

The solidification effects on diffusion experiments –Numerical simulation–

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Abstract

In order to evaluate the solidification effects on diffusion experiments by the long capillary method, numerical simulations using commercial codes were carried out. We calculated sample deformation due to solidification and concentration profiles after solidification with two commercial codes, MARC for a non-linear deformation analysis, and ProCAST for a casting simulation. The calculated results of the sample deformation and of the concentration profile change on solidification were similar qualitatively to the experimental results, but the calculated value of the sample deformation was much smaller than that of the experiments. It was found that the flow due to solidification shrinkage should be considered.

Introduction

As mentioned in Sec.3.(11), the solidification affects on diffusion measurements, and these effects should be examined. The experimental study was carried out in Sec.3.(11). Here, we analyzed the effect using commercial codes, MARC for a non-linear deformation analysis and ProCAST for a casting simulation. First, the change of the temperature profile during a experiment was calculated, and the sample deformation due to the change of the temperature profile (especially on solidification) was computed with these codes. The concentration profile after solidification was calculated from the sample deformation. We compared the two commercial codes to choose a suitable code for this analysis.

Analytical system

A calculation was performed for a diffusion couple of Ag-Ag_{0.95}Au_{0.05}, which was 1 or 2 mm diameter and 20 mm length (10 mm each); the configuration of calculation was taken to be 2-dimensional with axial symmetric, as shown in Figure 1. T1, T2, and T3 were points of the temperature measurement in experiments.

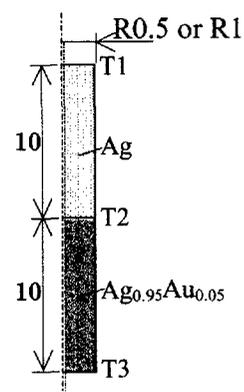


Figure 1
Configuration of calculation

The change of the temperature profile at the boundary was given from the experimental data. The upper and the lower ends were considered to be adiabatic. The elastic modulus was considered to be temperature dependent. For example, it was 100 GPa under the solidus temperature and 10 Pa over the solidus temperature in MARC. Poisson's ratio was determined as 0.3. The effect of the solidification shrinkage was considered by the thermal expansion coefficient, which was calculated from the density change with the variation of temperature. The deformation analysis of a sample was carried out with some constraint conditions at the bottom and at the surface of the sample.

Comparison between MARC and ProCAST

Table 1 shows features of MARC and ProCAST. MARC is a non-linear deformation code. It has a good deformation analysis part, but it is separated from thermal analysis part. It also doesn't have flow analysis. ProCAST is a casting simulation code. It can perform thermal and flow analysis coupled with deformation analysis at once. But the performance of the deformation analysis was found to have some problems, for example, the digital output can't be obtained for the calculated deformation, the concentration profile due to the deformation can't be calculated, and so on.

Table 1 Comparison between MARC and ProCAST

	MARC	ProCAST
Main use	Non-linear deformation analysis	Flow and solidification analysis for casting
Analytical method	Finite element method	Finite element method
Analysis	Thermal and deformation analysis are not coupled each other.	Thermal, flow and deformation analysis are coupled.
Deformation analysis	Satisfied	Having some problems
Flow analysis	Impossible	Possible

Analysis with MARC

It was confirmed that the displacement at the top was changed due to the constraint condition. The largest displacement was obtained under the condition, in which the bottom was restricted with axial direction and the surface was restricted with radial and axial direction after solidification. The displacement calculated for 2 mm diameter sample was larger than that for 1 mm diameter sample, as shown in Figure 2. However, the displacement at the middle was much smaller than that at the top, and even though in the largest displacement case, the displacement was much smaller than that in the experiments (0.5 – 1 mm at the center).

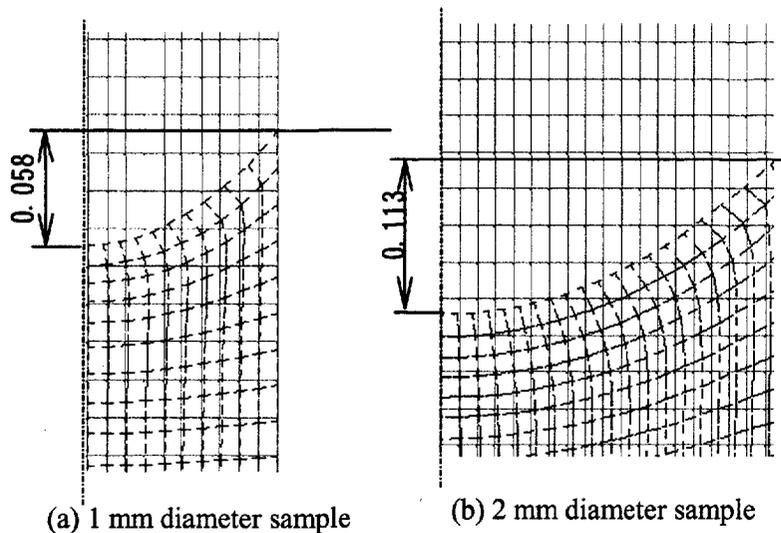


Figure 2 Displacement due to solidification at the top (unit in mm)

Analysis with ProCAST

The flow analysis was coupled with the thermal and deformation analysis. The downward flow on solidification shrinkage was observed at the center, but it couldn't be included into the displacement and into the change of the concentration profile. Therefore, the calculated displacement was much smaller than the experimental results.

Conclusions

The calculated displacement by deformation due to volume change on solidification was much smaller than the experimental results. It was found that the flow in the central portion generated due to solidification shrinkage has to be considered to explain the experimental results, as shown in Figure 3. It was confirmed that the deformation after solidification was negligibly small.

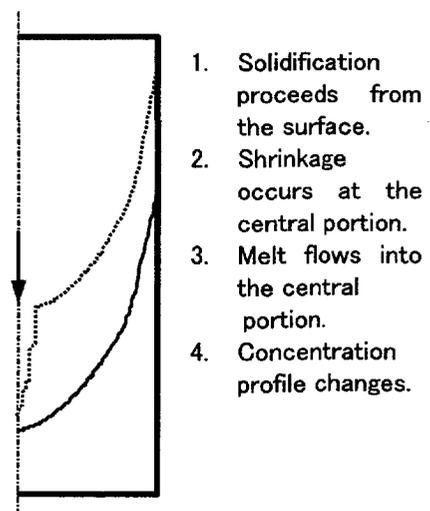


Figure 3 Mechanism of concentration change due to solidification