Hg – Te (Mercury – Tellurium)

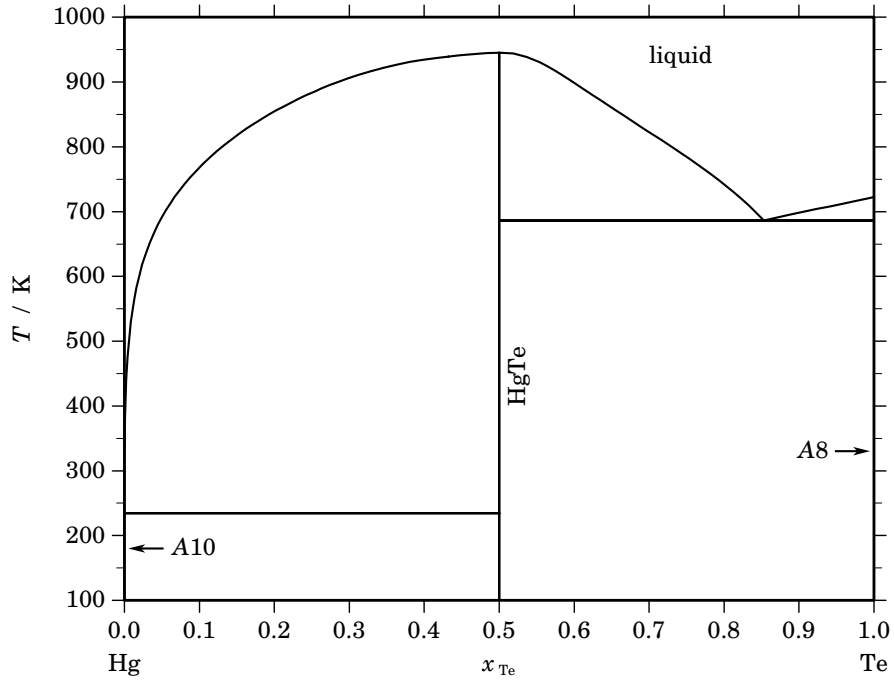

Fig. 1. Calculated phase diagram for the system Hg-Te.

The Hg-Te system is of interest because of the semimetallic compound HgTe which forms continuous solid solutions with the semiconducting compound CdTe. The resulting Cd-Hg tellurides are infrared sensitive semiconductors with wavelengths which can be tailored by means of the Cd-Hg composition ratio. Reviews and thermodynamic datasets for the Hg-Te system have been prepared by [1995Sha, 1995Yan] and the assessment of [1995Yan] is selected here because it is based on the SGTE element data. The data for the phase equilibria which have been used in the optimisation are based mainly on [1965Bre, 1967Str, 1971Dzi, 1980Har]. Partial pressure data for Hg [1963Gol, 1965Bre, 1981Su, 1989Sha] and Te [1965Bre] in the equilibrium of the liquid with the HgTe compound have been included in the assessment. Except for these partial pressure data no other thermodynamic data have been available for the liquid. The partial pressures and in addition results from EMF experiments [1964Ter] have been used to determine the Gibbs energy of formation of the HgTe compound. The terminal phases as well as the the HgTe compound have been modelled as stoichiometric since no solubility data have been available. The liquid has been described with an associate model using the species Hg, Te and HgTe.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Hg,HgTe,Te)_1$
$A10$	$A10$	αHg	$hR1$	$R\overline{3}m$	RHOMBO_A10	$(Hg,Te)_1$
HgTe	$B3$	ZnS	$cF8$	$F\overline{4}3m$	HGTE	Hg_1Te_1
$A8$	$A8$	γSe	$hP3$	$P3_121$	TRIGONAL_A8	Te_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Te}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid $\rightleftharpoons$ HgTe	congruent	945.4	0.500	0.500		−17430
liquid $\rightleftharpoons$ HgTe + $A8$	eutectic	686.3	0.853	0.500	1.000	−14214
liquid $\rightleftharpoons$ $A10$ + HgTe	eutectic	234.3	0.000	0.000	0.500	−2295

Table IIIa. Integral quantities for the liquid phase at 950 K.

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)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−3608	−1609	2.104	−1040	−0.599	1.807
0.200	−5954	−3441	2.645	−2002	−1.515	4.252
0.300	−7709	−5637	2.181	−2884	−2.898	7.406
0.400	−9017	−8499	0.545	−3701	−5.051	9.574
0.500	−9935	−11717	−1.875	−4460	−7.638	2.745
0.600	−9689	−12403	−2.857	−4373	−8.452	5.765
0.700	−8228	−9546	−1.387	−3403	−6.466	16.123
0.800	−6258	−5793	0.489	−2305	−3.672	13.180
0.900	−3742	−2654	1.145	−1174	−1.558	5.885
1.000	0	0	0.000	0	0.000	0.000

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

Table IIIb. Partial quantities for Hg in the liquid phase at 950 K.

x_{Hg}	ΔG_{Hg} [J/mol]	ΔH_{Hg} [J/mol]	ΔS_{Hg} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Hg}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Hg}}$ [J/(mol·K)]	a_{Hg}	γ_{Hg}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−871	96	1.018	−39	0.142	0.896	0.995
0.800	−1921	521	2.571	−159	0.716	0.784	0.980
0.700	−3167	1744	5.170	−350	2.204	0.670	0.957
0.600	−4543	4773	9.807	−509	5.560	0.563	0.938
0.500	−6982	276	7.640	−1507	1.877	0.413	0.826
0.400	−15978	−20129	−4.369	−8740	−11.988	0.132	0.331
0.300	−20474	−36465	−16.833	−10964	−26.843	0.075	0.250
0.200	−23917	−33459	−10.044	−11205	−23.426	0.048	0.242
0.100	−29722	−28400	1.391	−11534	−17.754	0.023	0.232
0.000	$-\infty$	−24748	∞	−11984	−13.435	0.000	0.219

Reference state: Hg(liquid)

Table IIIc. Partial quantities for Te in the liquid phase at 950 K.

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}
0.000	$-\infty$	−15242	∞	−10790	−4.686	0.000	0.255
0.100	−28239	−16954	11.879	−10052	−7.266	0.028	0.280
0.200	−22086	−19290	2.943	−9373	−10.439	0.061	0.305
0.300	−18308	−22861	−4.793	−8798	−14.803	0.098	0.328
0.400	−15727	−28407	−13.348	−8489	−20.966	0.137	0.341
0.500	−12889	−23710	−11.390	−7414	−17.153	0.196	0.391
0.600	−5496	−7252	−1.848	−1461	−6.095	0.499	0.831
0.700	−2980	1991	5.232	−163	2.267	0.686	0.980
0.800	−1843	1123	3.122	−80	1.267	0.792	0.990
0.900	−855	206	1.118	−23	0.242	0.897	0.997
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Te(liquid)

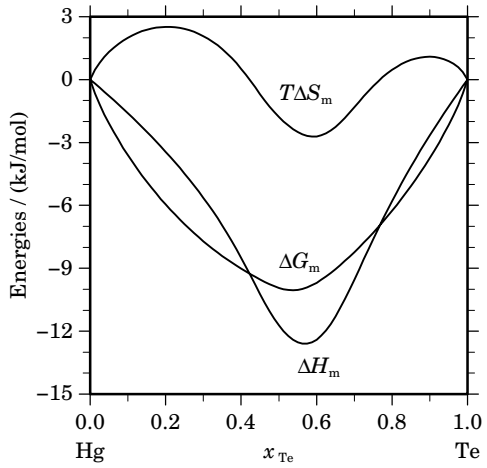

Fig. 2. Integral quantities of the liquid phase at T=950 K.

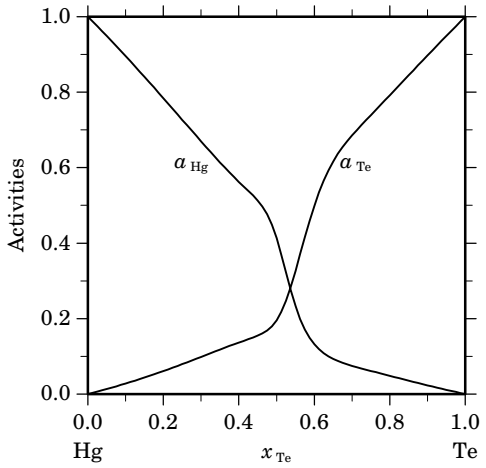

Fig. 3. Activities in the liquid phase at T=950 K.

Table IV. Standard reaction quantities at 298.15 K for the compounds per mole of atoms.

Compound	x_{Te}	$\Delta_{\mathrm{f}}G^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}H^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}S^{\circ}$ / (J/(mol·K))	$\Delta_{\mathrm{f}}C^{\circ}_{P}$ / (J/(mol·K))
Hg_1Te_1	0.500	−18594	−21769	−10.648	0.925

References

[1963Gol] P. Goldfinger, M. Jeunehomme: Trans. Faraday Soc. **59** (1963) 2851–2867.
[1964Ter] J. Terpilowski, E. Ratajzak: Bull. Acad. Pol. Sci. **12** (1964) 335–338.
[1965Bre] R.F. Brebrick, A.J. Strauss: J. Phys. Chem. Solids **26** (1965) 989–1002.
[1967Str] A.J. Strauss, quoted as private communication by: T.C. Harman in: "Physics and Chemistry of II/VI Compounds", M. Aven, J.S. Prener, eds, North Holland Publ. Comp., Amsterdam, 1967, p. 769.
[1971Dzi] E.Z. Dziuba: J. Cryst. Growth **8** (1971) 221–222.
[1980Har] T.C. Harman: J. Electron. Mater. **9** (1980) 945–961.
[1981Su] C. Su, P. Liao, T. Tung, R. Brebrick: High Temp. Sci. **14** (1981) 181–195.
[1989Sha] Y. Sha, K. Chen, R. Fang, R. Brebrick: J. Electrochem. Soc. **136** (1989) 3037–3041.
[1995Sha] R.C. Sharma, Y.A. Chang, C. Guminski: J. Phase Equilibria **16** (1995) 338–347.
[1995Yan] J. Yang, N.J. Silk, A. Watson, A.W. Bryant, B.B. Argent: Calphad **19** (1995) 399–414.