TCS Permanent Magnetic Materials Database (TCPMAG1)

Technical Information

Available Starting with Thermo-Calc Version 2022a

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Contents

About the TCS Permanent Magnetic Materials Database (TCPMAG)

The TCS Permanent Magnetic Materials Database (TCPMAG) is a thermodynamic and properties database for rare-earth permanent magnetic materials. It can be used for a wide range of compositions from pure Nd2Fe14B to very complex NdFeB-based commercial permanent magnetic materials. It can be used for calculating phase diagrams and thermodynamic properties of assessed systems, but also for predicting phase equilibria, curie temperatures and simulating solidification processes for a wide range of composition.

TCS Permanent Magnetic Materials Database (TCPMAG) is developed to be used with our entire suite of products: Thermo-Calc, the Add-on Modules, and all available SDKs.

In addition to thermodynamic data, it has thermophysical properties data available for:

- Molar volume of liquid and all solid phases
- Viscosity of liquid
- Surface tension of liquid

The current version of the database is TCPMAG1.

The CALPHAD Method

The Thermo-Calc databases are developed with the CALPHAD approach based on various types of experimental data and theoretical values (e.g. those from first-principles calculations). It is based on the critical evaluation of binary, ternary, and for some databases, important higher order systems. This enables predictions to be made for multicomponent systems and alloys of industrial importance. Among these, the thermodynamic database is of fundamental importance.

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

Use Case Examples

There are examples available to both demonstrate the *validation* of the database and to showcase the types of *calculations* that can be used for different materials or application area.

The TCS Permanent Magnetic Materials Database (TCPMAG) enables predictions (such as multicomponent phase equilibria calculations, equilibrium solidification simulations, and Scheil solidification simulations) to be made for multicomponent systems and alloys of industrial importance. This means it can be used to extrapolate to higher-order systems by combining several critically assessed systems.

Combining Databases

It is possible to combine several databases to make calculations using Thermo-Calc. For more information related to a specific type of problem, contact one of our support specialists at info@thermocalc.com. The experts are available to make recommendations on the most suitable database to use for your needs.

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.
- 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

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

TCPMAG1 Elements, Systems, Phases and Properties

Included Elements

There are six (6) elements included in the database.

B	Ce	Fe	La	Nd	Pr

Assessed Systems and Phases

A hybrid approach of experiments, first-principles calculations and CALPHAD modeling have been used to obtain thermodynamic descriptions of the constituent binary and ternary systems over the whole composition and temperature ranges.

All the stable solution phases and intermetallic compounds that exist in each assessed system are included. Note that in most cases phases having the same crystal structure had been merged as the same phase.

The database contains:

- 15 assessed binary systems
- 11 assessed ternary systems
- 19 phases

In Console Mode, you can list phases and constituents in the Database (TDB) module and the Gibbs (GES) module. For some phases, supplementary information is included in the definitions. To show the information, it is recommended in the Database (TDB) module to use the command LIST_SYSTEM with the option `Constituents`.

Properties Data

A variety of properties data is included with the TCS Permanent Magnetic Materials Database (TCPMAG).

- Molar volume of liquid and all solid phases
- Viscosity of liquid
- Surface tension of liquid

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.

Properties Data

Below is a summary of the available parameters and variables for the databases when working in Thermo-Calc. There are differences when you are working in Console Mode versus Graphical Mode as well as if you use the TC-Python SDK. More details are described in the online help.

Property	*Model Parameters*	*Variables to Show or Plot in Console Mode and TC-Python*
Surface tension	SIGM, XI	`SURF(LIQUID)`
Dynamic viscosity	VISC	`DVIS(LIQUID)`
Kinematic viscosity		`KVIS(LIQUID)`
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

TCPMAG1 Systems

In this section:

TCPMAG1 Assessed Binary Systems

	Ce	Fe	La	Nd	Pr
B	x	x	x	x	x
Ce		x	x	x	x
Fe			x	x	x
La				x	x
Nd					x

TCPMAG1 Assessed Ternary Systems

Assessed Ternaries				
B-Ce-Fe	B-Ce-Nd	B-Fe-La	B-Fe-Nd	B-Fe-Pr
Ce-Fe-La	Ce-Fe-Nd	Ce-Fe-Pr	Ce-La-Pr	Fe-La-Nd
Fe-Nd-Pr				

TCPMAG1 Phases

In this section:

Common Phases for Permanent Magnetic Alloys

TCPMAG1 Models for the Included Phases

The following lists common phase names and the corresponding Thermo-Calc database phase names for some key permanent magnetic alloys.

LIQUID	*Liquid phase, which covers the melt of permanent magnetic materials*
T1	Re2Fe14B based phase, which covers (Nd, La, Ce, Pr)0.1176471(Fe)0.8235294 (B)0.0588235 compositions
T2	ReFe4B4 based phase, which covers (Nd, La, Ce, Pr)0.121844(Fe)0.439078 (B)0.439078 compositions
Fe2Re	Fe2Re Laves phase, which covers (Ce, Nd, Pr)2Fe compositions
DHCP	Rare-earth rich phase, which covers (Ce, La, Nd, Pr)

TCPMAG1 Models for the Included Phases

Phase	*Prototype*	*Pearson Symbol*	*Space Group Symbol*	*Sublattices*
B4RE	UB4	tP20	P4/mbm	(B)0.8(CE,LA,ND,PR)0.2
B5RE2	Pr2B5	mS56	C2/c	(B)0.714286(CE,ND,PR)0.285714
B66ND	YB66	cF1936	Fm-3c	(B)0.985075(ND)0.014925
B6RE	CaB6 (D21)	cP7	Pm-3m	(B)0.857143(B,CE,LA,ND,PR)0.142857
BCC_A2	Body-Centered Cubic (W, A2, bcc)	cI2	Im-3m	(B,CE,FE,LA,ND,PR)1.0(VA)3.0
BETA_RHOMBO_B	beta-B (R-105)	hR105	R-3m	(B)1.0
DHCP	alpha-La (A3')	hP4	P6_3/mmc	(CE,LA,ND,PR)1.0
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	cF4	Fm-3m	(B,CE,FE,LA,ND,PR)1.0(VA)1.0
FE17RE2	Zn17Th2	hR57	R-3m	(FE)0.894737(CE,LA,ND,PR)0.105263
FE17RE5	Nd5Fe17	hP264	P6_3/mmc	(FE)0.772727(CE,LA,ND,PR)0.227273
FE2B	Khatyrkite (Al2Cu, C16)	tI12	I4/mcm	(FE)0.666667(B)0.333333
FE2RE	Cu2Mg Cubic Laves (C15)	cF24	Fd-3m	(FE)0.666667(CE,ND,PR)0.333333
FEB	FeB (B27)	oP8	Pnma	(FE)0.5(B)0.5
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	hP2	P6_3/mmc	(FE)1.0(VA)0.5
LA1B9	Unknown Structure			(LA)0.1(B)0.9
LIQUID	Liquid			(B,CE,FE,LA,ND,PR)1.0

Phase	*Prototype*	*Pearson Symbol*	*Space Group Symbol*	*Sublattices*
T1	Nd2Fe14B	tP68	P4_2/mnm	(FE)0.8235294(CE,LA,ND,PR)0.1176471 (B)0.0588235
T2	Nd19Fe68B68	tP310	P4_2/n	(FE)0.439078(CE,LA,ND,PR)0.121844 (B)0.439078
T3	Pr5Co2B6	hR39	R-3m	(FE)0.153846(CE,ND,PR)0.384615 (B)0.461539

TCPMAG1 Properties

Model Descriptions

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Examples

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