N – Ta (Nitrogen – Tantalum)

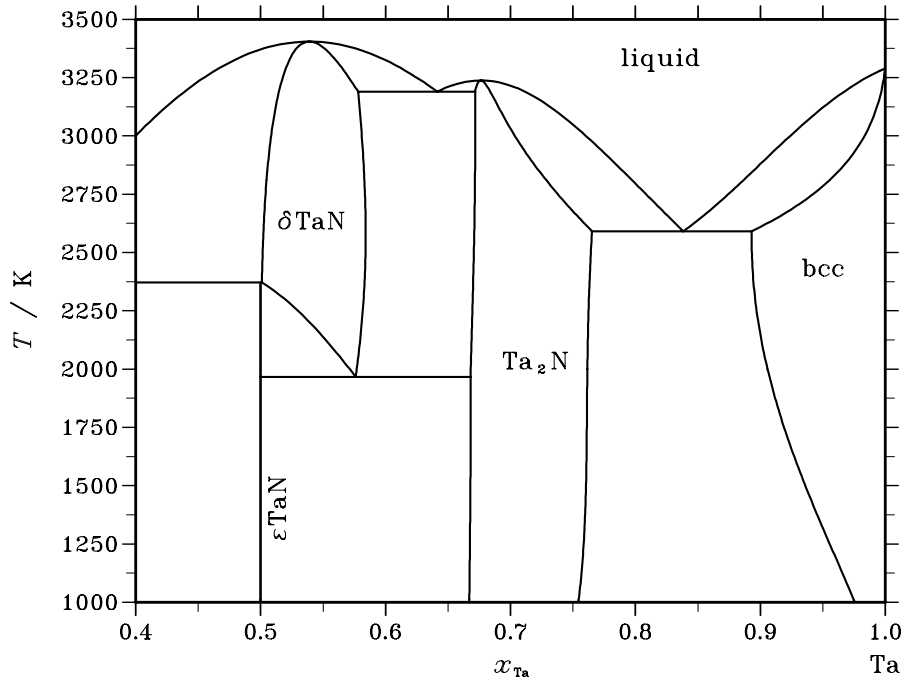

Fig. 1. Calculated phase diagram for the system N-Ta.

N and Ta are both alloying elements in steels and other alloys. Ta is a strong carbide and nitride former and this is used for hardening together with other carbide/nitride formers. The solubility of N in solid and liquid Ta is rather high. There are the usual hexagonal and cubic nitrides modelled as interstitial solution of N in hcp-Ta and in fcc-Ta, respectively. In addition a stoichiometric nitride, ϵTaN, is stable. The gas phase is omitted from the calculated phase diagram in Fig. 1. The assessment has been reported in [98Fri].

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(N,Ta)_1$
ϵTaN	$\cdots$	$\cdots$	$hP6$	$P62m$	EPS	Ta_1N_1
δTaN	$B1$	NaCl	$cF8$	$Fm\overline{3}m$	FCC_A1	$Ta_1(N,\Box)_1$
Ta_2N	$L'3$	Fe_2N	$hP3$	$P6_3/mmc$	HCP_A3	$Ta_2(N,\Box)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$Ta_1(N,\Box)_3$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ta}			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ δTaN	congruent	3404.6	0.539	0.539		−37485
liquid $\rightleftharpoons$ Ta_2N	congruent	3238.1	0.676	0.676		−23878
liquid $\rightleftharpoons$ δ TaN + Ta_2N	eutectic	3189.6	0.641	0.578	0.672	−28590
liquid $\rightleftharpoons$ Ta_2N + bcc	eutectic	2591.1	0.838	0.765	0.893	−27356
liquid + δTaN $\rightleftharpoons$ ϵTaN	peritectic	2371.2	0.306	0.501	0.500	−30529
δTaN $\rightleftharpoons$ ϵTaN + Ta_2N	eutectoid	1966.9	0.576	0.500	0.668	−15574

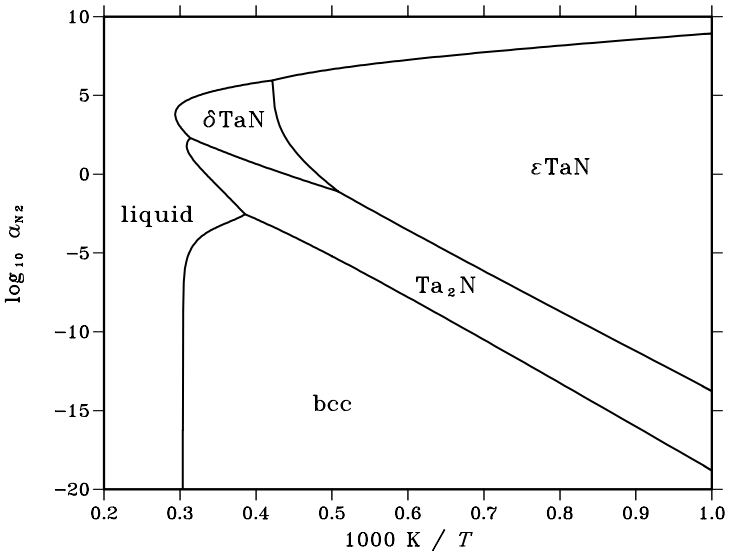

Fig. 2. Calculated temperature-activity phase diagram. Reference state: $\frac{1}{2}N_2$(gas, 0.1 MPa).

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

Compound	x_{Ta}	$\Delta_{\mathrm{f}}G^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}H^{\circ}$ / (J/mol)	$\Delta_{\mathrm{f}}S^{\circ}$ / (J/(mol·K))	$\Delta_{\mathrm{f}}C_P^{\circ}$ / (J/(mol·K))
ϵTaN	0.500	−112995	−128795	−52.997	−0.402

References

[98Fri] K. Frisk: J. Alloys Comp. **278** (1998) 216–226.