Database Description:

Thermodynamic Database for Aluminium Alloys for Additive Manufacturing: IAL

The IAL database covers the alloying elements: Al, Ar, B, Bi, C, Ce, Cr, Cu, Fe, Hf, Li, Mg, Mn, Mo, N, O, Nb, Nd, Ni, P Pb, Sc, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr.

It is based on the COST 507 database for light alloys, that was developed in the framework of the EU project COST 507 (see the description below). The purpose of IAL is to provide phase equilibria for Al-powder alloys for additive manufacturing, and for heat treatments of additively manufactured Al-parts. Additions to the COST 507 database have been made as described below.

Several alloys for additive manufacturing have additions of Sc and/or Zr to form strengthening precipitates. The alloying element Sc and the Al-Sc binary system were therefore added using the description of Cacciamani et al. [1]. Data for the ternary Al-Sc-Zr system from the work of Bo et al. [2] were included. The descriptions of these systems are only accurate for the Al-rich side and should not be used outside this range.

Additive manufacturing by laser powder bed fusion (LPBF) requires adaptation of powder alloy compositions since rapid solidification creates novel microstructures. For Al-alloys hot-cracking is often an issue. Calculations can aid in finding new types of alloy compositions. The IAL database can be used to find alloys with narrow melting ranges; and with alloying elements that permit precipitation hardening. Such an approach resulted in a new type of Al-alloy for additive manufacturing by laser powder bed fusion [3,4]. New information from these alloys on the phase equilibria was implemented in the database [5].

The calculated phase fractions in an Al-0.8%Cr-5%Mn-0.6%Zr alloy (wt%) are shown in Fig.1. below. When this material is printed by LPBF rapid solidification creates a supersaturated liquid, and the Al3Zr and Al6Mn phases are suppressed. This supersaturation is taken into account in Fig.2 where the solidification according to a Scheil calculation is plotted. Fig.2. shows that the alloy has a very narrow melting interval and can be expected to be printable without hot cracks. Small additions of Fe and Si, that are inevitable in commercial material, will cause a dip in the Scheil curve at the end of solidification which implies a larger melting interval. Experiments showed that the alloy can be printed crack-free [3-5].

Alloys based on the Al-Mg-Si system are commonly used for additive manufacturing since they are printed crack-free. It is well known that it is the metastable β'' precipitate (Mg_5Si_6) rather than the stable Mg_2Si precipitate that contributes to peak hardening of these alloys. To be able to apply the IAL database to precipitation calculations the two metastable β'' (Mg_5Si_6) and β' (Mg_9Si_5) phases were added to the database following the work of [6]. In a heat treatment simulation, the time when β'' is replaced by β' is an indication of the peak hardening time for the applied temperature, see the example calculation below. This calculation was performed using the PRISMA software and was compared with results of experiments and calculations of Du et al. [7]. Fig.3 shows how the volume fraction of the metastable phases evolves on heat treatment at 250°C, and Fig.4 shows the number density. The calculation suggests a short heat treatment (approximately 10 minutes) to obtain a high fraction of β''. The high number density of β'' provides a high hardening contribution. The simulations compare well with the results of Du et al.[7]. A dedicated mobility database was used to perform these calculations: IALMOB.

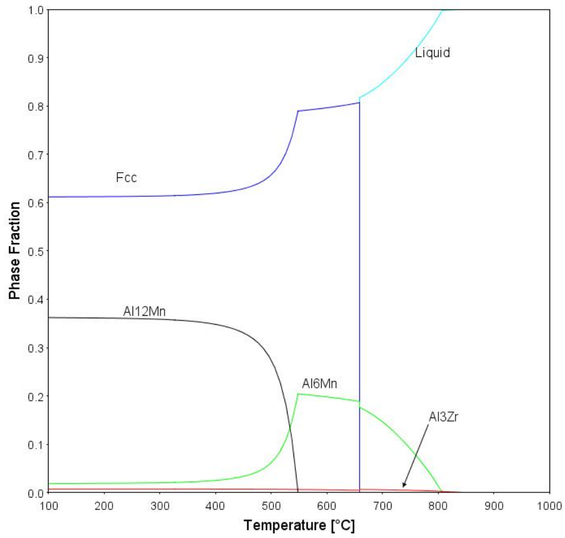

Fig.1. Calculated phase fractions in an Al-0.8%Cr-5%Mn-0.6%Zr alloy.

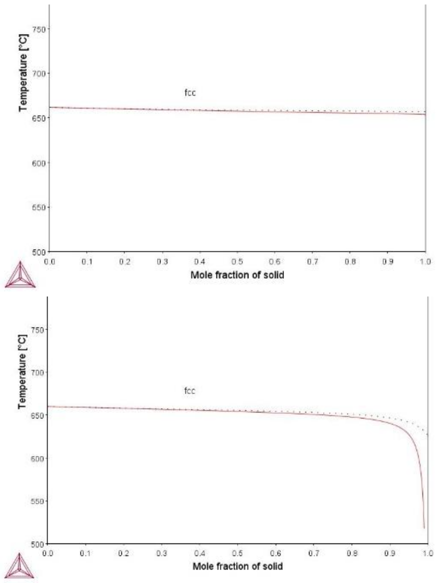

Fig 2. Scheil calculation for a Al-0.8Cr-5Mn-0.6Zr alloy assuming that precipitation of Al3Zr and Al6Mn from the melt is suppressed. The upper figure shows the calculation for Al-0.8Cr-5Mn-0.6Zr, and the lower figure for an alloy including 0.16%Fe and 0.17%Si.

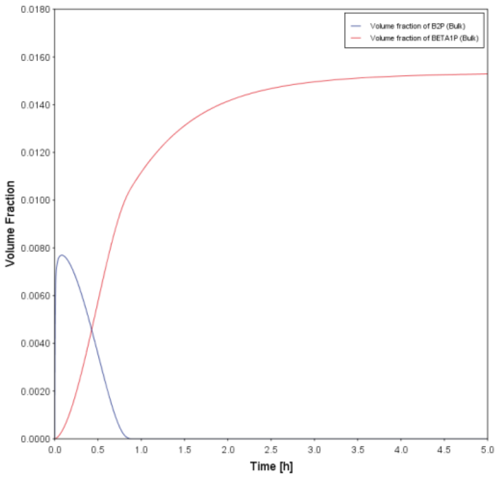

Fig.3. Calculated precipitation sequence for an Al-0.72Mg-0.57Si alloy heat treated at 250ºC. The blue curve shows precipitation of β’’ and the red curve shows precipitation of β’.

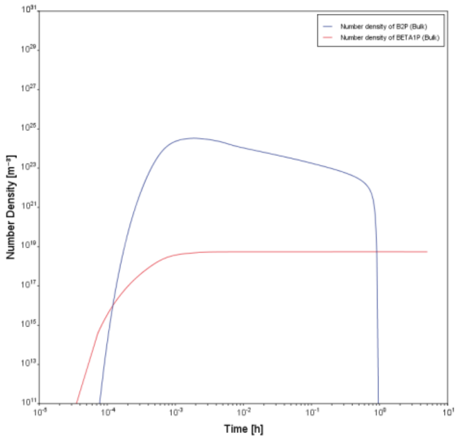

Fig.4. The number densities of β’’and β’ from the calculation shown in Fig.2.

References:

1. G.Cacciamani et al., Intermetallics 7 (1999) 101-108
2. H.Bo et al, Computational Materials Science, 133 (2017) 82-92
3. Karin Frisk, S. Bengtsson, L. Nyborg, B. Mehta, A new aluminum alloy for Additive Manufacturing (AM); "New powder, method for additive manufacturing of components made from the new powder and article made therefrom" EP4259363; 2024-12-25
4. Mehta, B., Nyborg, L., Frisk, K., Hryha, E., "Al–Mn–Cr–Zr-based alloys tailored for powder bed fusion-laser beam process: Alloy design, printability, resulting microstructure and alloy properties", Journal of Materials Research, 2022, 37(6), pp. 1256–1268. DOI:10.1557/s43578-022-00533-1
5. Mehta B., Frisk K., Nyborg L., "Role of Cr in Mn-rich precipitates for Al–Mn–Cr–Zr-based alloys tailored for additive manufacturing", (2024) Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 84, art. no. 102667, https://doi.org/10.1016/j.calphad.2024.102667
6. Powoden-Karadeniz et al., "CALPHAD modeling of metastable phases in the Al-Mg-Si system", CALPHAD 42 (2012) 94-104.
7. Q.Du et al., "Modeling over-ageing in AL-Mg-Si alloys by a multi-phase CALPHAD-coupled Kampmann-Wagner Numerical model", Acta Materialia 122 (2017) 178-186.

COST 507 Database Information:

The COST 507 database is an open database that can be found for download here: OpenCalphad. There is also a report available that documents some of the assessments. There is a huge amount of work collected in this database, and it was developed as a collaboration between several partners.

DATABASE INFORMATION FROM THE DEVELOPMENT TEAM:

The database may be used freely but at your own risk.

The assessed binary systems are:

B-HF, B-TI, C-HF, AL-ZN, CU-NI, CU-SI, CU-ZN, MG-NI, CU-Y, SI-SN, SI-ZN, AL-B, AL-C, AL-N, AL-SI, AL-SN, AL-Y, B-C, B-N, B-SI, B-TI, C-SI, MG-Y, MG-ZN, MG-SI, SI-Y, SN-ZN, MN-ZR, NI-V, SN-ZR, V-ZR, CR-MG, CR-SI, CR-ZN, CU-FE, CU-MG, SI-ZR, AL-CE, AL-ND, CE-MG, AL-FE, FE-MG, MG-MN, MN-SI, AL-MN, C-TI, CR-MN, FE-SI, N-TI, CR-CU, CR-ZR, CU-ZR, MG-ZR, SI-TI, AL-CR, AL-CU, AL-LI, AL-MG, AL-MO, AL-NB, AL-TA, AL-TI, AL-V, Al-W, AL-ZR, CR-TI, CU-LI, FE-TI, LI-MG, LI-ZR, MN-TI, MO-TI, NB-TI, SI-V, TA-TI, TI-V, TI-W, CR-V, MN-V, FE-MN,

The assessed ternary systems are:

B-HF-TI, AL-N-TI, AL-CU-MG, AL-SI-ZN, CU-MG-SI, CU-MG-Y, AL-C-SI, AL-MG-SI, AL-MG-ZN, CU-MG-ZN, AL-SN-ZN, AL-SN-ZN, AL-MG-MN, AL-FE-SI, AL-MN-SI, AL-FE-MN, CR-CU-ZR, AL-CR-TI, AL-CU-LI, AL-LI-MG, AL-MO-TI, AL-NB-TI, AL-TA-TI, AL-TI-V, AL-TI-W.