ME-Al1.2 database contains edited and newly assessed thermodynamic data for Al-base alloys. It is validated for various thermokinetic simulations in precipitation hardened alloys (e.g AA2xxx, AA6xxx, AA7xxx), as well as solidification modeling (Scheil-Gulliver calculation). More sophisticated applications of the database include the prediction of the cluster phase solvus temperatures, determination of dispersoid phase amounts (e.g. various AlFeMnSi phases) or influence of more exotic alloying elements (e.g. Li, Sc, Sn).

Composition range used for database validation

Element	Max. content [wt.%]	Element	Max. content [wt.%]	Element	Max. content [wt.%]
Cr	5	Mn	5	Ti	2
Cu	5	Ni	2	Zn	5
Fe	5	Sc	5	Zr	2
Li	5	Si	10		
Mg	5	Sn	2		

Major updates compared to the previous version (ME-Al1.1) include:

- Optimization of liquidi and solidi in multi-component Al-base alloys
- Optimization of phase stabilities in 7xxx Al-base alloys
- Extension of Al-base systems assessments to the Fe-rich side

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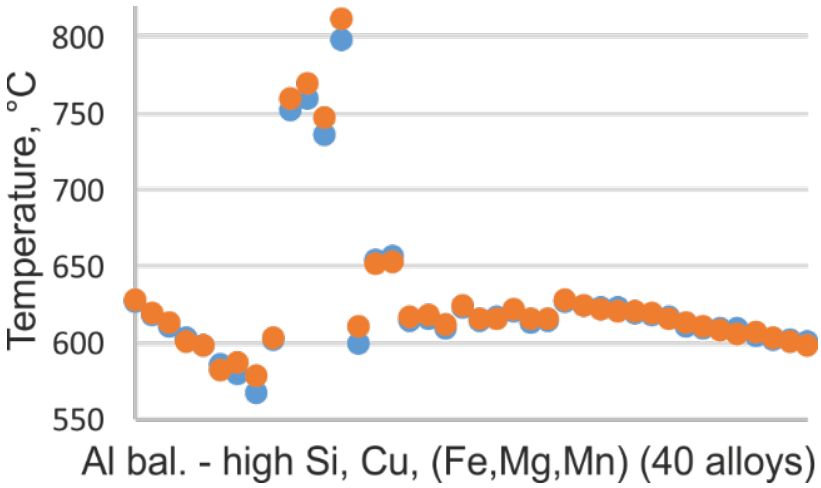
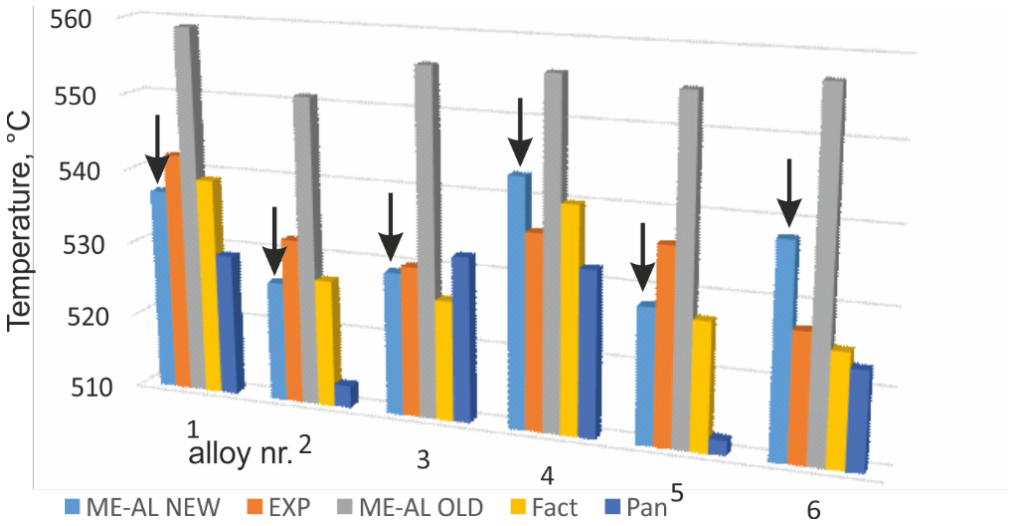
Optimization of liquidi and solidi in multi-component Al-base alloys

Phase descriptions in the multi-component Al-Mg-Si-Cr-Cu-Fe-Mn system are improved for close agreement of experimental and calculated solidus temperatures in 6xxx and 7xxx Al-alloys (now less than 10°C difference between experiment and thermodynamic computation).



Liquidus temperatures of 40 Al-alloys. Comparison of experimental data with computation with ME-Al1.2. The largest difference.



Solidus temperatures of representative 7xxx variations, comparison of experiments (Kolb2016) and competitive databases. The improvements in ME-Al1.2 compared to earlier versions are significant, putting the MatCalc Engineering database towards the top of commercially available thermodynamic multi-component Al-databases.

Optimization of phase stabilities in multi-component 7xxx Al-base alloys

Previous database versions could not reproduce the relative phase stabilities of Cu-containing MgZn2 Laves-phase (Eta, η; Database reference: LC14_ZN2MG) and Cu-containing Al-Mg-Zn-based T-phase (Tau, τ; Database reference: MGALCUZN_T) in Al-Mg-Zn based 7xxx alloys appropriately. The stability of MGALCUZN_T formulated by the 4-sublattice description (Mg)26(Al,Mg)6(Al,Cu,Mg,Zn)48(Al) was overrated. This problem is solved in the new database version. Relative LC14_ZN2MG / MGALCUZN_T stabilities as function of Mg:Zn ratios in AA7175 Al-alloy agree with experimentally observed phases (Lim2003) in homogenized (733K) and cooled samples of different Zn:Mg ratios.

Al-base, 733K	Cu	Mg	Zn	Zn:Mg	Phases exp.	Phases calc.
Alloy B	1.5	2.65	5.63	2.12	τ, η, S	S,τ (<728K), τ,η (<647K)
Alloy E	1.32	2.01	6.04	3	η	η (>441K<721K)

Extension of Al-base system assessments to the Fe-rich side

The full alloying range from Al-rich to Fe-rich compositions in the multi-component Al-Fe-Mn-Si is covered in the model descriptions of ME-Al1.2. For this, the following subsystem descriptions have been completed and agree with experiments and current Calphad assessments from the literature:

-) Al-Mn: Re-assessed Al8Mn5.

-) Al-Fe-Mn: extension adjusted accordingly.

-) Fe-Si: Model implementation of ordered B2-phase.

-) Al-Fe-Si

As a result of the modeling activities for ME-Al1.2, an earlier mentioned discrepancy (Marker2011) of liquidus and solidus temperatures in high-alloyed Al-Fe-Si with available thermodynamic assessments has been clarified. Improvement has been obtained with ME-Al1.2.

Literature:

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3) M.C.J. Marker, B. Skolyszewska-Kühberger, H. S. Effenberger, C. Schmetterer, K.W. Richter, Phase equilibria and structural investigations in the system Al-Fe-Si, Intermetallics 19 (2011) 1919.