TCSI1 - TCS Ultrapure Silicon Database, Version 1.2

TCSI1 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 impurity solubility in silicon is critically assessed in binary systems. The solubility in ternary and higher order systems can be calculated by Thermo-Calc through the extrapolation from binary systems.

The BINARY_DIAGRAM module is applicable in Si containing binary systems to calculate the impurity solubility in silicon.

- There are 34 elements included: 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.
- 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 in TCSAB 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 TCSAB (2015).

References

1. T. Yoshikawa, K. Morita, S. Kawanishi and T. Tanaka. *J. Alloy. Comp.,* 490 (2010) 31-41.
2. K. Tang, E.J. Øvrelid, G. Tranell and M. Tangstad. *Material. Trans.* 50 (2009) 1978-1984.
3. C. Bergman, *J Phase Equilibria*, 13 (1992) 113-119.

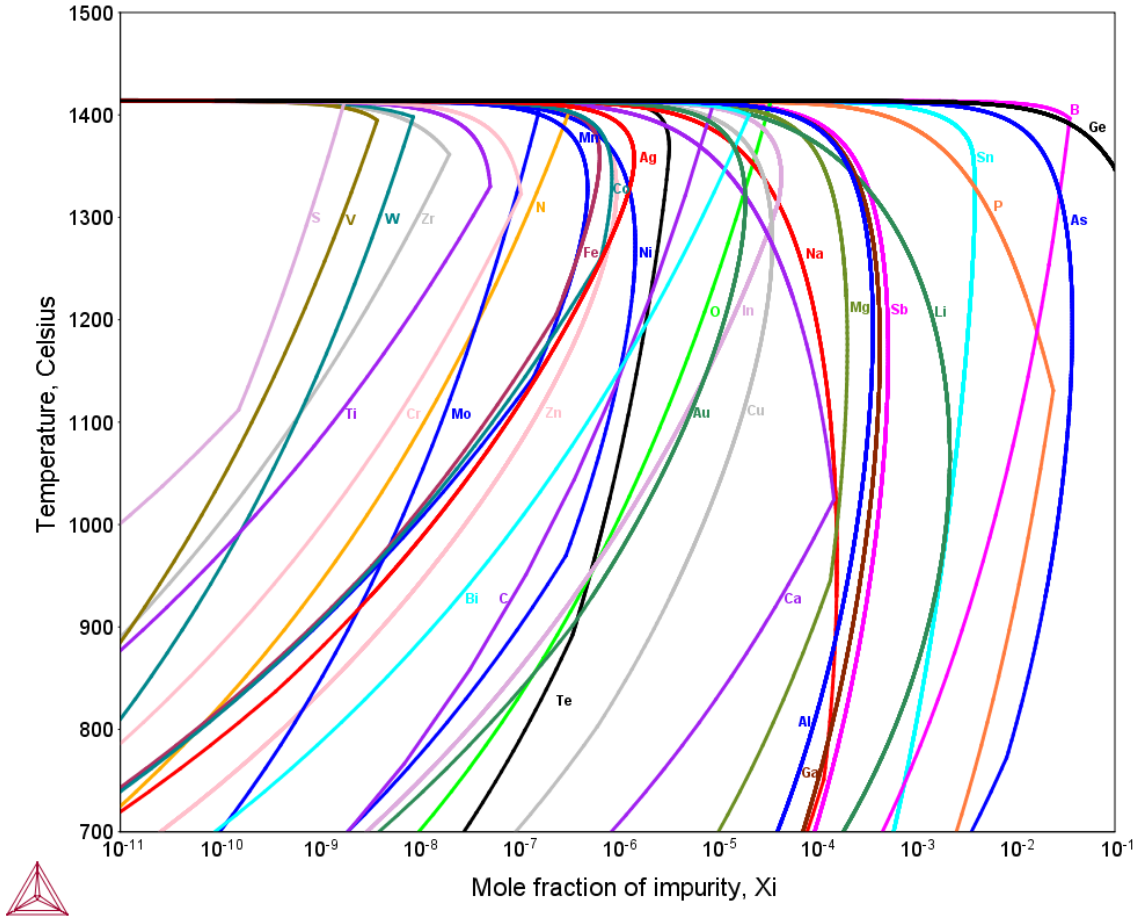

Fig.1. Calculated impurity solubility in Si-containing binaries using TCSI1.

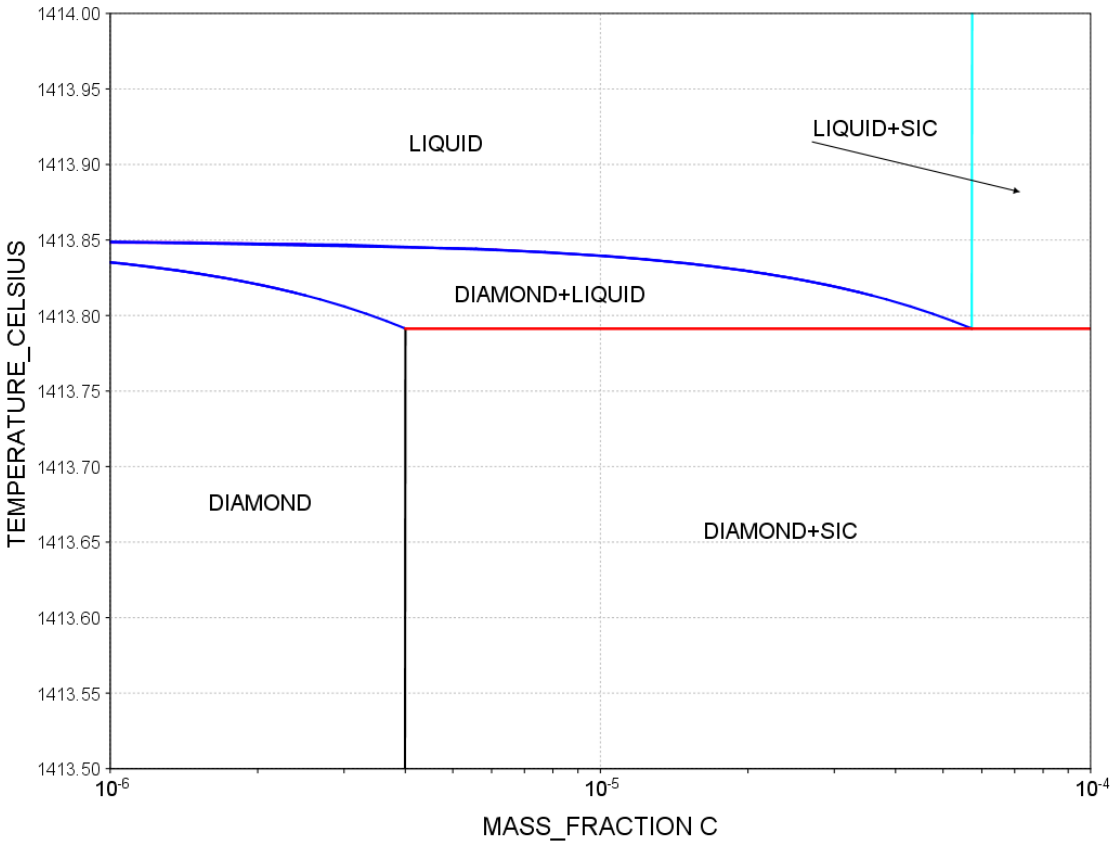

Fig. 2. TCSI1 predicted segregation coefficient (~ 0.07) between C content in the diamond phase (~ 4 ppmw) and that in the liquid phase (~ 57 ppmw) at the eutectic of diamond+SiC in the Si-C binary.

List of phases and corresponding 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 2 SUBL, SITES 93: 12: :B: CU SI B C:
CBCC_A12 2 SUBL, SITES 1: 1: :AL CO CR FE MG MN NI SI SN TI V ZN ZR: VA:
CUB_A13 2 SUBL, SITES 1: 1: :AG AL CO CR FE MG MN NI SI SN TI V ZN ZR: VA:
DHCP :AU IN SN:

FCC_A1 2 SUBL, SITES 1: 1: :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:
GRAPHITE :B C:
HCP_A3 2 SUBL, SITES 1: 0.5: :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:
HCP_ZN 2 SUBL, SITES 1: 0.5: :AG AL CR CU GA IN MG SI SN ZN: VA:
HEXAGONAL_A8 :TE:
LAVES_C14 2 SUBL, SITES 2: 1: :MN TI: MN TI:
LAVES_C15 2 SUBL, SITES 2: 1: :CR CU MG TI ZR: CR CU MG TI ZR:
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 2 SUBL, SITES 12: 7: :LI: SI:	QUARTZ :SIO2:
MG2SI_C1 2 SUBL, SITES 2: 1: :MG: GE SI SN:	TRIDYMITE :SIO2:
MN11SI19 2 SUBL, SITES 11: 19: :MN: AL SI:	SIP 2 SUBL, SITES 1: 1: :SI: P:
MOSI2_C11B 2 SUBL, SITES 1: 2: :MO: SI:	SIS 2 SUBL, SITES 1: 1: :SI: S:
M3SI_A15 2 SUBL, SITES 3: 1: :MO: SI:	SIS2 2 SUBL, SITES 1: 2: :SI: S:
M5SI3_D8M 3 SUBL, SITES 4: 1: 3: :MO: MO SI: MO SI:	SI2TE3_LT 2 SUBL, SITES 2: 3: :SI: TE:
SI3N4 2 SUBL, SITES 3: 4: :SI: N:	SI2TE3_HT 2 SUBL, SITES 2: 3: :SI: TE:
NASI_HT 2 SUBL, SITES 1: 1: :NA: SI:	SI2TI_C54 2 SUBL, SITES 2: 1: :GE SI: TI:
NASI_LT 2 SUBL, SITES 1: 1: :NA: SI:	FEB_B27 2 SUBL, SITES 1: 1: :TI ZR: SI GE:
NI2SI_HT 3 SUBL, SITES 1: 1: 1: :CU NI: NI VA: AL SI:	A6B5_OI44 2 SUBL, SITES 5: 6: :GE SN SI: V TI:
NI3SI2 2 SUBL, SITES 3: 2: :FE NI: SI:	SI2W_C11B 2 SUBL, SITES 2: 1: :SI: W:
AB_B31 2 SUBL, SITES 1: 1: :FE NI: GE SI ZN:	SI3W5_D8M 2 SUBL, SITES 3: 5: :SI: W:
NISI2 2 SUBL, SITES 2: 1: :AL CU SI ZN: CU FE MN NI:	SI2ZR_C49 2 SUBL, SITES 2: 1: :SI GE: ZR:
CRISTOBALITE :SIO2:	ALB2_C32 2 SUBL, SITES 1: 2: :AL: B:

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: