MODELLING OF PHASE EQUILIBRIA IN AlCu5Mg1 ALLOYS

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### Introduction

- Casting of Al-alloys is one of the most important features of Al technology and the increasing use of process modelling software to design and optimise castings makes it important that the thermo-physical and physical properties of Al alloys are well characterised, as they are critical input for almost all types of process models.

Obtaining these properties at low temperatures can be a time-consuming and expensive procedure if all relevant properties are considered. Experimental measurement becomes more problematical at high temperature, especially if the liquid phase is involved. To this end it is highly desirable to calculate thermo-physical and physical properties over the whole solidification range for as wide a range of alloys as possible.

Tools that utilize thermodynamic modeling to explore the equilibrium and phase relationships in complex materials are being used increasingly in industrial practice. It has been the extensive validation of calculated results against experiment. This means that properties can now be calculated for many alloys where no experimental information exists. The calculations utilise well-established material models and consider the effect of microstructure.

- It seen that the properties during solidification are intrinsically controlled not only by the properties of the liquid and solid phases themselves, but also by the fraction solid vs. temperature behaviour. Sharp deviations from smoothly changing behaviour are the result of discontinuities in the rate of solid transformed, which is amply demonstrated for a Al-alloy, where sharp changes in fraction solid vs. temperature (Fig. 2) cause sharp changes in the enthalpy vs. temperature plot (Fig. 3).

Verification of this predictions against multi-component alloys of many types has shown that they provide results that are very close to experimental observation.

The present paper provides examples of calculations for stable phase formation in the solid state. A feature of the JMatPro is that great store has been placed on using models that, as far as possible, are based on sound physical principles rather than purely statistical methods. Previous work has shown that excellent results can be obtained for the phases formed during solidification, as well as their composition and temperature range of formation. Such modelling can be further extended to calculate thermo-physical and physical properties over the complete relevant temperature range for a wide range of alloys. A key factor in the success of the approach has been the extensive validation of calculated results against experiment. This means that properties can now be calculated for many alloys where no experimental information exists. The calculations utilise well-established material models and consider the effect of microstructure.

### Results

The investigated materials were aluminium-copper-magnesium alloys with the chemical composition shown in Table 1.

<table>
<thead>
<tr>
<th>TYPE OF SAMPLE</th>
<th>% Si</th>
<th>%Cu</th>
<th>%Mg</th>
<th>%Zn</th>
<th>%Mn</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlCu5Mg1</td>
<td>0.002</td>
<td>0.14</td>
<td>0.08</td>
<td>5.153</td>
<td>0.002</td>
</tr>
<tr>
<td>Mg5wt.% alloy</td>
<td>0.164</td>
<td>0.001</td>
<td>0.001</td>
<td>0.009</td>
<td></td>
</tr>
</tbody>
</table>

Results from a computer programme JMatPro for calculating materials properties have been presented. Figures 1-7 have been calculated using JMatPro.

### Conclusion

The present paper provides examples of calculations for stable phase formation in the solid state. A feature of the JMatPro is that great store has been placed on using models that, as far as possible, are based on sound physical principles rather than purely statistical methods. Previous work has shown that excellent results can be obtained for the phases formed during solidification, as well as their composition and temperature range of formation. Such modelling can be further extended to calculate thermo-physical and physical properties over the complete relevant temperature range for a wide range of alloys. A key factor in the success of the approach has been the extensive validation of calculated results against experiment. This means that properties can now be calculated for many alloys where no experimental information exists. The calculations utilise well-established material models and consider the effect of microstructure.

Tools that utilize thermodynamic modeling to explore the equilibrium and phase relationships in complex materials are being used increasingly in industrial practice. Thermodynamic modeling helps toward the understand-ing of changes in phase constitution of a material as a function of composition or temperature. This methodology immediately provides results for enthalpy and specific heat (Cp) during the solidification process as well as the fraction solid transformed and amounts and compositions of each individual phase formed during solidification.

It seen that the properties during solidification are intrinsically controlled not only by the properties of the liquid and solid phases themselves, but also by the fraction solid vs. temperature behaviour. Sharp deviations from smoothly changing behaviour are the result of discontinuities in the rate of solid transformed, which is amply demonstrated for a Al-alloy, where sharp changes in fraction solid vs. temperature (Fig. 2) cause sharp changes in the enthalpy vs. temperature plot (Fig. 3).

Verification of this predictions against multi-component alloys of many types has shown that they provide results that are very close to experimental observation.

### REFERENCES