# **Ta – W** (Tantalum – Tungsten)

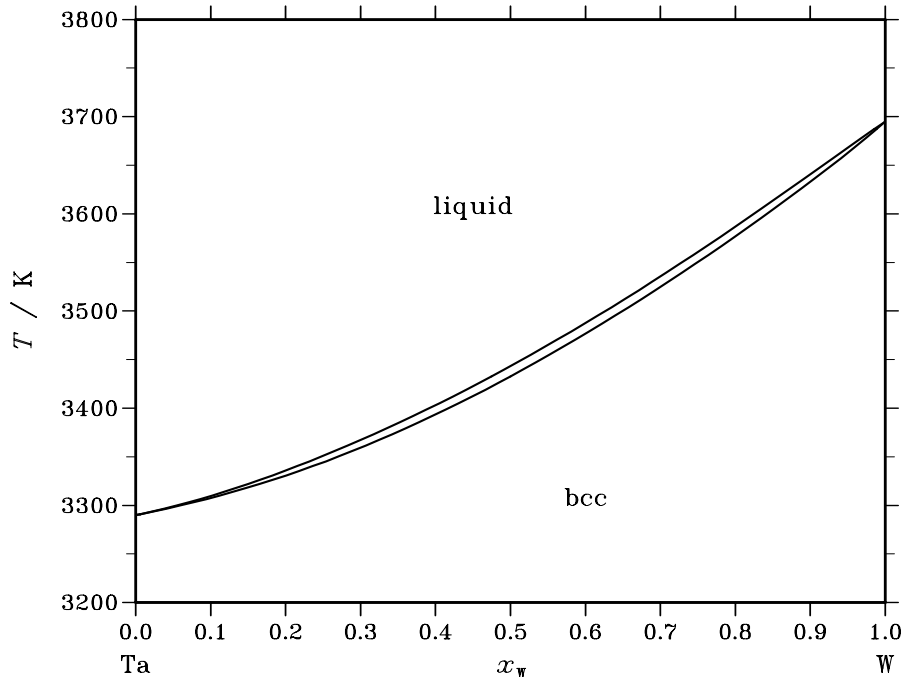


**Fig. 1.** Calculated phase diagram for the system Ta-W.

Tantalum and tungsten are important additions to many alloys, such as superalloys and refractory alloys. The Ta-W system is fairly simple with only two condensed stable phases, liquid and bcc. Few experimental data are available for this system beyond isothermal melting data and partial Gibbs energy data for Ta in the bcc phase. [01Kau] supplemented these data with first principles calculations. Several thermodynamic descriptions are available for this system. The assessment of [95Fer] is based solely on the available experimental information while the assessment of [01Kau] is based on the results of the first principles calculations and consideration of the experimental phase diagram information. The excess enthalpy of the bcc phase from the description of [95Fer] is only half that predicted by the first principles calculation. The description of [01Kau] also reproduces the Ta partial Gibbs energy data well for Ta concentrations larger than 0.3, thus is recommended.

**Table I.** Phases, structures and models.

| Phase | Struktur-bericht | Prototype | Pearson symbol | Space group | SGTE name | Model |
|---|---|---|---|---|---|---|
| liquid | | | | | LIQUID | $(Ta,W)_1$ |
| bcc | $A2$ | W | $cI2$ | $Im\overline{3}m$ | BCC_A2 | $(Ta,W)_1$ |

**Table IIa.** Integral quantities for the liquid phase at 3800 K.

| $x_{\mathrm{W}}$ | $\Delta G_{\mathrm{m}}$ [J/mol] | $\Delta H_{\mathrm{m}}$ [J/mol] | $\Delta S_{\mathrm{m}}$ [J/(mol·K)] | $G_{\mathrm{m}}^{\mathrm{E}}$ [J/mol] | $S_{\mathrm{m}}^{\mathrm{E}}$ [J/(mol·K)] | $\Delta C_P$ [J/(mol·K)] |
|---|---|---|---|---|---|---|
| 0.000 | 0 | 0 | 0.000 | 0 | 0.000 | 0.000 |
| 0.100 | −12830 | −1461 | 2.992 | −2559 | 0.289 | 0.886 |
| 0.200 | −21251 | −3546 | 4.659 | −5441 | 0.499 | 1.576 |
| 0.300 | −27612 | −5899 | 5.714 | −8311 | 0.635 | 2.068 |
| 0.400 | −32101 | −8165 | 6.299 | −10837 | 0.703 | 2.364 |
| 0.500 | −34582 | −9987 | 6.472 | −12682 | 0.709 | 2.462 |
| 0.600 | −34776 | −11011 | 6.254 | −13512 | 0.658 | 2.364 |
| 0.700 | −32294 | −10880 | 5.635 | −12994 | 0.556 | 2.068 |
| 0.800 | −26602 | −9238 | 4.570 | −10792 | 0.409 | 1.576 |
| 0.900 | −16843 | −5730 | 2.925 | −6572 | 0.222 | 0.886 |
| 1.000 | 0 | 0 | 0.000 | 0 | 0.000 | 0.000 |

Reference states: Ta(liquid), W(liquid)

**Table IIb.** Partial quantities for Ta in the liquid phase at 3800 K.

| $x_{\mathrm{Ta}}$ | $\Delta G_{\mathrm{Ta}}$ [J/mol] | $\Delta H_{\mathrm{Ta}}$ [J/mol] | $\Delta S_{\mathrm{Ta}}$ [J/(mol·K)] | $G_{\mathrm{Ta}}^{\mathrm{E}}$ [J/mol] | $S_{\mathrm{Ta}}^{\mathrm{E}}$ [J/(mol·K)] | $a_{\mathrm{Ta}}$ | $\gamma_{\mathrm{Ta}}$ |
|---|---|---|---|---|---|---|---|
| 1.000 | 0 | 0 | 0.000 | 0 | 0.000 | 1.000 | 1.000 |
| 0.900 | −3111 | 371 | 0.917 | 217 | 0.041 | 0.906 | 1.007 |
| 0.800 | −6627 | 1011 | 2.010 | 424 | 0.155 | 0.811 | 1.013 |
| 0.700 | −11319 | 1207 | 3.296 | −50 | 0.331 | 0.699 | 0.998 |
| 0.600 | −18013 | 249 | 4.806 | −1873 | 0.558 | 0.565 | 0.942 |
| 0.500 | −27614 | −2576 | 6.589 | −5714 | 0.826 | 0.417 | 0.835 |
| 0.400 | −41192 | −7978 | 8.740 | −12241 | 1.122 | 0.272 | 0.679 |
| 0.300 | −60164 | −16670 | 11.446 | −22125 | 1.435 | 0.149 | 0.496 |
| 0.200 | −86883 | −29363 | 15.137 | −36033 | 1.755 | 0.064 | 0.320 |
| 0.100 | −127385 | −46767 | 21.215 | −54634 | 2.070 | 0.018 | 0.177 |
| 0.000 | $-\infty$ | −69596 | $\infty$ | −78598 | 2.369 | 0.000 | 0.083 |

Reference state: Ta(liquid)

**Table IIc.** Partial quantities for W in the liquid phase at 3800 K.

| $x_{\mathrm{W}}$ | $\Delta G_{\mathrm{W}}$ [J/mol] | $\Delta H_{\mathrm{W}}$ [J/mol] | $\Delta S_{\mathrm{W}}$ [J/(mol·K)] | $G_{\mathrm{W}}^{\mathrm{E}}$ [J/mol] | $S_{\mathrm{W}}^{\mathrm{E}}$ [J/(mol·K)] | $a_{\mathrm{W}}$ | $\gamma_{\mathrm{W}}$ |
|---|---|---|---|---|---|---|---|
| 0.000 | $-\infty$ | −10303 | $\infty$ | −22855 | 3.303 | 0.000 | 0.485 |
| 0.100 | −100294 | −17951 | 21.669 | −27543 | 2.524 | 0.042 | 0.418 |
| 0.200 | −79748 | −21773 | 15.257 | −28898 | 1.875 | 0.080 | 0.401 |
| 0.300 | −65627 | −22481 | 11.354 | −27588 | 1.344 | 0.125 | 0.418 |
| 0.400 | −53232 | −20786 | 8.539 | −24282 | 0.920 | 0.185 | 0.464 |
| 0.500 | −41550 | −17399 | 6.355 | −19650 | 0.592 | 0.268 | 0.537 |
| 0.600 | −30499 | −13033 | 4.596 | −14360 | 0.349 | 0.381 | 0.635 |
| 0.700 | −20350 | −8398 | 3.145 | −9081 | 0.180 | 0.525 | 0.750 |
| 0.800 | −11532 | −4207 | 1.928 | −4482 | 0.072 | 0.694 | 0.868 |
| 0.900 | −4561 | −1170 | 0.892 | −1232 | 0.016 | 0.866 | 0.962 |
| 1.000 | 0 | 0 | 0.000 | 0 | 0.000 | 1.000 | 1.000 |

Reference state: W(liquid)

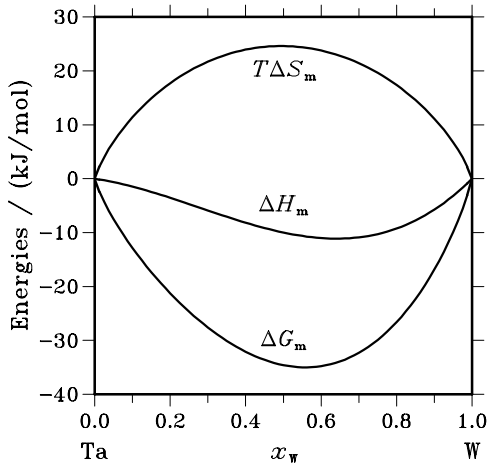


**Fig. 2.** Integral quantities of the liquid phase at $T$=3800 K.

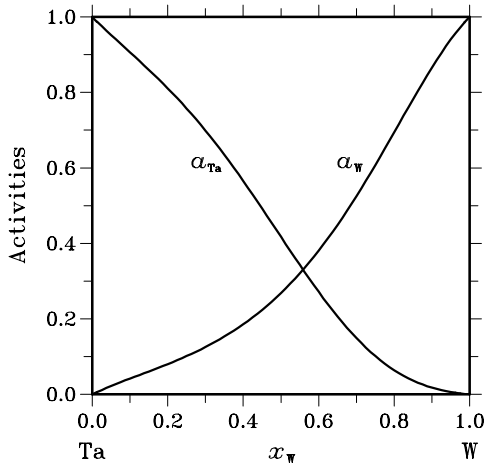


**Fig. 3.** Activities in the liquid phase at $T$=3800 K.

**Table IIIa.** Integral quantities for the stable phases at 2000 K.

| Phase | $x_{\mathrm{W}}$ | $\Delta G_{\mathrm{m}}$ [J/mol] | $\Delta H_{\mathrm{m}}$ [J/mol] | $\Delta S_{\mathrm{m}}$ [J/(mol·K)] | $G^{\mathrm{E}}_{\mathrm{m}}$ [J/mol] | $S^{\mathrm{E}}_{\mathrm{m}}$ [J/(mol·K)] | $\Delta C_P$ [J/(mol·K)] |
|---|---|---|---|---|---|---|---|
| bcc | 0.000 | 0 | 0 | 0.000 | 0 | 0.000 | 0.000 |
| | 0.100 | −7462 | −2318 | 2.572 | −2057 | −0.131 | 0.466 |
| | 0.200 | −12896 | −5070 | 3.913 | −4575 | −0.248 | 0.829 |
| | 0.300 | −17369 | −7900 | 4.734 | −7210 | −0.345 | 1.088 |
| | 0.400 | −20810 | −10452 | 5.179 | −9619 | −0.416 | 1.244 |
| | 0.500 | −22981 | −12370 | 5.306 | −11455 | −0.457 | 1.296 |
| | 0.600 | −23567 | −13298 | 5.134 | −12375 | −0.461 | 1.244 |
| | 0.700 | −22192 | −12881 | 4.656 | −12034 | −0.423 | 1.088 |
| | 0.800 | −18409 | −10763 | 3.823 | −10088 | −0.337 | 0.829 |
| | 0.900 | −11597 | −6588 | 2.505 | −6191 | −0.198 | 0.466 |
| | 1.000 | 0 | 0 | 0.000 | 0 | 0.000 | 0.000 |

Reference states: Ta(bcc), W(bcc)

**Table IIIb.** Partial quantities for Ta in the stable phases at 2000 K.

| Phase | $x_{\mathrm{Ta}}$ | $\Delta G_{\mathrm{Ta}}$ [J/mol] | $\Delta H_{\mathrm{Ta}}$ [J/mol] | $\Delta S_{\mathrm{Ta}}$ [J/(mol·K)] | $G^{\mathrm{E}}_{\mathrm{Ta}}$ [J/mol] | $S^{\mathrm{E}}_{\mathrm{Ta}}$ [J/(mol·K)] | $a_{\mathrm{Ta}}$ | $\gamma_{\mathrm{Ta}}$ |
|---|---|---|---|---|---|---|---|---|
| bcc | 1.000 | 0 | 0 | 0.000 | 0 | 0.000 | 1.000 | 1.000 |
| | 0.900 | −1464 | 276 | 0.870 | 288 | −0.006 | 0.916 | 1.017 |
| | 0.800 | −3017 | 630 | 1.823 | 694 | −0.032 | 0.834 | 1.043 |
| | 0.700 | −5404 | 350 | 2.877 | 528 | −0.089 | 0.723 | 1.032 |
| | 0.600 | −9394 | −1276 | 4.059 | −900 | −0.188 | 0.568 | 0.947 |
| | 0.500 | −15803 | −4958 | 5.423 | −4277 | −0.340 | 0.387 | 0.773 |
| | 0.400 | −25531 | −11408 | 7.061 | −10293 | −0.557 | 0.215 | 0.538 |
| | 0.300 | −39659 | −21339 | 9.160 | −19638 | −0.850 | 0.092 | 0.307 |
| | 0.200 | −59764 | −35461 | 12.152 | −33000 | −1.230 | 0.027 | 0.137 |
| | 0.100 | −89358 | −54485 | 17.437 | −51069 | −1.708 | 0.005 | 0.046 |
| | 0.000 | $-\infty$ | −79124 | $\infty$ | −74532 | −2.296 | 0.000 | 0.011 |

Reference state: Ta(bcc)

**Table IIIc.** Partial quantities for W in the stable phases at 2000 K.

| Phase | $x_W$ | $\Delta G_W$ [J/mol] | $\Delta H_W$ [J/mol] | $\Delta S_W$ [J/(mol·K)] | $G_W^E$ [J/mol] | $S_W^E$ [J/(mol·K)] | $a_W$ | $\gamma_W$ |
|---|---|---|---|---|---|---|---|---|
| bcc | 0.000 | $-\infty$ | −19832 | $\infty$ | −17108 | −1.362 | 0.000 | 0.357 |
| | 0.100 | −61450 | −25669 | 17.890 | −23160 | −1.254 | 0.025 | 0.248 |
| | 0.200 | −52413 | −27871 | 12.271 | −25650 | −1.111 | 0.043 | 0.214 |
| | 0.300 | −45287 | −27149 | 9.069 | −25266 | −0.942 | 0.066 | 0.219 |
| | 0.400 | −37934 | −24216 | 6.859 | −22697 | −0.759 | 0.102 | 0.255 |
| | 0.500 | −30160 | −19781 | 5.189 | −18633 | −0.574 | 0.163 | 0.326 |
| | 0.600 | −22257 | −14557 | 3.850 | −13763 | −0.397 | 0.262 | 0.437 |
| | 0.700 | −14706 | −9256 | 2.725 | −8775 | −0.240 | 0.413 | 0.590 |
| | 0.800 | −8070 | −4588 | 1.741 | −4359 | −0.114 | 0.616 | 0.769 |
| | 0.900 | −2957 | −1266 | 0.846 | −1205 | −0.030 | 0.837 | 0.930 |
| | 1.000 | 0 | 0 | 0.000 | 0 | 0.000 | 1.000 | 1.000 |

Reference state: W(bcc)

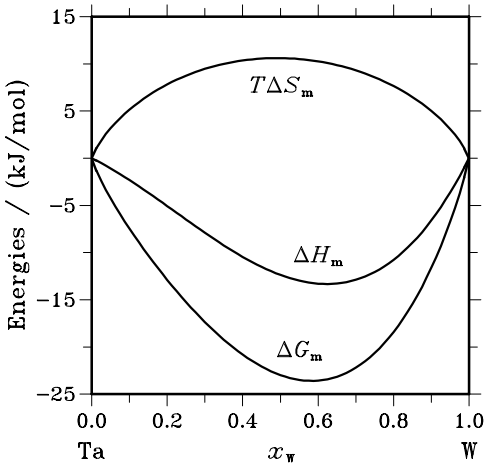


**Fig. 4.** Integral quantities of the stable phases at $T$=2000 K.

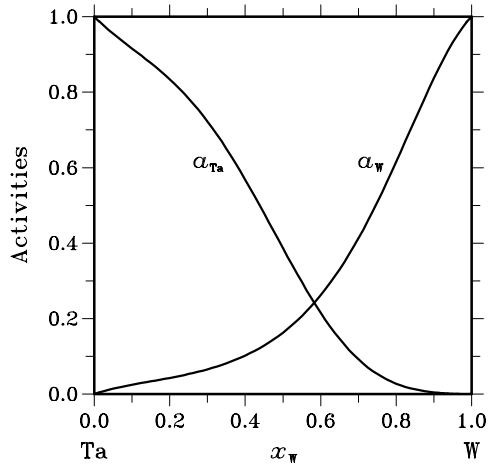


**Fig. 5.** Activities in the stable phases at $T$=2000 K.

## References

[95Fer] A. Fernández Guillermet, W. Huang: personal communication (1995), referenced by K. Frisk: Z. Metallkd. **90** (1999) 704–711.

[01Kau] L. Kaufman, P.E.A. Turchi, W. Huang, Z.-K. Liu: Calphad **25** (2001) 419–433.