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The Study of Micro-segregation in Al-Cu Alloys Using Thermal Analysis and Numerical Modeling

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1- Introduction

One of the most important phenomena occurring during solidification is microsegregation which is the non-uniform distribution of alloying elements in the scale of dendrite arm spacing or grain size. There are numerous theoretical models which can be used to predict the microsegregation level and solidification path with different degrees of sophistication. Recently Fredriksson and his colleagues proposed a new model for solidification that considers the effect of excess vacancies formed during solidification. According to their model as the solidification rate changes, the excess vacancy content changes and several solidification characteristics such as melting temperature and latent heat of solidification change.

The aim of the current research is to consider the effect of excess vacancies on the microsegregation in Al-Cu alloys at low cooling rates. For this purpose, the thermodynamic (phase diagram) and kinetic (diffusion coefficient) data were modified to include the effect of excess vacancies. The kinetic (diffusion coefficient) data is modified for the first time in the present paper.

2- Experimental

Al-Cu binary alloys containing 2.2, 3.7, and 4.8 wt.% copper were used as the experimental alloys. Solidification tests were performed using a DTA furnace with the possibility of quenching samples during solidification. Samples were heated to 700°C, kept at this temperature for 10min and then cooled at 0.008 and 0.083 K/s. Samples were quenched from a predetermined temperature during solidification. The microstructure of the samples was evaluated by conventional metallography methods. The concentration profile in the primary phase was measured using SEM/EDS technique according to the method developed by Gungor.

equilibrium content of vacancies in the solid.

In order to model the microsegregation, Fick's second law was solved separately in the solid and liquid according to the numerical scheme presented by Tanzilli and Heckel. The diffusion coefficient was modified according to Eq. 1 to consider the effect of excess vacancies in the numerical modeling.

$$D_S^{NEq} = V^* D_S^{Eq} \qquad (1)$$

Where D_S^{NEq} and D_S^{Eq} are non-equilibrium and equilibrium diffusion coefficients in the solid, respectively.

3- Results and Discussions

According to the thermal analysis results the solidification sequence for all samples consisted of nucleation and growth of primary α_{Al}. This phase continues to grow until the solidification process is finished with the eutectic reaction.

According to the thermal analysis results, by increasing the cooling rates, the undercooling (for both primary and eutectic solidification) increases which can be estimated by a semi-empirical function as shown in Eq. 2.

$$\Delta T = k_U \left(\frac{dT}{dt}\right)^{n_U} \qquad (2)$$

where k_U and n_U are free variables which can be determined based on experimental conditions. In the present study k_U and n_U were calculated for primary undercooling as k_{UP}=4.48 and n_{UP}=0.14 and for the eutectic undercooling k_{UE}= 6.62 and n_{UE}=0.09 by least square method. Eq. (2) was used to construct a semi-empirical phase diagram which is used to compare with the CALPHAD results. Kinetic phase diagram was calculated based on the Fjellstedt and Fredriksson CALPHAD model and presented in Fig. 1.

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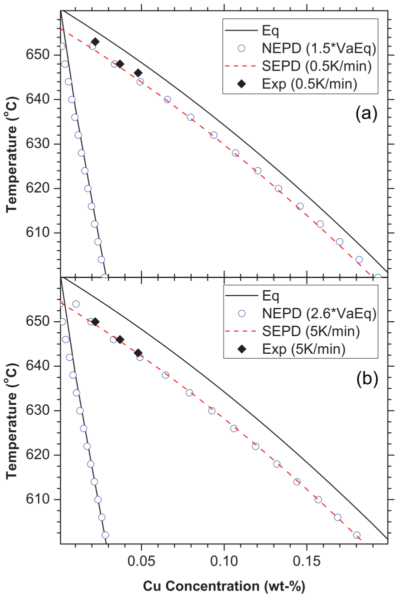

Fig. 1 Equilibrium (Eq) and non-equilibrium (NEPD) phase diagrams calculated by CALPHAD method compared to the semi-empirical phase diagram (SEPD) and experimental results for (a) 0.008; (b) 0.083 K/s

The calculated concentration profiles in the primary phase for the alloy containing 4.8 wt.% copper are presented in Fig. 2 and are compared to the experimental profiles and the Scheil equation curve. According to this figure it is obvious that the modification of the phase diagram alone (NEPD curves) improves the consistency between the experimental and modeling results but not to a satisfactory level. However, modification of diffusion coefficient (NEPD-DyDi) caused better correlation between the experimental and modeling results specially at 0.083 K/s cooling rate. Furthermore, the best consistency between the experimental and modeling results is obtained when the vacancy sink is considered (NEPD-DyDiXt).

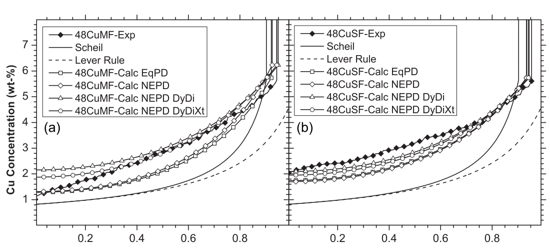

Fig. 2 Calculated concentration profiles for the alloy containing 4.8 wt.% copper compared with experimental profile and Scheil equation curve

4- Conclusions

Microsegregation in the Al-Cu binary alloys containing 2.2, 3.7, and 4.8 wt.% copper was investigated using thermal analysis and theoretical modeling. Experimental solidification tests were performed using a DTA furnace with the possibility of quenching samples during solidification at slow cooling rates of 0.008 and 0.083 K/s. The solidification was modeled with three different input data including equilibrium thermodynamic and kinetic data called EqPD, non-equilibrium thermodynamic and equilibrium kinetic data called NEPD (developed by Fjlldestdt and Fredriksson), and non-equilibrium thermodynamic and kinetic data called NEPD-DyDiXt (developed in the present study). The results were compared with the experiments and it was shown that the developed NEPD-DyDiXt model shows the best consistency with the experimental results.

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