Thermodynamic database ME-Ni1.3

MatCalc Engineering

RELEASE NOTES

ME-Ni1.3 database contains edited and newly assessed thermodynamic data for Ni-base superalloys. It is validated for various thermokinetic simulations in multi-component wrought and cast alloy systems (e.g Fe-Cr-alloyed Ni-base superalloys), as well as solidification modeling (Scheil-Gulliver calculation). More sophisticated applications of the database include the description of precipitate evolution in a variety of single-crystal Ni-base superalloys or estimation of the multimodal precipitate size distributions in these systems.

Composition range used for database validation (min. 55 wt.% Ni)

Element	Max. content [wt.%]	Element	Max. content [wt.%]	Element	Max. content [wt.%]
Al	15	La	0.5	Si	2
B	1	Mn	25	Ta	10
C	1	Mo	5	Ti	5
Co	25	N	1	V	0.5
Cr	25	Nb	1	W	15
Cu	0.5	O	0.5	Y	0.1
Fe	20	Re	7	Zr	0.5
Ge	10	Ru	7		
Hf	1	S	0.1		

Major updates compared to the previous version (ME-Ni1.2) include:

- Assessment of Germanium into the database for simulations of advanced brazing alloys
- Improvement of the Boron effect on solidus temperatures

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Assessment of Germanium into the database for simulations of advanced brazing alloys

Germanium partitioning in Ni-matrix and gamma-prime phase is a relevant information in the framework of advanced brazing alloys design for superalloys. In ME-Ni1.3, the following Ge-containing binary systems have been assessed. **pov**=Povoden-Karadeniz, systems with new parametrisation, written in bold style. prel.=preliminary. pov=parameters refined.

Ge-Al	Dong13
Ge-B	**pov**
Ge-Co	Long09
Ge-Cr	Liu10, pov
Ge-Hf	**pov**
Ge-Mo	**pov**
Ge-Ni	Jin12, pov
Ge-Re	**pov**
Ge-Ru	Long09
Ge-Si	Long09
Ge-Ru-Si	Long09
Ge-Ta	**pov, prel.**
Ge-Ti	**pov**
Ge-W	**pov**
Ge-Zr	**pov**
Al-Ge-Ni	**pov**

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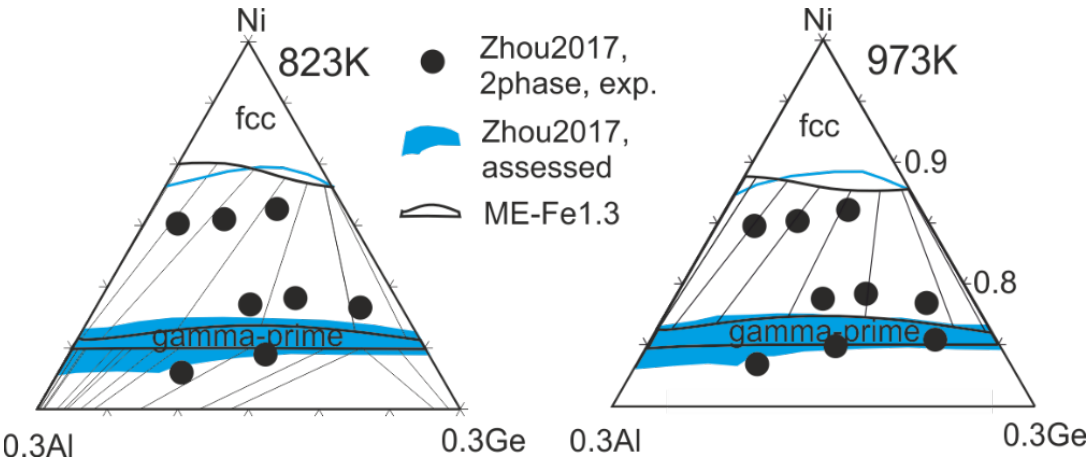
A system of main control of phase stabilities in Ge-containing Ni-base brazing alloys and modified superalloy parent specifications is the Al-Ge-Ni system. There is a new Calphad assessment available (Zhou2017). However, for the reproduction of the experimental phase diagram, these authors used extremely high, unrealistic interaction energies between Al, Ge and Ni in bcc and ordered B2-phase (excess mixing enthalpies less than 500 kJ and more than 100xT entropic contributions. In contrast, ME-Ni1.3 leads to a good reproduction of the experimental phase diagram without such fitting. This also concerns ternary mixing energies of the fcc-Ni base. In this case, up to 100 kJ of interaction energies were chosen, whereas ME-Fe employs an excess energy of only 30kJ.



Comparison of experimental gamma-prime – fcc-Ni phase boundaries and modeling by Zhou 2017 and the ones using ME-NI1.3 in Ni-Al-Ge in the Ni-corner.

Assessment of Boron influence on phase stabilities

The Boron effect on the decrease of solidus temperatures in high Cr-Co-Mo alloyed Ni-base superalloys has been overrated in precious database versions. The decrease of 150°C has been reduced to around 50°C in the new database. Alloy matrix parameters have been refined, and Co-, Mo-, and Ni-solubilites in borides CR5B3 and M3B2 have been assessed.

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Literature:

1) C. Zhou, J. Cui, C. Guo, C. Li, Z. Du, Thermodynamic description of the Al-Ge-Ni system over the whole composition and temperature ranges, Calphad 58 (2017) 138.

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