O – Y (Oxygen – Yttrium)

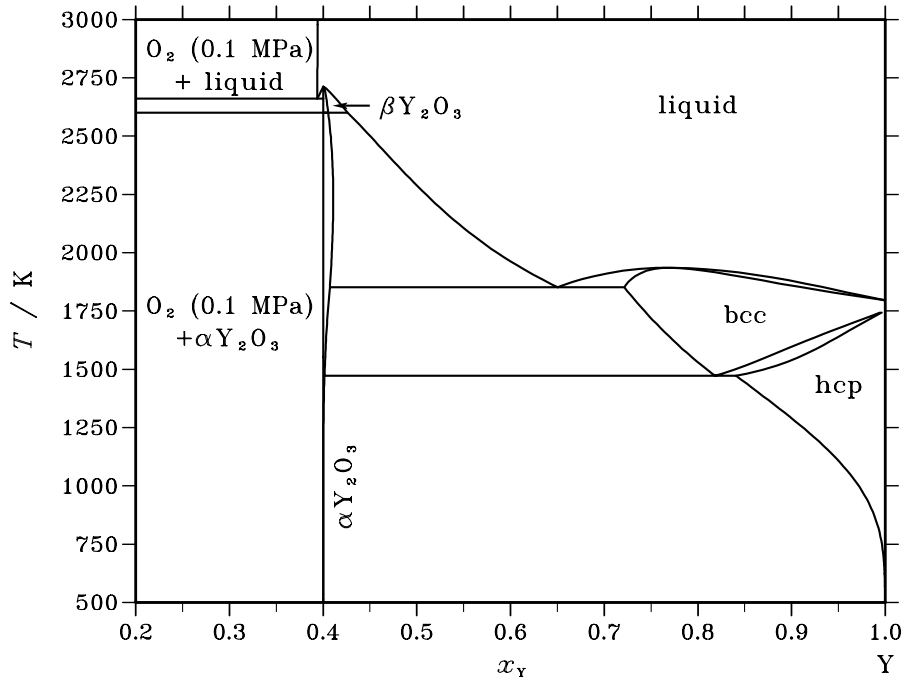

Fig. 1. Calculated phase diagram for the system O-Y.

Yttria (Y_2O_3) is a super-refractory oxide that finds use in a variety of applications including optics and electronics. Yttria is an additive for liquid phase sintering of Si_3N_4, SiC and other covalently bonded structural ceramics. It is also used to stabilise cubic and tetragonal zirconia, which find numerous applications such as gas sensors, solid state electrolytes and thermal barrier coatings. From available thermodynamic descriptions [89Ran, 96Gro, 96Lys, 98Swa] the assessment of [98Swa] is based on the most extensive experimental database including latest calorimetric measurements [90Lav, 93Gav, 93Mor, 95Kol]. Apart from phase equilibrium data, thermodynamic data derived from emf and vapour pressure measurements and from equilibration of Y-O solid solutions with Ti-O solid solutions were also used in [98Swa]. The description recommended here is based mainly on [98Swa] with small adjustments [04Fab] due to a revision of the SGTE data for pure Y. Metallic Y phases with hcp and bcc structure were found to contain up to 15 and 25 at.% of oxygen, respectively. Both phases are treated as interstitial solid solutions. Narrow homogeneity ranges in cubic and hexagonal Y_2O_3 are described by the Wagner-Schottky model. The liquid phase is described by a two-sublattice partially ionic liquid model.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					IONIC_LIQUID	$Y_p^{3+}(O^{2-},O,\square)_q$
αY_2O_3	$D5_3$	Mn_2O_3	$cI80$	$Ia\overline{3}$	Y2O3R	$Y_2^{3+}(O^{2-},\square^{2-})_3$
βY_2O_3	···	···	$hP*$	$P\overline{3}m1$	Y2O3H	$Y_2^{3+}(O^{2-},\square^{2-})_3$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$Y_1(O,\square)_3$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$Y_1(O,\square)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_Y			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ βY_2O_3	congruent	2711.6	0.400	0.400		−18400
liquid $\rightleftharpoons$ gas + βY_2O_3	gas-eutectic	2661.1	0.394	0.000	0.400	−18151
gas + βY_2O_3 $\rightleftharpoons$ αY_2O_3	gas-peritectic	2600.0	0.000	0.400	0.400	−5000
βY_2O_3 $\rightleftharpoons$ αY_2O_3 + liquid	metatectic	2600.0	0.405	0.405	0.426	−4955
liquid $\rightleftharpoons$ bcc	congruent	1935.5	0.771	0.771		−14692
liquid $\rightleftharpoons$ αY_2O_3 + bcc	eutectic	1851.8	0.650	0.407	0.721	−18034
bcc $\rightleftharpoons$ αY_2O_3 + hcp	eutectoid	1472.1	0.818	0.401	0.841	−7890

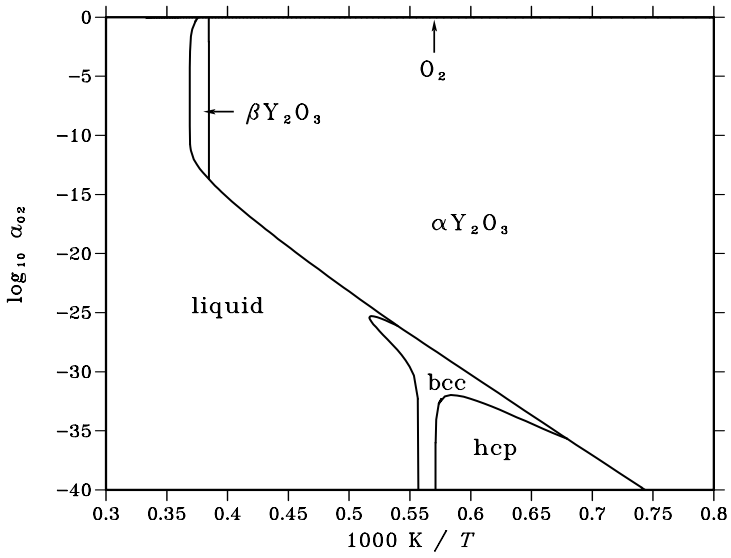

Fig. 2. Calculated temperature-activity phase diagram. Reference state: $\frac{1}{2}O_2$(gas, 0.1 MPa).

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

Compound	x_Y	$\Delta_f G^\circ$ / (J/mol)	$\Delta_f H^\circ$ / (J/mol)	$\Delta_f S^\circ$ / (J/(mol·K))	$\Delta_f C_P^\circ$ / (J/(mol·K))
αY_2O_3	0.400	−369131	−386911	−59.635	1.223
βY_2O_3	0.400	−364705	−381911	−57.712	1.223

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