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# MODELLING OF PHASE EQUILIBRIA IN AlCu5Mg1 ALLOYS

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**Summary:** Al-based alloys were one of the first material types to which thermodynamic phase diagram calculations were applied. Since then improvements in modelling and the increase in computing power has enabled very accurate predictions to be made for phase equilibria in real multicomponent alloys.
**Keywords:** ternary phase diagram, JMatPro, aluminium-copper-magnesium alloys.

## 1. INTRODUCTION

Aluminium alloys are used in automotive, aerospace, construction, and shipbuilding industry because of their combination of high strength, low density, durability, machinability, availability and the cost is also very attractive compared to competing materials [1]. AlCuMg alloys developed in the early years in the aeronautical field, they have been then considered for a wide range of different applications, even though, due to their high specific strength, they are mainly considered as a substitute of iron-based materials for structural parts in the transportation industry [2]. Several compositions are presently standardized and new alloys based on that metallic system are now being considered and developed.

For many years the prime sources of information regarding phase equilibria in Al-alloys have been the compendia of Mondolfo [1] and Philips [3]. These books provide extensive information concerning the behavior of binary and ternary systems and, to a certain degree, higher order systems. Such work enables a reasonable understanding of many known alloys. However, while providing broad information on particular alloy systems, equilibrium phase diagrams fall short in providing detailed information on how multi-component alloys behave, particularly for the case of new alloys and in understanding what may happen as compositions vary within the composition specification of known alloys. 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 optimize castings makes it important that the thermo-physical and physical properties of Al alloys are well characterized, 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 [4–7].

## 2. EXPERIMENTAL

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

*Table 1. Chemical composition of the investigated alloy (in mass%).*

| TYPE OF SAMPLE | % Ti | %Fe | %Si | %Cu | %Zn | %Mg | %V | %Cr | %Mn |
|---|---|---|---|---|---|---|---|---|---|
| AlCu5Mg1 | 0.002 | 0.14 | 0.08 | 5.353 | 0.067 | 1.064 | 0.001 | 0.001 | 0.009 |

DSC analyses have been performed in a differential scanning calorimeter type Shimadzu DSC-50 under protective argon atmosphere, at a scanning rate of 10ºC/min, to the maximum temperature of 725ºC. This method has produced DSC - curve on which basis the transition enthalpy (the activation energies of the transformations responsible for the thermal effects) was calculated.

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From the testing results it can be seen that addition of the copper and magnesium induces a modification of the microstructure. If a result is a better dispersion of insoluble components, porosity and nonmetal inclusions, it will improve mechanical properties [8]. The effect of the magnesium and titanium content on the microstructure was monitored quantitatively, using an automatic device for image analysis, QUANTIMET 500MC, and linear measuring method. Using automatic image analysis, we were able to measure volume fractions of the α-solid solution and the eutectic.

In these alloys aluminium is the primary constituent and in the cast alloys the basic structure consists of cored dendrites of aluminium solid solution, with a variety of constituents at the grain boundaries or interdendritic spaces forming a brittle, more or less continuous network of eutectics. Copper has been the most common alloying element almost since the beginning of the aluminium industry, and a variety of alloys in which copper is the major addition, were developed. Magnesium is usually combined with copper [9].

## 3. RESULTS AND DISCUSSION

Recently the application of so-called 'Scheil-Gulliver' modelling via a thermodynamic modelling route has led to the ability to predict a number of critical thermo-physical properties for a variety of alloy types during solidification. The limit to the SG simulation is that some back diffusion will take place. However, if the degree is small, good results will still be obtained and comparison of experimentally determined solidification behavior and SG calculations for Al-alloys match very well [4]. Thermodynamic modeling helps toward the understanding of changes in phase constitution of a material as a function of composition or temperature.

Computer program called JMatPro was developed to augment the thermodynamic calculation by incorporating various theoretical materials models and properties databases that allow a quantitative calculation for the requisite materials property to be made within a larger software structure. Results from a computer program JMatPro for calculating materials properties have been presented. Figures 1–7 have been calculated using JMatPro.

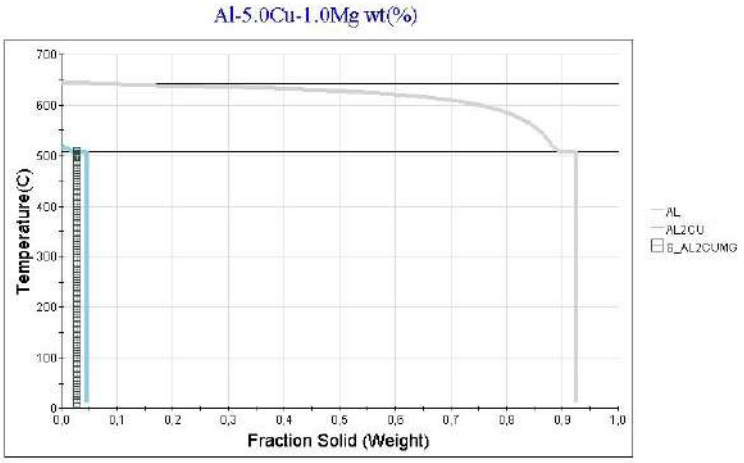


*Figure 1. Fraction solid vs. temperature curve calculated for an Al-Cu5wt.%-Mg5wt.% alloy*

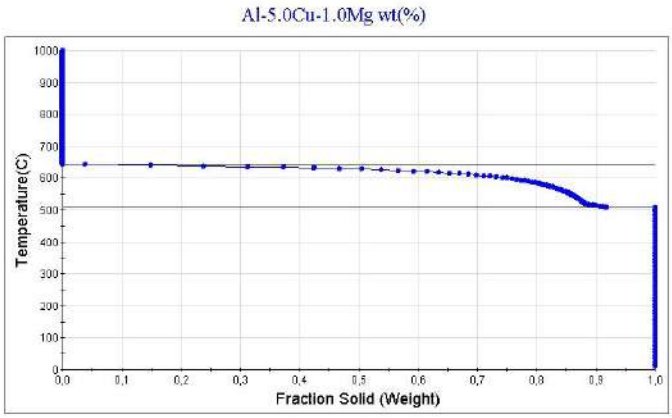


*Figure 2. Fraction α solid vs. temperature curve calculated for an Al-Cu5wt.%-Mg5wt.% alloy*

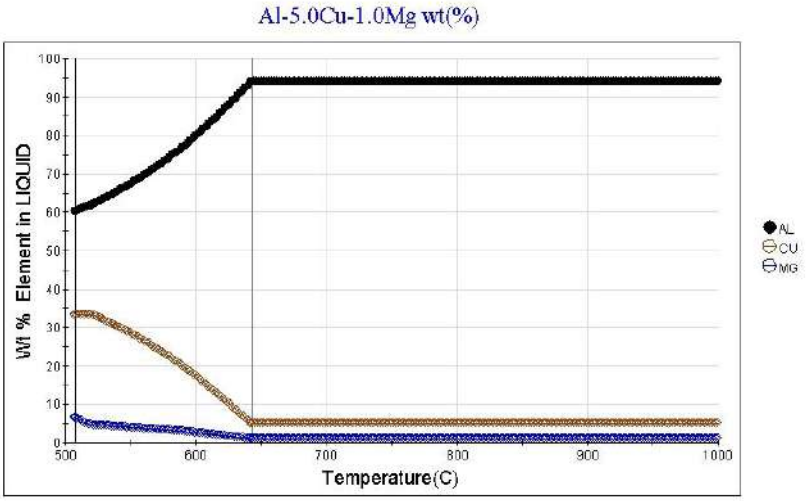


*Figure 3. Composition profiles of Cu and Mg in liquid for an Al-Cu5wt.%-Mg5wt.% alloy*

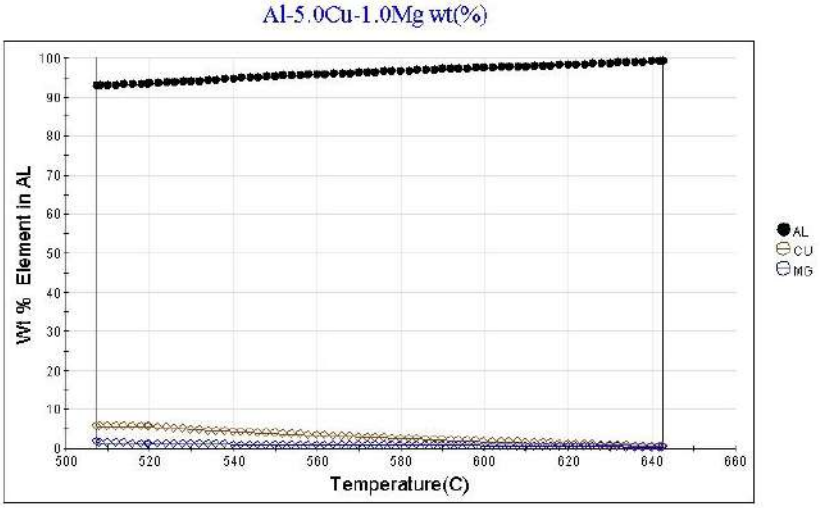


*Figure 4. Composition profiles of Cu and Mg in primary Al for an Al-Cu5wt.%-Mg5wt.% alloy*

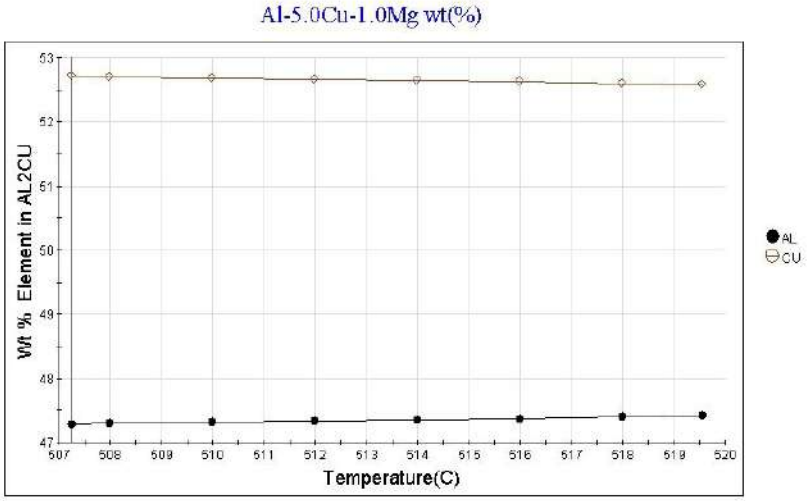


*Figure 5. Composition profiles of Cu and Al in $CuAl_2$ for an Al-Cu5wt.%-Mg1wt.% alloy*

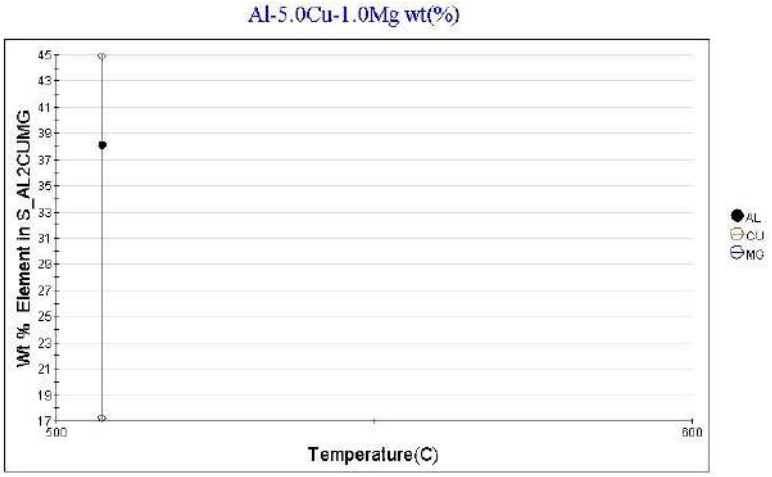


*Figure 6. Composition profiles of Cu, Mg and Al in $CuMgAl_2$ for an Al-Cu15wt.%-Mg1wt.% alloy*

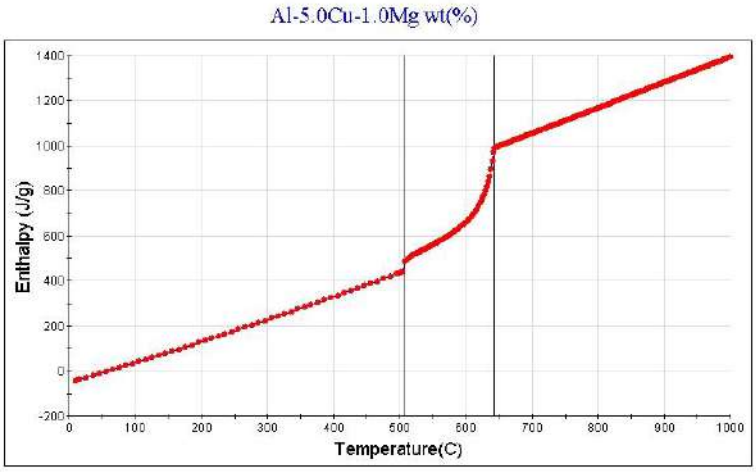


*Figure 7. Calculated enthalpy vs. temperature for an Al-Cu15wt.%-Mg1wt.% alloy during solidification*

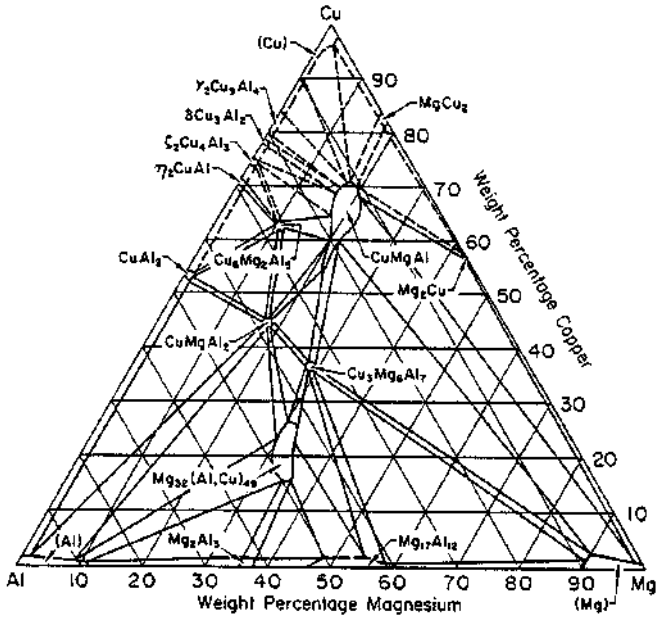


*Figure 8. Isothermal section at 430°C for the Al-Cu-Mg system. (Adapted from Metals Handbook, 8th Ed., Vol 8, American Society for Metals, Metals Park, Ohio, 1973)*

In the binary aluminium-copper system, the aluminium-rich part solid solution is in equilibrium with the intermetallic compound θ, with the approximate composition of $CuAl_2$. The addition of magnesium allows the formation of other intermetallic compounds, such as $CuMgAl_2$, $CuMg_4Al_6$, CuMgAl and $Cu_6Mg_2Al_5$, as shown in the isothermal section at 430°C of the ternary system Al-Cu-Mg in Figure 8. The liquidus, solidus and solvus isotherms are shown in Figure 9**.** To explain this, we will consider an alloy containing 5% Cu and 1% Mg. This composition is located at the circle in each of the isothermal projections. To visualize the relation of this composition and the isotherms in Figure 9. the relation of the liquidus, solidus and solvus projections to the three-dimensional ternary phase diagram is shown. It is seen that, for this composition, the alloy is liquid above 650°C (point a); in a two-phase liquid-solid region between 570°C (point b) and 650°C; it is a single-phase α region between 570°C and 500°C (point c); and it is in the three-phase region below 500°C where the α–solid solution is in equilibrium with the compounds $Al_2Cu$ and $Al_2CuMg$.

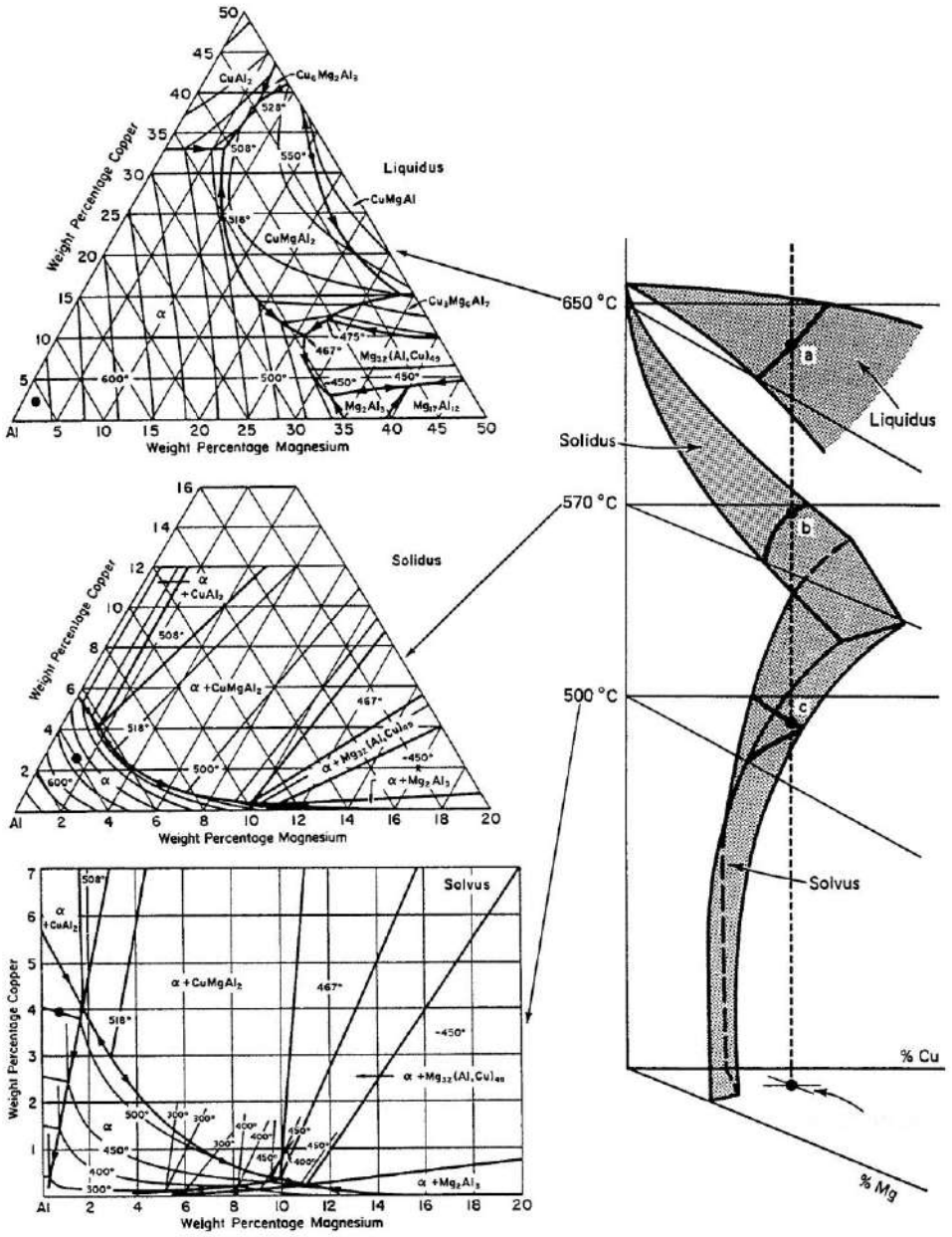


*Figure 9. The relation between the projection of the liquidus, solidus and solvus isotherms and the three-dimensional phase diagram. The temperatures noted are for an AlCuMg alloy containing 1% Mg*

Where phases exist over a wide range of stoichiometries, which is the usual case for metallic materials, other mathematical models are used which account for the effect of composition changes on Gibbs energy. Any appearance of secondary phases can be easily taken into account in this approach with the assumption that no back diffusion occurs in them. Therefore, all transformations can be accounted for, including the final eutectic solidification. For many cases, equilibrium calculations provide valuable information for processing, liquidus and solidus temperatures, solubility curves etc.Mathematical model calculates composition profiles of Cu and Mg in primary phase and in liquid and takes into account diffusion in solid phase due to the compositional gradients. A comparison between experimentally observed values 92.3wt.% of the weight fractions of the α-solid solution and those calculated using the present model 92.53wt.%, is very good. The average difference between predicted values and those observed experimentally is of the order of 0.25%.

Table 2 shows the agreement between calculated and experimentally determined critical temperatures by DSC.

*Table 2. Comparison between experimentally determined DSC results and calculated using JMatPro for Al-Cu5wt.%-Mg1wt.% alloy (temperatures all in ºC)*

| type of sample Al-Cu5-Mg1 | Liquidus | α h.s.start | $CuAl_2$ | α h.s.+$CuAl_2$+ $CuMgAl_2$ | Solidification end |
|---|---|---|---|---|---|
| Eksperiment | - | 647.8 | 524.5 | 508.3 | 508.3 |
| JMatPro-calculated | 642.6 | 642 | 518 | 507.25 | 507.25 |

## 4. 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 utilize 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 understanding 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 ($C_p$) during the solidification process as well as the fraction solid transformed and amounts and compositions of each individual phase formed during solidification.

It was 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 behavior. Sharp deviations from smoothly changing behavior 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.

## 5. REFERENCES

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МОДЕЛОВАЊЕ ФАЗНЕ РАВНОТЕЖЕ AlCu5Mg1 ЛЕГУРА

**Сажетак:** Легуре алуминијума представљају један од првих материјала на којем је примијењен модел за прорачун фазног дијаграма. Захваљујући напретку у моделовању, данас је могуће поуздано и брзо прорачунати равнотежне фазне дијаграме за вишекомпонентне легуре. Помоћу компјутерског програма JMatPro урадили смо прорачун физичких и механичких својстава za Al-Cu5-Mg1 легуру.

**Кључне ријечи:** тројни фазни дијаграм, алуминијум-бакар-магнезијум легуре.

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