## Cr-Ru Cr-Ta

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\*Indicates key paper. #Indicates presence of a phase diagram.

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# The Cr-Ta (Chromium-Tantalum) System

51.996

180.9479

#### By M. Venkatraman and J.P. Neumann The University of Wisconsin-Milwaukee

## **Equilibrium Diagram**

The assessed Cr-Ta phase diagram shown in Fig. 1 is based primarily on the investigations by [48Kub2], [52Duw], [59Gri1], [61Aul], [67Geb], [69Rud], and [73Koc], which are in reasonable agreement with each other. The diagram, which closely resembles the Cr-Nb phase diagram, exhibits a single intermediate phase,  $Cr_2Ta$ ; this phase forms a eutectic with each of the terminal solid solutions, (Cr) and (Ta). The assessed diagram is similar to the one presented by [69Rud]. It has now been firmly established that  $Cr_2Ta$  melts congruently and not peritectically as shown in the earlier review by [Hansen], who took the phase diagram from [48Kub1] and [48Kub2]. The formula  $Cr_3Ta_2$ , which had been assigned by [48Kub1] and [48Kub2] to the intermediate phase, is incorrect.

The values of the congruent melting temperature of  $Cr_2Ta$  reported by various investigators, are in good

## Cr-Ta







Table 1 Cr-Ta Crystal Structure Data

| Phase        | Composition,<br>at.% Ta | Stability<br>range, °C | Pearson<br>symbol | Space<br>group | Strukturbericht designation | Prototype         |
|--------------|-------------------------|------------------------|-------------------|----------------|-----------------------------|-------------------|
| (Cr)         | 0 to 4                  | <1863                  | cI2               | Im3m           | A2                          | W                 |
| $Cr_2Ta(HT)$ |                         | 1660 to 2020           | hP12              | $P6_3/mmc$     | C14                         | MgZn <sub>2</sub> |
| $Cr_2Ta(LT)$ |                         | $<\!\!1695$            | cF24              | Fd3m           | C15                         | MgCu <sub>2</sub> |
| (Ta)         | 73 to 100               | <3020                  | <b>cI</b> 2       | Im3m           | A2                          | W L               |

agreement: 2015 °C [58Ell], 2020 °C [59Gri1], 2020 °C [69Rud], 2040 °C [73Koc]. A value of 2020  $\pm$  20 °C is selected.

The composition and temperature of the eutectic L  $\rightleftharpoons$  (Cr) + Cr<sub>2</sub>Ta have been determined by [48Kub2], [59Gri1], [69Rud], and [73Koc]. Giving more weight to the more recent temperature determinations by [69Rud] and [73Koc], a temperature of 1760 ± 20 °C is selected. [48Kub2] and [59Gri1] reported a eutectic temperature of 1700 °C. The selected value of 13 at.% Ta for the composition of the eutectic was reported by [48Kub2], [59Gri1], and [73Koc]. According to [69Rud], the composition is 10.5 at.% Ta.

For the eutectic L  $\rightleftharpoons$  Cr<sub>2</sub>Ta + (Ta), the determinations of composition and temperature by [59Gri1], [69Rud], and [73Koc] agree, within the stated uncertainties, with the selected values of 50 ± 4 at.% Ta and 1965 ± 20 °C.

The adopted melting temperatures of Cr and Ta are 1863  $^{\circ}$ C and 3020  $^{\circ}$ C, respectively.

The intermediate phase  $Cr_2Ta$  exhibits two modifications, both of them Laves phases [52Duw, 59Gri1, 61Aul, 64Fes, 65Gus, 69Rud, 73Koc]. The high-temperature form,  $Cr_2Ta(HT)$ , has the hexagonal MgZn<sub>2</sub>-type (C14) structure, whereas the low-temperature form,  $Cr_2Ta(LT)$ , has the cubic  $MgCu_2$ -type (C15) structure. The transformation between these two forms is sluggish, which explains the wide range of transformation temperatures that have been reported in the literature: 1375 to 1590 °C [52Duw], 1805 °C [59Gri1], 1600 to 1640 °C [64Fes], 1660 to 1695 °C [69Rud], and 1640 to 1740 °C [73Koc]. The results by [69Rud], shown in Fig. 2, are preferred. They indicate that the transformation temperature increases from 1660 °C at the Cr-rich side to 1695 °C at the Ta-rich side.

Lattice parameter measurements as a function of composition of the  $Cr_2Ta$  phase [64Fes, 65Gus, 69Rud, 73Koc] indicate that the homogeneity range of both modifications extends over several atomic percent. These investigations supersede the earlier study by [59Gri1], who reported a very small homogeneity range. The partial phase diagram shown in Fig. 2 is based on [69Rud]. Further information concerning the  $Cr_2Ta$  phase is given in the section "Crystal Structures".

Partial diagrams of the adopted terminal solid solution regions (Cr) and (Ta) are given in Fig. 3 and Fig. 4, respectively. Figure 3 is based primarily on the X-ray and metallographic studies by [61Aul], whereas Fig. 4 is taken mainly from the analogous investigations by [67Geb].

## **Crystal Structures**

The crystal structures of the phases that occur in the Cr-Ta system are given in Table 1.

Based on their studies of the Cr-rich region of the Cr-Ta system, [59Gri2] and [60Gri] claim the existence of five allotropic forms of pure Cr. These findings have been refuted by other investigators and the existence of only one form of Cr, the bcc modification, is accepted here.

According to [73Koc], an additional intermediate phase with the stoichiometric composition of  $Cr_3Ta_2$  occurs at 40 at.% Ta. This phase has the hexagonal MgNi<sub>2</sub>-type (C36) structure with lattice parameters of a = 0.4963 nm and c = 1.626 nm; it decomposes peritectoidally at 1825 °C into  $Cr_2Ta(HT)$  and (Ta) [73Koc]. The existence of this phase is questionable, because it has not been corroborated by other investigators.

The atomic volume of Ta is approximately 50% larger than that of Cr, that is, 0.018 nm<sup>3</sup>/atom as compared to 0.012 nm<sup>3</sup>/atom. In agreement with this fact, it has been observed that the lattice parameters of all phases in the Cr-Ta system increase with increasing Ta content [61Aul, 69Rud, 73Koc]. The lattice parameters of the hexagonal Cr<sub>2</sub>Ta(HT) phase are approximately a = 0.494nm and c = 0.810 nm [52Duw, 58Ell, 69Rud]. According to [69Rud], the *a* parameter increases from 0.491 nm at the Cr-rich side to 0.498 nm at the Ta-rich side, whereas the *c* parameter increases from 0.805 nm to 0.816 nm. The lattice parameter of the cubic  $Cr_2Ta(LT)$  phase is  $a = 0.697 \pm 0.003$  nm [52Duw, 73Koc]. According to [73Koc], it increases from a = 0.694 nm at the Cr-rich side to a = 0.700 nm at the Ta-rich side.

### Thermodynamics

By means of calorimetric and activity measurements, [64Fes] obtained the following thermodynamic values for  $Cr_2Ta(LT)$ :

- Gibbs energy of formation at 1472 K:
  - $\Delta G = -9.2 \pm 0.5 \text{ kJ/mol of atoms}$
- Enthalpy of formation at 1693 K:

 $\Delta H = -8.5 \pm 0.5 \text{ kJ/mol of atoms}$ 

• Entropy of formation at 1472 K:

 $\Delta S = +0.4 \pm 0.7 \text{ J/K} \cdot \text{mol of atoms}$ 

Combining the value for the enthalpy of formation of  $Cr_2Ta$  at 1693 K, obtained by [64Fes], with an estimated value for the specific heat between 298 and 1693 K, [70Mar] obtained a value of  $\Delta H = -9.0 \pm 1.0$  kJ/mol of atoms for the standard enthalpy of formation of  $Cr_2Ta$  at 298 K.

Using Miedema's model, [82Boe] calculated the enthalpy of formation of  $Cr_2Ta$  as  $\Delta H = -9$  kJ/mol of atoms, in good agreement with the experimental value by [64Fes].



### Magnetism

The influence of Ta on the Nèel temperature of Cr was studied by [69Ara] and [73Ara] by means of electrical resistivity measurements on alloys quenched from 1400 K. The Nèel temperature of Cr is lowered by additions of Ta from 311.5 K for pure Cr to 213 K at 1.5 at.% Ta. The effect of Ta is similar to that of V and Nb [73Ara].

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\* Indicates key paper

#Indicates presence of a phase diagram.

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# The Mg-Po (Magnesium-Polonium) System

24.305

(209)

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The equilibrium phase diagram of the Mg-Po system has not been determined. The melting points of pure Mg and Po are 650 and 254 °C, respectively.

[60Wit] prepared the MgPo intermetallic compound by the "micro technique" (a selective distillation technique).

The structure was determined by powder X-ray diffraction and was analyzed as being the NiAs type (see Tables 1 and 2). However, [67Per], in his review of binary Mg compounds, classified MgPo as the MgTe type.

It appears that the solid solubility of Po in (Mg) and vice-versa is negligible.

Crystal structures and lattice parameters are shown in Tables 1 and 2, respectively.

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