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Journal of Alloys and Compounds 433 (2007) 108–113

Journal of ALLOYS AND COMPOUNDS

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Predictive calculation of phase formation in Al-rich Al–Zn–Mg–Cu–Sc–Zr alloys using a thermodynamic Mg-alloy database

J. Gröbner [a], L.L. Rokhlin [b], T.V. Dobatkina [b], R. Schmid-Fetzer [a,*]

[a] *Institute of Metallurgy, Clausthal University of Technology, Robert-Koch Strasse 42, D-38678 Clausthal-Zellerfeld, Germany*
[b] *Baikov Institute of Metallurgy and Materials Science, Leninsky prosp. 49, 119991 GSP-1, Moscow, Russia*

Received 19 April 2006; received in revised form 6 June 2006; accepted 7 June 2006
Available online 14 July 2006

Abstract

Three series of Al-rich alloys in the system Al–Zn–Mg–Cu–Sc–Zr and the subsystems Al–Zn–Mg–Cu–Sc and Al–Zn–Mg–Sc were studied by thermodynamic calculations. Phase formation was compared with experimental data obtained by DTA and microstructural analysis. Calculated phase diagrams, phase amount charts and enthalpy charts together with non-equilibrium calculations under Scheil conditions reveal significant details of the complex phase formation. This enables consistent and correct interpretation of thermal analysis data. Especially the interpretation of liquidus temperature and primary phase is prone to be wrong without using this tool of computational thermodynamics. All data are predictions from a thermodynamic database developed for Mg-alloys and not a specialized Al-alloy database. That provides support for a reasonable application of this database for advanced Mg-alloys beyond the conventional composition ranges.

Keywords: Aluminium alloys; Al–Zn–Mg–Cu–Zr–Sc system; Phase diagrams; Thermodynamic modeling

1. Introduction

A correct interpretation of the phases in the solidification microstructures can be a challenging task for multi-component commercial Al-alloys. A most important tool is provided by making use of the pertinent phase diagrams. A thermodynamic calculation of these diagrams is the only feasible approach for truly multi-component alloys. This approach is based on the Calphad method [1,2]. In this work it will be shown that a thermodynamic database originally developed for Mg-alloys gives correct results for selected multi-component Al-alloys. This is a consequence of the fact that all phase diagrams are implemented in composition ranges from 0 to 100%. The ongoing development of this thermodynamic database for Mg-alloys was described in detail previously [3] and specific problems of database quality assurance were recently given [4].

The base of the present thermodynamic calculation is formed by four ternary systems implemented from the literature: Al–Mg–Zn [5], Al–Cu–Mg [6], Al–Cu–Zn [7] and Cu–Mg–Zn [8]. These ternary subsystems build the edges of a quaternary system Al–Cu–Mg–Zn, which corresponds to more than 99 wt.% of the pertinent alloy compositions. For the additional microalloying elements Sc and Zr (each 0.3 wt.%) no thermodynamic description of the entire multi-component phase diagrams is needed. The entire ternary system Al–Mg–Sc was described by an optimization published by our group some years ago [9]. The binary systems Mg–Zr [10] and Cu–Zr [11] were taken from the literature. The missing binary systems Cu–Sc, Sc–Zn, Sc–Zr and Zn–Zr were estimated without interaction parameters. No parameter fitting to experimental data of the pertinent multi-component Al-alloys was used. The calculations are all predictions from the Al–Mg–Cu–Sc–Zn–Zr subset of the Mg-database. All calculations were performed using the software "Pandat" [12].[1]

Some results of the experimental investigations of commercial Al-alloys containing Cu, Mg, Zn, Sc and Zr and the experimental methods were published in more detail by Rokhlin et al. [13]. The alloys for this investigation were prepared by melting

* Corresponding author. Tel.: +49 5323 72 2150; fax: +49 5323 72 3120.
E-mail address: schmid-fetzer@tu-clausthal.de (R. Schmid-Fetzer).

[1] PANDAT, Software for Multicomponent Phase Diagram Calculation, Computherm LLC, 437 S. Yellowstone Drive, Suite 217, Madison, WI 53719, USA.

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doi:10.1016/j.jallcom.2006.06.032

of the high purity metals in appropriate proportions in an electrical resistance furnace in Al_2O_3 crucibles. Characterization of the alloys was done using differential thermal analysis, light microscopy, X-ray diffraction phase analysis and X-ray spectral analysis. Differential thermal analysis (DTA) of the alloys was performed by heating and cooling at a rate of 3 K/min. The temperature was registered using a chromel/alumel thermocouple. In construction of the presented phase diagram sections the thermal signals were selected either from the cooling curves or heating curves, depending what was assumed to be more reliable. The chemical contents of Zn, Cu, Zr and Sc were analyzed after DTA analysis. The deviation from the charge was not more than 5% relative error. The microstructures of alloys shown below were prepared after slow DTA cooling of samples.

The purpose of this work is to provide a correct interpretation of the phases formed in the solidification microstructures considering the calculated phase diagrams and some more thermodynamically calculated properties. Additionally, it is demonstrated that, due to its design, the Mg-alloy database gives correct results for selected multi-component Al-alloys.

2. Phase formation predicted from thermodynamic calculations compared with experimental data

2.1. The quaternary alloy system Al–Zn–Mg–Sc

Alloys in the Al–Zn–Mg–Sc system with constant 5 wt.% Mg and 0.5 wt.% Sc were prepared. The results of thermal analysis are compared with the calculated vertical phase diagram section in Fig. 1. The experimentally observed secondary crystallization of (Al) and solidus line is well predicted by calculation. The primary crystallization of Al_3Sc forms only miniscule amounts, as demonstrated in the calculated phase amount chart of the alloy Al–15Zn–5Mg–0.5Sc in Fig. 2. These small amounts are not detectable by DTA, because the heat effect during solidification is negligibly small. Thus, the "primary" DTA signal actually

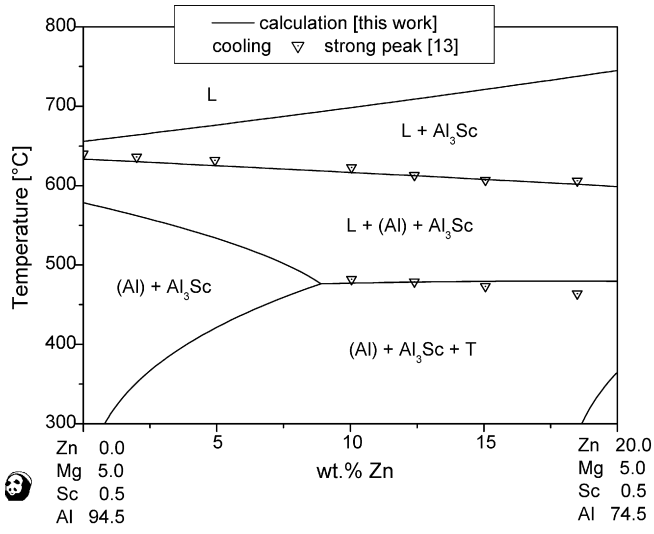

Fig. 1. Calculated vertical section of the Al–Zn–Mg–Sc phase diagram for constant 5 wt.% Mg and 0.5 wt.% Sc including thermal signals from [13].

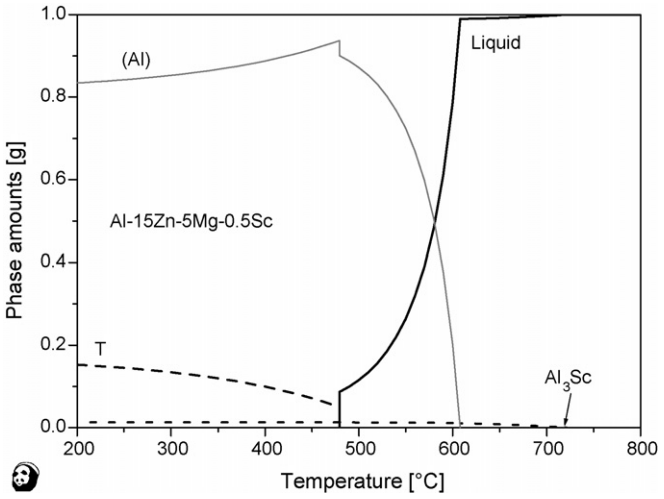

Fig. 2. Calculated equilibrium phase amounts of alloy Al–15Zn–5Mg–0.5Sc (wt.%) show the extremely small amount of primary Al_3Sc phase, not detectable in thermal analysis.

corresponds to the secondary precipitation. However, the small amounts of primary Al_3Sc phase may be important for grain refining of the alloy, rendering the combined information of the phase diagram and the phase amount chart in Figs. 1 and 2 most significant.

2.2. The quinary alloy system Al–Zn–Mg–Cu–Sc

With addition of Cu commercially important five-component alloys Al–Zn–Mg–Cu–Sc can be prepared. The results of thermal analysis are compared with the calculated vertical section of alloys with constant 8 wt.% Zn, 2 wt.% Cu and 0.3 wt.% Sc in Fig. 3. Similar to Fig. 1, the calculation reproduces the experimentally observed secondary crystallization of (Al) and the solidus line well. The primary crystallization of Al_3Sc is

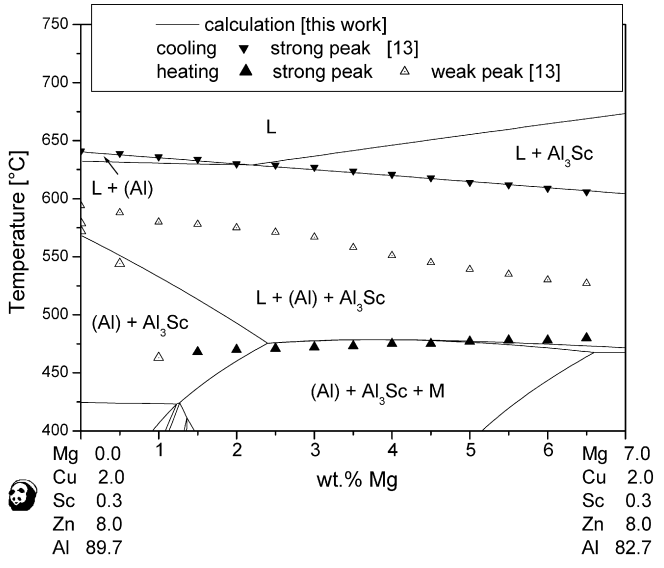

Fig. 3. Calculated vertical section of the Al–Zn–Mg–Cu–Sc phase diagram for constant 8 wt.% Zn, 2 wt.% Cu and 0.3 wt.% Sc including thermal signals from [13].