TCSI1: TCS Ultrapure Silicon Database

Database name:	TCS Si-based alloys Database	*Database acronym:*	TCSI
Database owner:	Thermo-Calc Software AB	*Database version:*	1.2

TCSI is a thermodynamic database for the application of solar grade silicon materials. It is developed using the CALPHAD approach based on experimental and First Principles results. The database focuses on the impurity solubility in silicon with diamond structure within a 34-element framework. The database can also be used with the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA).

Included Elements (34)

Ag	Al	As	Au	B	Bi	C	Ca	Co	Cr	Cu	Fe	Ga	Ge	In	Li	Mg
Mn	Mo	N	Na	Ni	O	P	S	Sb	Si	Sn	Te	Ti	V	W	Zn	Zr

Critically Assessed Systems

Generally, only the diamond phase and Si-rich corner is critically assessed in each Si-containing binary system. The BINARY_DIAGRAM module is applicable in Si containing binary systems to calculate the impurity solubility in silicon. The solubility in ternary and higher order systems can be calculated by Thermo-Calc through the extrapolation from binary systems.

- The solubility of impurity X in diamond Si of all Si-X binaries is assessed.
- Besides the diamond phase, at least the liquid and the corresponding stable silicide phase with highest Si content is included in each Si-X binary, except for X = As, Ga and Sb.
- Two assessed Si-free binaries i.e. Al-B and Al-P are included.
- The Si-Al-C ternary is included.
- The following 17 binaries (Si-M1) using the excess Gibbs energy of the diamond phase transited from Yoshikawa et al (2010), where M1 = Ag, Al, Au, B, Bi, Co, Cr, Cu, Fe, Ga, In, Mn, Ni, Sb, Sn, Ti, Zn.
- The diamond in the following 13 binaries (Si-M2) was optimized to reproduce the M2 solubility in Si published in Tang et al. (2009), where M2 = As, Ca, Li, Mg, Mo, N, Na, O, P, S, V, W, Zr.
- The thermodynamic description of the Ge-Si binary was taken from Bergman [1992].
- The Si-C binary was reassessed in 2015.

Calculation Examples

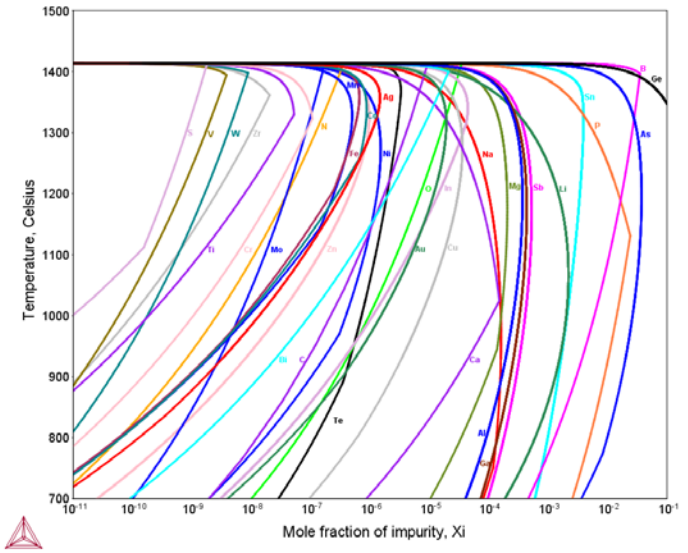

Figure 1. Calculated impurity solubility in Si-containing binaries using TCSI1.

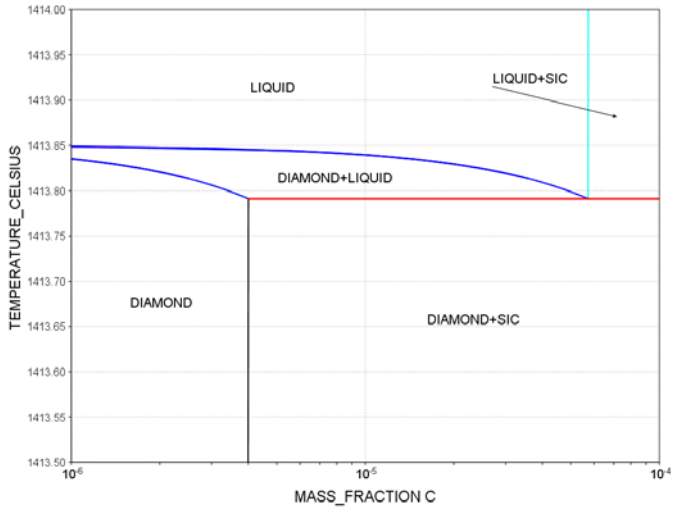

Figure 2. TCSI1 predicted segregation coefficient (~ 0.07) between C content in the diamond phase (~ 4 ppmw) and that in the liquid phase (~ 57 ppmw) at the eutectic of diamond+SiC in the Si-C binary.

References

[1992, Bergman] C. Bergman, R. Chastel, R. Castanet, Thermodynamic investigation on the Si-Ge binary system by calorimetry and Knudsen cell mass spectrometry. *J. Phase Equilibria*. **13**, 113–118 (1992).

[2010, Tang] K. Tang, E. J. Øvrelid, G. Tranell, M. Tangstad, Critical assessment of the impurity diffusivities in solid and liquid silicon. *JOM*. **61**, 49–55 (2010).

[2010, Yoshikawa] T. Yoshikawa, K. Morita, S. Kawanishi, T. Tanaka, Thermodynamics of impurity elements in solid silicon. *J. Alloys Compd.* **490**, 31–41 (2010).

Phases and Phase Models

TCSI1 contains 84 solution phases and intermetallic compounds.

- Compounds having the same crystal structure might have been merged into one phase.
- In Console Mode, you can list phases and constituents in the Database module and the GES module. For some phases, supplementary information is included in the definitions. In order to show the information, it is recommended to use “List-System” with the option of “Constituents” in the Database module.

The table lists the most common phases in TCSI. The following section details the phases and phase models.

DIAMOND_A4	LIQUID	GAS	BCC_A2	FCC_A1	HCP_A3
BETA_RHOMBO_B	RED_P	CBCC_A12	GRAPHITE	LAVES_C14	LAVES_C15
RHOMBOHEDRAL_A7	SIB3	SIB6	CASI2	COSI2_C1	CRSI2_C40
CUSI_ETA	FESI2_H	FESI2_L	LI12SI7	MG2SI_C1	MN11SI19
MOSI2_C11B	M3SI_A15	M5SI3_D8M	SI3N4	NASI_HT	NASI_LT
NISI2	CRISTOBALITE	QUARTZ	SIP	SIS	SI2TE3_HT
SI2TE3_LT	SI2TI_C54	AB_B31	A6B5_OI44	SI3W5_D8M	SI2ZR_C49
GE3TI5	ALB12	ALP_ZNS	AL4C3	AL4C4SI	AL8C7SI

Phases and Phase Models

DIAMOND_A4 :AG AL AS AU B BI C CA CO CR CU FE GA GE IN LI MG MN MO N NA NI O P S SB SI SN TI V W ZN ZR:
LIQUID :AG AL AS AU B BI C CA CO CR CU FE GA GE IN LI MG MN MO N NA NI P S SB SI SIO2 SIS2 SI2TE3 SN TE TI V W ZN ZR:
GAS:G :C N N2 N3 O2 SI SI2 SI3 S S1SI1 S2 S2SI1 S3 S4 S5 S6 S7 S8 P P2 P3 P4 SIN SI2N SIP SIP2 SI2P SI2P2:
ALPHA_RHOMBO_B :B:
BCC_A2 2 SUBL, SITES 1: 3: :AG AL AS AU B BI CA CO CR CU FE GA GE IN MG MN MO NA NI O P S SB SI SN TI V W ZN ZR: VA:

BCT_A5 :AG AL BI GA GE IN NI SB SN TI ZN:	
BETA_RHOMBO_B :B: CU SI B C:	2 SUBL, SITES 93: 12:
CBCC_A12 :AL CO CR FE MG MN NI SI SN TI V ZN ZR: VA:	2 SUBL, SITES 1: 1:
CUB_A13 :AG AL CO CR FE MG MN NI SI SN TI V ZN ZR: VA:	2 SUBL, SITES 1: 1:
DHCP :AU IN SN:	
FCC_A1 :AG AL AS AU B BI CA CO CR CU FE GA GE IN MG MN MO NA NI O P S SB SI SN TI V W ZN ZR: VA:	2 SUBL, SITES 1: 1:
GRAPHITE :B C:	
HCP_A3 :AG AL AS AU B BI CA CO CR CU FE GA GE IN MG MN MO NA NI SB SI SN TI V W ZN ZR: O VA:	2 SUBL, SITES 1: 0.5:
HCP_ZN :AG AL CR CU GA IN MG SI SN ZN: VA:	2 SUBL, SITES 1: 0.5:
HEXAGONAL_A8 :TE:	
LAVES_C14 :MN TI: MN TI:	2 SUBL, SITES 2: 1:
LAVES_C15 :CR CU MG TI ZR: CR CU MG TI ZR:	2 SUBL, SITES 2: 1:
MONOCLINIC :S:	
OMEGA :ZR:	

ORTHORHOMBIC_A20 :FE ZR:	
ORTHORHOMBIC_GA :GA:	
ORTHORHOMBIC_S :S:	
RED_P :AS P:	
RHOMBOHEDRAL_A10 :ZN:	
RHOMBOHEDRAL_A7 :AS BI GE IN P SB SN ZN:	
TETRAGONAL_A6 :BI GA IN SN ZN:	
TETRAGONAL_U :FE ZR:	
TET_ALPHA1 :BI IN SN:	
WHITE_P :P:	
SIB3 :B: SI: B SI:	3 SUBL, SITES 6: 2: 6:
SIB6 :B: SI: B SI:	3 SUBL, SITES 210: 23: 48:
SIBX :B: SI: B SI:	3 SUBL, SITES 61: 1: 8:
SIC :C: SI:	2 SUBL, SITES 1: 1:
CASI :CA: SI:	2 SUBL, SITES 1: 1:

CA3SI4 :CA: SI:	2 SUBL, SITES 0.43: 0.57:
CA14SI19 :CA: SI:	2 SUBL, SITES 0.42: 0.58:
CASI2 :CA: SI:	2 SUBL, SITES 0.33: 0.67:
CO3SI_D019 :CO: SI:	2 SUBL, SITES 3: 1:
CO2SI_C37 :CO SI: CO SI:	2 SUBL, SITES 2: 1:
CO2SI_BETA :CO SI: CO SI:	2 SUBL, SITES 2: 1:
COSI_B20 :CO SI: CO SI:	2 SUBL, SITES 1: 1:
COSI2_C1 :CO: SI:	2 SUBL, SITES 1: 2:
CRSI2_C40 :CR SI V : AL CR SI:	2 SUBL, SITES 1: 2:
CUSI_ETA :CU MN NI ZN: SI:	2 SUBL, SITES 0.76: 0.24:
FESI2_H :FE NI: AL MG SI:	2 SUBL, SITES 3: 7:
FESI2_L :FE NI: AL SI:	2 SUBL, SITES 1: 2:
FESI_B20 :FE MN NI CR: AL MG SI GE:	2 SUBL, SITES 1: 1:
LI22SI5 :LI: SI:	2 SUBL, SITES 22: 5:
LI13SI4 :LI: SI:	2 SUBL, SITES 13: 4:

LI7SI3 :LI: SI:	2 SUBL, SITES 7: 3:
LI12SI7 :LI: SI:	2 SUBL, SITES 12: 7:
MG2SI_C1 :MG: GE SI SN:	2 SUBL, SITES 2: 1:
MN11SI19 :MN: AL SI:	2 SUBL, SITES 11: 19:
MOSI2_C11B :MO: SI:	2 SUBL, SITES 1: 2:
M3SI_A15 :MO: SI:	2 SUBL, SITES 3: 1:
M5SI3_D8M :MO: MO SI: MO SI:	3 SUBL, SITES 4: 1: 3:
SI3N4 :SI: N:	2 SUBL, SITES 3: 4:
NASI_HT :NA: SI:	2 SUBL, SITES 1: 1:
NASI_LT :NA: SI:	2 SUBL, SITES 1: 1:
NI2SI_HT :CU NI: NI VA: AL SI:	3 SUBL, SITES 1: 1: 1:
NI3SI2 :FE NI: SI:	2 SUBL, SITES 3: 2:
AB_B31 :FE NI: GE SI ZN:	2 SUBL, SITES 1: 1:
NISI2 :AL CU SI ZN: CU FE MN NI:	2 SUBL, SITES 2: 1:
CRISTOBALITE :SIO2:	

QUARTZ :SIO2:	
TRIDYMITE :SIO2:	
SIP :SI: P:	2 SUBL, SITES 1: 1:
SIS :SI: S:	2 SUBL, SITES 1: 1:
SIS2 :SI: S:	2 SUBL, SITES 1: 2:
SI2TE3_LT :SI: TE:	2 SUBL, SITES 2: 3:
SI2TE3_HT :SI: TE:	2 SUBL, SITES 2: 3:
SI2TI_C54 :GE SI: TI:	2 SUBL, SITES 2: 1:
FEB_B27 :TI ZR: SI GE:	2 SUBL, SITES 1: 1:
A6B5_OI44 :GE SN SI: V TI:	2 SUBL, SITES 5: 6:
SI2W_C11B :SI: W:	2 SUBL, SITES 2: 1:
SI3W5_D8M :SI: W:	2 SUBL, SITES 3: 5:
SI2ZR_C49 :SI GE: ZR:	2 SUBL, SITES 2: 1:
ALB2_C32 :AL: B:	2 SUBL, SITES 1: 2:
ALB12 :AL: B:	2 SUBL, SITES 1: 12:

ALP_ZNS :AL: P:	2 SUBL, SITES 0.5: 0.5:
GE3TI5 :TI: GE:	2 SUBL, SITES 5: 3:
AL4C3 :AL SI: C:	2 SUBL, SITES 4: 3:
AL4C4SI :AL: SI: C:	3 SUBL, SITES 4: 1: 4:
AL8C7SI :AL: SI: C:	3 SUBL, SITES 8: 1: 7: