Thermo-Calc Software

TCS Permanent Magnetic Materials Database (TCPMAG)

Examples Collection

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Contents

About the Database Examples

There are examples available to demonstrate both the *validity* of the database itself as well as to demonstrate some of its *calculation* capabilities when combined with Thermo-Calc software and its Add-on Modules and features.

For each database, the type and number of available examples varies. In some cases an example can belong to both a validation and calculation type.

- *Validation* examples generally include experimental data in the plot or diagram to show how close to the predicted data sets the Thermo-Calc calculations are. It uses the most recent version of the software and relevant database(s) unless otherwise specified.
- *Calculation* examples are intended to demonstrate a use case of the database. This might be showing a binary or ternary system calculated in a phase diagram, or demonstrate how the database and relevant software features would be applied to a heat treatment application, process metallurgy, soldering process, and so forth. In the case of heat treatment, it might include the result of calculating solidification segregation, determining homogenization temperature and then predicting the time needed to homogenize. There are many other examples specifically related to each database.

Where relevant, most references related to each example set are included at the end of the individual section. You can also find additional references specific to the database itself when using the database within Thermo-Calc. You can also contact us directly should you have any questions.

If you are interested in sharing your own examples using Thermo-Calc products in unique or surprising ways, or if you want to share your results from a peer reviewed paper, send an email to info@thermocalc.com.

TCS Permanent Magnetic Materials Database (TCPMAG) Resources

Information about the database is available on our website and in the Thermo-Calc software online Help.

- **Website**: On our website the information is both searchable and the database specific PDFs are available to download.
- **Online Help**: Technical database information is included with the Thermo-Calc software online Help. When in Thermo-Calc, press F1 to search for the same information as is contained in the PDF documents described. Depending on the database, there are additional examples available on the website.

Database Specific Documentation

- The *TCS Permanent Magnetic Materials Database (TCPMAG) Technical Information* PDF document contains version specific information such as the binary and ternary assessed systems, and the phases and models. It also includes details about the properties data (e.g. viscosity, surface tension, etc.), and a list of the included elements, and summaries of the database revision history by version.
- The *TCS Permanent Magnetic Materials Database (TCPMAG) Examples Collection* PDF document contains a series of validation examples using experimental data, and a set of calculation examples showing some of the ways the database can be used.

Go to the Permanent Magnetic Materials page on our website where you can access an examples collection and the technical information plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to Permanent Magnets including links to resources such as examples, publications, and more.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

TCPMAG Validation Examples

Some diagrams are calculated with earlier versions of the database. Negligible differences might be observed if these are recalculated with the most recent version. The diagrams are updated when there are considerable or significant improvements.

In this section:

Phase Stability Predictions

The TCS Permanent Magnetic Materials Database (TCPMAG) can be used to calculate phase equilibria, including phase fractions and compositions, to reliably account for phase transformations. All the stable solution phases and intermetallic compounds that exist in the assessed and their extrapolated systems are included in the current database.

TCPMAG2 is able to predict the stable phases for a given composition and condition within the recommended composition range of the database.

Ce-Nd-Fe-B

The table below shows the calculated phases in $(Ce_{1-x}Nd_x)_{16}Fe_{78}B_6$ alloys compared with experimentally determined ones. TCPMAG2 is able to predict the phase types at each given composition correctly and predict the transition from Fe_2Re to $ReFe_4B_4$ (T2) phase at around x=0.5-0.6. In the table, GB is the *grain boundary* phases.

	x=0	*x=0.1*	*x=0.2*	*x=0.3*	*x=0.4*	*x=0.5*	*x=0.6*	*x=0.7*
Exp. from [2017Zha]	$Re_2Fe_{14}B$ Fe_2Re GB	$Re_2Fe_{14}B$ Fe_2Re GB	$Re_2Fe_{14}B$ Fe_2Re GB	$Re_2Fe_{14}B$ Fe_2Re GB	$Re_2Fe_{14}B$ Fe_2Re GB	$Re_2Fe_{14}B$ Fe_2Re GB	$Re_2Fe_{14}B$ $ReFe_4B_4$ GB	$Re_2Fe_{14}B$ $ReFe_4B_4$ GB
Cal.	$Re_2Fe_{14}B$ Fe_2Re $ReFe_4B_4$	$Re_2Fe_{14}B$ Fe_2Re $ReFe_4B_4$	$Re_2Fe_{14}B$ Fe_2Re $ReFe_4B_4$	$Re_2Fe_{14}B$ Fe_2Re $ReFe_4B_4$	$Re_2Fe_{14}B$ Fe_2Re $ReFe_4B_4$	$Re_2Fe_{14}B$ Fe_2Re $ReFe_4B_4$ Dhcp	$Re_2Fe_{14}B$ $ReFe_4B_4$ Dhcp	$Re_2Fe_{14}B$ $ReFe_4B_4$ Dhcp

Ce-Co-Fe-B

To understand the phase equilibria and explore promising magnetic phases, Wang et al. [2016Wan] studied the Ce-Co-Fe-B diffusion couples and key alloys at 900 °C by SEM/WDS and XRD. Three magnetic phases $Ce_2(Co,Fe)_{14}B$ (T1), $CeCo_4B$ and $Ce_3(Co,Fe)_{11}B_4$ were determined. In this example, the step diagram for $Ce_2Fe_{14}B$-Co and phase equilibrium calculations were made to compare with the experimental results on diffusion couple and key alloys.

For $Ce_2Fe_{14}B$-Co, with increasing Co content, the stable phases changing from T1 to T1+BCC → BCC+$Fe_{17}Re_2$+$ReCo_4B$ → FCC+$ReCo_4B$+$Fe_{17}Re_2$ and reach the FCC phase at Co end.

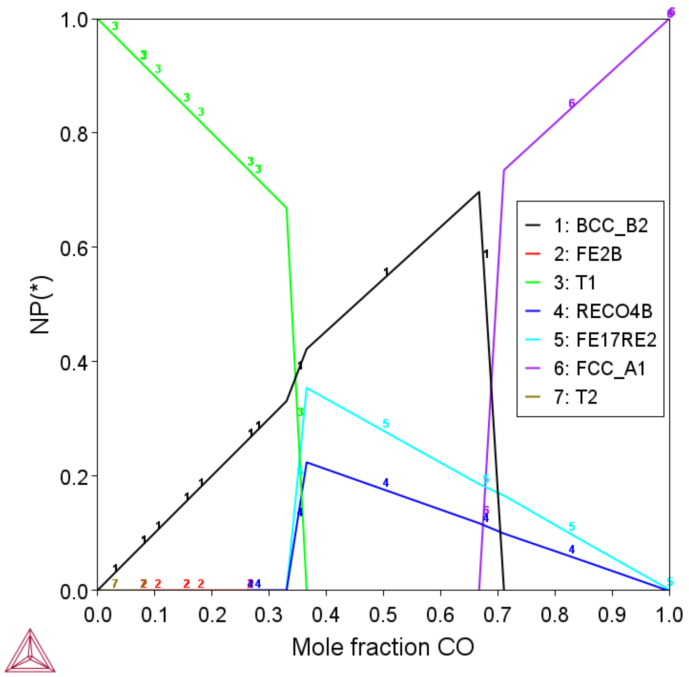

Figure 1: Calculated $Ce_2Fe_{14}B$-Co step diagram at 900 °C.

The following table shows the calculated phase equilibrium at 900 °C on the key alloys compared with the experimental results from [2016Wan].

Comparison A	Phase Name	Composition (mol%)			
		Ce	Fe	Co	B
Nominal		15	66	12	7
Exp.	T1	12	71	11	6
	$ReCo_4B$	16	54	15	15
	Fe_2Re	36	41	23	0
Calc.	T1	11.8	70.8	11.5	5.9
	$ReCo_4B$	16.7	48.4	18.3	16.7
	Fe_2Re	33.3	49.9	16.8	0
	T2	12.2	43.9	0	43.9

Comparison B	Phase Name	Composition (mol%)			
		Ce	Fe	Co	B
Nominal		12	32	50	6
Exp.	$Fe_{17}Re_2$	11	37	52	0
	$ReCo_4B$	17	13	54	16
	BCC	0	57	43	0
Calc.	$Fe_{17}Re_2$	10.5	38.1	51.4	0
	$ReCo_4B$	16.7	17.3	49.4	16.7
	BCC	0	57.9	42.1	0

Dy-Fe-Nd-B

The following figure shows the calculated $Nd_2Fe_{14}B$-$Dy_2Fe_{14}B$ isopleth compared with the one investigated by Grieb et al. [1989Gri] by means of metallography, XRD and DTA. They reported unlimited solid solubility above 800 °C for T1 phase $(Dy,Nd)_2Fe_{14}B$ and on the increasing temperatures of formation measured. According to the authors, there is stable peritectic formation of Fe + L = T1 on the Nd-rich side and the stable peritectic formation Dy_2Fe_{17} + L = T1 on the Dy-rich side.

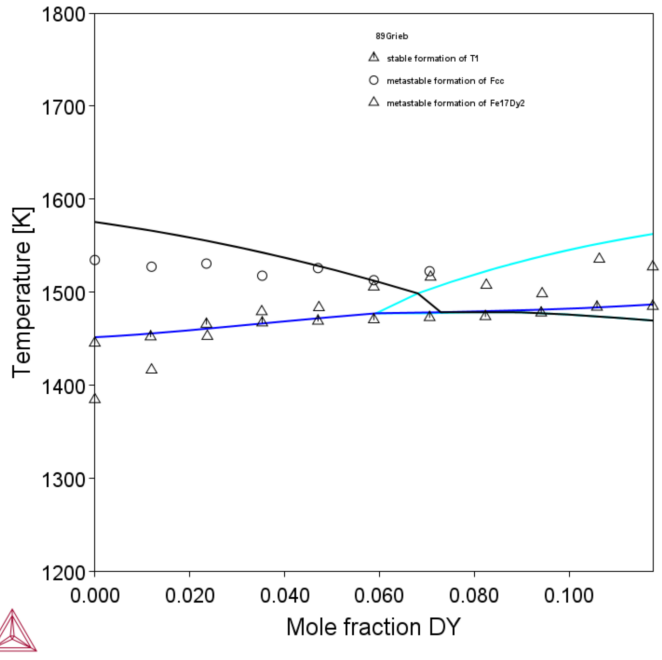

Figure 2: Calculated $Nd_2Fe_{14}B$-$Dy_2Fe_{14}B$ isopleth compared with experimental data from [1989Gri].

References

[1989Gri] B. Grieb, G. Schneider, E.-T. Henig, G. Petzow, Structural Investigations and Constitution along Fe 14 (Nd 1-x (Tb or Dy) x) 2 B. Int. J. Mater. Res. 80, 515–519 (1989).

[2016Wan] T. Wang, D. Kevorkov, M. Medraj, Phase Equilibria and Magnetic Phases in the Ce-Fe-Co-B System. Materials (Basel). 10, 16 (2016).

[2017Zha] L. Z. Zhao, H. Y. Yu, W. T. Guo, J. S. Zhang, Z. Y. Zhang, M. Hussain, Z. W. Liu, J. M. Greneche, Phase and Hyperfine Structures of Melt-spun Nanocrystalline (Ce 1–x Nd x) 16 Fe 78 B 6 Alloys. IEEE Trans. Magn. 53, 1–5 (2017).

Curie Temperature Predictions

Curie temperature is one of the important properties for permanent magnetic materials. The Curie temperature (Tc) is a critical temperature, above which certain materials lose their permanent magnetic properties. Considering the high-temperature range of practical usage of traction motors of cars up to 450 K, it has been in high demand to find a way to supplement the high-temperature performance of Nd-Fe-B magnets or to design a new champion magnet desirably with higher Curie temperatures with a good structure stability [2020Mat].

The TCS Permanent Magnetic Materials Database (TCPMAG) includes magnetic parameters for phases with magnetic properties. Thus, it can be used to predict the curie temperatures of a magnetic phase as a function of the chemical composition of typical industrial alloys. The figure below shows the comparison of calculated and measured curie temperature for (Ce,La,Nd,Pr)2Fe14B (T1) phase. In all cases, the differences are less than 5%.

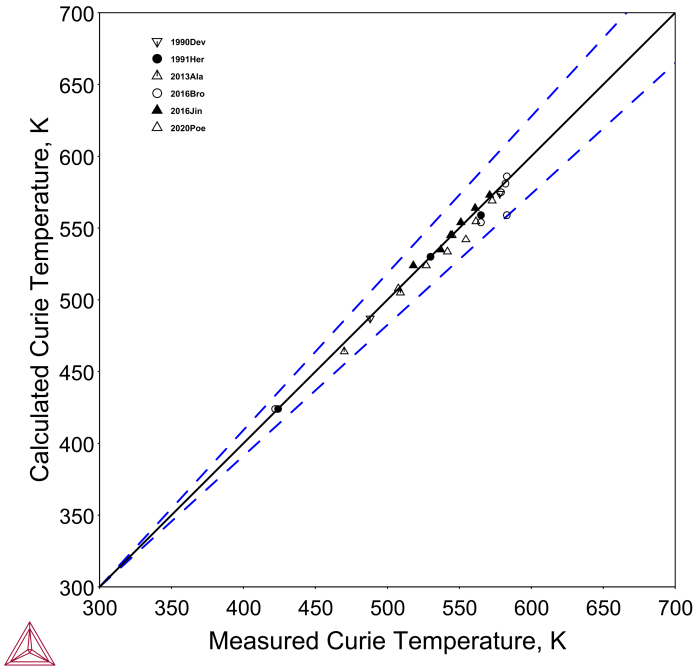

Figure 3: Comparison of calculated vs experimental Curie temperatures.

Reference

[2020Mat] M. Matsumoto, H. Akai, Calculating Curie temperatures for rare-earth permanent magnets: Ab initio inspection of localized magnetic moments in d -electron ferromagnetism. Phys. Rev. B. 101, 144402 (2020).

Heat Capacity of $Nd_2Fe_{14}B$ (T1)

The TCS Permanent Magnetic Materials Database (TCPMAG) can be used to calculate a variety of thermodynamic properties. The plot below compares the calculated heat capacity of $Nd_2Fe_{14}B$ (T1) with the experimental data. The calculated heat capacity is consistent with the experimental data.

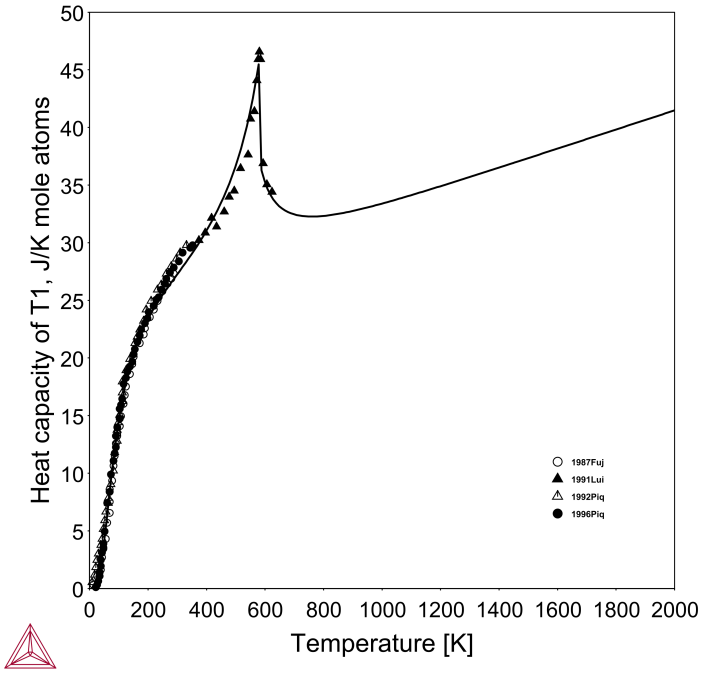

Figure 4: Calculated heat capacity of $Nd_2Fe_{14}B$ (T1) with experimental data.

TCPMAG Calculation Examples

Some diagrams are calculated with earlier versions of the database. Negligible differences might be observed if these are recalculated with the most recent version. The diagrams are updated when there are considerable or significant improvements.

In this section:

Binary Phase Diagrams

You can use the TCS Permanent Magnetic Materials Database (TCPMAG) to plot binary phase diagrams in Thermo-Calc. Each assessed binary system is modeled to accurately describe experimental phase diagram data available in the literature. These examples show a selection of the important assessed systems that are the building blocks of the database itself when applying the CALPHAD method.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

Fe-B

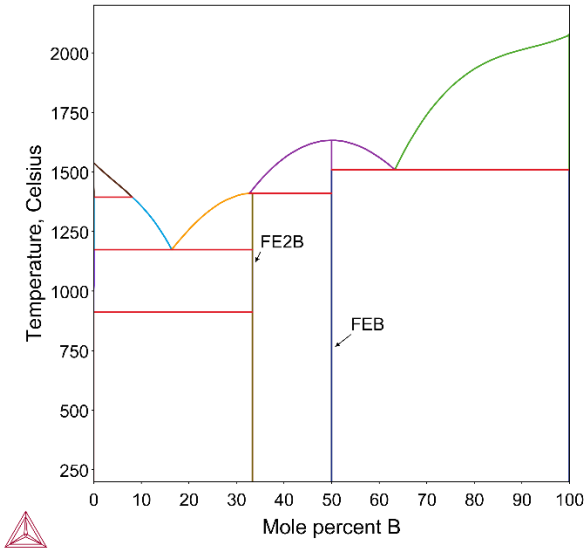

Figure 5: Calculated Fe-B phase diagram.

Fe-Nd

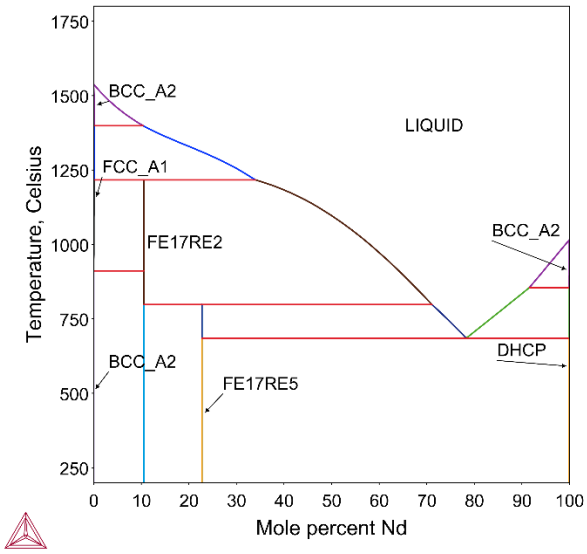

Figure 6: Calculated Fe-Nd phase diagram.

Nd-B

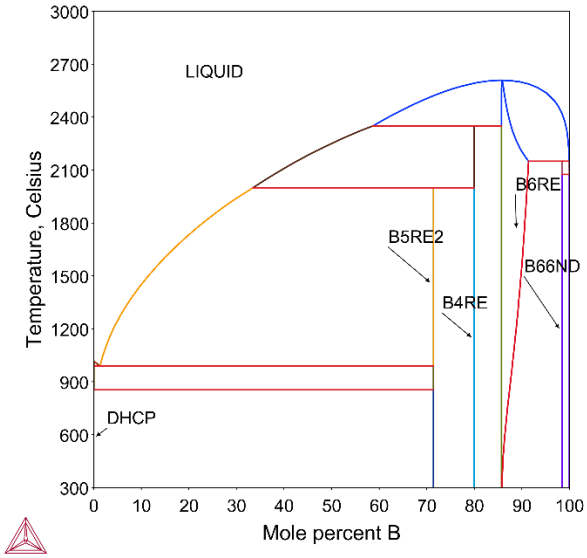

Figure 7: Calculated Nd-B phase diagram.

Nd-Pr

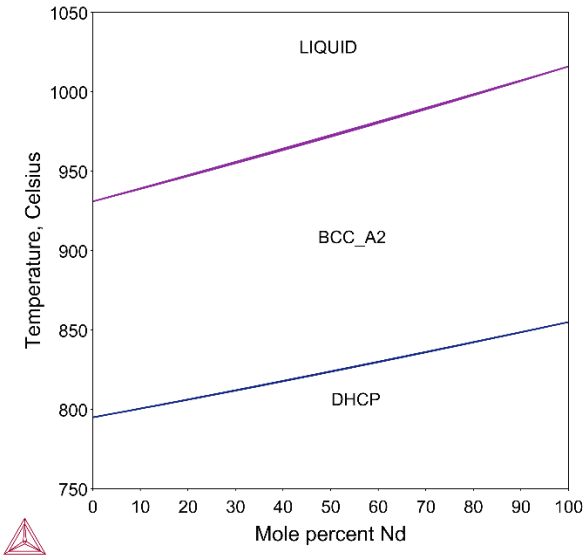

Figure 8: Calculated Nd-Pr phase diagram.

Ternary Phase Diagrams

You can use the TCS Permanent Magnetic Materials Database (TCPMAG) to plot ternary phase diagrams in Thermo-Calc. Each assessed ternary system is modeled to accurately describe experimental phase diagram data available in the literature. These examples show a selection of the important assessed systems that are the building blocks of the database itself when applying the CALPHAD method.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

When working in Thermo-Calc with ternary diagrams you use either the Ternary Calculator (in Graphical Mode) or the Ternary module (in Console Mode). The fundamental calculation engine is the same but you access the settings in different ways.

Fe-Nd-B

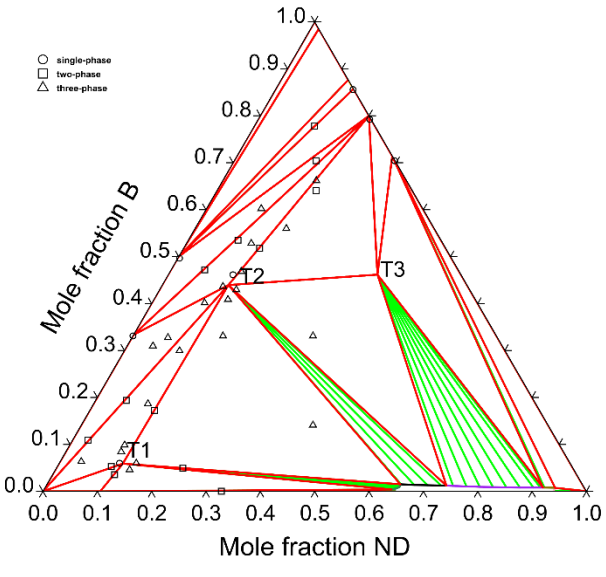

Figure 9: Calculated Fe-Nd-B isothermal section at 1173 K with experimental data from [1985Bus] and [1986Bus].

Fe-Nd-B

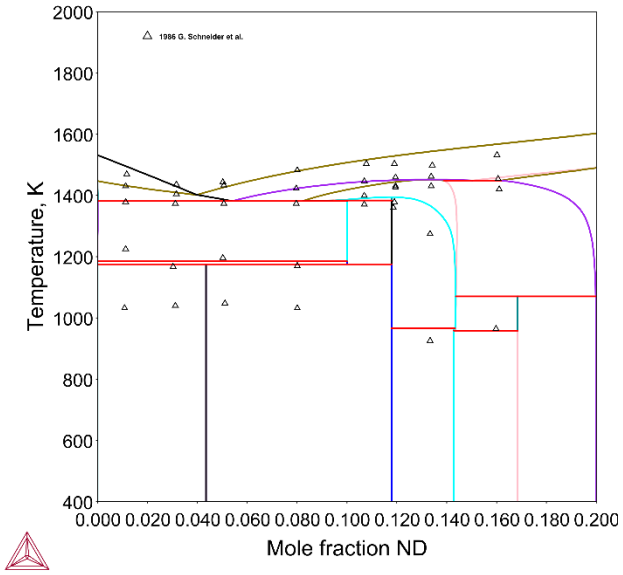

Figure 10: Calculated vertical section of Fe-Nd-B at 80 at. % Fe with experimental data from [1986Sch].

Ce-Fe-B

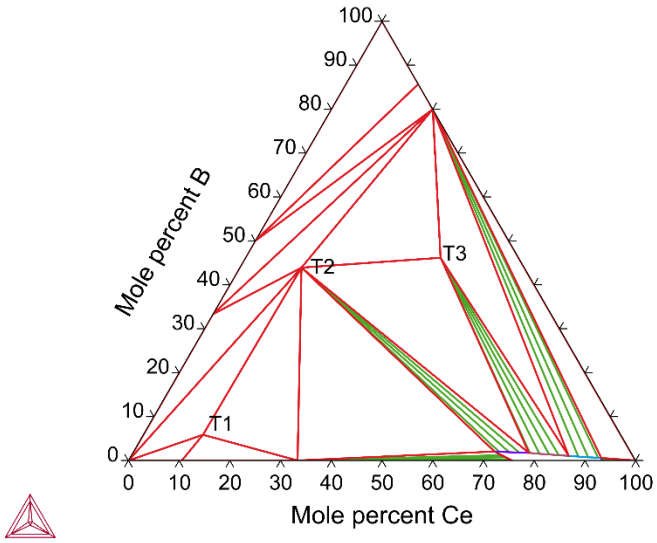

Figure 11: Calculated Ce-Fe-B isothermal section at 973 K.

Fe-Pr-B

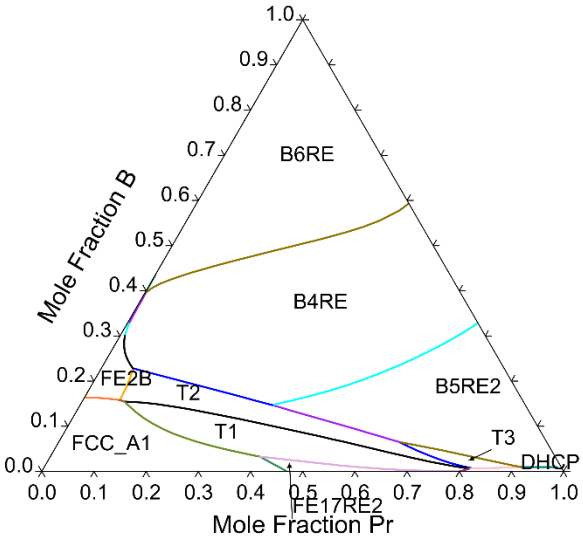

Figure 12: Calculated Fe-Pr-B liquidus projection.

References

[1985Bus] K. H. J. Buschow, D. B. De Mooij, H. M. Van Noort, The Fe- Rich Isothermal Section of Nd-Fe-B at 900 C. Philips J. Res. 40, 227–238 (1985).

[1986Bus] K. H. J. Buschow, D. B. De Mooij, J. L. C. Daams, H. M. Van Noort, Phase relationships, magnetic and crystallographic properties of Nd-Fe-B alloys. J. Less Common Met. 115, 357–366 (1986).

[1986Sch] G. Schneider, E.-T. Henig, G. Petzow, H. H. Stadelmaier, Phase Relations in the System Fe-Nd-B. Zeitschrift für Met. 77, 755–761 (1986).

TCPMAG Surface Tension of Nd-Fe-B and B-Co-Fe Alloys

The surface tension thermophysical property data is included with the TCS Permanent Magnetic Materials Database (TCPMAG).

For more information about the various thermophysical models, and when in Thermo-Calc, press F1 to search the online help. The details are found under a *General Reference* section.

You can find information on our website about the properties that can be calculated with Thermo-Calc and the Add-on Modules. Additional resources are added on a regular basis so keep checking back or subscribe to our newsletter.

Nd-Fe-B

Noguchi et al. [2021Nog] have measured the surface tension of Nd-rich ternary Nd-Fe-B alloys by means of a constrained drop method. The calculations show good agreement with these measurements.

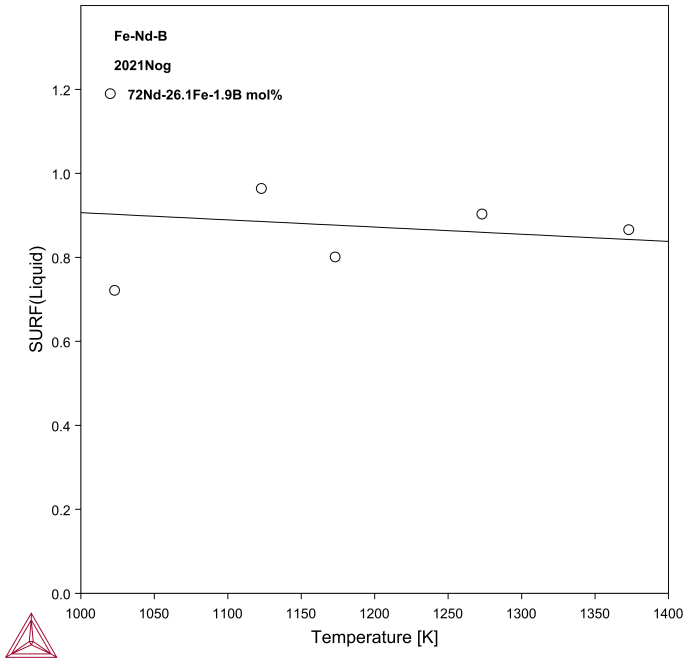

Figure 13: Calculated surface tension of Nd-Fe-B ternary alloy compared with experimental data from [2021Nog].

B-Co-Fe

Sidorov et al. [2000Sid] measured the surface tension of B-Co-Fe alloy using the sessile drop method and the magnetic susceptibility. The calculation shows a good agreement with the reported measurements.

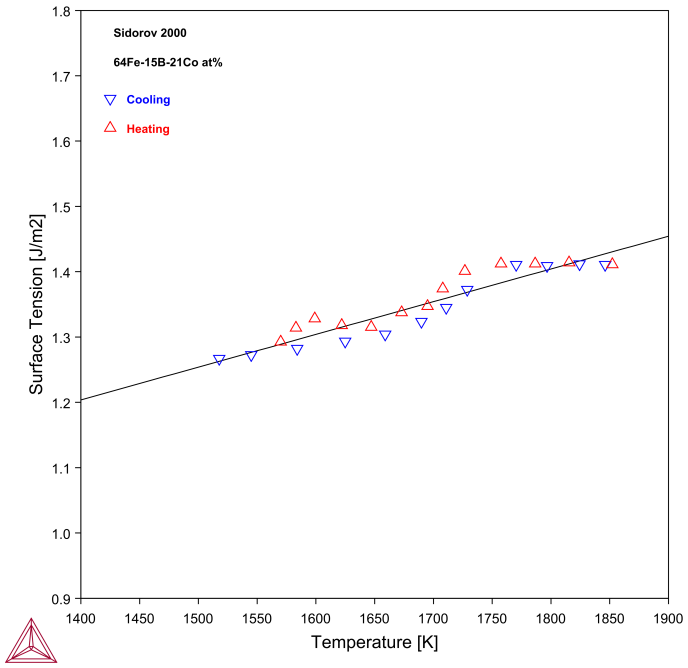

Figure 14: Calculated surface tension of B-Co-Fe ternary alloy compared with experimental data from [2000Sid].

References

[2000Sid] V. E. Sidorov, M. Calvo-Dahlborg, U. Dahlborg, P. S. Popel, S. Chernoborodova, Physical properties of some iron based alloys in liquid and amorphous states. J. Mater. Sci. 35, 2255–2262 (2000).

[2021Nog] D. Noguchi, O. Takeda, H. Zhu, S. Sugimoto, Surface tension measurement of Nd−Fe−B−X melts (X = O, Cu, Ga, In) as simulated substances of Nd-rich phase in Nd magnet. J. Magn. Magn. Mater. 539, 168407 (2021).