Mg – O (Magnesium – Oxygen)

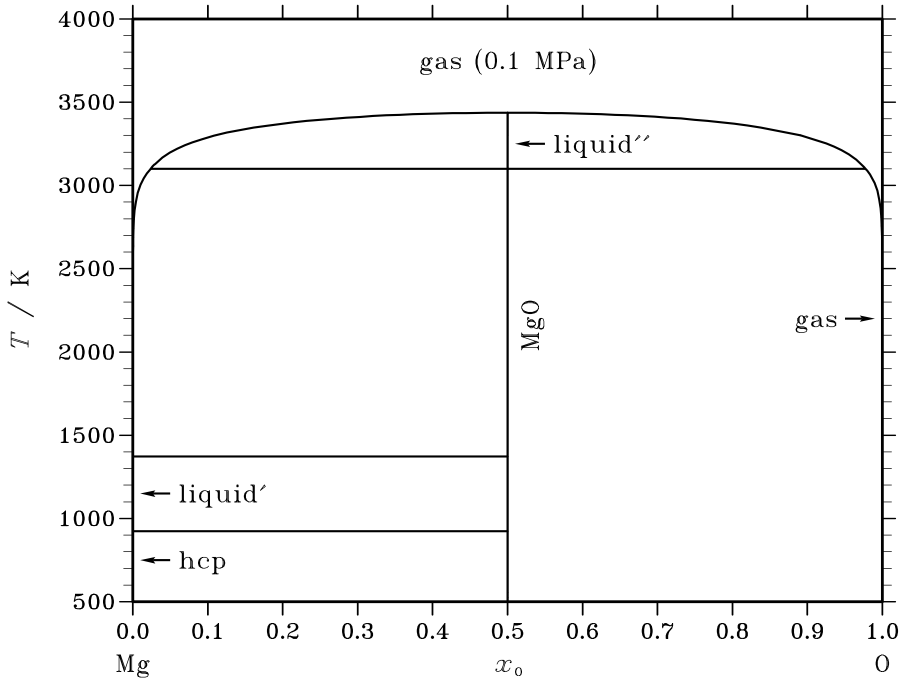

Fig. 1. Calculated phase diagram for the system Mg-O.

The Mg-O system is encountered in many industrially important systems. MgO is a major constituent of many slags, ceramics and rock-forming minerals. The review of experimental data for the Mg-O system was given by [87Wri]. The thermodynamic description of this system including the gas phase and taking into account the oxygen solubility in liquid Mg was presented by [93Hal]. The only stable compound in the system is MgO, periclase. It is an essentially stoichiometric compound which melts congruently at 3100 K [87Wri]. The temperature of melting was confirmed by in situ X-ray measurements [97Dub]. The solubility of O in solid and liquid Mg is very low and difficult to measure [87Wri]. The correlation between enthalpy and entropy of dissolution of O in liquid metal and enthalpy of formation of oxide was used by [93Hal]. The thermodynamic data for Mg and MgO are well established except for the enthalpy of fusion of MgO [87Gar, 87Wri, 96Bel]. Metallic and oxide liquid are described as a single phase exhibiting a very wide miscibility gap using a two-sublattice ionic liquid model. The gas phase is assumed to consist of the species Mg, Mg_2, MgO, O, O_2 and O_3. The MgO and hcp phases are treated as stoichiometric phases.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					IONIC_LIQ	$Mg_p^{2+}(O^{2-},\Box)_2$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$Mg_1(O,\Box)_1$
MgO	$B1$	NaCl	$cF8$	$Fm\overline{3}m$	HALITE	$(Mg^{2+},\Box)_1O_1^{2-}$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_O			$\Delta_r H$ / (J/mol)
gas ⇌ liquid″	congruent	3436.8	0.500	0.500		−331252
liquid″ ⇌ MgO	congruent	3100.0	0.500	0.500		−38503
gas + MgO ⇌ liquid′	degenerate	1372.9	0.000	0.500	0.000	−128270
liquid′ + MgO ⇌ hcp	degenerate	923.0	0.000	0.500	0.000	−8477

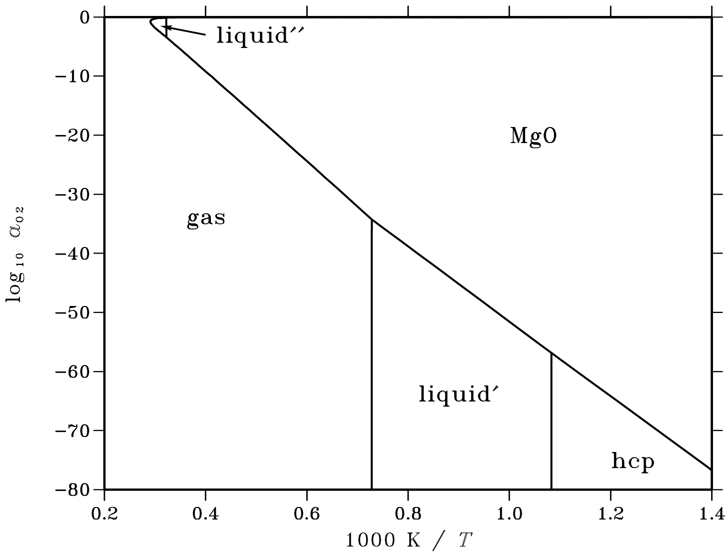

Fig. 2. Calculated temperature-activity phase diagram. Reference state: $\frac{1}{2}O_2$(gas, 0.1 MPa).

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

Compound	x_O	$\Delta_f G^\circ$ / (J/mol)	$\Delta_f H^\circ$ / (J/mol)	$\Delta_f S^\circ$ / (J/(mol·K))	$\Delta_f C_P^\circ$ / (J/(mol·K))
MgO	0.500	−284664	−300800	−54.120	−1.167

References

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