is taken to be cylindrical or spherical. The radius of the cylinder or sphere is an important parameter that determines the distance on which solute elements must diffuse; the larger the radius the slower the homogenizing kinetics. For more details on the ALCAN phase diagram and long range diffusion routines used in this study the reader can refer to [2, 3].

This approach has been used to simulate the casting structure of an aerospace AA7449 alloy (see Table 1) cast in a laboratory using the Aluminum Association TP-1 grain refiner test crucible [4]. A typical segregation pattern of the alloy is presented in Fig.1. In the model, a 50-70 μm (60 μm) diameter cylindrical geometry has been chosen to describe this microstructure; the corresponding solidification rate is 0.55 $^{\circ}\text{C/s}$. In the calculations, care must be taken to mesh the dendritic cylinder with sufficiently small enough radius increments. Starting from the center of the cylinder, we have used the following meshing: 0.305 μm for the first 90 increments and 0.061 μm for the next 50 increments. Using these input parameters, the concentration gradients after solidification have been computed using the above mentioned model; they are presented in Fig. 2. A heat up of 20 $^{\circ}\text{C/mn}$ has then been applied to the as cast microstructure in order to simulate the expected differential calorimetric first melting peak of the as cast structure; this peak corresponds to the melting of the high solute area at the periphery of the dendritic cylinder. As shown in Fig. 3, this predicted first melting peak is in good agreement with the experimental one.

Table 1: Composition range of 7449 according to the Aluminum Association

	Si	Fe	Cu	Mn	Mg	Zn	Ti+Zr
min	0	0	1.4	0	1.8	7.5	0
max	0.12	0.15	2.1	0.2	2.7	8.7	0.25

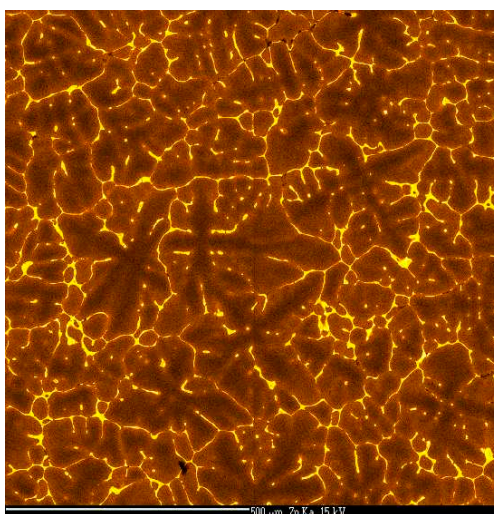


Fig. 1: Microprobe mapping of Zinc concentration within 7449 TP-1 cast sample (length of the scale: 500 μm).

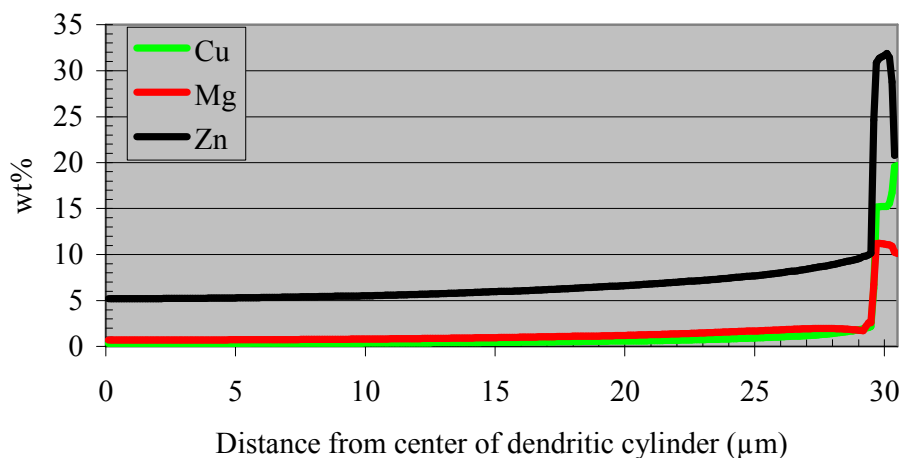


Fig. 2: Predicted concentration gradients after solidification.

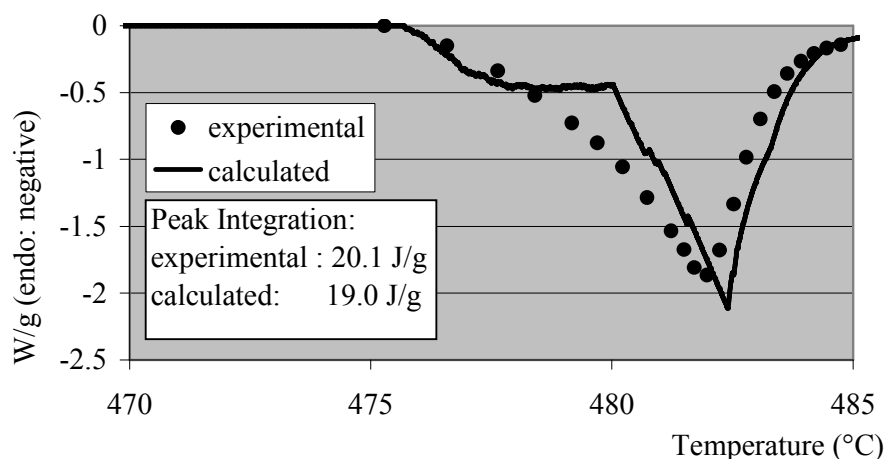


Fig. 3: Simulated and predicted DSC first melting peak of an as cast 7449 alloy. The heating rate in the calorimeter is 20°C/mn.

3. Simulation of the homogenization kinetics

The evolution of composition gradients has been simulated during on homogenization consisting in a linear heating up of 40°C/h up to 472°C followed by a holding of 10h at 472°C. It is simulated using the exact same long range diffusion routine used for solidification and are illustrated in Fig. 4. The corresponding predicted and measured incipient melting temperatures and integrated enthalpies for the DSC first melting peak are compared in Fig. 5. On the overall, a good agreement is achieved indicating that the proposed physical description of the phenomena occurring during solidification and homogenizing is acceptable. From Fig. 4-5, it can be noticed that a significant amount of homogenization occurs during the heat up at 472°C. Very quickly (after 0.5h at 472°C), the only soluble phase left to dissolve is the Al_2CuMg phase (also called S phase); this is in agreement with previous observations in 7xxx alloys [5]. As shown in Fig. 6, the S phase volume fraction decreases rapidly with time during the holding at 472°C. The simulations also allow making a relation between the residual S phase volume fraction and the enthalpy of the first melting peak (see Fig. 7); such a correlation should apply for 7xxx alloys when the S phase is the only soluble phase left in the alloy during homogenizing (no T or M present).

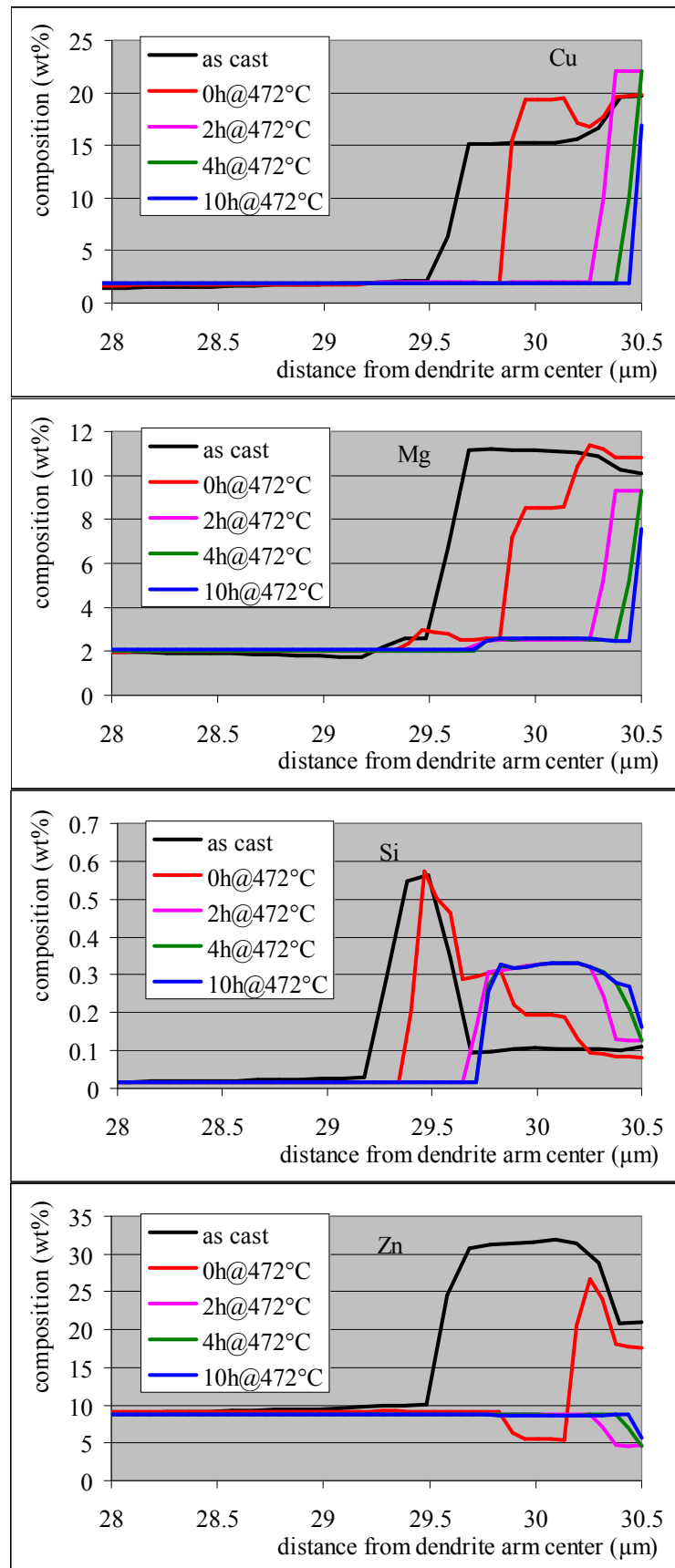


Fig. 4: Simulated composition gradient evolution during homogenization at 472°C.

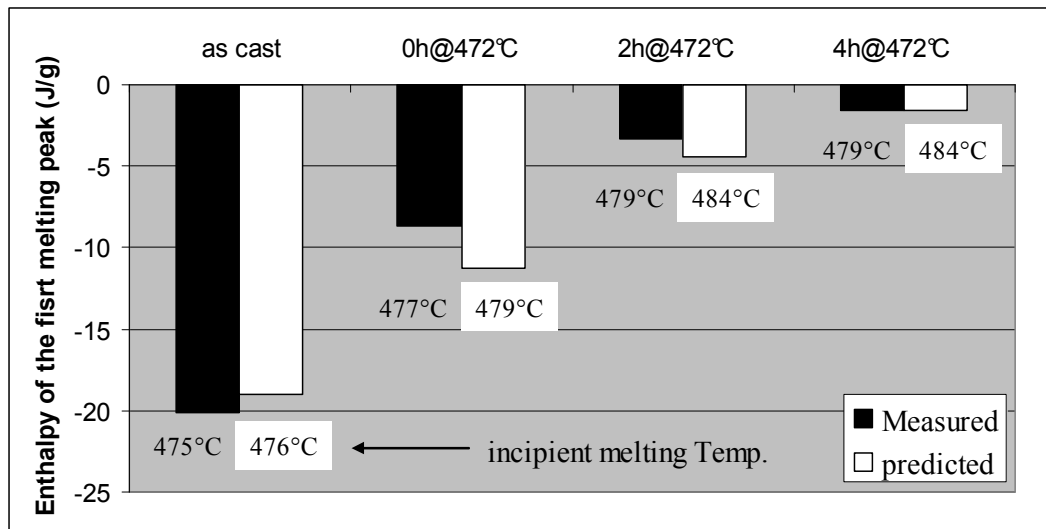


Fig. 5: Simulated and predicted incipient melting temperatures and enthalpies of the first melting peak during a calorimetric heat up at a rate of 20°C/mn.

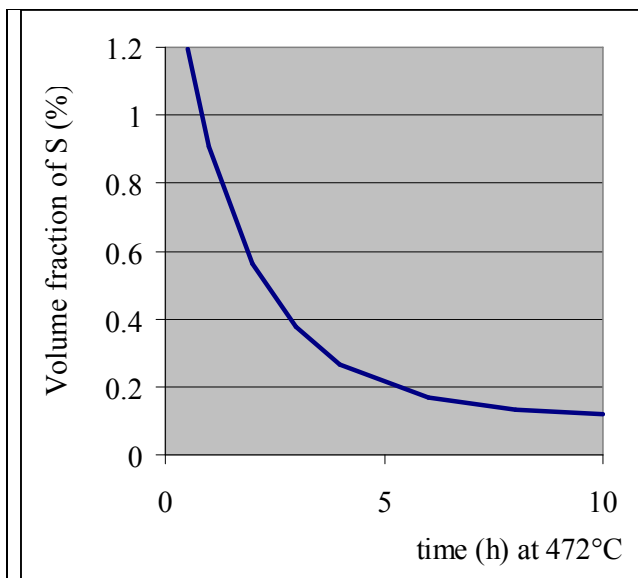


Fig. 6: Predicted evolution of the S phase dissolution kinetics during a homogenizing at 472°C.

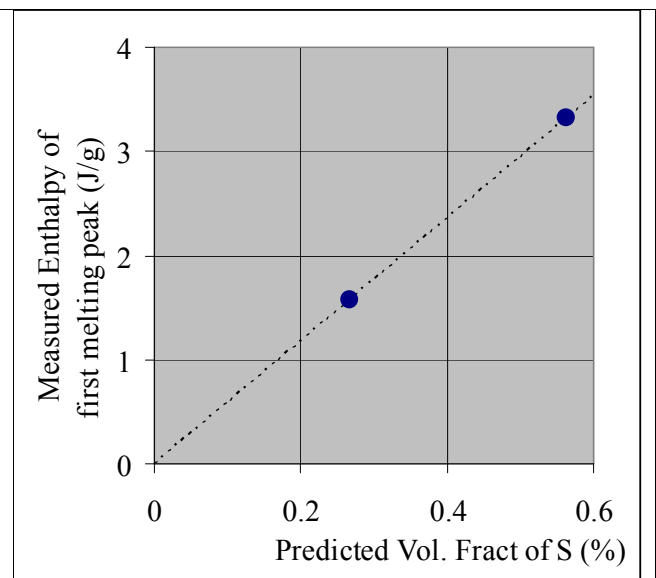


Fig. 7: Relation between the enthalpy of the first incipient melting peak and the volume fraction of coarse S phase remaining in the microstructure during homogenization. This relation has been established for a calorimeter heating rate of 20°C/mn; it can be applied if the S phase is the only soluble phase left.

4. Conclusions and perspectives

It is possible to reproduce the homogenizing kinetics and associated incipient melting temperature of a 7000 aluminum alloy with models based on phase diagrams, segregation during solidification and long range diffusion within the dendrites. The validation of the model has been made with measurement of the temperature and enthalpy of the first melting calorimetry peak on laboratory cast samples that are not or partially homogenized. A good overall agreement has been obtained.

For a multi-component alloy, the homogenizing simulation is not analytical and must be tackled numerically: as illustrated in the previous paragraph, the evolution of the composition gradient within the dendrite during a heat treatment is not simple, due to the interplay between the phase diagram, the resulting concentration in solid solution and the diffusion inside the solid diffusion.

As mentioned, meshing of the dendrite must be refined enough near the dendrite periphery in order to capture the detail of the concentration gradient evolution and the respective impact of the melting peak enthalpy. In order to accelerate the calculation, it is advisable to parallelize the computation of the simultaneous equilibrium calculations that must be performed in each volume cell of the dendrite.

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