pTM 2020-06-14
Thermo Calc
VS Distributions

Constants $Rpg := 8.314$ J/K/mol $T0K := 273.15$ $PC := \frac{1}{760}$

Temperature $Tg := 625 + T0K$ $P := 20$

Energy $\Delta GSi(Tg) := 383.673 \cdot 1000 - Tg \cdot 267.7$ $\Delta GGe(Tg) := 348.9456 \cdot 1000 - Tg \cdot 282.4$

SiGe $\Omega i$ $\Omega i := 5060$

Flows $\phi T := 20$ $\phi Ge := \phi T \cdot 0.1$ $\phi H2 := 20000 - \phi T$

Partial Pressures $pzT := \frac{\phi T}{\phi H2 + \phi T} \cdot \frac{P}{PC}$ $pzH2 := \frac{\phi H2}{\phi H2 + \phi T} \cdot \frac{P}{PC}$ $pzGe := \frac{\phi Ge}{\phi H2 + \phi T} \cdot \frac{P}{PC}$

$pzSi(pzGe) := pzT - pzGe$

Solid Mole Fraction $x(pzGe, pSi, pGe) := \frac{pzGe - pGe}{pzSi(pzGe) - pSi + pzGe - pGe}$

Activities $aSi(pzGe, pSi, pGe) := (1 - x(pzGe, pSi, pGe)) \cdot e^{\frac{\Omega i}{Rpg \cdot Tg} \cdot x(pzGe, pSi, pGe)^2}$

$aGe(pzGe, pSi, pGe) := x(pzGe, pSi, pGe) \cdot e^{\frac{\Omega i}{Rpg \cdot Tg} \cdot (1 - x(pzGe, pSi, pGe))^2}$

Equilibrium Constants $KSi(pzGe, pSi, pGe) := \frac{aSi(pzGe, pSi, pGe) \cdot [2 \cdot (pzSi(pzGe) - pSi)]^2}{pSi}$

$KGe(pzGe, pSi, pGe) := \frac{aGe(pzGe, pSi, pGe) \cdot [2 \cdot (pzGe - pGe)]^2}{pGe}$

Kp $KSi0 := e^{-\frac{\Delta GSi(Tg)}{Rpg \cdot Tg}}$ $KGe0 := e^{-\frac{\Delta GGe(Tg)}{Rpg \cdot Tg}}$

Guess $pSi := 10^{-1}$ $pGe := \frac{pSi}{10}$

Solve Block

Given

$KSi(pzGe, pSi, pGe) = KSi0$

$KGe(pzGe, pSi, pGe) = KGe0$

$f(pzGe) := Minerr(pSi, pGe)$

$f(pzGe) := \begin{pmatrix} NaN \\ NaN \end{pmatrix}$ on error $f(pzGe)$

$pzT \cdot 101325 = 1.54 \times 10^6$

$pzSi(pzGe) \cdot 101325 = 1.39 \times 10^6$

$pzGe \cdot 101325 = 1.54 \times 10^5$

Check function

$f(0.1) = \begin{pmatrix} 15.09981 \\ 0.09968 \end{pmatrix}$

Program

$$MX := \left| \begin{array}{l} N \leftarrow 100 \\ \text{for } I \in 1 .. 99 \\ \quad \left| \begin{array}{l} pzSi \leftarrow \dfrac{\phi T}{\phi H2 + \phi T} \cdot \dfrac{P}{PC} \cdot \dfrac{N - I}{N} \\ pzGe \leftarrow \dfrac{\phi T}{\phi H2 + \phi T} \cdot \dfrac{P}{PC} \cdot \dfrac{I}{N} \\ sol \leftarrow f(pzGe) \\ MAT_{I,0} \leftarrow I \\ MAT_{I,1} \leftarrow pzSi \\ MAT_{I,2} \leftarrow pzGe \\ MAT_{I,3} \leftarrow sol_0 \\ MAT_{I,4} \leftarrow sol_1 \\ MAT_{I,5} \leftarrow \dfrac{pzGe}{pzSi + pzGe} \\ MAT_{I,6} \leftarrow \dfrac{pzGe - sol_1}{pzSi - sol_0 + pzGe - sol_1} \end{array} \right. \\ MAT \end{array} \right.$$

Slope

$N0 := 20 \quad N := 50$

$$lnXX := \left| \begin{array}{l} \text{for } I \in N0 .. N \\ \quad Buffer_I \leftarrow \ln\left(MX_{I,5}\right) \\ Buffer \end{array} \right. \qquad lnYY := \left| \begin{array}{l} \text{for } I \in N0 .. N \\ \quad Buffer_I \leftarrow \ln\left(MX_{I,6}\right) \\ Buffer \end{array} \right.$$

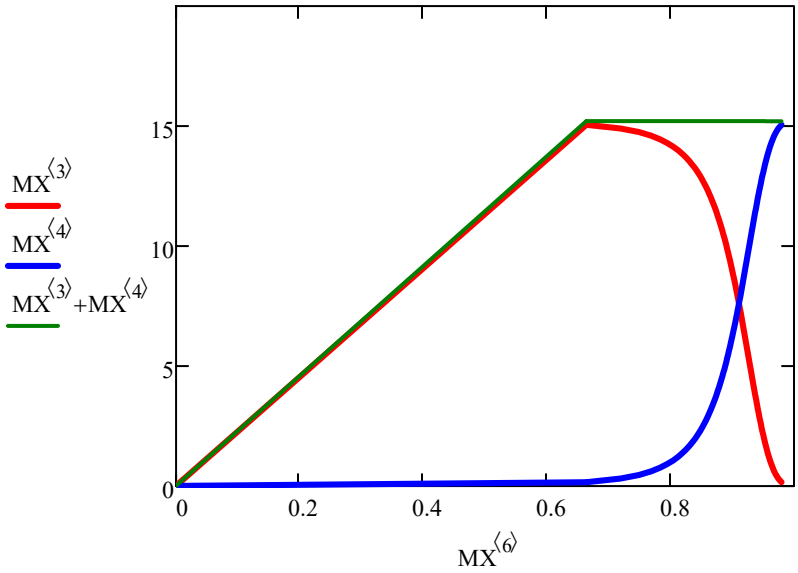
$lnX := submatrix(lnXX, N0, N, 0, 0)$ $\quad lnY := submatrix(lnYY, N0, N, 0, 0)$

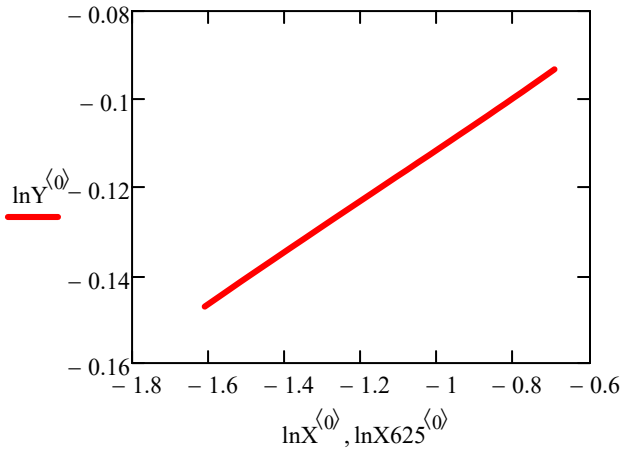
$slp := slope(lnX, lnY)$ $\quad slp = 0.059$

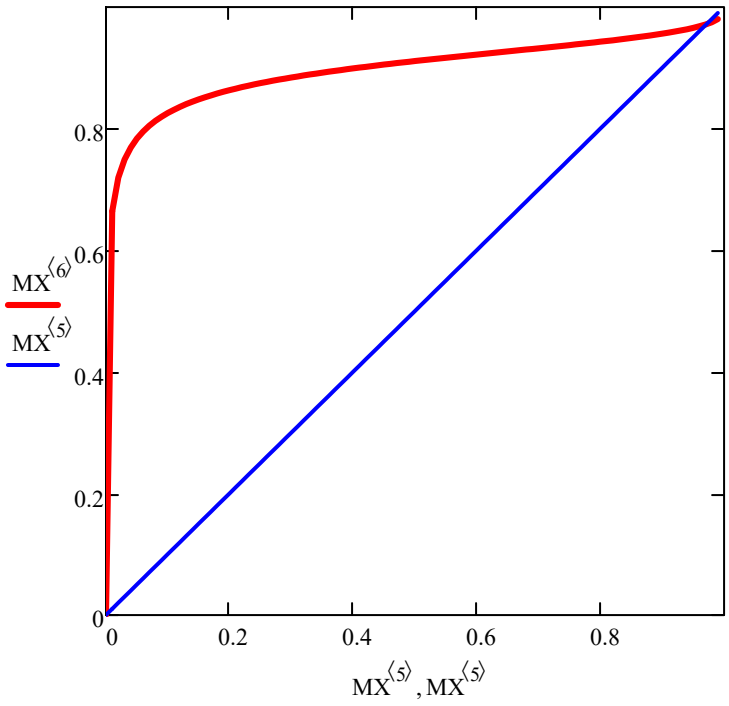
Export

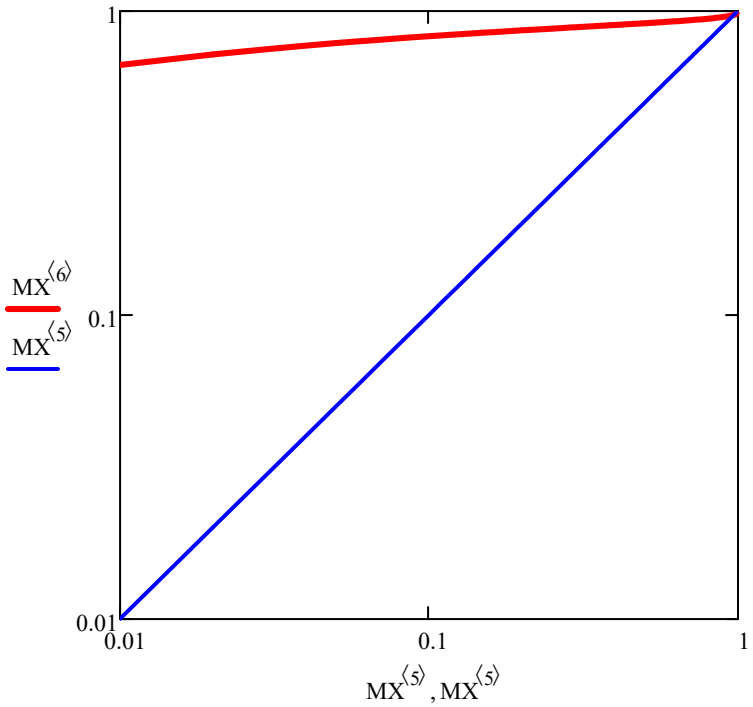
$Filepath := "C:\Temp\SiGe-650C-0.02.xlsx"$

$Dummy := WRITEEXCEL(MX, Filepath)$


MX⟨3⟩
MX⟨4⟩
MX⟨3⟩+MX⟨4⟩
15
10
5
0
0
0.2
0.4
0.6
0.8
MX⟨6⟩


lnY⟨0⟩
− 0.08
− 0.1
− 0.12
− 0.14
− 0.16
− 1.8
− 1.6
− 1.4
− 1.2
− 1
− 0.8
− 0.6
lnX⟨0⟩, lnX625⟨0⟩


0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
MX⟨6⟩
MX⟨5⟩
MX⟨5⟩ , MX⟨5⟩


1
0.1
0.01
0.01
0.1
1
MX⟨6⟩
MX⟨5⟩
MX⟨5⟩ , MX⟨5⟩

MX =

| | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1 | 1 | 15.048 | 0.152 | 15.0478 | 0.15161 | 0.01 |
| 2 | 2 | 14.896 | 0.304 | 14.89579 | 0.30346 | 0.02 |
| 3 | 3 | 14.744 | 0.456 | 14.74378 | 0.45535 | 0.03 |
| 4 | 4 | 14.592 | 0.608 | 14.59178 | 0.60726 | 0.04 |
| 5 | 5 | 14.44 | 0.76 | 14.43977 | 0.75918 | 0.05 |
| 6 | 6 | 14.288 | 0.912 | 14.28777 | 0.91111 | 0.06 |
| 7 | 7 | 14.136 | 1.064 | 14.13577 | 1.06304 | 0.07 |
| 8 | 8 | 13.984 | 1.216 | 13.98376 | 1.21498 | 0.08 |
| 9 | 9 | 13.832 | 1.368 | 13.83176 | 1.36692 | 0.09 |
| 10 | 10 | 13.68 | 1.52 | 13.67976 | 1.51886 | 0.1 |
| 11 | 11 | 13.528 | 1.672 | 13.52776 | 1.67081 | 0.11 |
| 12 | 12 | 13.376 | 1.824 | 13.37576 | 1.82276 | 0.12 |
| 13 | 13 | 13.224 | 1.976 | 13.22376 | 1.97471 | 0.13 |
| 14 | 14 | 13.072 | 2.128 | 13.07175 | 2.12667 | 0.14 |
| 15 | 15 | 12.92 | 2.28 | 12.91975 | 2.27862 | ... |