

## Carbon – Molybdenum – Uranium

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### Introduction

Mixed carbides of uranium are candidate fuel materials for fast breeder reactors. The fuel pellets are enclosed in stainless steel clad tubes. During reactor operation, transport of carbon may occur to or from the cladding through the fuel-clad interface. The difference in carbon potential between the fuel and the cladding strongly influences carbon transport. Variation in the carbon content of the stainless steel cladding can adversely affect the mechanical integrity of the steel. Thus, data on the carbon potentials of the fuel and the cladding are useful in understanding and predicting the carbon transport phenomenon. As uranium undergoes fission, a number of fission products are formed with different affinities for formation of binary and ternary carbides. Thus, fission products with high yield, in particular, with participation of molybdenum, may alter the carbon balance as well as the carbon potential of the fuel, and consequently influence cladding carburization [1996Ana]. With a view to the optimization of alloy compositions in the preparation of these materials, information about phase relations in the corresponding ternary system C–Mo–U is of great importance. But up to now, this information has errors and is not complete. It is presented in literature via the invariant equilibrium data [1968Ale, 1973Ale2, 1975Uga2, 1984Ale], liquidus surface projection [1964Chu, 1975Uga2, 1968Ale], a series of isothermal sections [1962Cra, 1963Rud, 1964Chu, 1964Str, 1975Hol, 1975Uga1, 1984Ale, 1984Hol1, 1984Hol2, 1989Lin, 1994Mch] and temperature-composition sections [1964Str, 1967Chu, 1973Ale2, 1973Ale3, 1975Uga2, 1989Lin, 1994Mch]. Phase contents of the alloys and crystal structures of the intermediate phases were studied by [1962Cra, 1962Kat, 1963Rud, 1964Str, 1964Cro, 1965Dec, 1966Ans, 1967Chu, 1968Ale, 1970Bow, 1971Uch, 1973Ale1, 1973Ale2, 1973Ale3, 1973Ale4, 1973–1974Nar, 1974Iva, 1975Ale, 1985Ara, 1986Jei, 1988Jon]. Thermodynamic properties were obtained experimentally by [1974Nar, 1975Uga2, 1996Ana]. The experimental methods used and the temperature and composition ranges studied are shown in Table 1. Physical properties of the C–Mo–U alloys are presented in [1967Chu, 1970Bow, 1971Uch, 1972Lor, 1985Ara]. The C–Mo–U system was reviewed in [1963Bri, 1964Far, 1967Far, 1968Ale, 1975Hol, 1984Hol1, 1984Hol2, 1994Mch]. However, further amendments to the character of the phase equilibria are necessary, in particular concerning the constitution of the liquidus, solidus and solvus surfaces as well as the reaction scheme for the whole range of compositions. Discrepancies between the isothermal and temperature-composition sections need to be solved.

### Binary Systems

The C–U and Mo–U constituent binary systems are accepted from [Mas2]. The constitution of the C–Mo system as a whole has been accepted from [Mas2], but with the addition of the  $\beta'$ ,  $\text{Mo}_2\text{C}$  ( $h_1$ ) ordered phase after [1988Epi].

### Solid Phases

Crystallographic data relating to the unary, binary and ternary phases are listed in Table 2. The solubilities of the third component in each of the binary C–U, C–Mo and Mo–U phases were found to be no more than 0.1 at.%. Two ternary phases with crystal structures different from any of the unary and binary phases were found, namely  $\tau_1$ ,  $\text{UMoC}_{2-x}$  ( $x = 0.25$  to  $0.5$ ) and  $\tau_2$ ,  $\text{UMoC}_2$ . They melt, respectively, incongruently at  $\sim 2227^\circ\text{C}$  [1975Uga2] and congruently at  $\sim 2350^\circ\text{C}$  [1967Chu].

### Invariant Equilibria

A partial reaction scheme is presented in Fig. 1. It was compiled on the basis of data relating to reactions involving the liquid phase as presented in [1968Ale, 1973Ale2, 1975Uga2], as well solid state reactions from [1984Ale]. Carbon poor and carbon rich compositions of the  $\epsilon$ , UC phase are labeled as  $\epsilon'$  and  $\epsilon''$ ,

respectively. Invariant reactions in the binary systems are presented according to the accepted versions, with addition of the reaction  $(\beta\text{U}) \rightleftharpoons (\alpha\text{U}) + \varepsilon$  in the C–U system ( $e_{18}$ ,  $\sim 668^\circ\text{C}$ ) taken from [1984Ale], and information relating to invariant temperatures in the C–Mo system from [1985Dan, 1988Vel]. All the four-phase invariant temperatures need experimental determination as they were evaluated on the basis of comparing of phase equilibria at different temperatures.

The compositions of the liquid phase taking part in the invariant equilibria are shown in Table 3. They were determined on the basis of the liquidus surface projection from [1964Chu, 1968Ale, 1973Ale2, 1975Uga2], (see “Liquidus, Solidus and Solvus Surfaces”).

### Liquidus, Solidus and Solvus Surfaces

The partial liquidus surface projection is shown in Fig. 2. It is based on the experimental results of [1964Chu, 1968Ale, 1973Ale2] as well as on the data of [1975Uga2], including both their own experimental results and an assessment of the literature data. Corrections to the invariant points in the edge binary systems have been made to maintain consistency with the accepted corresponding phase diagrams. Temperatures of invariant four-phase reactions are corrected according to the accepted reaction scheme (Table 3, Fig. 1). The  $U_5$  point was shifted towards the uranium corner in comparison to [1968Ale] owing to the location of  $p_4$  in the accepted Mo–U phase diagram. The positions of the curves  $U_1U_4$  and  $U_3U_4$  are reproduced according to data of this work. The composition of the phase  $\tau_1$  taking part in equilibria with the liquid is given as  $\text{UMoC}_{1.7}$  whereas in some publications in the literature it varies from  $\text{UMoC}_{1.75}$  to  $\text{UMoC}_{1.5}$  (Table 2). Thus, the carbon content of this phase can vary from 42.9 to 46.7 at.%, with a constant U:Mo ratio of 1:1. The  $\tau_1$  phase field of primary crystallization is placed outside of its composition range because of the incongruent formation of this phase. The position of the point  $p_1$  is located on the intersection of monovariant curve  $U_1U_2$  with the extension of the  $\tau_1\tau_2$  tie line. As a whole, the liquidus surface projection, like the solidus and solvus surface projections need further experimental determination.

### Isothermal Sections

An isothermal section at  $2000^\circ\text{C}$  for the whole range of compositions is presented in Fig. 3 based on the data of [1967Chu] with amendments to maintain consistency with the accepted binary phase diagrams and in accordance with the reaction scheme and the temperature – composition sections. The extent of the liquid and molybdenum solid solution regions in the Mo–U system as well as the liquid region in the C–U system are enlarged compared with the section given in [1967Chu]. In the C–Mo system the  $\delta$  and  $\eta$  phases are presented instead of the  $\text{Mo}_3\text{C}_2$  phase. Both the  $\tau_1$  and  $\tau_2$  phases are included in Fig. 3, whereas [1967Chu] presented just the  $\text{UMoC}_2$  phase with a carbon content ranging from  $\sim 43.7$  to 50 at.% C. The composition of the  $\tau_1$ ,  $\text{UMoC}_{2-x}$  phase is about 43.7 at.% C ( $x \approx 0.45$ ). From the reaction scheme one can conclude that at  $2000^\circ\text{C}$  the  $\tau_2 + \varepsilon + \tau_1$  and  $\tau_2 + \tau_1 + \beta$  three-phase as well as the  $\tau_2 + \beta$ ,  $\tau_1 + \tau_2$  and  $\varepsilon + \tau_2$  two-phase equilibria must exist, while the  $\beta + (\text{Mo}) + \tau_1$ ,  $\tau_1 + \varepsilon + (\text{Mo})$  and  $(\text{Mo}) + \varepsilon + (\gamma\text{U})$  equilibria cannot (in the corresponding range of compositions the liquid phase region must be presented). The  $\text{UC}_2$  phase which is presented in [1967Chu] is replaced by  $\varepsilon''$  (the carbon rich  $\varepsilon$  phase) while the UC phase is labeled as  $\varepsilon'$ . The liquid phase field in the ternary system in Fig. 3 is widened considerably compared with [1967Chu] owing to the presence of the corresponding field in the  $\text{UMoC}_2$ –Mo temperature–composition section [1973Ale2] at  $2000^\circ\text{C}$ .

The isothermal section at  $1800^\circ\text{C}$  (Fig. 4) is also constructed on the basis of [1967Chu] taking into account the accepted binary phase diagrams, the reaction scheme and the temperature–composition sections. Comparing with [1967Chu], the liquid phase field is widened, the  $\mu$  phase is added, the UC and  $\text{UC}_2$  phases are replaced by  $\varepsilon'$  and  $\varepsilon''$  phases, respectively. In the C–Mo system the  $\text{Mo}_3\text{C}_2$ -based phase is replaced by the  $\eta$  phase. The composition of the  $\tau_1$ ,  $\text{UMoC}_{2-x}$  phase is shown with  $x = 0.3$  (about 45.9 at.% C) after [1966Ans] and [1985Ara] (Table 2). The liquid phase region stretches deep inside the ternary system, as found in the UC–Mo at  $1800^\circ\text{C}$  (Fig. 4). From the reaction scheme it follows that at this temperature, the  $\tau_2 + \varepsilon + \tau_1$ ,  $\tau_2 + \tau_1 + \beta$  and  $\beta + (\text{Mo}) + \tau_1$  three-phase fields, as well as the  $\tau_2 + \beta$ ,  $\tau_1 + \tau_2$  and  $\varepsilon + \tau_2$  must exist while  $\tau_1 + \beta + (\text{Mo})$  and  $(\text{Mo}) + (\gamma\text{U}) + \varepsilon$  three-phase equilibria cannot be present. Structure modifications of the  $\beta$  phase are designated as  $\beta'$  and  $\beta''$ , but it was not determined which modification takes

part in the three-phase equilibrium with the  $\tau_1$  phase and (Mo). The corresponding phase field is labeled  $\tau_1 + \beta + (\text{Mo})$ .

[1963Rud] presented a partial isothermal section in the UC–Mo–C corner for 1600°C. Equilibria were presented that involved the metastable  $\omega$ ,  $\text{UMo}_2\text{C}_2$  phase which formed from the melt being found at temperatures between 1500°C and 1800°C, whilst the existence of the  $\tau_1$  phase was not taken into account. Therefore the corresponding figure is not shown in this assessment.

The isothermal section for 1525°C (Fig. 5) is presented after [1989Lin, 1994Mch] with some amendments for consistency with the accepted binary phase diagrams. According to the accepted C–U phase diagram, the  $\epsilon$  phase possesses a visible homogeneity range (from 48.5 to 50 at.% C) at this temperature, which is not shown in [1989Lin, 1994Mch]. In order to be consistent with the accepted binary phase diagrams the extent of liquid phase field is increased in the both C–U and Mo–U systems somewhat - from 8 to 12 at.% and from 34 to 37 at.%, respectively. The composition of  $\tau_1$  is presented as  $\text{UMoC}_{1.7}$ .

The assessed isothermal section for 1500°C was first published by [1964Chu]. It was compiled on the basis of available literature data. Only one ternary phase,  $\text{UMoC}_2$ , was included in the diagram. Equilibria involving the  $\text{UC}_2$  and  $\text{Mo}_3\text{C}_2$  phases were shown, although it was established later that at this temperature, they do not take part in equilibria. An assessed isothermal section for 1500°C was published by [1975Uga1] (with reference to experimental data), [1975Hol] and [1984Hol1, 1984Hol2] (with references to [1966Ans, 1975Ale, 1975Uga2]). The constitution of the section presented in [1975Hol, 1984Hol1, 1984Hol2] is the same, while the data of [1975Uga1] differ from them by the presence of equilibria involving the  $\text{UC}_2$  and  $\text{MoC}_{1-x}$  phases as well as by the extent of liquid phase region in the U rich corner deep into the ternary system. Taking into account the constitution of the accepted binaries, the isothermal section at 1500°C is redrawn in Fig. 6. The character of phase equilibria at this temperature differs from those at 1525°C by the disappearance of the  $\kappa$  phase following its dissociation at  $1516 \pm 10^\circ\text{C}$  in the C–U binary system.

The metallographic characteristics of the microstructures of the uranium-based alloys with up to 2 mass% of Mo and up to 2 mass% of C, after annealing at 800°C and step-annealing at 675°C, were obtained by [1962Cra]. The possible effects of the microstructural condition of these alloys during irradiation were discussed. An isothermal section of the U–UC–Mo partial system at 900°C was presented by [1963Rud], Fig. 7. It was established, that a wide  $\epsilon + (\gamma\text{U}) + (\text{Mo})$  three-phase field occupies most of this part of the diagram. Isothermal sections in the concentration range of up to 45 at.% C and 25 at.% Mo at temperatures of 650, 585 and 550°C were constructed on the basis of experimental results from [1964Str]. It was concluded that carbon added to Mo–U alloys removes uranium from the metallic matrix through the formation of UC and enriches the matrix in molybdenum. The solubility of molybdenum in UC at 650°C was estimated to be about 1.8 at.%. Isothermal sections in the U–UC–Mo composition range and the temperature range 1100–550°C were constructed theoretically by [1984Ale] to show the development of the phase equilibria. Data relating to the Mo–U and C–U forming edge binary systems as well as the experimentally determined isothermal section for 900°C from [1963Rud] were used.

### Temperature – Composition Sections

The  $\text{UMoC}_2$ –Mo temperature-composition section is presented in Fig. 8 based on [1973Ale2] with corrections according to the constitution of the accepted boundary binary systems as well as of the reaction scheme, liquidus surface and isothermal sections. In comparison with [1973Ale2], fields containing the  $\beta'$  phase have been added and the positions of the  $L + \tau_2$ ,  $L + \tau_1$ ,  $L + \beta$  and  $L + (\text{Mo})$  fields have been changed considerably. The  $\tau_1 + \beta$  ( $\beta'$ ) two-phase region is placed in the range of molybdenum content of about 1 at.%. From the isothermal sections for different temperatures it follows that position of this region shifts towards the molybdenum side with increasing temperature.

The UC–Mo temperature-composition section is presented in (Fig. 9) based mainly on [1973Ale2]. Some corrections according to constitution of the forming C–U system are carried out, in particular, the  $\epsilon + \mu$ ,  $\epsilon + \mu + (\text{Mo})$ ,  $\epsilon + (\text{C})$  and  $\epsilon + (\text{C}) + (\text{Mo})$  fields are added. In contrast to the work of [1967Chu], the authors of [1973Ale2] determined that the UC–Mo system contains the  $\tau_1$  phase rather than the  $\tau_2$  phase, and consequently, the phase fields have been amended.

The  $U_{50}Mo_{50}$ -C temperature-composition section is shown in Fig. 10. It is based mainly on the data of [1975Uga2] (reproduced in [1989Lin, 1994Mch]) with modifications to be consistent with the accepted Mo-U binary system and the ternary phase diagram. This section was also reported in [1967Chu], but the  $\tau_1$  phase was not presented and the  $\tau_2$  phase was demonstrated as possessing a visible homogeneity range (up to 3 at.% carbon). In Fig. 10, the narrow by temperature  $L + \epsilon$  two-phase field is added; the  $L / L + \epsilon$  and  $L + \epsilon / L + \epsilon + (Mo)$  fields increase in temperature with increasing carbon content. Following the reaction scheme, the temperatures of the horizontal lines at the Mo-U system side representing the invariants  $U_4$  and  $U_5$  are changed to 1530°C (instead of 1830°C) and 1185°C (instead of ~1265°C), respectively.

Partial temperature-composition sections at 5 and 15 at.% C for molybdenum contents of up to 40 and 30 at.%, respectively, are presented in Figs. 11 and 12 after [1964Str]. They illustrate the character of the phase equilibria in the solid state from the C-U side of the system. Also in this article, schematic partial temperature-composition sections at 2 mass% (up to 25 at.% Mo) and at 4 mass% (up to 10 at.% Mo) for temperatures up to 750°C were shown. However, they need further investigation. The  $UC_2$ - $UMoC_2$  section was presented in [1973Ale3], but it also needs further study owing to contradictions with isothermal sections of the ternary system and the accepted C-U binary system. The authors of this work also have investigated a series of alloys along the  $U_2C_3$ - $UMoC_2$  and  $UMoC_2$ - $Mo_{58}C_{42}$  sections. Some of the lattice parameters obtained for the  $\eta$ ,  $MoC_{1-x}$  phase are presented in Table 2.

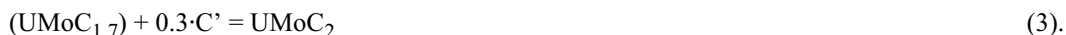
### Thermodynamics

[1996Ana] measured the carbon potential in the  $\epsilon + (Mo) + \tau_1$  and the  $\epsilon + \tau_1 + \tau_2$  three-phase fields using the methane-hydrogen gas equilibration technique. Graphite was the standard state and the temperature range used was 700°C to 900°C (973 to 1173 K). The results for these fields are presented in Figs. 13 and 14, respectively. The chemical potential of carbon was calculated from the equilibrium using the expression  $\Delta\mu_C = R \cdot T \cdot \ln a_C = \Delta_f G^\circ (CH_4) + R \cdot T \cdot \ln (p_{CH_4}/p_{H_2}^2)$  (1)

From a least squares regression analysis of the data, the expression for  $\Delta\mu_C = -52.21 - 19 \cdot T (\pm 7.3) \text{ kJ} \cdot \text{mol}^{-1}$  for the  $\epsilon + (Mo) + \tau_1$  three-phase field and  $\Delta\mu_C = -17.77 - 2 \cdot T (\pm 4.6) \text{ kJ} \cdot \text{mol}^{-1}$  for the  $\epsilon + \tau_1 + \tau_2$  field were obtained. The chemical potentials of carbon in these fields were established by the respective reactions



and



Here  $C'$  refers to carbon in a state with an activity less than unity with respect to graphite as the reference state. The thermodynamic properties of the  $\tau_1$  and  $\tau_2$  phases are given in Table 4. The Gibbs energy of formation of the  $\tau_2$  phase was obtained by [1974Nar] from emf measurements using a three phase mixture of  $\tau_2 + \epsilon + (Mo)$  as the electrode, but according to later phase equilibrium studies, these phases are not in equilibrium and therefore their data are found to be in error.

### Notes on Materials Properties and Applications

Mixed uranium carbides containing molybdenum are the prospective components for nuclear fuel. [1972Lor, 1996Ana] have predicted that about 2 at.% Mo would be produced in a mixed carbide fuel when the burn up exceeds 10 at.%. Further, these authors have indicated that the ternary carbides  $UMoC_{1.7}$  and  $UMoC_2$  may form in irradiated UC fuel when the concentration of Mo is about 2 at.%. Microhardness of the phase constituents of alloys have been measured by [1967Chu]. Using a high temperature neutron diffractometer, [1970Bow] determined the lattice parameters of the  $UMoC_2$  compound in the temperature range from 925 to 2100°C. Some of the data are listed in Table 2. Anisotropic thermal expansion was measured. The coefficients of thermal expansion are equal to (units of  $10^{-6} \text{ C}^{-1}$ ):  $\alpha_{11} = 8.6 \pm 0.2$ ,  $\alpha_{22} = 15.5 \pm 0.5$ ,  $\alpha_{33} = 9.9 \pm 2.6$ . Thermal expansion coefficients for  $UMoC_2$  were also determined by [1971Uch] using X-ray diffraction technique in the temperature range from 20 to 1100°C. The values obtained are ( $10^{-6} \text{ C}^{-1}$  units):  $\alpha_{11} = 7.7 \pm 0.6$ ,  $\alpha_{22} = 12.5 \pm 0.7$ ,  $\alpha_{33} = 3.4 \pm 1.0$ . They are lower than the data of [1970Bow], and differ most in the behavior of the  $c$ -axis ( $\alpha_{33}$ ), which the authors of [1970Bow] reported as expanding more rapidly than the  $a$ -axis ( $\alpha_{11}$ ). [1971Uch] attributed this to the higher temperature range

covered by [1970Bow], since it is believed that in general the thermal expansion coefficient increases with temperature. [1985Ara] have determined the thermal conductivities of  $\text{UMoC}_2$  and  $\text{UMoC}_{1.7}$  from thermal diffusivities measured in the temperature range from 477 to 1227°C. The pellets were preliminarily sintered at 1800°C for 5 h. The measured bulk densities were  $10.2 \text{ g}\cdot\text{cm}^{-3}$  and  $10.6 \text{ g}\cdot\text{cm}^{-3}$  for  $\text{UMoC}_2$  and  $\text{UMoC}_{1.7}$ , respectively. Figure 15 shows the thermal diffusivities. These values are not corrected for porosity. Thermal diffusivities for these compounds increase gradually with increasing temperature. The thermal conductivities were calculated by using the thermal diffusivity data, the heat capacity and the density of the samples. Figure 16 presents the thermal conductivities of  $\text{UMoC}_{1.7}$  corrected to 100% theoretical density in the temperature range from 477 to 1227°C. The thermal conductivities also increase as the temperature increases, but their temperature dependence was a little larger than that of the thermal diffusivities, which was mainly due to the heat capacity values estimated in [1985Ara]. The thermal conductivity of  $\text{UMoC}_2$  is slightly higher than that of  $\text{UMoC}_{1.7}$  especially at lower temperatures.

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**Table 1:** Investigations of the C-Mo-U Phase Relations, Structures and Thermodynamics

Reference	Method/Experimental Technique	Temperature/Composition/Phase Range Studied
[1962Cra]	Optical microscopy, replica electron microscopy of slowly cooled alloys	U rich corner
[1962Kat]	Metallography, X-ray diffraction	1000°C; UC-Mo, $UC_2$ -Mo
[1963Rud]	X-ray diffraction, metallography	Whole range of compositions
[1964Str]	Metallography, X-ray diffraction	500-950°C, isopleths at 5 and 15 at.% C, 2 and 4 mass% C, 0 to 25 at.% Mo
[1964Cro]	Single-crystal X-ray diffraction	$UMoC_2$
[1965Dec]	Metallography	U rich corner
[1966Ans]	X-ray diffraction, metallography	Annealed at 1800°C, $UMoC_{1.7}$
[1967Chu]	Metallography, X-ray diffraction	Whole range of compositions
[1968Ale]	Single-crystal X-ray diffraction, optical microscopy	UC- $UMoC_2$ -Mo-U-UC phase region
[1970Bow]	High-temperature neutron diffractometry	800-2100°C, $UMoC_2$
[1971Uch]	High-temperature X-ray diffraction	$UMoC_2$



Reference	Method/Experimental Technique	Temperature/Composition/Phase Range Studied
[1973Ale1]	Metallography, X-ray diffraction	Isopleths $\text{UMoC}_2$ -C, $\text{UMoC}_2$ -U:Mo = 1:1
[1973Ale2]	Metallography, X-ray diffraction	UC- $\text{UMoC}_2$ - $\text{Mo}_2\text{C}$ -Mo-U phase region. Partial liquidus surface
[1973Ale3]	Metallography, X-ray diffraction	The $\text{UC}_2$ - $\text{UMoC}_2$ , $\text{UMoC}_2$ - $\text{Mo}_{58}\text{C}_{42}$ , $\text{U}_2\text{C}_3$ - $\text{UMoC}_2$ sections
[1973Ale4]	X-ray diffraction (single crystal)	$\text{UMoC}_{2-x}$
[1974Nar]	Chemical analysis, X-ray diffraction, electron probe, metallography, standard Gibbs free energy of formation determination (emf studies)	$\text{UMoC}_{2-x}$ ( $x = 0, 0.25$ to $0.5$ ). $\Delta_f G^\circ$ ( $\text{UMoC}_2$ )
[1974Iva]	Crystal structure studies	$\text{UMoC}_2$
[1975Ale] as quoted by [1986Jei]	Crystal structure studies	$\text{UMoC}_{1.5}$
[1975Uga1]	Free energy determination, thermodynamic activity calculation	Three-phase and two-phase fields across the system.
[1975Uga2]	Free energy estimation, metallography, X-ray diffraction	1500-2000°C
[1985Ara]	X-ray diffraction, chemical analysis	$\text{UMoC}_2$ , $\text{UMoC}_{1.7}$
[1986Jei]	X-ray Guinier studies	$\text{UMoC}_{1.5}$
[1988Jon]	Mild hydrolysis, thermal analysis, X-ray diffraction, Rietveld neutron powder diffraction	$\text{UMoC}_2$
[1989Lin] as quoted by [1994Mch]	Phase equilibria experimental studying	Whole range of compositions
[1996Ana]	Methane-hydrogen gas equilibrium technique - C activity	700-900°C, $\text{UMoC}_{1.7}$ , $\text{UMoC}_2$

**Table 2:** Crystallographic Data of Solid Phases

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
(C) (diamond)	$cF8$ $Fd\bar{3}m$ C (diamond)	$a = 356.69$	at 25°C, 60 GPa [Mas2]
(C) (graphite) < 3827	$hP4$ $P6_3/mmc$ C (graphite)	$a = 246.12$ $c = 670.90$	at 25°C [Mas2] sublimation point

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
(Mo) < 2623	$cI2$ $Im\bar{3}m$ W	$a = 314.70$	at 25°C [Mas2] $x = 0, 0 < y \leq 0.011, T = 2205 \pm 9^\circ\text{C}$ [Mas2]
$U_x\text{Mo}_{1-x-y}\text{C}_y$		$a = 336.93$	$y = 0, 0 < x \leq 0.03,$ $T = 1284 \pm 2^\circ\text{C}$ [Mas2] $y = 0, x = 0.645$ [2001Pov]
( $\gamma$ U) 1135 - 776 $U_{1-x-y}\text{Mo}_x\text{C}_y$	$cI2$ $Im\bar{3}m$ W	$a = 352.4$          $a = 436$	[Mas2] $x = 0, 0 < y \leq 0.0022$ to $0.0037,$ $T = 1119 \pm 1^\circ\text{C}$ [Mas2] $y = 0, 0 < x \leq 0.42,$ $T = 1284 \pm 2^\circ\text{C}$ [Mas2] $x = 0.36, y = 0, T = 900^\circ\text{C}$ [1963Rud]
( $\beta$ U) 776 - 668 $U_{1-x-y}\text{Mo}_x\text{C}_y$	$tP30$ $P4_2/mnm$ $\beta$ U	$a = 1075.9$ $c = 565.6$	[Mas2] $x = 0, 0 < y \leq 0.0002, T = 772^\circ\text{C}$ [Mas2] $y = 0, 0 < x < 0.02,$ $T = 668^\circ\text{C}$ [Mas2]
( $\alpha$ U) < 668	$oC4$ $Cmcm$ $\alpha$ U	$a = 285.37$ $b = 586.95$ $c = 495.48$	at 25°C [Mas2] [1963Rud]
$U_{1-x-y}\text{Mo}_x\text{C}_y$		$a = 285.8$ $b = 587.6$ $c = 494.7$	$x = 0, 0 < y \leq 6 \cdot 10^{-5}, T = 660^\circ\text{C}$ [Mas2] $y = 0, 0 < x \leq 0.007,$ $T = \sim 570^\circ\text{C}$ [Mas2]
$\beta, \text{Mo}_2\text{C} (h_2)$ 2537 - 1650	$hP3$ $P6_3/mmc$ $\text{Fe}_2\text{N}$	$a = 299.6$ to $301.2$ $c = 473.1$ to $478.6$          $a = 299.6$ $c = 473.8$          $a = 300.6$ $c = 473.4$          $a = 299.0$ to $301.0$ $c = 473.0$ to $477.8$	27 to 36 at.% C [Mas2], [1988Epi], [1988Vel]          $T = 255^\circ\text{C}$ [V-C2]          at 33.5 at.% C, quenched from $T = 2000^\circ\text{C}$ [1965Rud]    at 30 to 34 at.% C, $T = 2200^\circ\text{C}$ [V-C2]
$\beta', \text{Mo}_2\text{C} (h_1)$ 1960 - 1190	$hP12$ $P\bar{3}1m$ $\text{Mo}_2\text{C}$	$a = 519$ $c = 472.4$          $a = 526$ $c = 480$	ordered $\beta$ phase, labeled as “ $\epsilon$ - $\text{Mo}_2\text{C}$ ” in [1988Epi]          $T = 1700^\circ\text{C}$ [1988Epi]

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
$\beta''$ , Mo <sub>2</sub> C (r <sub>2</sub> ) ≤ 1380	<i>oP12</i> <i>Pbcn</i> PbO <sub>2</sub>	$a = 473.0$	at ~32.5 at.% C [Mas2], [V-C2]
		$b = 602.7$	
		$c = 519.8$	
		$a = 473.5$ $b = 602.5$ $c = 521.0$	
		$a = 473.2$ $b = 604.8$ $c = 518.8$	labeled as “ $\beta'$ -Mo <sub>2</sub> C” [1988Vel] $T = 20^\circ\text{C}$ [1988Epi] $T = 227^\circ\text{C}$ [V-C2]
		$a = 476.2$ $b = 607.2$ $c = 521.6$	$T = 727^\circ\text{C}$ [V-C2]
$\beta'''$ , Mo <sub>2</sub> C (r <sub>1</sub> ) < 1220	<i>o**</i>	$a = 946.6$ $b = 2415.2$ $c = 4167.5$	at ~33.5 at.% C [Mas2] labeled as “ $\beta$ -Mo <sub>2</sub> C” [1988Vel]
$\delta$ , MoC <sub>1-x</sub> 2605 - 1956	<i>oF8</i> <i>Fm<math>\bar{3}m</math></i> NaCl		37 to 43 at.% C [V-C, Mas2]
			labeled as “ $\alpha$ -MoC <sub>1-x</sub> ” [1973Ale3]
		$a = 426.6$ to 428.1	39.7 to 43 at.% C [1988Vel]
		$a = 426.7$	at 41 at.% C [1965Rud]
		$a = 428.1$	at 43 at.% C [1965Rud]
U <sub>y</sub> Mo <sub>x</sub> C <sub>1-x-y</sub>		$a = 426.2$	in the alloy U <sub>2.3</sub> Mo <sub>55</sub> C <sub>42.7</sub> annealed at $T = 2050^\circ\text{C}$ [1973Ale3]
		$a = 426.8$	in the alloy U <sub>9.85</sub> Mo <sub>45</sub> C <sub>45.15</sub> annealed at $T = 2050^\circ\text{C}$ [1973Ale3]
		$a = 427.6$	in the as-cast alloy U <sub>2.3</sub> Mo <sub>55</sub> C <sub>42.7</sub> [1973Ale3]
		$a = 428.2$	in the as-cast alloy U <sub>9.85</sub> Mo <sub>45</sub> C <sub>45.15</sub> [1973Ale3]
$\eta$ , MoC <sub>1-x</sub> 2530 - 1647	<i>hP8</i> <i>P6<sub>3</sub>/mmc</i> TiAs	$a = 301.2$	37 to 40 at.% C [Mas2]
		$c = 1463.4$	at 39 at.% C [1988Vel]
		$a = 301.2$ $c = 1465$	at 39 at.% C [1965Rud]

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
$\gamma$ , MoC < 1220	$hP2$ $P\bar{6}m2$ WC	$a = 289.8$ $c = 280.9$  $a = 290.6$ $c = 282.2$	50 at.% C [Mas2] [V-C2]  [1988Vel]
$\epsilon$ , UC (I) < 2585 1.013 bar	$cF8$ $Fm\bar{3}m$ NaCl	$a = 495.98$  $a = 496.2$	47 to 66 at.% C [Mas2] [E] [1963Rud]
UC (II) > $2.7 \cdot 10^5$ bar	$o^{**}$	-	[1987Ben]
$\mu$ , $U_2C_3$ 1823 - ~850	$cI40$ $\bar{I}43d$ $Pu_2C_3$	-	60 at.% C [Mas2]
$\kappa$ , $UC_2$ 1793 - 1516	$tI6$ $I4/mmm$ $CaC_2$	$a = 351.7$ $c = 598.7$  $a = 352.4$ $c = 599.9$  $a = 351.9$ to $352.41$ [S] $c = 597.87$ to $599.62$  $a = 352.7$ $c = 598.0$  $a = 352.0$ $c = 598.5$  $a = 352.2$ $c = 598.8$	62 to 65.5 at.% C [Mas2] [E]  [H]  [1963Rud]  [1967Rea]  [1987Jon]
$UC_2$ 2434 - 1762	$cF12$ $Fm\bar{3}m$ $CaF_2?$	$a = 545.0$	actually, “ $UC_2$ ” phase represents the $\epsilon$ ,UC phase in equilibrium with graphite [1993But, 2001Che]
$\lambda$ , $U_2Mo$ $\leq 1252$ (?)	$tI6$ $I4/mmm$ $MoSi_2$	$a = 342.7$ $c = 985.4$	32.5 to 34 at.% Mo [Mas2] [E]

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
* $\tau_1$ , $\text{UMoC}_{2-x}$ $\lesssim 2227$	$m^{**}$	$a = 562.6$ $b = 323.8$ $c = 1166.1$ $\beta = 109.7^\circ$	$x = 0.25$ to $0.5$ $x = 0.3$ , $T = 1800^\circ\text{C}$ [1966Ans]
		$a = 532$ $b = 324$ $c = 1100$ $\beta = 108.5^\circ$	$x = 0.33$ [1968Ale]
		$a = 562.8$ $b = 323.8$ $c = 1165.5$ $\beta = 109.5^\circ$	$x = 0.5$ [1973Ale4, 1975Ale, 1986Jei]
		$a = 564$ $b = 324$ $c = 1166$ $\beta = 109.8^\circ$	$x = 0.3$ , $T = 1800^\circ\text{C}$ [1985Ara]
		$a = 561.8$ $b = 324.35$ $c = 1164.9$ $\beta = 109.63^\circ$	$x = 0.5$ [1986Jei]

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
* $\tau_2$ , $\text{UMoC}_2$ $\lesssim 2350$	$oP4$ $Pnma$ $\text{UCrC}_2$	$a = 562.5$ $b = 324.9$ $c = 1098.0$	[1964Cro]
		$a = 562.6$ $b = 324.0$ $c = 1095.7$	at room temperature [1970Bow]
		$a = 566.5$ $b = 328.5$ $c = 1102.0$	$T = 925^\circ\text{C}$ [1970Bow]
		$a = 571.5$ $b = 334.2$ $c = 1110.0$	$T = 2000^\circ\text{C}$ [1970Bow]
		$a = 563.0$ $b = 325.3$ $c = 1101.0$	[1971Uch]
		$a = 562.5$ $b = 324.9$ $c = 1099.0$	[1974Iva]
		$a = 561.2$ $b = 324.1$ $c = 1095.6$	[1988Jon]
$\omega$ , $\text{UMo}_2\text{C}_2$ 1800 - 1500	-	-	Metastable [1963Rud]
$\chi$ , $\text{UMoC}$ > 1800	-	-	Metastable [1964Chu]

**Table 3:** Invariant Equilibria

Reaction	$T$ [°C]	Type	Phase	Composition (at.%)		
				C	Mo	U
$\text{L} \rightleftharpoons \tau_2$	$\sim 2350$	congruent	L $\tau_2$	50 50	25 25	25 25
$\text{l} \rightleftharpoons \tau_2 + \beta$	2270	$e_5$	L	-	-	-
$\text{l} \rightleftharpoons \tau_2 + (\text{C})$	2200	e	L	-	-	-
$\text{l} + \tau_2 \rightleftharpoons \tau_1$	2170	$p_1$	L	$\sim 42$	$\sim 29$	$\sim 29$
$\text{l} \rightleftharpoons \varepsilon + \tau_2$	2160	$e_7$	L	-	-	-

Reaction	$T$ [°C]	Type	Phase	Composition (at.%)		
				C	Mo	U
$L + \tau_2 \rightleftharpoons \varepsilon + \tau_1$	?	$U_1$	L	~ 45	~ 18	~ 37
$L + \tau_2 \rightleftharpoons \tau_1 + \beta$	$2100 \pm 50$	$U_2$	L	~ 39	~ 44	~ 17
$L + \beta \rightleftharpoons (\text{Mo}) + \tau_1$	$1900 \pm 20$	$U_3$	L	~ 33	~ 46	~ 21
$L + \tau_1 \rightleftharpoons \varepsilon + (\text{Mo})$	1530	$U_4$	L	~ 20	~ 43	~ 37
$L + (\text{Mo}) \rightleftharpoons (\gamma\text{U}) + \varepsilon$	1185	$U_5$	L	~ 3	~ 29	~ 68
$(\beta\text{U}) \rightleftharpoons (\alpha\text{U}) + (\gamma\text{U}) + \varepsilon$	640	$E_1$	-	-	-	-
$(\gamma\text{U}) \rightleftharpoons \lambda + \varepsilon$	590	$e_{20}$	-	-	-	-
$(\gamma\text{U}) \rightleftharpoons \lambda + \varepsilon + (\text{Mo})$	$580 \pm 7$	$E_2$	-	-	-	-
$(\gamma\text{U}) + \varepsilon \rightleftharpoons \lambda + (\alpha\text{U})$	570	$U_6$	-	-	-	-

**Table 4:** Thermodynamic Properties of Single Phases

Phase	Temperature Range [°C]	Property, per mole of atoms [J, mol, K]	Comments
$\tau_1$ , $\text{UMoC}_{1.7}$	25 - 1827	$\Delta_f G^\circ = -168824 - 2.89 \cdot T$ ( $\pm 17000$ )	[1975Uga2] approximation
	700 - 900	$\Delta_f G^\circ = -146632 - 15.0 \cdot T$ ( $\pm 8200$ )	[1996Ana] methane-hydrogen gas equilibration technique
$\tau_2$ , $\text{UMoC}_2$	727 - 927	$\Delta_f G^\circ = -274658 + 90.0 \cdot T$	[1973-1974Nar] derived from galvanic cell measurements
	25 - 1827	$\Delta_f G^\circ = -193970 - 2.89 \cdot T$	[1975Uga2] approximation
	700 - 900	$\Delta_f G^\circ = -151961 - 13.7 \cdot T$ ( $\pm 8100$ )	[1996Ana] methane-hydrogen gas equilibration technique
	25	$S^\circ = 93.05$	[1975Uga2] estimation

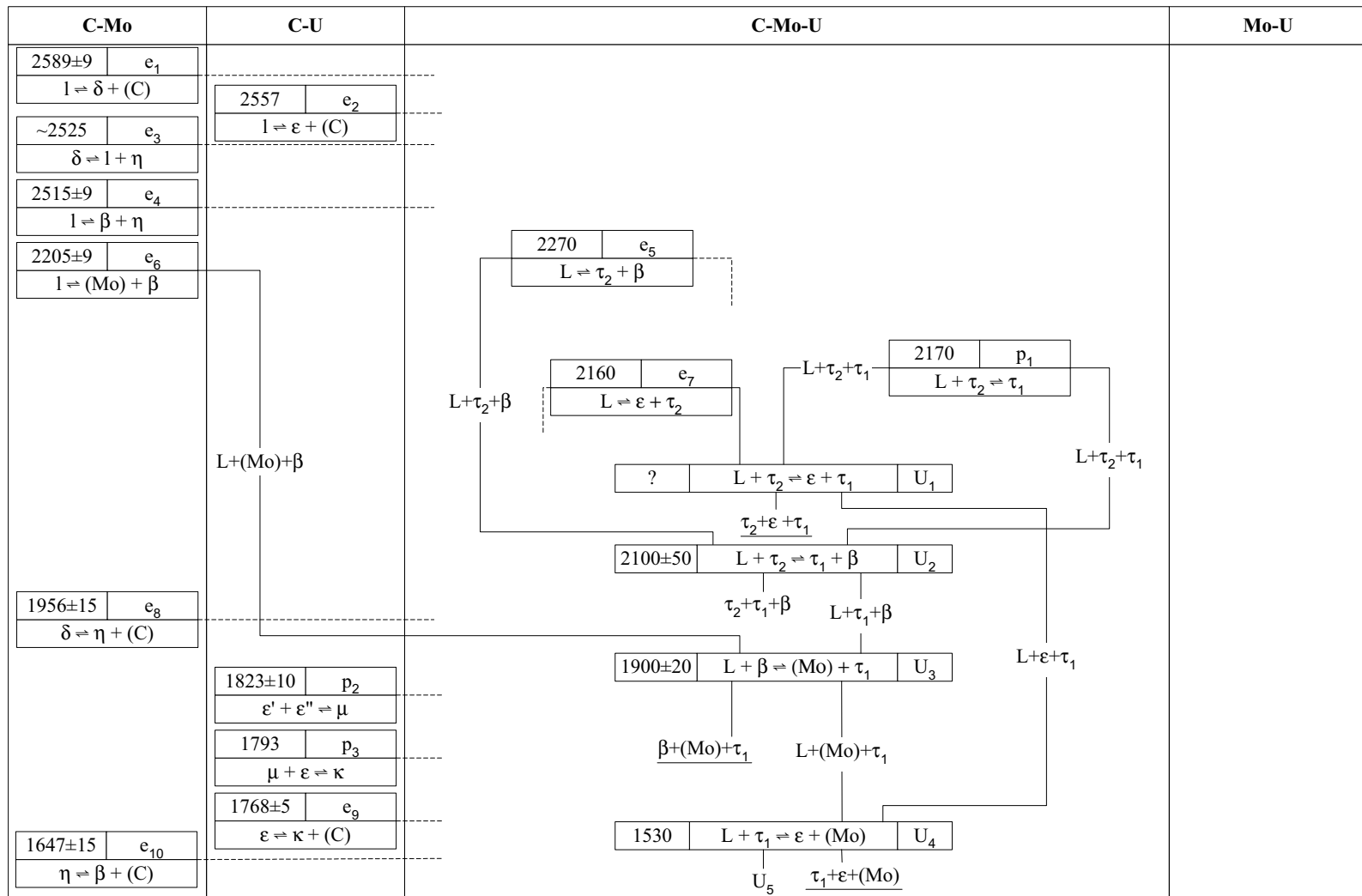


Fig. 1a: C-Mo-U. Partial reaction scheme



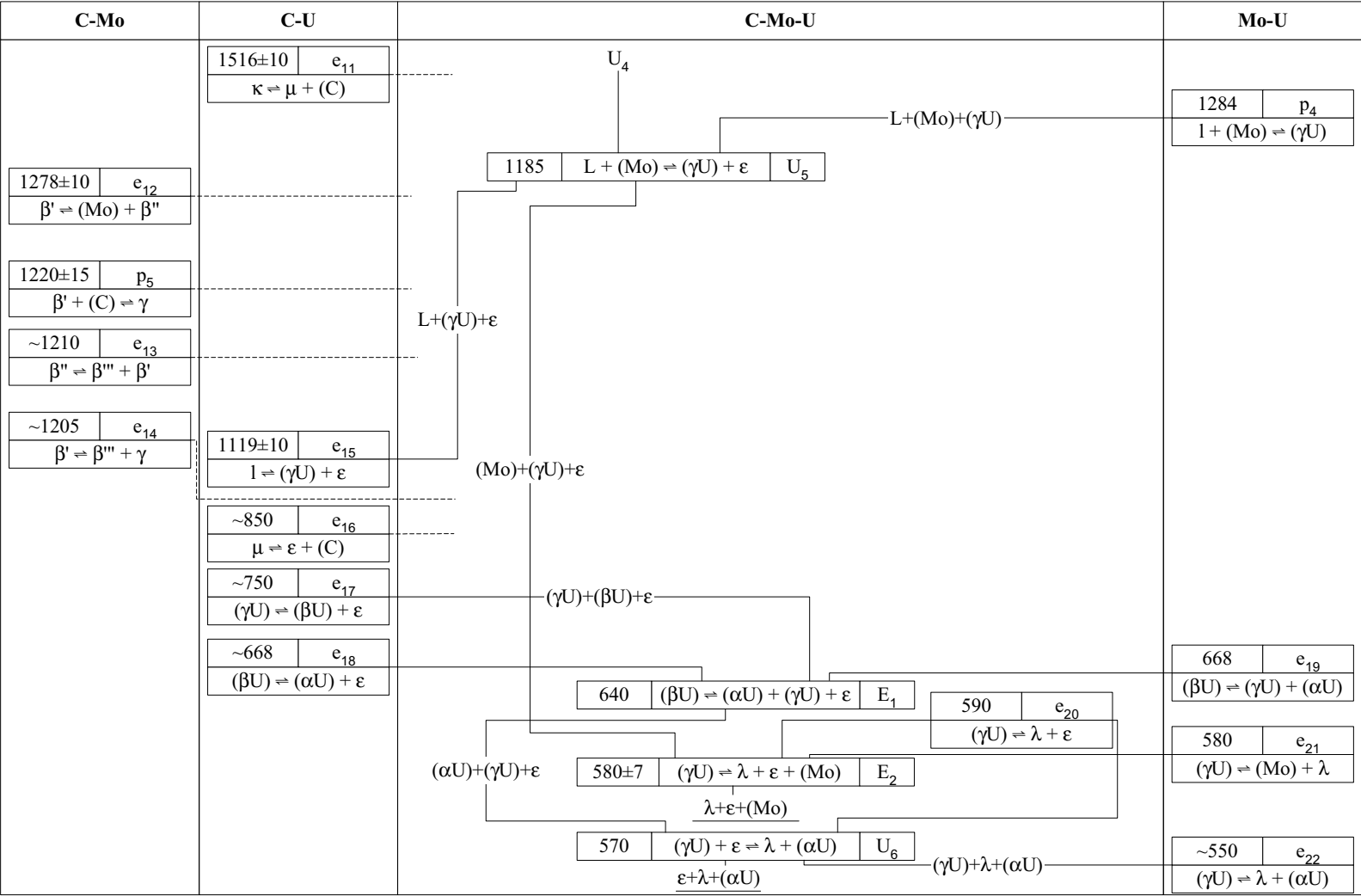
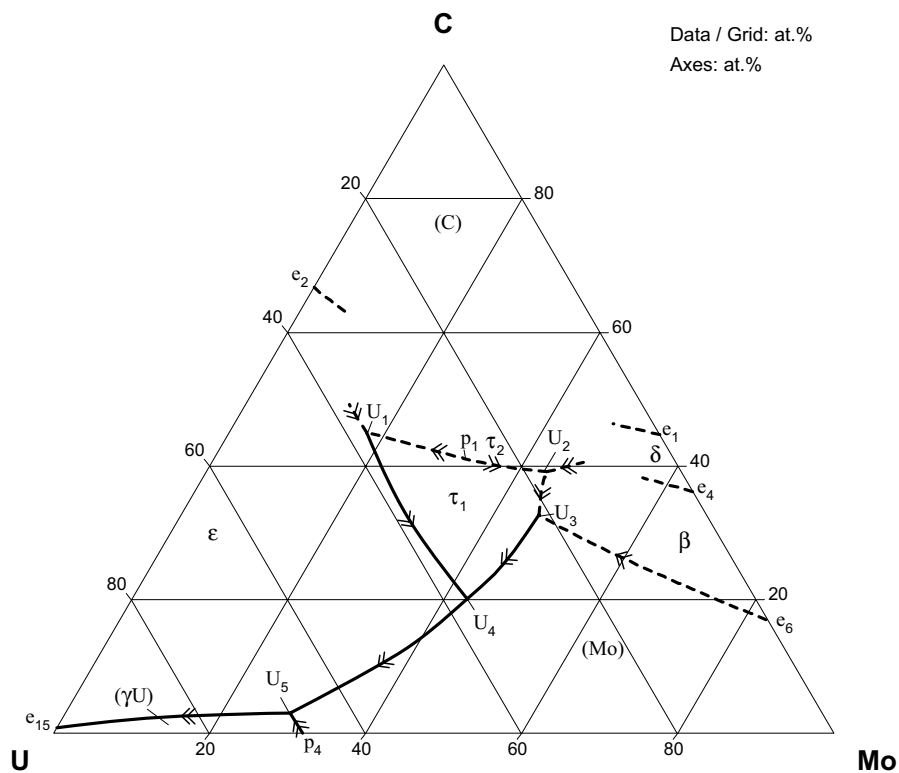
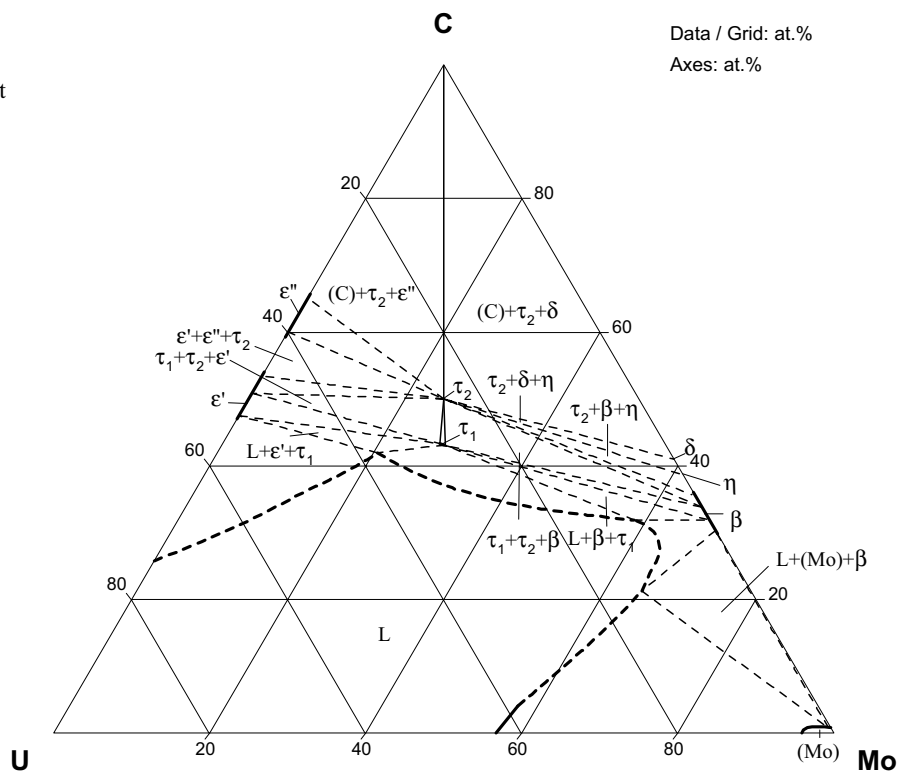


Fig. 1b: C-Mo-U. Partial reaction scheme

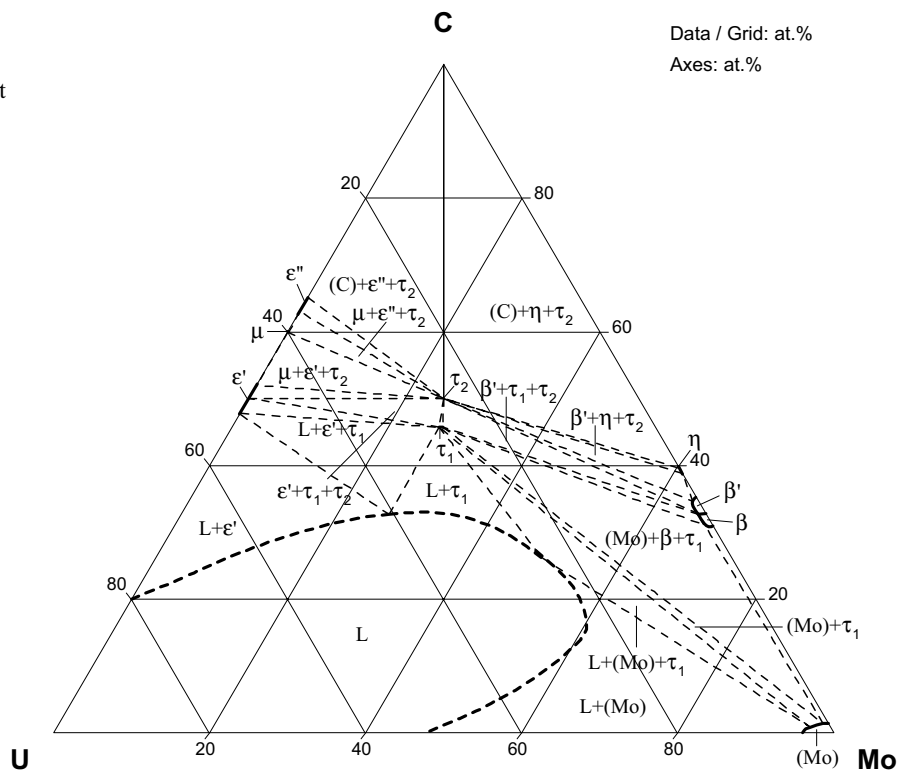
**Fig. 2: C-Mo-U.**  
Partial liquidus  
surface projection



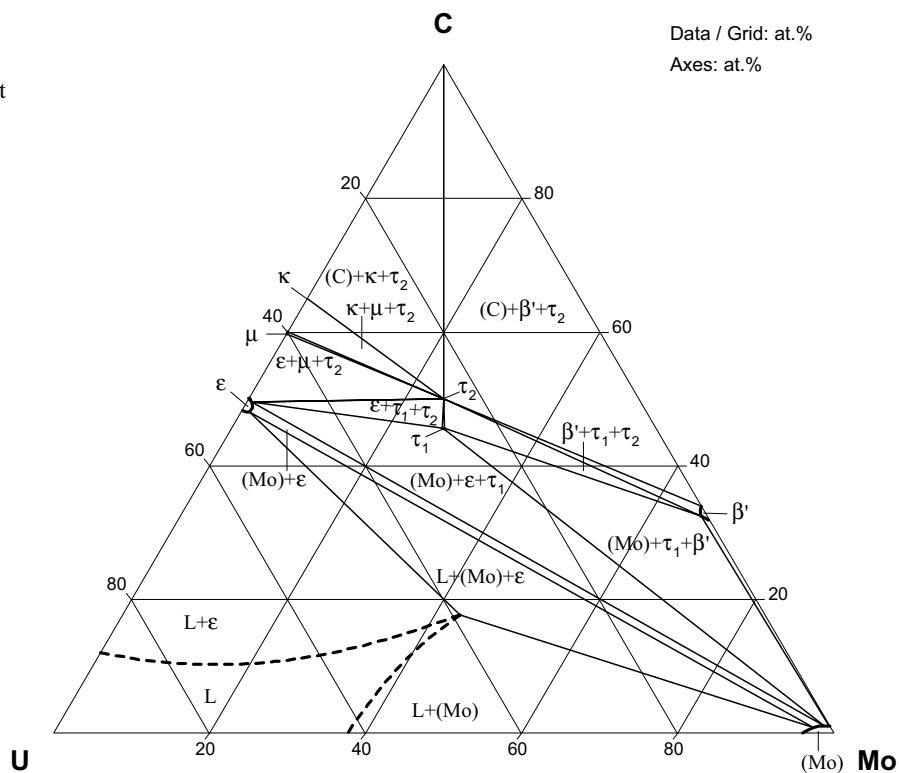
**Fig. 3: C-Mo-U.**  
Isothermal section at  
2000°C



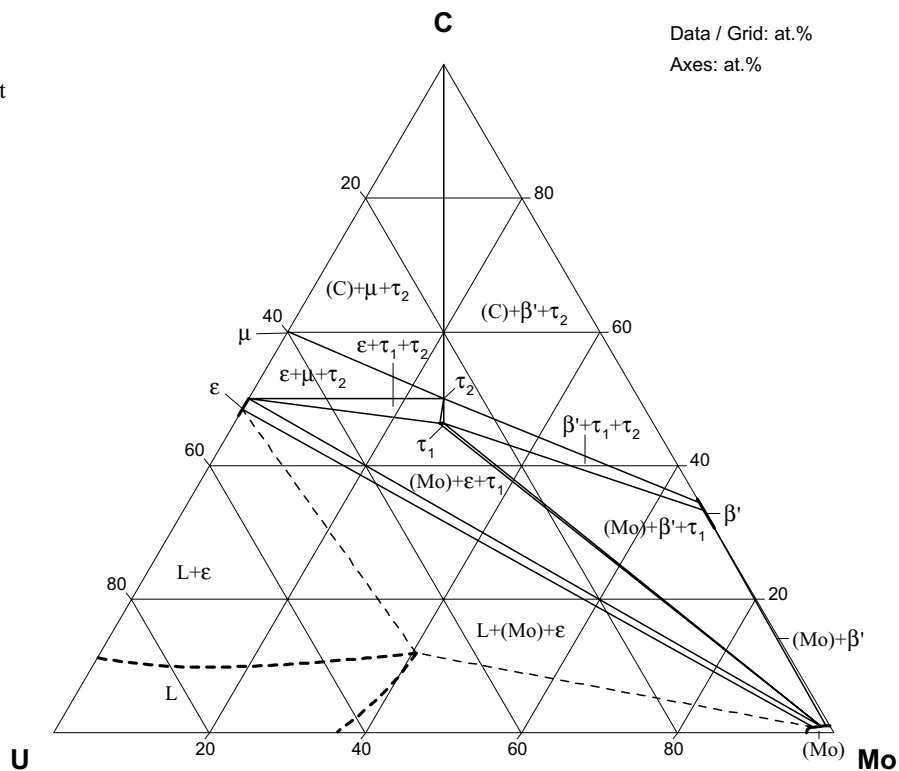
**Fig. 4: C-Mo-U.**  
Isothermal section at  
1800°C



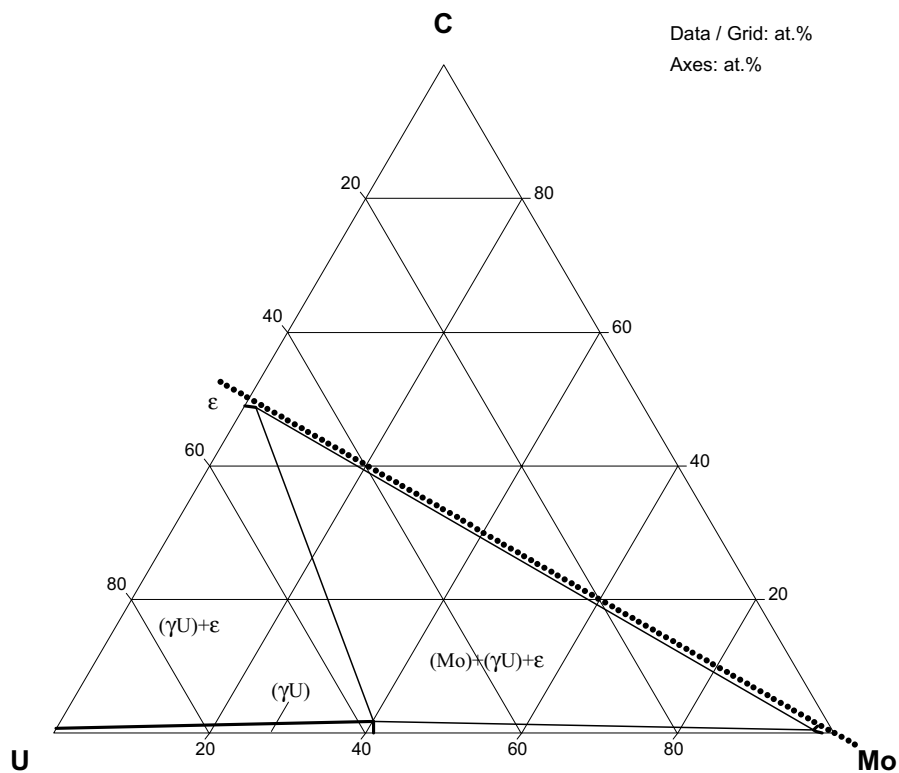
**Fig. 5: C-Mo-U.**  
Isothermal section at  
1525°C



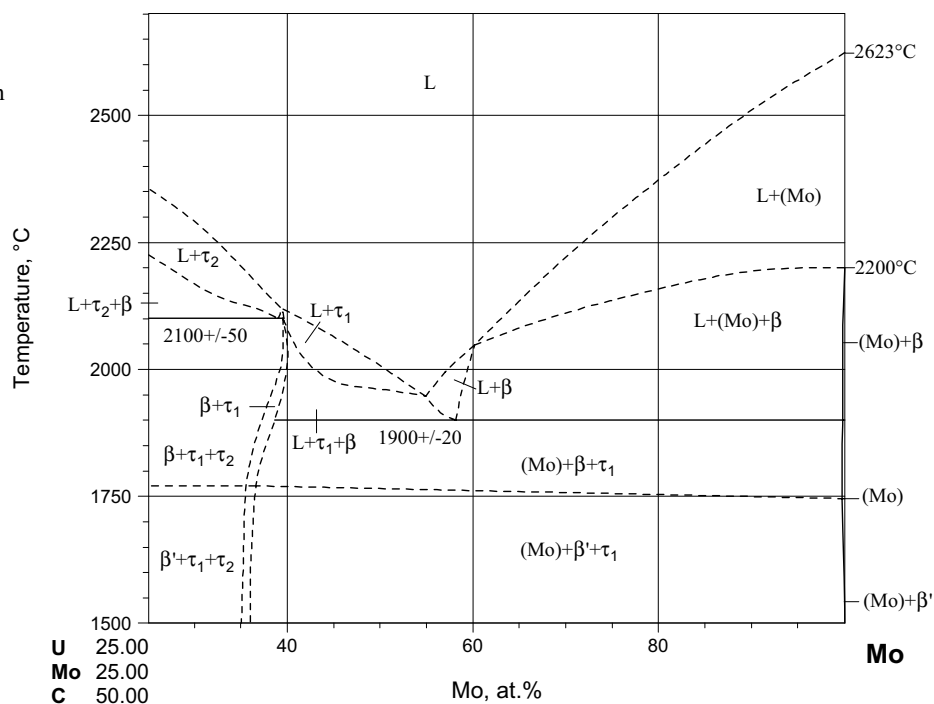
**Fig. 6: C-Mo-U.**  
Isothermal section at  
1500°C



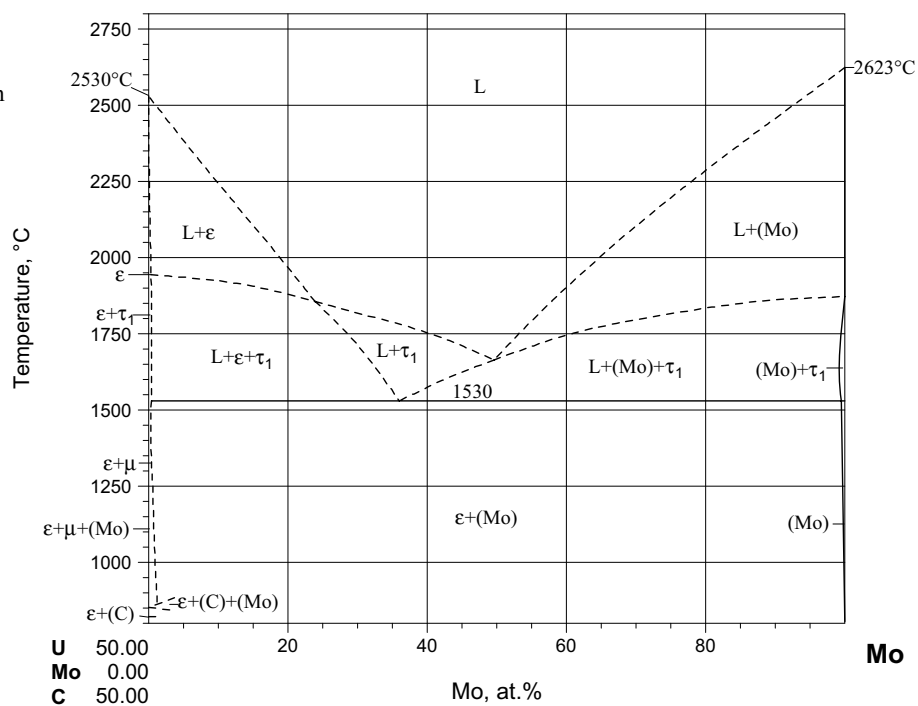
**Fig. 7: C-Mo-U.**  
Partial isothermal  
section at 900°C



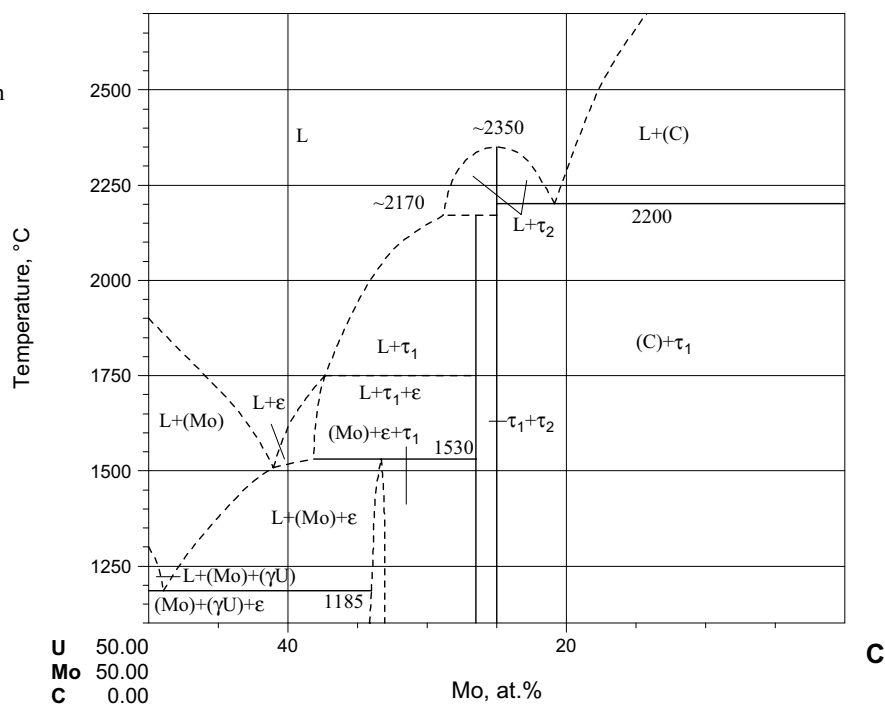
**Fig. 8: C-Mo-U.**  
Temperature -  
composition section  
UMoC<sub>2</sub> - Mo



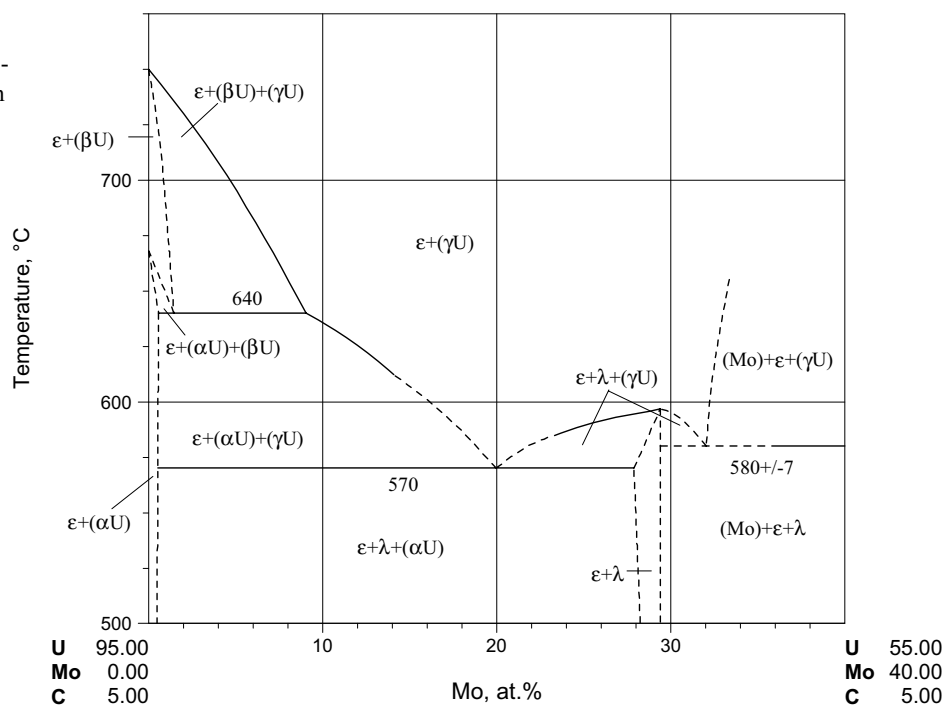
**Fig. 9: C-Mo-U.**  
Temperature -  
composition section  
UC - Mo



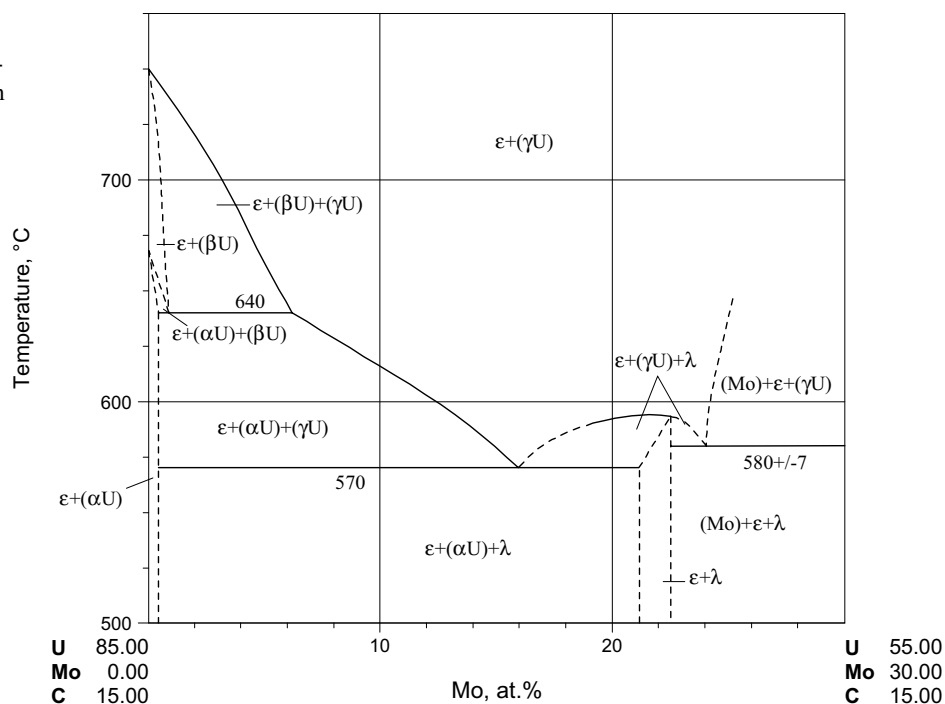
**Fig. 10: C-Mo-U.**  
Temperature -  
composition section  
 $U_{50}Mo_{50}C$



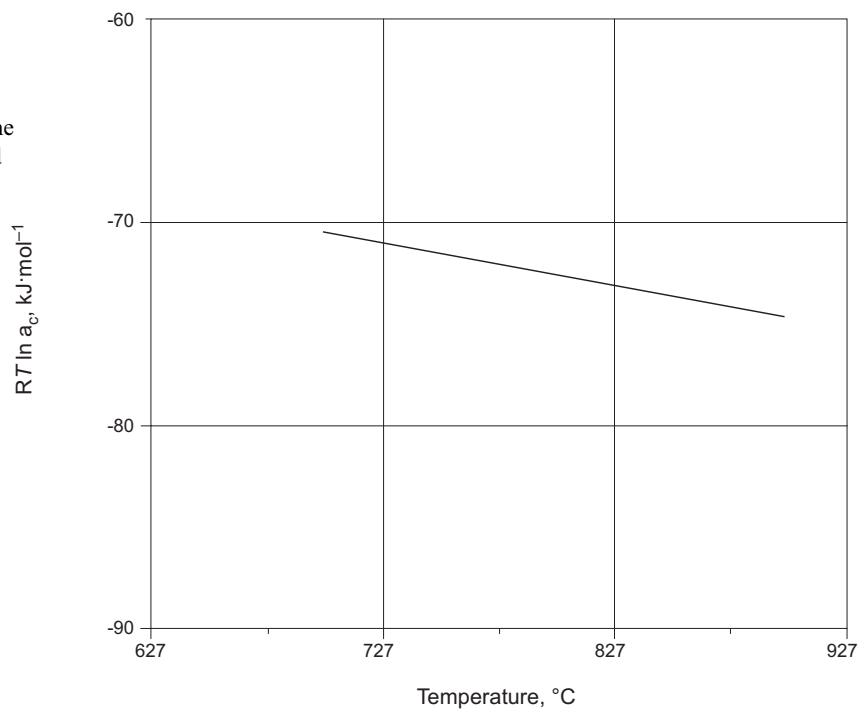
**Fig. 11: C-Mo-U.**  
Partial temperature -  
composition section  
at 5 at.% C



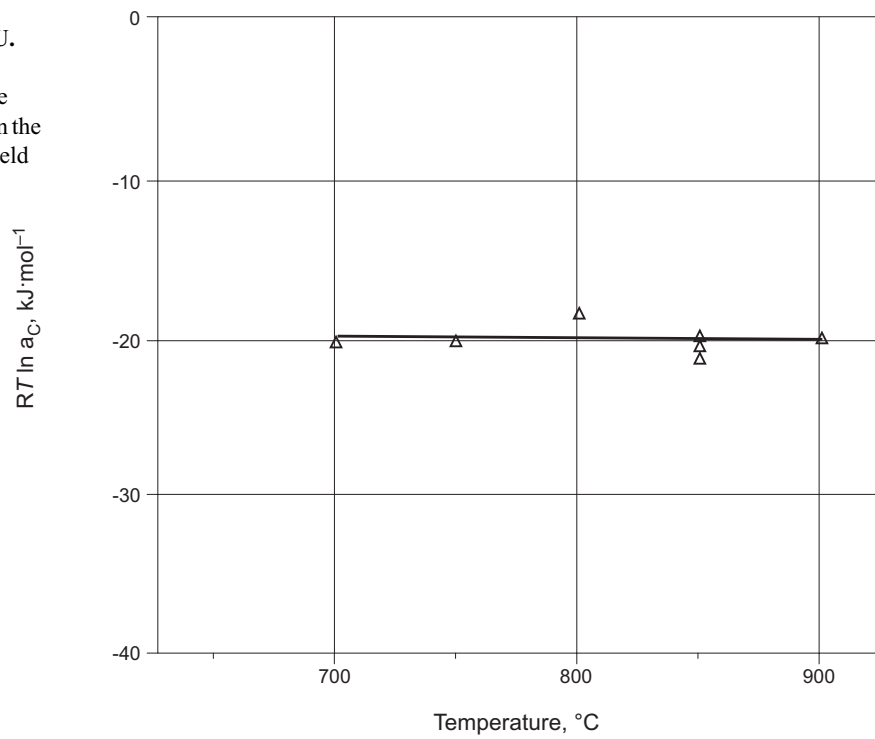
**Fig. 12: C-Mo-U.**  
Partial temperature-  
composition section  
at 15 at.% C



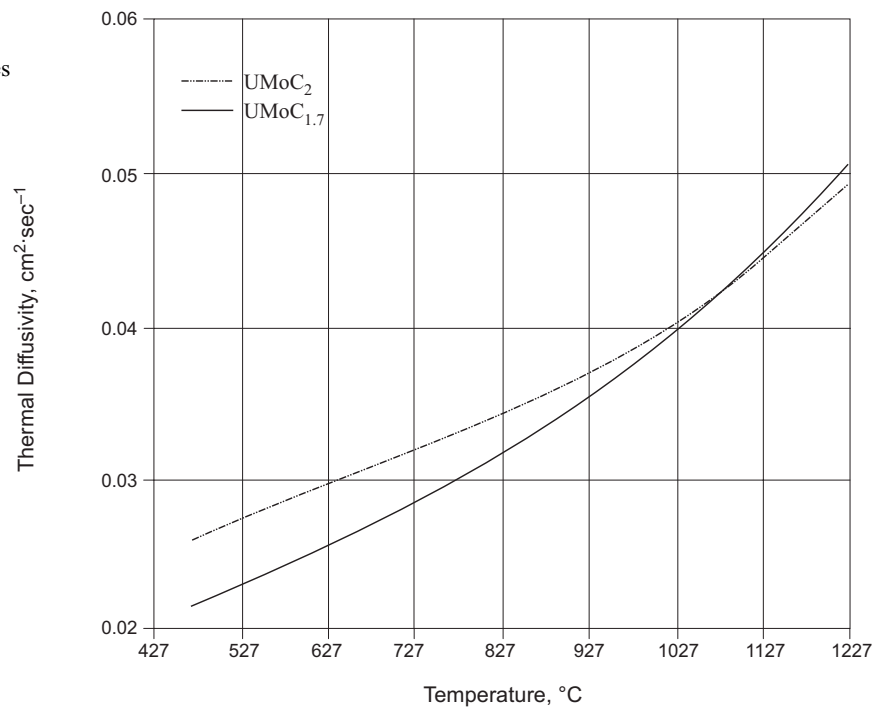
**Fig. 13: C-Mo-U.**  
Temperature  
dependence of the  
carbon potential in the  
three-phase field  
 $\epsilon + (Mo) + \tau_1$



**Fig. 14: C-Mo-U.**  
Temperature  
dependence of the  
carbon potential in the  
three-phase field  
 $\epsilon + \tau_1 + \tau_2$



**Fig. 15: C-Mo-U.**  
Thermal diffusivities  
of  $\text{UMoC}_2$  and  
 $\text{UMoC}_{1.7}$





**Fig. 16: C-Mo-U.**  
Thermal  
conductivities of  
 $\text{UMoC}_2$  and  $\text{UMoC}_{1.7}$   
normalized to 100%  
theoretical density

