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Thermodynamic Properties of Se-Te(l) Described by an Extension of the Two Domain Model

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Abstract

The two domain model of Se-Te liquid is developed further than heretofore. Explicit equations are obtained for the excess Gibbs energy of mixing, the chemical potentials, the enthalpy of mixing, the relative constant pressure heat capacity, and the partial and total pressures. A generally satisfactory fit is obtained for the experimental activity of Te and enthalpy of mixing at 733 K, the relative heat capacity as a function of temperature, and for the total pressure for 99, 60, and 27 at.% Se between about 780 and 1130 K. This is done while leaving unchanged the site fraction of H or (Te-like) and L (or Se-like) domains previously used to fit a number of physical properties.

Keywords

chemical potential, thermodynamic modeling, thermodynamic properties

1. Introduction

Se-Te liquid has been the subject of a number of thermodynamic and physical measurements, which have been described by Tsuchiya[1] and Tsuchiya and Seymour[2] with a “Two Domain” model. This model envisions the liquid as consisting of two types of domain or cluster each of which contains twenty atoms, are of the same composition, and which are distributed at random. The domains differ in structure. One type called H dominates at high temperature and has the tri-coordinated structure of tellurium. The other low temperature L type has the dicoordinated structure of selenium. Among the properties described,[1] are the Knight shift, magnetic susceptibility, molar volume, temperature coefficient of expansion, electrical conductivity, which changes from semiconducting to metallic with increasing temperature, thermoelectric power, and sound velocity. In all these cases the behavior is assumed to depend only on the site fractions of domains which in turn depend on the difference in the Gibbs energies of the H and L domains. From this model, equations have been given[1,3] for the enthalpy and heat capacity of mixing which do not seem to follow from thermodynamic arguments. The enthalpy of mixing does not go to zero at 100 at.% Se as it should.[1] Equations for the chemical potentials are not given. These are needed to determine the partial pressures of tellurium and selenium species over the liquid. Another analysis has been given which does give equations for both the enthalpy of mixing and the component activities. We reserve discussion to section 4 on Results. The purpose here is to extend the formulation of the model and specify a general form for its composition and temperature dependence. The experimental enthalpy of mixing, relative heat capacity, activity of tellurium, and total pressure are then fit without changing the parameters that determine the site fraction of domains and therefore the property descriptions given by Tsuchiya.[1]

2. The Two Domain Thermodynamic Model

The Gibbs energy of the two domain model was originally written[1] as:

$$G = CG_H + (1 - C)G_L + (RT/m)(C \ln(C) + (1 - C) \ln(1 - C)) \quad (\text{Eq 1})$$

where C is the site fraction of tellurium-like or H domains and $(1 - C)$ is that of selenium-like or L domains, G_H and G_L are the corresponding Gibbs energies of the domains, and m is the number of atoms in each domain, which was determined to be 20 by Tsuchiya.[1] This form results from the random mixing of two equi-sized domains. The equilibrium value for the site fraction of H domains, C , is the solution of $\partial G/\partial C = 0$ and is given by

$$\frac{C}{1 - C} = \exp(-m(G_H - G_L)/RT) = \exp(-mG_{HL}/RT) \quad (\text{Eq 2})$$

where

$$G_{HL} = G_H - G_L \quad (\text{Eq 3})$$

These Gibbs energies are written here as

$$G_{HL} = (A_{HL} + X_{Te}B_{HL}); G_L = X_{Te}X_{Se}(A_L + X_{Se}B_L) \quad (\text{Eq 4})$$

where A_{HL} ; B_{HL} ; A_L ; and B_L are all functions of temperature and independent of composition, the X 's are atom fractions and where, following Tsuchiya, we omit the factor $X_{Te}X_{Se}$ in G_{HL} .

Here we start with the Gibbs energy of mixing as

$$\Delta G_M = X_{Te}RT \ln(X_{Te}) + X_{Se}RT \ln(X_{Se}) + \Delta G_M^x \quad (\text{Eq 5})$$

The excess Gibbs energy of mixing is obtained by subtracting the values of Eq 1 at $X_{Te} = 0$ and 1 from Eq 1 to give,

$$\begin{aligned} \Delta G_M^x = & C G_{HL} + G_L + (RT/m)(C \ln(C) + (1 - C)\ln(1 - C)) \\ & - X_{Se} \left[C_0 G_{HL}(0, T) + \frac{RT}{m} (C_0 \ln(C_0) + (1 - C_0)\ln(1 - C_0)) \right] \\ & - X_{Te} \left[C_1 G_{HL}(1, T) + \frac{RT}{m} (C_1 \ln(C_1) + (1 - C_1)\ln(1 - C_1)) \right] \end{aligned} \quad (\text{Eq 6})$$

where for brevity C_0 means that C , which is a function of X_{Te} and T , is evaluated at $X_{Te} = 0$ while C_1 means it is evaluated at 1 and similarly for $G_{HL}(0, T)$ and $G_{HL}(1, T)$.

When $X_{Te} = 0$ or 1 then $\Delta G_M^x = 0$ so that ΔG_M^x is a Gibbs energy of mixing from the pure liquid elements. Finally, when the domains each have zero Gibbs energy so that $G_H = G_L = 0$, then $C = 1/2$ at all temperatures and compositions, the excess Gibbs energy for the solution is zero, and the Gibbs energy is that for an ideal solution. When $G_H = G_L \neq 0$, then again $C = 1/2$ at all temperatures and compositions but the equations reduce to those of a subregular solution.

The general form for the temperature dependence of the parameters of Eq 4 adopted here is that generally used for high temperature properties of condensed phases,

$$\begin{aligned} A_{HL} &= A_{HL1} + A_{HL2}T + A_{HL3}T^2 \\ B_{HL} &= B_{HL1} + B_{HL2}T + B_{HL3}T^2 \\ A_L &= A_{L1} + A_{L2}T + A_{L3}T^2 + A_{L4}T \ln(T) + A_{L5}/T \\ B_L &= B_{L1} + B_{L2}T + B_{L3}T^2 + B_{L4}T \ln(T) + B_{L5}/T \end{aligned} \quad (\text{Eq 7})$$

The temperature dependence of A_{HL} and B_{HL} are limited to just beyond what is required to obtain Tsuchiya's function for C but is easily extended if that should prove necessary. A standard thermodynamic equation gives the enthalpy of mixing as

$$\Delta H_M = -T^2 \partial(\Delta G_M^x/T) / \partial T \quad (\text{Eq 8})$$

For our model this leads to

$$\begin{aligned}\Delta H_M &= C(G_{HL} - TG'_{HL}) + (G_L - TG'_L) \\ &\quad - X_{Se}C_0 [G_{HL}(0, T) - TG'_{HL}(0, T)] \\ &\quad - X_{Te}C_1 [G_{HL}(1, T) - TG'_{HL}(1, T)]\end{aligned}$$

(Eq 9)

Here the prime superscript stands for the temperature derivative and C_0 and C_1 have the meanings given after Eq 6. With the definitions of G_{HL} and G_L given in Eq 4 and those of the parameters therein given by Eq 7 the enthalpy of mixing can be written explicitly as,

$$\begin{aligned}\Delta H_M &= C[A_{HL1} + X_{Te}B_{HL1} - (A_{HL3} + X_{Te}B_{HL3})T^2] \\ &\quad + X_{Te}X_{Se}[A_{L1} + X_{Se}B_{L1} - (A_{L4} + X_{Se}B_{L4})T \\ &\quad - (A_{L3} + X_{Se}B_{L3})T^2 + 2(A_{L5} + X_{Se}B_{L5})/T] \\ &\quad - X_{Se}C_0(A_{HL1} - A_{HL3}T^2) \\ &\quad - X_{Te}C_1 - [A_{HL1} + B_{HL1} - (A_{HL3} + B_{HL3})T^2]\end{aligned}$$

(Eq 10)

The constant pressure heat capacity of mixing follows as the temperature derivative of the enthalpy of mixing,

$$\begin{aligned}\Delta C_{P,M} &= C'(G_{HL} - TG'_{HL}) - CTG''_{HL} - TG''_L \\ &\quad - X_{Se}C'_0[G_{HL}(0, T) - TG'_{HL}(0, T)] \\ &\quad + X_{Se}C_0TG''_{HL}(0, T) \\ &\quad - X_{Te}C'_1[G_{HL}(1, T) - TG'_{HL}(1, T)] \\ &\quad + X_{Te}C_1TG''_{HL}(1, T) \\ &\quad \text{where as before } ' = \partial/\partial T \text{ and now } '' = \partial^2/\partial T^2\end{aligned}$$

(Eq 11)

Again the heat capacity can be written explicitly as

$$\begin{aligned}\Delta C_{P,M} &= C' [A_{HL1} - A_{HL3}T^2 + X_{Te}(B_{HL1} - B_{HL3}T^2)] \\ &\quad - 2CT(A_{HL3} + X_{Te}B_{HL3}) \\ &\quad - X_{Te}X_{Se}[2A_{L3}T + A_{L4} - 2A_{L5}/T^2 \\ &\quad + X_{Se}(2B_{L3}T + B_{L4} - 2B_{L5}/T^2)] \\ &\quad - X_{Se}C'_0[A_{HL1} - A_{HL3}T^2] + 2X_{Se}C_0TA_{HL3} \\ &\quad - X_{Te}C'_1[A_{HL1} + B_{HL1} - (A_{HL3} + B_{HL3})T^2] \\ &\quad + 2X_{Te}C_1T(A_{HL3} + B_{HL3})\end{aligned}$$

(Eq 12)

It is interesting in its own right and will be useful in our discussion in section 4 on Results to have the heat capacity in a different but equivalent form. What is needed for the purpose of comparison is not the

relative constant pressure heat capacity but the constant pressure heat capacity, which is obtained by dropping the last two lines in Eq 12. Then using the standard thermodynamic relations,

$$\begin{aligned}\partial G_k / \partial T &= -S_k ; C_{P,k} = T \partial S_k / \partial T ; \\ H_k &= G_k + T S_k ; k = H \text{ or } L,\end{aligned}$$

(Eq 13)

in the truncated version of Eq 12 along with Eq 2 for C one obtains the heat capacity as

$$C_p = C C_{P,H} + (1 - C) C_{P,L} + m C (1 - C) (H_H - H_L)^2 / RT^2$$

(Eq 14)

The first two terms of Eq 14 can be viewed as conventional contributions to the heat capacity such as those from atomic vibrations while the last term is the contribution due to the changing value of C with temperature, a feature of the two domain model.

Finally, the excess chemical potentials are obtained with the formulae

$$\begin{aligned}\mu_{Te}^x &= RT \ln \gamma_{Te} = \Delta G_m^x + X_{Se} \partial (\Delta G_m^x) = \partial X_{Te} \\ \mu_{Se}^x &= RT \ln \gamma_{Se} = \Delta G_m^x - X_{Te} \partial (\Delta G_m^x) = \partial X_{Te}\end{aligned}$$

(Eq 15)

where γ_{Te} and γ_{Se} are the activity coefficients of components of Te and Se, respectively. For the model here

$$\begin{aligned}\mu_{Te}^x &= C(A_{HL} + B_{HL}) + X_{Se}^2(A_L + X_{Se}B_L) \\ &+ (RT/m)(C \ln(C) + (1 - C) \ln(1 - C)) \\ &- C_1(A_{HL} + B_{HL}) - (RT/m)(C_1 \ln(C_1) \\ &+ (1 - C_1) \ln(1 - C_1)) \\ \mu_{Se}^x &= CA_{HL} + X_{Te}^2(A_L + X_{Se}B_L) \\ &+ (RT/m)(C \ln(C) + (1 - C) \ln(1 - C)) \\ &- C_0 A_{HL} - (RT/m)(C_0 \ln(C_0) + (1 - C_0) \ln(1 - C_0))\end{aligned}$$

(Eq 16)

With the excess chemical potentials and through them the activity coefficients determined, the partial pressures of diatomic tellurium and selenium are given by

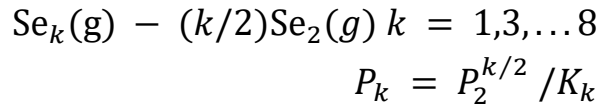
$$P_{Te_2} = (X_{Te} \gamma_{Te})^2 P_{Te_2}^0 ; P_{Se_2} = (X_{Se} \gamma_{Se})^2 P_{Se_2}^0$$

(Eq 17)

where $P_{Te_2}^0$ and $P_{Se_2}^0$ are the partial pressures of the diatomic species in the saturated vapors of the pure elements.

3. Remaining Input Data

Some additional data and assumptions are now discussed which are necessary in order to calculate the partial pressures in the vapor phase. We assume the vapor species are diatomic tellurium, SeTe, and selenium species Se_j with j running from 1 through 8 and with equilibria described by



(Eq 18)

The equilibrium constants are given in Table 1 and are from the critical compilation of Mills.[4]

The total vapor pressure[5] is

$$\log_{10}(P(\text{bar})) = -4989.5/T + 5.2135$$

(Eq 19)

Finally, an equation for the standard Gibbs energy of formation of $Se_2(g)$ from two $Se(l)$ has been constructed from the thermodynamic data in Mills[4] and is given by

$$\begin{aligned} \Delta G_f^o &= -8:3145T \ln(P_{Se_2}^o) \\ &= 25:6906T \ln(T) + .00132842T^2 - 314:251T \\ &\quad + 125100/T + 137405 \end{aligned}$$

(Eq 20)

The saturated vapor of pure tellurium is 99% Te_2 . As the temperature is decreased towards the melting point the vapor pressure drops[6] below the linear $\log(P)$ versus $1/T$ relation given by Brooks,[5] being about 15% lower in P at the melting point. In a third law analysis[7] of the tellurium crystal-liquid-vapor equilibrium the temperature above the melting point was divided into four intervals and the logarithm of the vapor pressure in each given as a linear function of $1/T$. These equations can be represented to better than 2% by the single equation,[8]

$$\begin{aligned} \log_{10} P(\text{bar}) &= 4:41420 - 5267.68/T - 368192.2/T^2 \\ &\quad 722.65 < T < 1434 \end{aligned}$$

(Eq 21)

Above 847 K this equation agrees with that given by Brooks to better than 2%. Below 847 K and with decreasing temperature it falls below Brooks' equation, as much as 15% at the melting point of 723 K. Since as noted above the saturated vapor is 99% diatomic tellurium $P_{Te_2}^o$ can be taken as equal to the total pressure.

Finally, the partial pressure of SeTe is given by

$$P_{SeTe} = (P_{Te_2} P_{Se_2} K_f^o)^{1/2}$$

(Eq 22)

Mass spectrograph-Knudsen cell measurements[9] between 1400 and 1640 K give

$$K_f^0 = 3.162 \exp(-1531/8:3145/T)$$

(Eq 23)

A second study from electron impact-Knudsen cell measurements[10] between 800 and 1000 K gives 2.596 for the pre-exponential factor and 15000 for the enthalpy. Between 733 and 1123 K these give an equilibrium constant about 1/3 to 1/5 that of Eq 23.

4. Results and Discussion

The difference in the Gibbs energies of the H and L domains was determined from Fig. 3 in Tsuchiya[1] which shows $m\Delta S_{\text{GHL}}$ and $m\Delta H_{\text{GHL}}$ versus X_{Te} . Taking $m = 20$ we find

$$G_{\text{HL}} = G_{\text{H}} - G_{\text{L}} = 3500 - (2.0 + 3.75X_{\text{Te}}) T$$

(Eq 24)

Table 1 Equilibrium constants for the selenium species equilibria described by Eq 18 $\log_{10} K = A/T + B + C \log T$

	K_1	K_3	K_4	K_5	K_6	K_7	K_8
A	8655	-1716	-4984	-10984	-14775	-17956	-21027
B	-2.585	1.428	5.336	12.06	16.83	20.96	25.877
C	-0.101	0.454	-0.119	-0.129	-0.478	-0.675	-1.015

Referring to Eq 4 and 7 one can see that that the three numbers in Eq 24 are the parameters, A_{HL1} , A_{HL2} , and B_{HL2} . We retain these values in what follows so that, as can be seen by Eq 2, the value of C as a function of X_{Te} and T is then fixed regardless of our specification of the parameters in G_{L} . Isotherms of C as a function of X_{Se} are shown in Fig. 1. As the temperature is increased from 733 to 1123 K, high values for the site fraction of the Te- like or H domains cover more and more of the composition range. According to the figure pure liquid Te contains about 10% of the L domain at 733 K.

Fits to the remaining thermodynamic properties were made with Eq 22 for the partial pressure of SeTe(g) and the following equation for G_{L} ,

$$G_{\text{L}} = X_{\text{Te}}X_{\text{Se}}[-16280. + 28.459T - 0.013600T^2 + X_{\text{Te}}(8033.1 - 4.6005T)]$$

(Eq 25)

The results are shown in the following figures. Figure 2 shows the activity coefficients at 733 K versus the atom fraction of Se. The curves are calculated. The circles for Te show experimental values obtained from emf measurements and given in table 2a of Ref 11. The squares for Se presumably were obtained by a Gibbs-Duhem integration.

Figure 3 shows the enthalpy of mixing of the liquid Se-Te liquid from liquid tellurium and selenium at 733 K as a function of the atom fraction of Se. The curve is calculated while the symbols represent drop calorimetry measurements from three studies.[12-14] Both experimental and calculated enthalpies show a minimum value of about -2550 J/g-atom at about 41 at.% Se. Calculated isotherms between 733 and 1123 K for the enthalpy of mixing are shown in Fig. 4. The calculated enthalpy of mixing becomes less negative with increasing temperature and eventually is positive over the entire composition range at 1023 and 1123 K.

In Ref 12, equations have been derived for the enthalpy of mixing and component activities based on a two domain model in which the domains are confined to the tellurium liquid and do not appear in the Se-Te liquid. The experimental activity of Te and the enthalpy of mixing at 733 K are both fit well but only to about 50 and 60 at.% Te, respectively. This is a limit recognized by the authors themselves. The calculated activity continues to increase beyond one and the enthalpy of mixing similarly continues to become more negative instead of approaching zero as the atom fraction of Te approaches one.

Figure 5 shows the relative constant pressure heat capacity versus temperature for 30, 50, and 70 at.% Se. The filled symbols are from measurements[15] with an adiabatic scanning calorimeter and are scaled from their Fig. 6. The matching open symbols are calculated. Although the calculated values are only in fair agreement with experiment, the qualitative features are correct. The 30 and 50 at.% compositions show maxima, that for 50 at.% occurring at the higher temperature. Both the experimental and calculated values for 70 at.% appear to be approaching a maximum beyond the upper temperature of the figure. Calculated isotherms are shown in Fig. 6 as a function of composition. The maximum relative heat capacity moves to higher atom fraction of Se with increasing temperature.

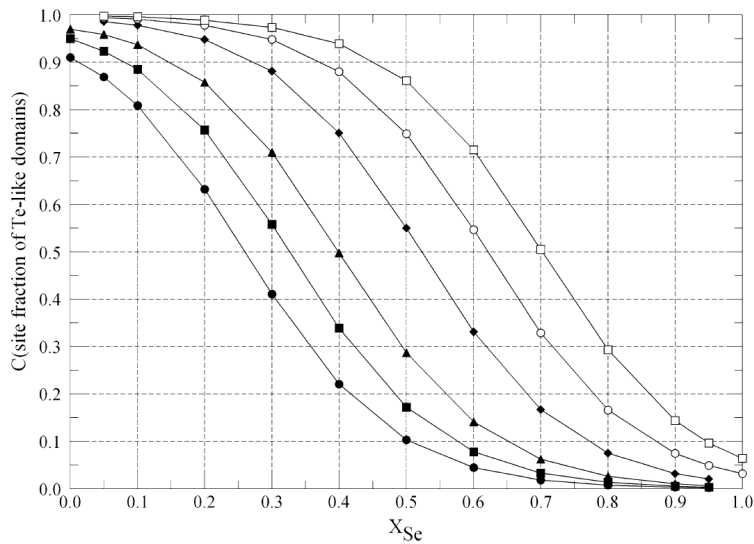


Fig. 1 Isotherms of the site fraction of H or Te-like domains in Se-Te liquid as a function of the atom fraction of Se. From top to bottom the temperatures are 1123, 1023, 923, 823, 773, and 733 K

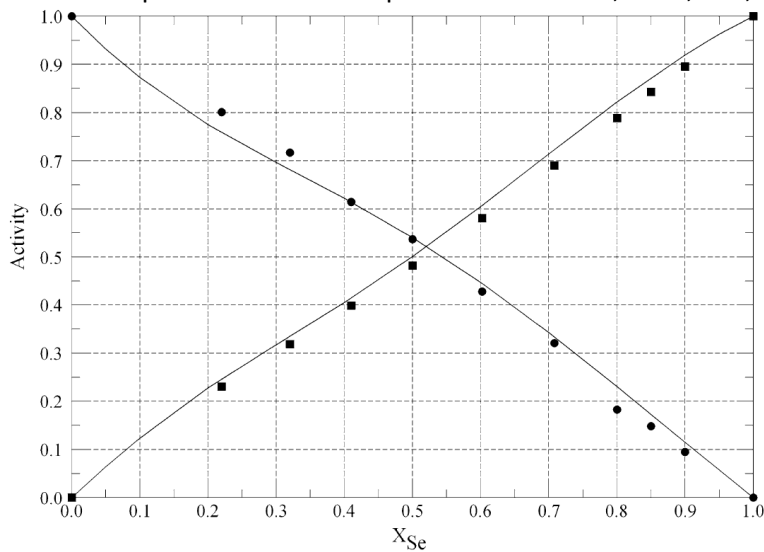


Fig. 2 Activity of Te and Se in Se-Te liquid at 733 K as a function of the atom fraction of Se. Curves are calculated. Circles for Te are from emf meas which are given in Table 2a in Ref 11. Squares obtained by Gibbs-Duhem integration in Ref 11

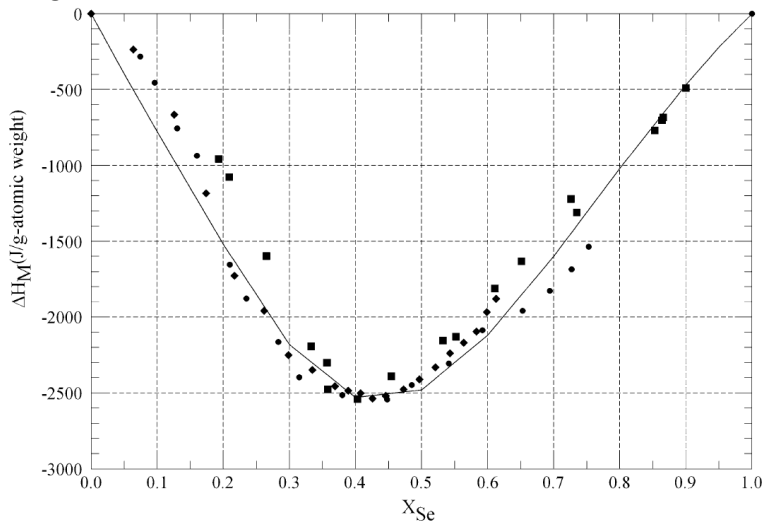


Fig. 3 Enthalpy of mixing of Se-Te liquid from its liquid elements at 733 K as a function of the atom fraction of Se. The curve is calculated. Symbols are from tabulated drop calorimetry measurements. Circles; Ref 12, Triangles; Ref 13, Squares; Ref 14

An analysis[16] of liquid tellurium with the two domain model has been made using Eq 14 for the heat capacity. Equation 2 was first used to fit the experimental Knight shift and fix the parameters of the Gibbs energy G_{HL} of Eq 3 and 4 and thus the value of C with temperature. Then since C was essentially unity at the highest temperatures of the experimental measurements, it was assumed the first two terms of Eq 14 for the heat capacity are dominant there. These values were extrapolated back to the lower temperatures and the excess of the experimental heat capacity over the extrapolated values assumed to be due to the last term of Eq 14. The model parameters were found to be

$$G_{HL} = 4200 - 6.5T; m = 14$$

(Eq 26)

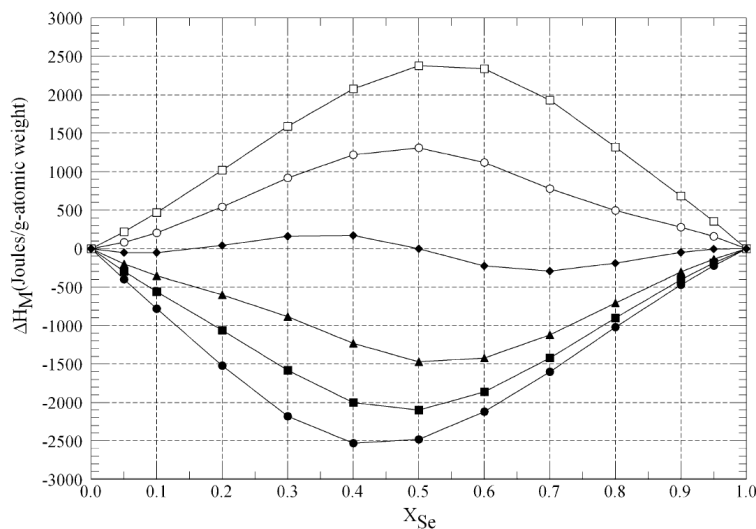


Fig. 4 Calculated isotherms for the enthalpy of mixing as a function of the atom fraction of Se. From top to bottom; 1123, 1023, 923, 823, 773, 733 K

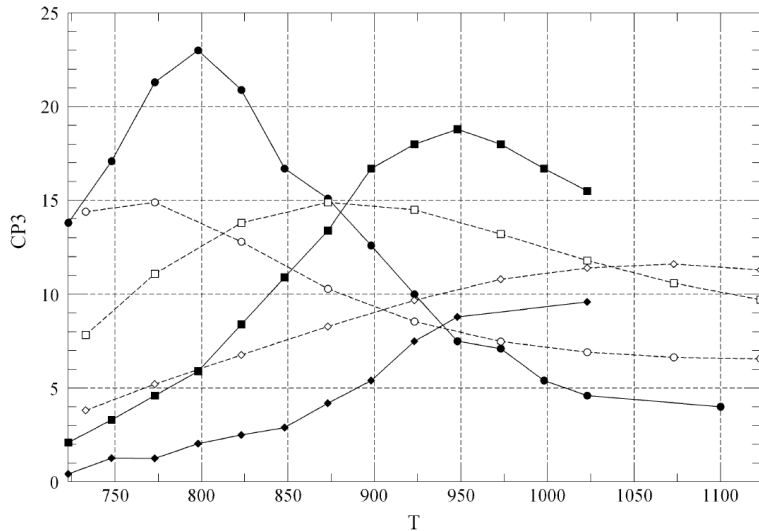


Fig. 5 Experimental constant pressure heat capacity of mixing from ref 15 for 30, 50, and 70 at.% Se as circles, squares, and diamonds, respectively, as a function of temperature. The calculated values are given by the corresponding open symbols along dashed curves

Ideally the results should be the same as those given by Eq 24 with $X_{Te} = 1$ but are only roughly the same.

Silica membrane pressure measurements have been reported[17] between 909 and 1111 K.

For 50 at.% Se values of 0.08 and 1.6 bar were obtained at the temperature limits compared to calculated values of 0.11 and 1.6 bar. For 62 at.% Se, values of 0.17 and 2.4 bar were obtained compared to calculated values of 0.15 and 2.4 bar, showing excellent agreement for both compositions. Extensive boiling point measurements have been made[18] for a range of liquid compositions and temperatures and the composition of the vapor determined. Tabulated values are given for liquid composition, temperature, total pressure, and vapor composition. The two phase, two component system has two degrees of freedom by the Gibbs phase rule. For our analysis we choose liquid composition and temperature as independent variables and calculate the remaining quantities to obtain the fractional difference between the experimental total pressures and our calculated values and similarly the fractional difference in the atom fraction of Se in the vapor phase. The calculated total pressure is between 10 and 20% lower than experiment from 0 and 70% Te for all temperatures. Between 70 and 100 at.% Te the fractional difference in the total pressure becomes more scattered but generally becomes more negative with increasing Te content, reaching 50 to 100% near 0 at.% Te. The fractional difference in atomic % Se in the vapor phase goes from 0 to -10% as the atomic fraction of Te increases from 0 to about 50 at.% then becomes increasingly positive with increasing at.% Te, reaching 70% near 100% Te. So by this measure there is fair agreement between experiment and calculation only for compositions above about 30 at.% Se. Figure 7 shows the experimental and calculated total pressures for nominal compositions of 99, 60, and 27 at.% Se. Compositions are grouped together which are the same within plus or minus 1 at.%. The agreement is good.

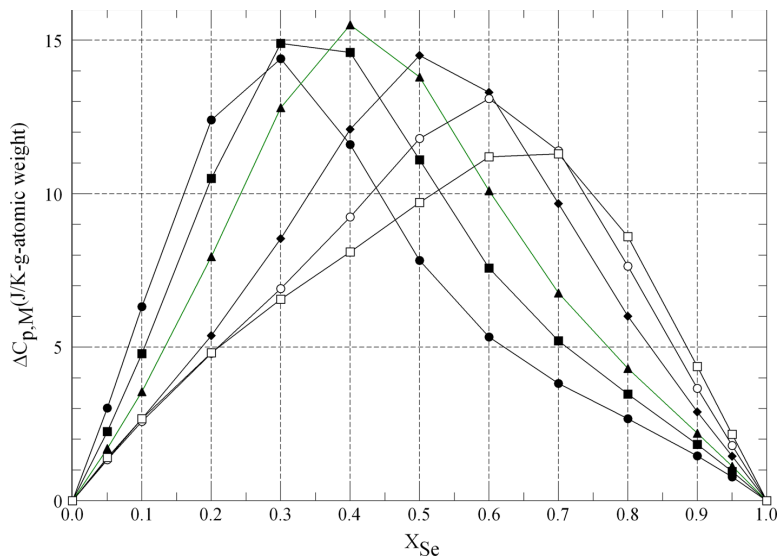


Fig. 6 Calculated isotherms for the constant pressure heat capacity of mixing as a function of composition. From top to bottom at $X_{Se} = 0:25, 733, 773, 823, 923, 1023, 1123$ K

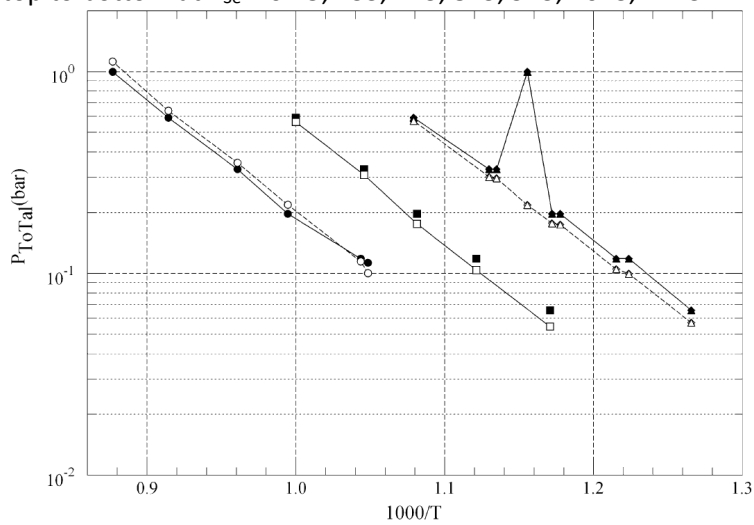


Fig. 7 Total pressure as a function of reciprocal temperature. Filled symbols are from Ref 18, open symbols are from calculation. Triangles are for 99, squares for 60, circles for 27 at.% Se

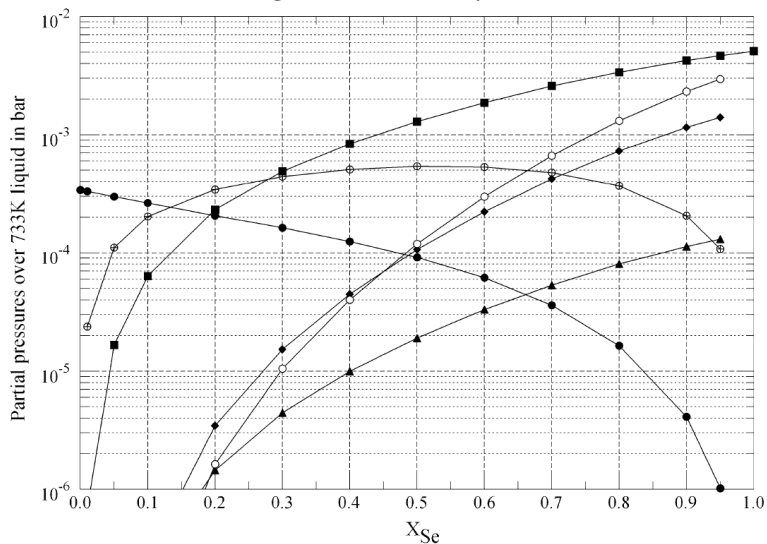


Fig. 8 Calculated partial pressures at 733 K as a function of the atom fraction of Se. At $X_{\text{Se}} = 0:60$ and from top to bottom, Se_2 , SeTe , Se_5 , Se_4 , Te_2 , Se_3

Partial pressures at 733 K are shown as a function of the atom fraction of Se in Fig. 8. Over most of the composition range Se_2 , and SeTe are the predominant species with Te_2 following below 50 at.% Se. Above 70 at.% Se Se_4 and Se_5 become important.

5. Summary

The two domain model previously applied to Se-Te liquid is given a more complete thermodynamic formulation and fits are obtained to the experimental activity of Te and enthalpy of mixing at 733 K, the relative constant pressure heat capacity, and the total pressure over an extensive range of composition and temperature. This is done while leaving unchanged that part of the model that has already been used to account for a large number of physical properties. This is accomplished by retaining the original[1] composition and temperature dependence of the difference in Gibbs energies of the Te-like and Se-like domains, G_{HL} , and the dependence of the fraction of domains, C , upon it. The fits are generally very good except for the calculated relative heat capacities, which are only qualitatively correct, and the total pressures at Se compositions below about 27 at.%.

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