Se – Te (Selenium – Tellurium)

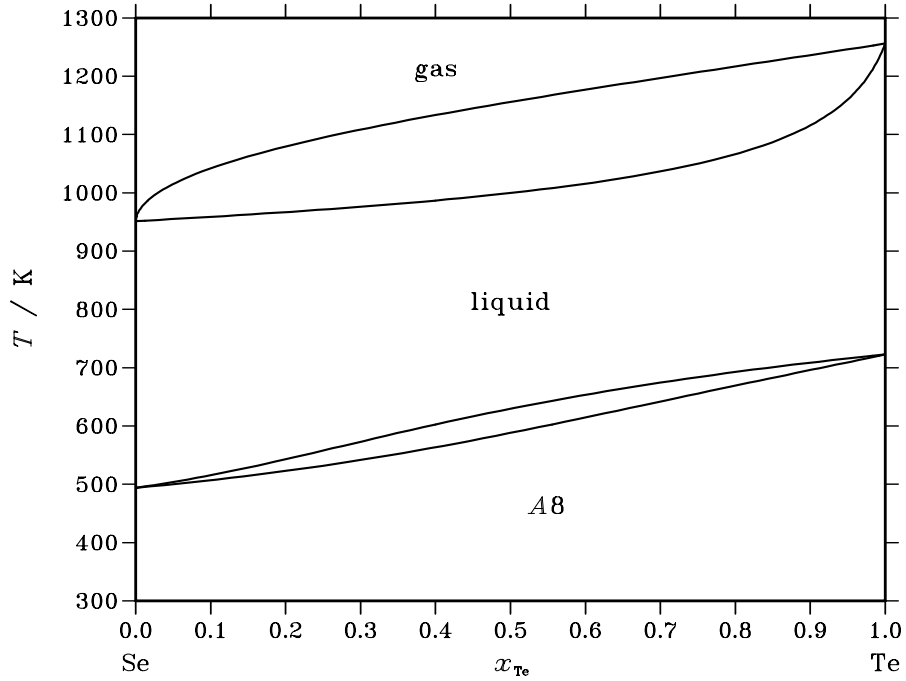

Fig. 1. Calculated phase diagram for the system Se-Te.

The Se-Te system has been studied by [86Mor] and assessed by [88Gho]. The system is apparently very simple because it presents complete mutual solubility in the liquid and solid phases. The structure of the liquid is rather complicated because it contains chains composed of Se and Te as in a polymer. [96Amz] proposed the "regular model with multiple connectivity" for the liquid state. In the liquid state Se is two-fold coordinated and in Te-melts metallic three-fold coordinated microdomains (Te(III)) coexist with semiconducting two-fold coordinated microdomains (Te(II)). The Se-Te system in the liquid state is now considered as a ternary system with Se, Te(II) and Te(III).

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Se,Te)_1$
$A8$	$A8$	γSe	$hP3$	$P3_121$	TRIGONAL_A8	$(Se,Te)_1$

Table IIa. Integral quantities for the liquid phase at 733 K.

x_{Te}	ΔG_{m} [J/mol]	ΔH_{m} [J/mol]	ΔS_{m} [J/(mol·K)]	$G_{\mathrm{m}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{m}}^{\mathrm{E}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−2112	−711	1.912	−131	−0.791	0.000
0.200	−3298	−1279	2.754	−248	−1.406	0.000
0.300	−4068	−1698	3.233	−345	−1.846	0.000
0.400	−4518	−1963	3.487	−417	−2.109	0.000
0.500	−4682	−2068	3.566	−457	−2.197	0.000
0.600	−4563	−2008	3.487	−462	−2.109	0.000
0.700	−4146	−1776	3.233	−424	−1.846	0.000
0.800	−3387	−1368	2.754	−338	−1.406	0.000
0.900	−2180	−778	1.912	−198	−0.791	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Se(liquid), Te(liquid)

Table IIb. Partial quantities for Se in the liquid phase at 733 K.

x_{Se}	ΔG_{Se} [J/mol]	ΔH_{Se} [J/mol]	ΔS_{Se} [J/(mol·K)]	$G_{\mathrm{Se}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Se}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Se}	γ_{Se}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−648	−71	0.788	−6	−0.088	0.899	0.999
0.800	−1392	−290	1.504	−32	−0.352	0.796	0.995
0.700	−2263	−669	2.175	−89	−0.791	0.690	0.986
0.600	−3301	−1219	2.841	−188	−1.406	0.582	0.970
0.500	−4565	−1951	3.566	−340	−2.197	0.473	0.946
0.400	−6142	−2877	4.455	−558	−3.164	0.365	0.913
0.300	−8188	−4007	5.704	−851	−4.306	0.261	0.870
0.200	−11040	−5354	7.757	−1231	−5.625	0.163	0.817
0.100	−15743	−6927	12.026	−1709	−7.119	0.076	0.755
0.000	$-\infty$	−8739	∞	−2297	−8.788	0.000	0.686

Reference state: Se(liquid)

Table IIc. Partial quantities for Te in the liquid phase at 733 K.

x_{Te}	ΔG_{Te} [J/mol]	ΔH_{Te} [J/mol]	ΔS_{Te} [J/(mol·K)]	$G_{\mathrm{Te}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Te}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Te}	γ_{Te}
0.000	$-\infty$	−7804	∞	−1362	−8.788	0.000	0.800
0.100	−15288	−6473	12.026	−1255	−7.119	0.081	0.814
0.200	−10920	−5234	7.757	−1111	−5.625	0.167	0.833
0.300	−8280	−4099	5.704	−942	−4.306	0.257	0.857
0.400	−6344	−3079	4.455	−760	−3.164	0.353	0.883
0.500	−4799	−2185	3.566	−574	−2.197	0.455	0.910
0.600	−3511	−1428	2.841	−398	−1.406	0.562	0.937
0.700	−2414	−820	2.175	−240	−0.791	0.673	0.961
0.800	−1474	−372	1.504	−114	−0.352	0.785	0.981
0.900	−673	−95	0.788	−30	−0.088	0.896	0.995
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Te(liquid)

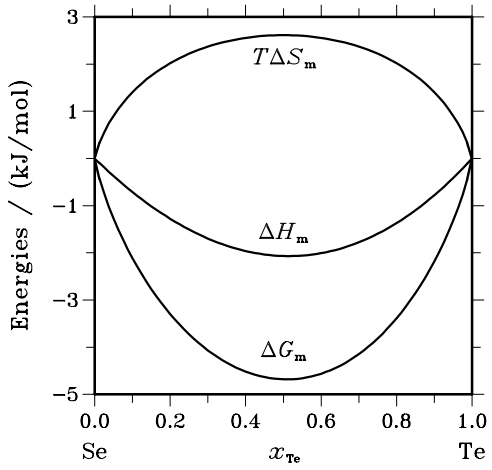

Fig. 2. Integral quantities of the liquid phase at T=733 K.

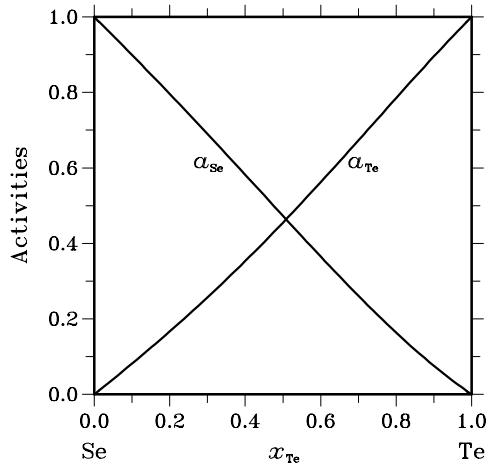

Fig. 3. Activities in the liquid phase at T=733 K.

Table IIIa. Integral quantities for the stable phases at 298 K.

Phase	x_{Te}	ΔG_{m} [J/mol]	ΔH_{m} [J/mol]	ΔS_{m} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{m}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{m}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
$A8$	0.000	0	0	0.000	0	0.000	0.000
	0.100	−860	−20	2.818	−54	0.115	0.000
	0.200	−1337	−36	4.366	−97	0.205	0.000
	0.300	−1641	−47	5.348	−127	0.269	0.000
	0.400	−1813	−53	5.903	−145	0.308	0.000
	0.500	−1869	−56	6.084	−151	0.320	0.000
	0.600	−1813	−53	5.903	−145	0.308	0.000
	0.700	−1641	−47	5.348	−127	0.269	0.000
	0.800	−1337	−36	4.366	−97	0.205	0.000
	0.900	−860	−20	2.818	−54	0.115	0.000
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Se($A8$), Te($A8$)

Table IIIb. Partial quantities for Se in the stable phases at 298 K.

Phase	x_{Se}	ΔG_{Se} [J/mol]	ΔH_{Se} [J/mol]	ΔS_{Se} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Se}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Se}}$ [J/(mol·K)]	a_{Se}	γ_{Se}
$A8$	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−267	−2	0.889	−6	0.013	0.898	0.998
	0.800	−577	−9	1.907	−24	0.051	0.792	0.990
	0.700	−938	−20	3.081	−54	0.115	0.685	0.978
	0.600	−1362	−36	4.452	−97	0.205	0.577	0.962
	0.500	−1869	−56	6.084	−151	0.320	0.470	0.941
	0.400	−2488	−80	8.080	−218	0.461	0.366	0.916
	0.300	−3279	−109	10.638	−296	0.628	0.266	0.887
	0.200	−4375	−142	14.202	−387	0.820	0.171	0.855
	0.100	−6195	−180	20.183	−490	1.038	0.082	0.821
	0.000	$-\infty$	−223	∞	−604	1.282	0.000	0.784

Reference state: Se($A8$)

Table IIIc. Partial quantities for Te in the stable phases at 298 K.

Phase	x_{Te}	ΔG_{Te} [J/mol]	ΔH_{Te} [J/mol]	ΔS_{Te} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Te}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Te}}$ [J/(mol·K)]	a_{Te}	γ_{Te}
$A8$	0.000	$-\infty$	−223	∞	−604	1.282	0.000	0.784
	0.100	−6195	−180	20.183	−490	1.038	0.082	0.821
	0.200	−4375	−142	14.202	−387	0.820	0.171	0.855
	0.300	−3279	−109	10.638	−296	0.628	0.266	0.887
	0.400	−2488	−80	8.080	−218	0.461	0.366	0.916
	0.500	−1869	−56	6.084	−151	0.320	0.470	0.941
	0.600	−1362	−36	4.452	−97	0.205	0.577	0.962
	0.700	−938	−20	3.081	−54	0.115	0.685	0.978
	0.800	−577	−9	1.907	−24	0.051	0.792	0.990
	0.900	−267	−2	0.889	−6	0.013	0.898	0.998
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Te($A8$)

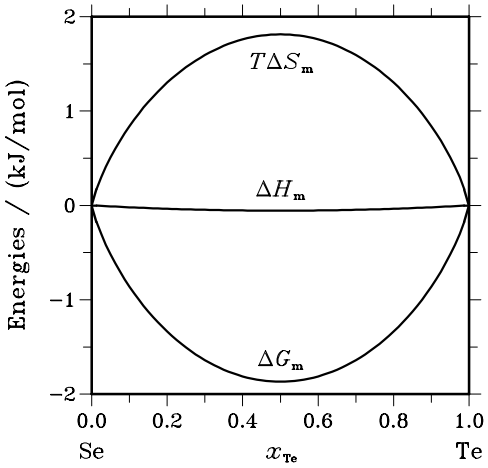

Fig. 4. Integral quantities of the stable phases at T=298 K.

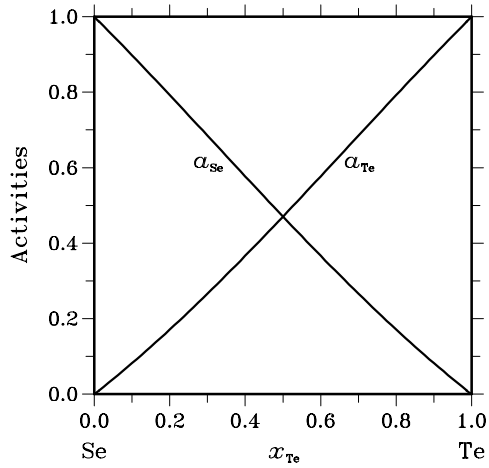

Fig. 5. Activities in the stable phases at T=298 K.

References

[86Mor] G. Morgant, B. Legendre: J. Therm. Anal. **31** (1986) 377–385.
[88Gho] G. Ghosh, H.L. Lukas, L. Delaey: Calphad **12** (1988) 295–299.
[96Amz] A. Amzil, M. Gilbert, C. Bichara, J.C. Mathieu: J. Phys. Cond. Mat. **8** (1996) 5281–5293.