Documenting thermodynamic databases

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Setting up a thermodynamic database

- Bibliography
- The real work: editing, optimising, validating, turning back, running crazy, asking for experiments, ab initio
- Reporting: topic of present talk

Why reporting ?

- Help the potential user of the database
- Help yourself in revision, extension

Ni database

Home | Introduction | Thermodynamic models | Phases of interest | Assessed systems

This documentation was developed by

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to report the constitution of a thermodynamic database
for the Ni based superalloys **NI24**,
supported by TCSAB, GE, A&D, and Snecma.

Current version : June 12, 2013

Johan Bratberg, Lina Kjellqvist, Andreas Markström, Hai-Lin Chen and Huahai Mao
from TCSAB has contributed to the database via the Ni20 and Ni24 projects.

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You must allow its use in order to get it work properly.

Ni database

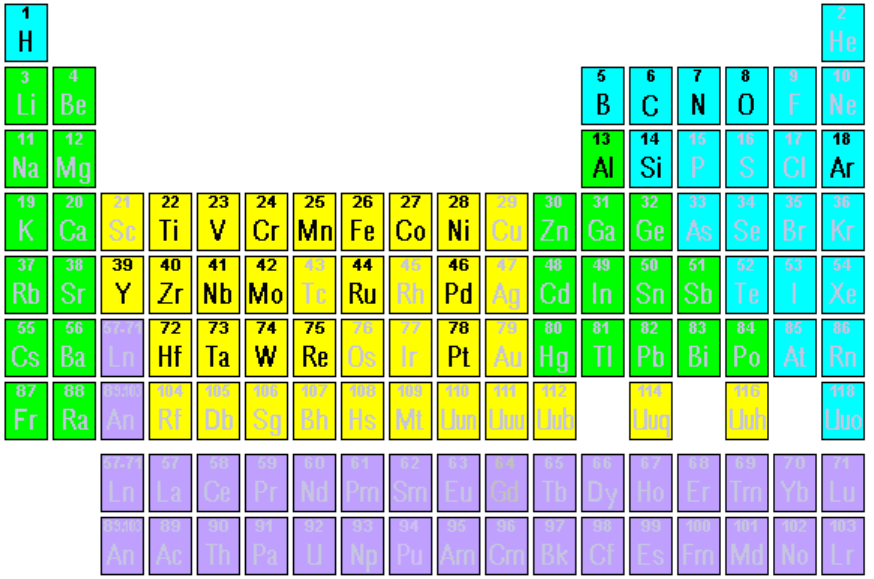
Home | Introduction | Thermodynamic models | Phases of interest | Assessed systems

To reach information on:

- elements
- binary systems
- ternary systems
- commented ternary systems

systems with **Al**, **Ar**, **B**, **C**, **Co**, **Cr**, **Fe**, **H**, **Hf**, **Mn**, **Mo**, **N**, **Nb**, **Ni**, **O**, **Pd**, **Pt**, **Re**, **Ru**, **Si**, **Ta**, **Ti**, **V**, **W**, **Y**, **Zr**

- via periodic table



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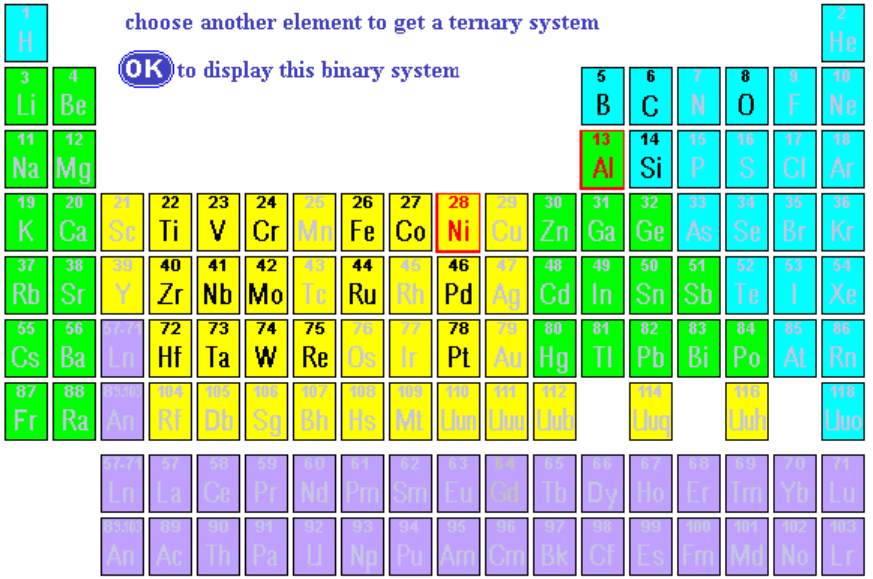
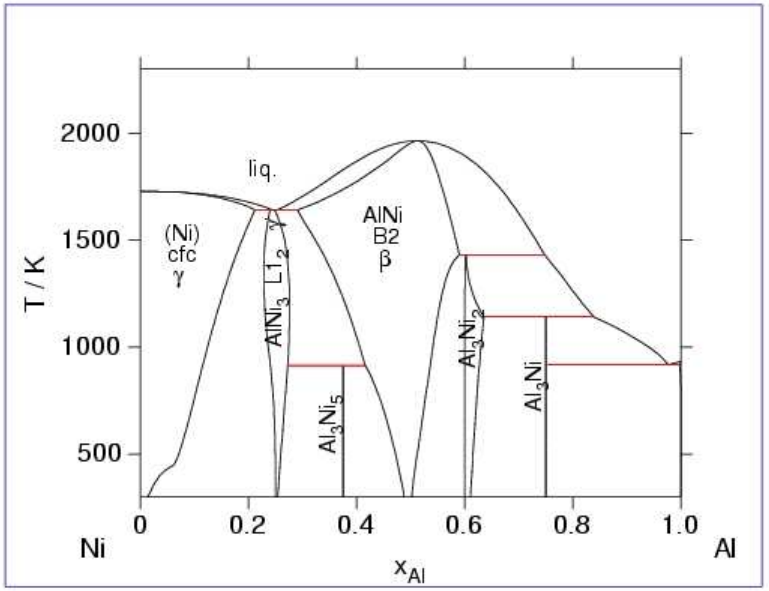
- via periodic table



Ni database

Binary system Al-Ni

Al Ni Al-B-Ni Al-C-Ni Al-Co-Ni Al-Cr-Ni Al-Fe-Ni Al-Hf-Ni Al-Mo-Ni Al-Nb-Ni Al-Ni-O Al-Ni-Pd Al-Ni-Pt
Al-Ni-Re Al-Ni-Ru Al-Ni-Si Al-Ni-Ta Al-Ni-Ti Al-Ni-V Al-Ni-W Al-Ni-Zr Binary syst. Ternary syst.
Periodic table



Source of the description

N. Dupin, Thèse, Institut National Polytechnique de Grenoble, France, 1995, p. 76-94; Ansara I, Dupin N, Lukas HL, Sundman B. J. of Alloys and Comp., 247, 20-30 (1997).

Comments

Slight modification of the low temperature equilibria between γ and γ' after N. Dupin, B. Sundman, A thermodynamic database for Ni-base superalloys, Scand. J. Metall., 30, 184-192 (2001).

During the NI17 project, the B2 phase description was modified when changing the lattice stability for the empty A2. The description of the Al_3Ni_2 and Al_3Ni phases has then also been odified in order to better account for the experimental results from Klaus Richter in the Al-Ni-Si ternary system.

Ni database

Home | Introduction | Thermodynamic models | Phases of interest | Assessed systems

Phases described by

usual name : liquid, γ, γ', Cr_3Si ...

database name : LIQUID, FCC_L12, BCC_A2...

prototype : Cu, NaCl, $MgCu_2$ ...

StrukturBericht : *A*1, *L*1$_2$, *A*2, *B*1, *C*14...

All phases in a table

List of the phases by default

last modification of this page by N. Dupin 2012-04-0

Usual name

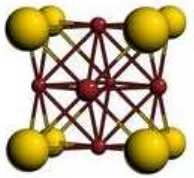
γ', Ni_3Al, Ni_3Fe, Co_3Ti, Ni_3Si-β1, Pd_3Ti, Pd_3Y, Pt_3Ti, Zr_3Al

Name in the database

FCC_L12_2

Crystallography

Prototype Cu_3Au ***StrukturBericht*** $L1_2$ ***Pearson*** *cP4* ***Space Group*** *Fm-3m*



Characteristics of the different sites for the prototype

Occupation	Multiplicity	Wickoff	Symmetry
Cu	3	c	4/mm.m
Au	1	a	m-3m

Thermodynamic modelling

$(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr)_{0.75}$
$(Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr)_{0.25}$ (B,C,N,O,VA)

Assessed systems where the phase is stable

Al-Ni Al-Pt Al-Zr Co-Ti Co-Pt Cr-Pd Cr-Pt Fe-Ni Fe-Pd Fe-Pt Mn-Ni Ni-Pt Ni-Si Pd-Ti Pd-Y Pt-Ti Al-Cr-Ni Al-Co-Ni Al-Ni-O Al-Ni-Ti

Comment

This phase is described with the same mathematical expression than the matrix γ and the carbides MC. It can be identify

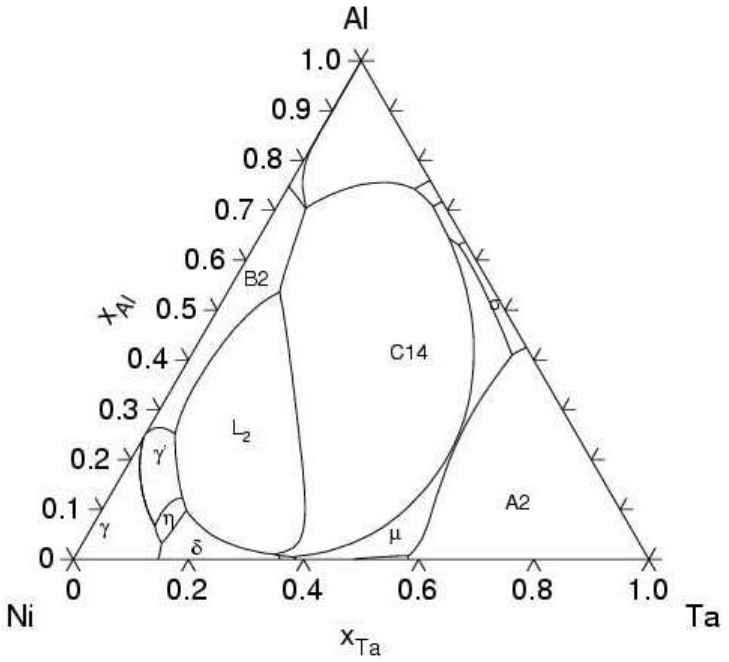
Ni database

Home | Introduction | Thermodynamic models | Phases of interest | Assessed systems

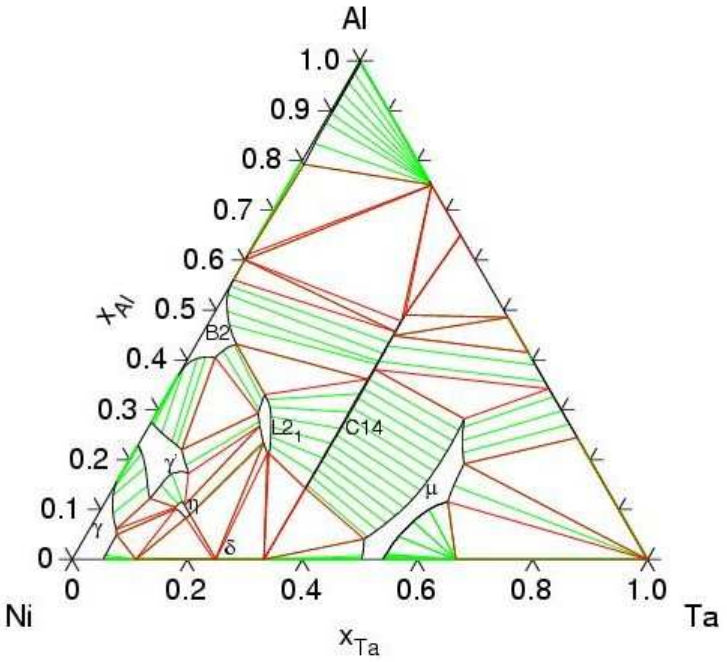
Ternary system Al-Ni-Ta

Al Ni Ta Al-Ni Al-Ta Ni-Ta Binary syst. Ternary syst. Periodic table

Projection of the monovariant lines of the liquidus



Isothermal section at 1273 K



Source of the description

Present work : NI13.

Ni database

Source of the description

Present work : NI13.

Comments

The previous description **Dupin** of this system has shown a big imprecision for the γ' composition in equilibrium with the γ phase at low temperature when comparing to **Dugue** made available since. The revision made during the present work (NI13) has allowed an important improvement on this point. The agreement with the experimental data at high temperature is slightly less than previousmy but still satisfactory.

Moreover, the model used for the phase Ni_6AlTa phase has been modified. It is now described as the Ni_3Ti isotypique phase. The description of this phase was reviewed during the nI17 project because it was becoming stable at low temperature in the binary Ni-Ta.

An important modification in the area less rich in Ni has also been introduced in order to describe the experimental results from Palm *et al.*. The Heusler phase, $AlNi_2Ta$, and the Laves phase, C14, as well as the extension of the mu phase have been introduced with a reasonable overal agreement.

An important disagreement has however not been resolved. The experimental equilibrium $AlNi+Ni_3Ta$ is less stable than $\gamma'+AlNi_2Ta$ in the calculation. The attempts to get the esperimental equilibrium induce important disagreements in the other fields and in particular in the Ni rich domain where the Ni_8Ta becomes too much stable. It is possible that this problem originates from the models used for the B2 and $AlNi_2Ta$ phases. This later is actually an ordered structure of the B2 state. In some systems, the transition between these two phases is of 2nd order (Al-Fe-Ti for instance). They should be described as a single phase with 4 sub-lattices.

Comparison with experimental data

Jia C.C. Jia, K. Ishida et T. Nishizawa, *Metall. Trans.*, **25A**, 473-485, 1994.
Nash P. Nash et D.R.F. West, *Met. Science*, **13**, 670-676, 1979.
Willemin P. Willemin, Thèse, INPG, Grenoble, 1986.
Hong Y.M. Hong, H. Nakayima and T. Suzuki, *ISIJ International*, **29**(1), 78-84, 1989.
Dupin N. Dupin, Thèse, INPG Grenoble, 1995.

Ni database

Jia C.C. Jia, K. Ishida et T. Nishizawa, *Metall. Trans.*, **25A**, 473-485, 1994.
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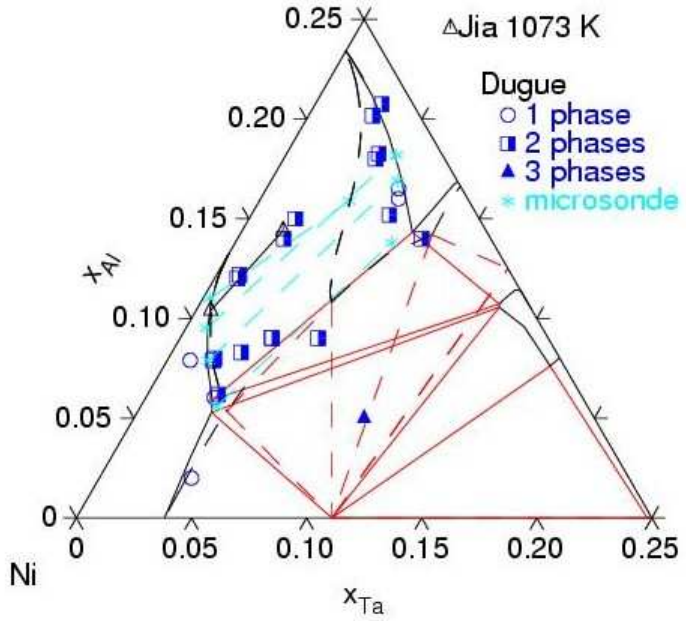
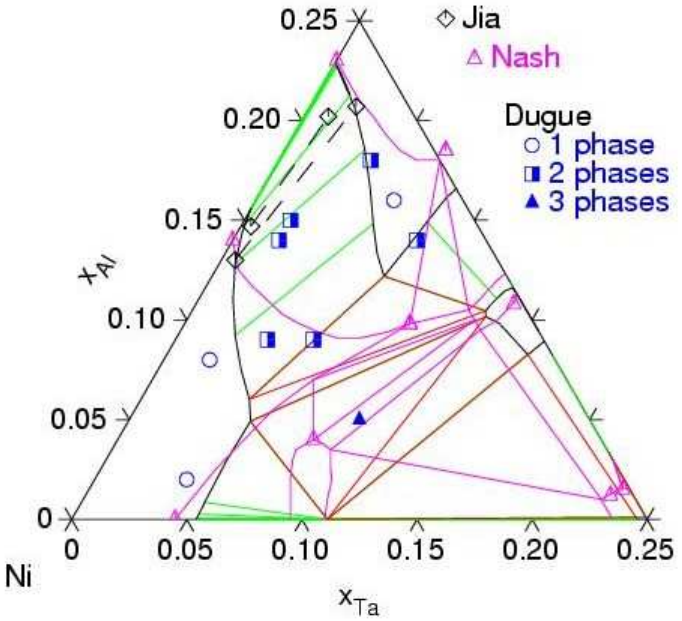
Dupin N. Dupin, Thèse, INPG Grenoble, 1995.
Dugue O. Dugué, Thèse, Ecole des Mines Paris, 1985.
Palm M. Palm, W. Sanders et G. Sauthoff, *Z. Metallkd.*, **87**(5), 390-398, 1996.



Calculated isothermal section at 1073 K compared to the experimental results at this temperature and top the previous description **Dupin** dashed.



Calculated isothermal section at 1273 K compared to the experimental results at this temperature and top the previous description **Dupin** dashed.

Ni database

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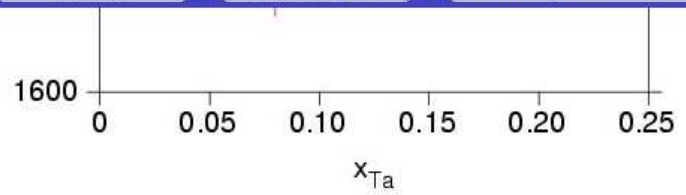
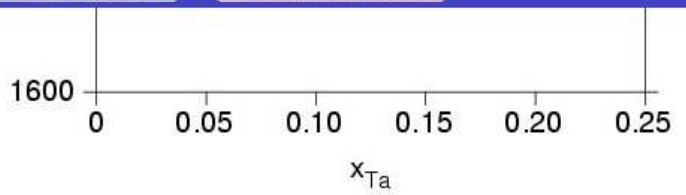
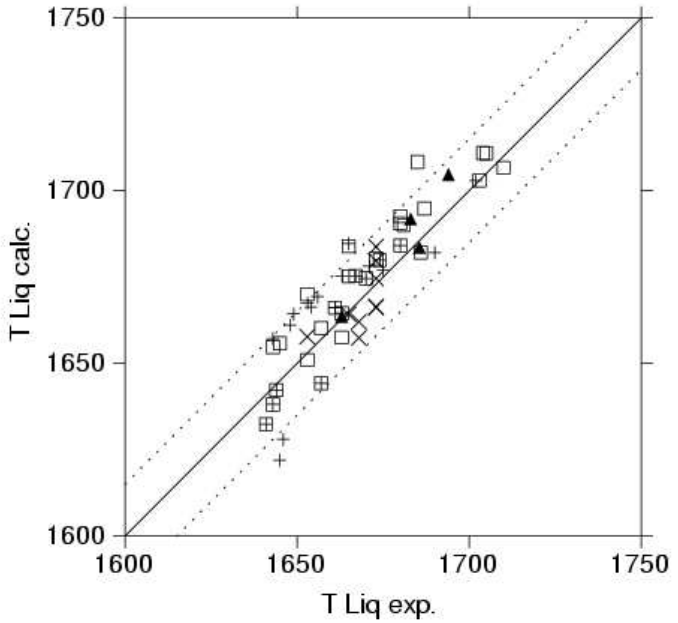
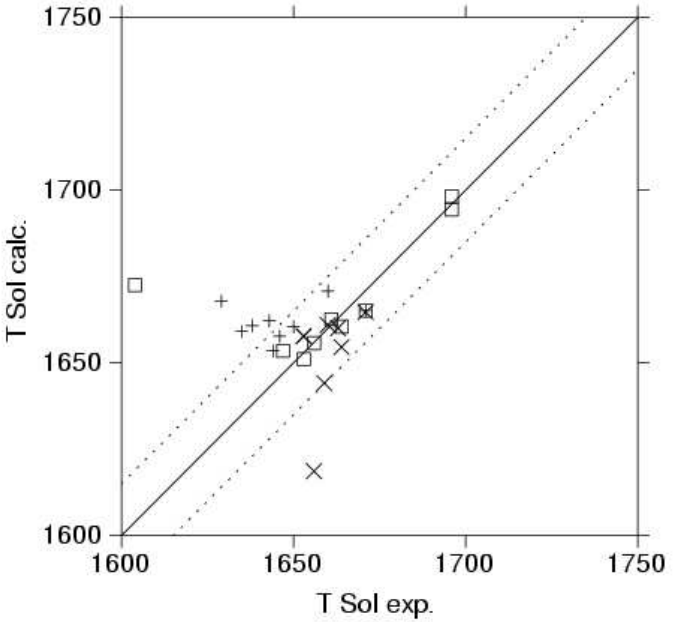






Comparison of the liquidus temperature calculated with the measured ones in the γ or γ' fields (the points where another phase appears during the calculation have not been considered).



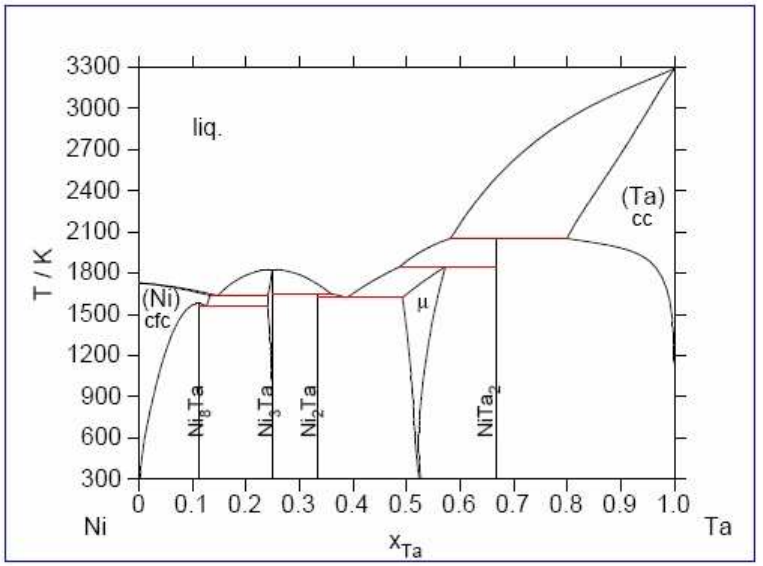
Comparison of the solidus temperatures calculated with the measured ones in the γ ou γ' field (the points where another phase appears during the calculation have not been considered).

Al Ni Ta Al-Ni Al-Ta Ni-Ta Top of this page Binary syst. Ternary syst. Periodic table

Ni database

Binary system Ni-Ta

Ni Ta Al-Ni-Ta B-Ni-Ta Co-Ni-Ta Cr-Ni-Ta Hf-Ni-Ta Mo-Ni-Ta Ni-Re-Ta Ni-Ta-W Binary syst. Ternary syst. Periodic table



Source of the description

I. Ansara, M. Selleby, Calphad, 1994, 18, 99-107

Comments

The original description has been modified :
-for the μ phase for model compatibility reason and
-for the liquid phase in order to take into account the mixing enthalpy in the liquid phase measured by Victor Vitusevych (Access, Aachen, communication privée 2004) run in order to check the ones previously reported by Schaeffer et al. (Canad. Metall. Quart., 1996, 35, 47-51) that turn out to be bad.

The description by Ansara and Selleby has been preferred to Pan and Jin's also close to Vitusevich mixing enthalpy in the liquid phase because it was the bases of available descriptions for important ternary systems (Al-Ni-Ta , Cr-Ni-Ta).

Comparisons with the previous description and data are shown herunder.

Some uncertainties remain in this system. The solvus, solidus and liquidus in the Ta rich area are not well known and difficult to study due to high temperatures. The only enthalpy of formation known experimentally is the one for Ni_2Ta. The stability of Ni_8Ta is not well known; Nash proposed a peritectoïd $\gamma+Ni_3Ta=Ni_8Ta$ that seems inconsistent with the solvus. The experimental determination of the enthalpy of formation of this compound as well as a better knowledge of the equilibria close to its decomposition temperature are desirable.

During the NI17 project, the model for the Ni_3Ta phase has been modified in order to be able to model some none-stoichiometry for this phase.

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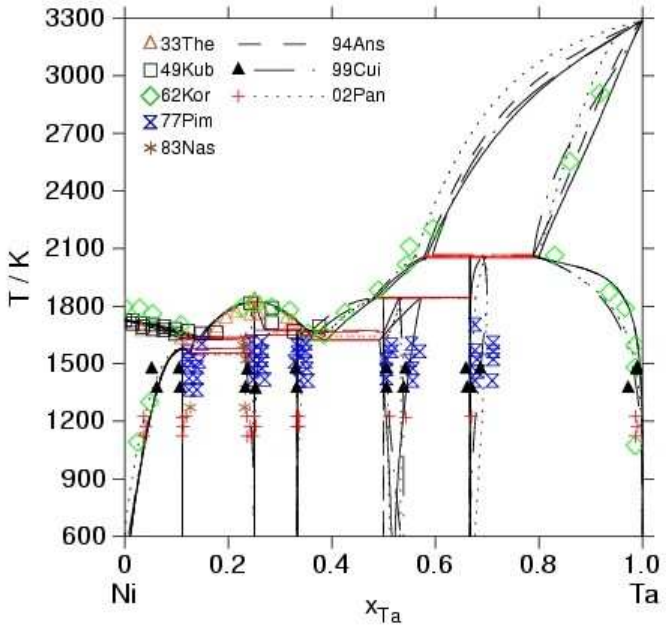
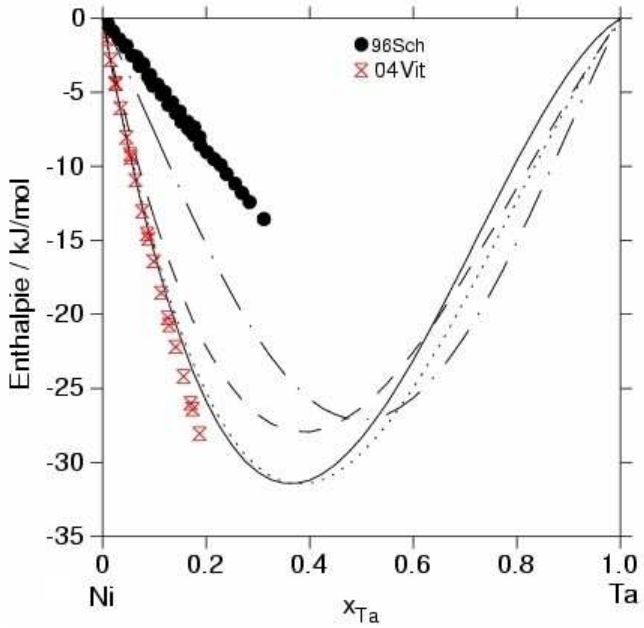
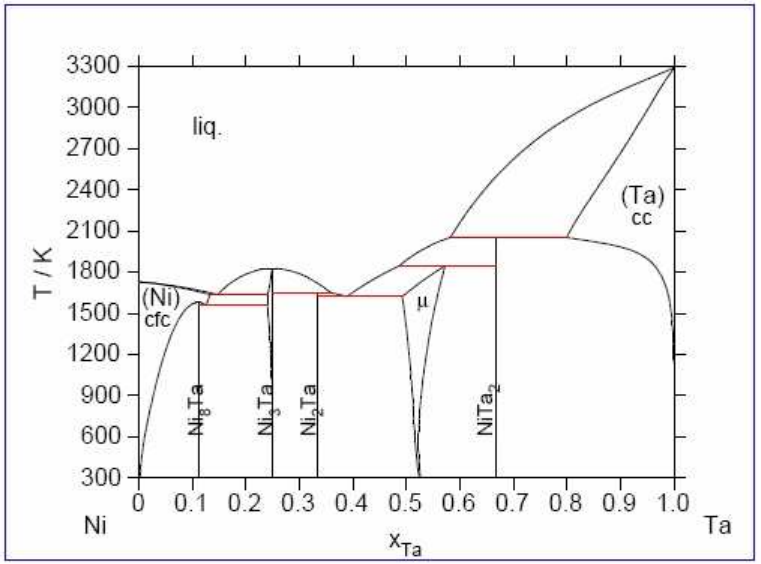




33Thes E. Therkelsen, *Met. Alloys*, 1933, **4**, 105-108
49Kub O. Kubaschewski, P.N. Habil, H. Speidel, *J. Inst. Metals*, 1949, **75**, 417-430
62Kor I.I. Kornilov, E.V. Plyaeva, *Izv. Neorg.*, 1962, **7**(3), 590-595
77Pim V.N. Pimeniv, Yu.E. Ugaste, K.A. Akkusharova, *Russ. Met.*, 1977, **1**, 155-159
83Nas P. Nash, D.R.F. West, *Met. Sci.*, 1983, **12**, 99-100
94Ans I. Ansara, M. Selleby, *Calphad*, 1994, **18**, 99-107
99Cui Y. Cui, Z. Jin, *Z. Metallk.*, 1999, **90** (3), 233-241
02Pan X. Pan, Z. Jin, *Transactions of Nonferrous Metals Society of China*, 2002 **12** (4), 748-753

Ni database



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Ni database

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Phases described by

usual name : liquid, γ, γ', Cr_3Si ...

database name : LIQUID, FCC_L12, BCC_A2...

prototype : Cu, NaCl, $MgCu_2$ ...

StrukturBericht : *A*1, $L1_2$, *A*2, *B*1, *C*14...

All phases in a table

List of the phases by default

last modification of this page by unknown before 2011-06-0

Usual name

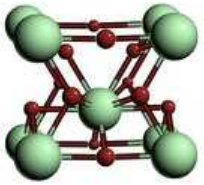
δ, Ni_3Ta, Ni_3Mo, Ni_3Nb, Pt_3Nb

Name in the database

NI3TA_D0A

Crystallography

Prototype Cu_3Ti ***StrukturBericht*** $D0_a$ ***Pearson*** *oP*8



Thermodynamic modelling

$(Al,Co,Cr,Fe,Ni,Nb,Pt)_3$ (Al,Fe,Mo,Nb,Ni,Pt,Ta,Ti,V,W)

Assessed systems where the phase is stable

Mo-Ni Nb-Ni Nb-Pt Ni-Ta

Ni database

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Phases described by

usual name : liquid, γ, γ', Cr_3Si ...

database name : LIQUID, FCC_L12, BCC_A2...

prototype : Cu, NaCl, $MgCu_2$ ...

StrukturBericht : *A*1, $L1_2$, *A*2, *B*1, *C*14...

All phases in a table

List of the phases by default

All the database phases.

By usual name alphabetical order; clicking on other column titles other ordering is given.

Name	Prototype	Pearson	S.Bericht	Model
AF				(Al_2O_3) (Fe_2O_3)
AL10V		*cF*116		$(Al)_{10}$ (V)
AL11CR2	Al_5Cr	*mP*48		$(Al)_{10}$ (Al) $(Cr)_2$
AL11MN4_HT	$Mn_6(Al_{0.5}Mn_{0.5})_{25}$	*oP*156		$(Al,Mn)_{29}$ $(Mn)_{10}$
AL11MN4_LT	$Al_{11}Mn_4$	*aP*15		$(Al)_{11}$ $(Fe,Mn)_4$
AL11RE4	$Al_{11}Mn_4$	*aP*15		$(Al)_{11}$ $(Re)_4$
AL11TI5				$(Al)_{17}$ $(Ti)_8$
AL12MN	$Al_{12}W$	*cI*26		$(Al)_{12}$ (Mn)
AL12W	$Al_{12}W$	*cI*26		$(Al)_{12}$ (Mo,Re,W)
also $Al_{12}Re$ and $Al_{12}Mo$				
AL13CO4	$Al_{13}Co_4$			$(Al)_{13}$ $(Co)_4$
*oP*102 and *mC*100				
AL13CR2	$Al_{45}V_7$	*mC*104		(Al) $(Cr)_2$
AL13FE4	$Al_{13}Fe_4$	*mS*102		$(Al)_{0.6275}$ $(Fe,Ru)_{0.235}$ $(Al,Si,VA)_{0.1375}$
AL21PD8	Al_3Ni_2	*hP*5	$D5_{19}$	$(Al)_{21}$ $(Pd)_8$
AL21PT5				$(Al)_{0.8077}$ $(Pt)_{0.1923}$
AL21PT8		*tI*116		$(Al)_{0.7241}$ $(Pt)_{0.2759}$
AL23V4	$Al_{23}V_4$	*hP*54		$(Al)_{23}$ $(V)_4$
AL2FE				$(Al)_2$ (Fe)
AL2N2TI3				$(Al)_2$ $(N)_2$ $(Ti)_3$

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Phases described by

- usual name : liquid, γ, γ', Cr_3Si ...
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- prototype : Cu, NaCl, $MgCu_2$ ...
- StrukturBericht : *A*1, $L1_2$, *A*2, *B*1, *C*14...

All phases in a table

List of the phases by default

undefined				
YSI2_HT	AlB_2	*hP*3	undefined	$(Si)_2$ (Y)
undefined				
ZR3Y4O12	Y_6OU_{12}	*hR*57	undefined	$(Zr^4)_3(Zr^4)_4(O^{-2})_{12}$
undefined				
ZR5SI4	Zr_5Si_4	*tP*36	undefined	$(Hf,Nb,Ti,Y,Zr)_5$ $(Si)_4$
ZRO2_MONO	ZrO_2	*mP*12	C43	$(Al^{+3},Cr^{+3},Hf^{+4},Ti^{+4},Y^{+3},Zr^{+4})_2(O^{-2},Va)_4$
Baddeleyite				
ZRO2_TETR	ZrO_2	*tP*6	undefined	$(Al^{+3},Cr^{+3},Fe^{+2},Hf^{+4},Mn^{+2},Mn^{+3},Ni^{+2},Ti^{+4},Y^{+3},Zr^{+4})_2(O^{-2},V$
undefined				
ZRSI2_C49	$ZrSi_2$	*oC*12	C49	(Zr,Hf,Nb) $(Si)_2$
undefined				
ZRSIO4				$(Si^{+4})_1(Zr^{+4})_1(O^{-2})_4$
undefined				
ZRTI2O6				$(Zr^{+4})_1(Ti^{+4})_2(O^{-2})_6$
undefined				
ZRTIO4_ALPHA				$(Zr^{+4})_1(Ti^{+4})_1(O^{-2})_4$
undefined				
ZRTIO4_BETA				$(Ti^{+4},Zr^{+4})_2(O^{-2})_4$
undefined				
Z_PHASE	undefined	undefined	undefined	(Cr,Fe) (Mo,Nb,V) (N,VA)

i. e. 458 phases described in the database.

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Ni database

Home | Introduction | Thermodynamic models | Phases of interest | Assessed systems

Phases described by

usual name : liquid, γ, γ', Cr_3Si ...

database name : LIQUID, FCC_L12, BCC_A2...

prototype : Cu, NaCl, $MgCu_2$ ...

StrukturBericht : *A*1, $L1_2$, *A*2, *B*1, *C*14...

All phases in a table

List of the phases by default

The phases dy default in the database.

By usual name alphabetical order. Clicking on other column titles other ordering is given.

Name	Prototype	Pearson	S.Bericht	Model
BCC_B2	W	*cI*2	A2	$(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr,VA)_{0.5}$ $(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr,VA)_{0.5}$ (B,C,N,C
The non-configurational contribution, BCC_A2, should not be rejected when this phase is kept.				
BCC_B2_2	CsCl	*cP*2	B2	$(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr,VA)_{0.5}$ $(Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr,VA)_{0.5}$ (B,C,N,O,VA
The non-configurational contribution, BCC_A2, should not be rejected when this phase is kept.				
BCT_D022	Al_3Ti	*tI*8	$D0_{22}$	$(Al,Cr,Fe,Mo,Ni,Pd,Pt,Ti,V)_3$ $(Al,Cr,Mo,Nb,Ni,Pd,Pt,Ta,Ti,V,Si)$
γ'', Al_3Nb, Al_3Ta, Al_3Ti, Al_3V, Ni_3V				
BETA_RHOMBO_B	B	*hR*105		$(B)_{93}$ $(B,C,Si)_{12}$
C14_LAVES	$MgZn_2$	*hP*12	C14	$(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Si,Re,Ru,Ta,Ti,W,Y,Zr)_2$ $(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Si,Re,Ru,Ta,Ti,W,Y,Zr)$
Al_2Hf, Al_2Zr, Co_2Ta, Cr_2Hf, Cr_2Ta, Cr_2Ti, Cr_2Zr, Re_2Hf, Mn_2Ta, Mn_2Ti, Mn_2Zr, Re_2Y, Re_2Zr				
CBCC_A12	Mn	*cI*58	A12	$(Al,Co,Cr,Fe,Hf,Mn,Mo,Ni,Ru,Si,Ta,Ti,V)_1(C,VA)_1$
CEMENTITE	Fe_3C	*oP*16	$D0_{11}$	$(Co,Cr,Fe,Mn,Mo,Ni,V,W)_3$ (C,N)
CHI_A12	α-Mn	*cI*58	A12	$(Cr,Fe,Ni,Re)_{24}$ $(Al,Cr,Hf,Mo,Nb,Ta,Ti,W,Zr)_{10}$ $(Cr,Fe,Mo,Nb,Ni,Re,Ta,W)_{24}$
Hf_5Re_{24}, Mo_2Re_8, Ta_3Re_7, Ti_5Re_{24}, WRe_3, Zr_5Re_{24}				
CORUNDUM	Al_2O_3	*hR*10	$D5_1$	$(Al^{+3},Cr^{+2},Cr^{+3},Fe^{+2},Fe^{+3},Mn^{+3},Ti^{+3},V^{+3})_2$ $(Cr^{+3},Fe^{+3},Ni^{+2},VA)$ $(O^{-2})_3$
CUB_A13	Mn	*cP*20	A13	$(Al,Co,Cr,Fe,Hf,Mn,Mo,Ni,Ru,Si,Ta,Ti,V)_1(C,VA)_1$
DIAMOND_A4	C	*cF*8	A4	(B,C,Si)
FCC_L12	Cu	*cF*4	A1	$(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr)_{0.75}$ $(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr)_{0.25}$ (B,C,N,O,V

When the global minimisation is used, the number attributed to this phase is given randomly. Only the filling of the different

Ni database

Home | Introduction | Thermodynamic models | Phases of interest | Assessed systems

Phases described by

usual name : liquid, γ, γ', Cr_3Si ...

database name : LIQUID, FCC_L12, BCC_A2...

prototype : Cu, NaCl, $MgCu_2$ ...

StrukturBericht : *A*1, $L1_2$, *A*2, *B*1, *C*14...

All phases in a table

List of the phases by default

MB_B33	BCr	*oC*8	B33	(Cr,Fe,Hf,Mo,Nb,Ni,Ta,Ti,V) (B)
CrB, NbB, NiB, TaB, VB				
MC_ETA	TiAs	*hP*8	B_i	(Mo,V,W) (C,VA)
MoC_{1-x} η				
MC_SHP	WC	*hP*2	B_h	(Mo,W) (C,N)
MoC, WC				
MU_PHASE	W_6Fe_7	*hR*13	$D8_5$	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Re,Ta,W) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Re,Ta,W)$_2$ (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Re,Ta,W)$_6$ (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Re,Ta,W)$_4$
The non-configurational contribution to the description of this phase, DIS_MU, should not be rejected when this phase is defin				
NI3TA_D0A	Cu_3Ti	*oP*8	$D0_a$	(Al,Co,Cr,Fe,Ni,Nb,Pt)$_3$ (Al,Fe,Mo,Nb,Ni,Pt,Ta,Ti,V,W)
δ, Ni_3Ta, Ni_3Mo, Ni_3Nb				
NI3TI_D024	Ni_3Ti	*hP*16	$D0_{24}$	(Al,Co,Cr,Fe,Hf,Ni,Pd,Pt,Ta,Ti,W,Zr)$_{0.75}$ (Al,Cr,Hf,Mo,Nb,Ni,Pd,Pt,Si,Ta,Ti,W
η, Ni_3Ti, Ni_6AlTa				
PI	β-Mn	*cP*20	A13	(Cr)$_{12.8}$ (Fe,Ni)$_{7.2}$ (N)$_4$
Only Stable in C-N-Ni if gas suspended				
P_PHASE	$Cr_9Mo_{21}Ni_{20}$	*oP*56		(Cr,Fe,Ni,Re)$_{24}$ (Cr,Fe,Mo,Ni,Re)$_{20}$ (Mo)$_{12}$
R_PHASE	$Co_5Cr_2Mo_3$	*hR*53		(Co,Cr,Fe,Ni,Re)$_{27}$ (Mo,W)$_{14}$ (Co,Cr,Fe,Mo,Ni,Re,W)$_{12}$
SIGMA	CrFe	*tP*30	$D8_b$	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W)$_{10}$ (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W)$_4$ (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W)$_{16}$
The non-configurational contribution to the description of this phase, DIS_SIG, should not be rejected when this phase is defin				
TAU	$Cr_{23}C_6$	*cF*116	$D8_4$	(Co,Hf,Ni,Re)$_{20}$ (B)$_6$ (B,VA)$_6$ (Al,Cr,Hf,Mo,Re,Ta,Ti,V,W,Zr)$_3$

i.e. 39 phases described by default in the database.

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Ni database

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Phases described by

usual name : liquid, γ, γ', Cr_3Si ...

database name : LIQUID, FCC_L12, BCC_A2...

prototype : Cu, NaCl, $MgCu_2$ ...

StrukturBericht : *A*1, $L1_2$, *A*2, *B*1, *C*14...

All phases in a table

List of the phases by default

All the phases by default.

By StukturBericht alphabetical order. Clicking on other column titles other ordering are given.

Name	Prototype	Pearson	S.Bericht	Model
FCC_L12	Cu	*cF*4	A1	$(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr)_{0.75}$ $(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr)_{0.25}$ (B,C,N,O,VA)
When the global minimisation is used, the number attributed to this phase is given randomly. Only the filling of the different sublattices allow to identify the different crystallographic structures described by this model.				
CBCC_A12	Mn	*cI*58	A12	$(Al,Co,Cr,Fe,Hf,Mn,Mo,Ni,Ru,Si,Ta,Ti,V)_1(C,VA)_1$
CHI_A12	α-Mn	*cI*58	A12	$(Cr,Fe,Ni,Re)_{24}$ $(Al,Cr,Hf,Mo,Nb,Ta,Ti,W,Zr)_{10}$ $(Cr,Fe,Mo,Nb,Ni,Re,Ta,W)_{24}$
Hf_5Re_{24}, Mo_2Re_8, Ta_3Re_7, Ti_5Re_{24}, WRe_3, Zr_5Re_{24}				
CUB_A13	Mn	*cP*20	A13	$(Al,Co,Cr,Fe,Hf,Mn,Mo,Ni,Ru,Si,Ta,Ti,V)_1(C,VA)_1$
PI	β-Mn	*cP*20	A13	$(Cr)_{12.8}$ $(Fe,Ni)_{7.2}$ $(N)_4$
Only Stable in C-N-Ni if gas suspended				
BCC_B2	W	*cI*2	A2	$(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr,VA)_{0.5}$ $(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr,VA)_{0.5}$ (B,C,N,O,V
The non-configurational contribution, BCC_A2, should not be rejected when this phase is kept.				
HCP_A3	Mg	*hP*2	A3	$(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr)$ $(B,C,N,O,VA)_{0.5}$
(α-Ti), (α-Zr), Re				
DIAMOND_A4	C	*cF*8	A4	(B,C,Si)
GRAPHITE	C	*hP*4	A9	(B,C)
FCC_L12_3	NaCl	*cF*8	B1	$(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr)_{0.75}$ $(Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Pd,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr)_{0.25}$ (B,C,N,O,VA)
When the global minimisation is used, the number attributed to this phase is given randomly. Only the filling of the different sublattices allow to identify the different crystallographic structures described by this model. A miscibility gap appearing betwe some of these carbides, another of these phase can appear, in particular when Zr and Ti or Hf are defined.				
HALITE	NaCl	*cF*8	B1	$(Al^{+3},C_a,C_v)^{+2}(C_a,C_v,F_a,F_v,Mn^{+2},Mn^{+3},Ni^{+2},Ni^{+3},Ti^{+2},Ti^{+3},V,V^{+2},V$

Ni database

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To reach information on:

elements

binary systems

ternary systems

commented ternary systems

systems with **Al**, **Ar**, **B**, **C**, **Co**, **Cr**, **Fe**, **H**, **Hf**, **Mn**, **Mo**, **N**, **Nb**, **Ni**, **O**, **Pd**, **Pt**, **Re**, **Ru**, **Si**, **Ta**, **Ti**, **V**, **W**, **Y**, **Zr**

via periodic table

Binary systems

The phase diagrams calculated at 10^5 Pa for the different assessed binary systems can be displayed thanks to the following list.

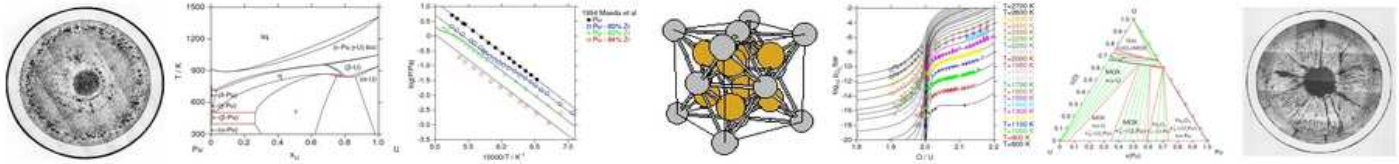
Al-B Al-C Al-Co Al-Cr Al-Fe Al-Hf+ Al-Mn Al-Mo Al-N Al-Nb+ Al-Ni Al-O Al-Pd+ Al-Pt* Al-Re+
Al-Ru+ Al-Si Al-Ta+ Al-Ti Al-V Al-W Al-Y Al-Zr+ B-C B-Co B-Cr B-Fe B-Hf B-Mn B-Mo+ B-N
B-Nb+ B-Ni B-O B-Pd+ B-Pt* B-Re* B-Ru* B-Si B-Ta+ B-Ti B-V B-W B-Y* B-Zr C-Co C-Cr C-Fe
C-Hf C-Mn C-Mo C-Nb C-Ni C-O C-Pd* C-Pt C-Re* C-Ru* C-Si+ C-Ta C-Ti C-V C-W C-Y C-Zr
Co-Cr+ Co-Fe+ Co-Hf* Co-Mn Co-Mo+ Co-N Co-Nb+ Co-Ni Co-O+ Co-Pd Co-Pt+ Co-Re* Co-Ru*
Co-Si Co-Ta+ Co-Ti Co-V+ Co-W+ Co-Y Co-Zr Cr-Fe+ Cr-Hf* Cr-Mn+ Cr-Mo Cr-N Cr-Nb Cr-Ni Cr-O
Cr-Pd+ Cr-Pt+ Cr-Re* Cr-Ru* Cr-Si Cr-Ta Cr-Ti Cr-V Cr-W Cr-Y Cr-Zr Fe-Hf* Fe-Mn Fe-Mo+ Fe-N
Fe-Nb+ Fe-Ni Fe-O Fe-Pd+ Fe-Pt Fe-Re* Fe-Ru* Fe-Si Fe-Ta+ Fe-Ti Fe-V+ Fe-W+ Fe-Y Fe-Zr
Hf-Mn Hf-Mo* Hf-N° Hf-Nb Hf-Ni+ Hf-O Hf-Pd* Hf-Pt* Hf-Re* Hf-Ru* Hf-Si Hf-Ta Hf-Ti Hf-V* Hf-W*
Hf-Y* Hf-Zr Mn-Mo+ Mn-N Mn-Nb Mn-Ni Mn-O Mn-Ru* Mn-Si Mn-Ta Mn-Ti Mn-V Mn-W* Mn-Y
Mn-Zr Mo-N Mo-Nb Mo-Ni Mo-O Mo-Pd Mo-Pt° Mo-Re* Mo-Ru* Mo-Si Mo-Ta* Mo-Ti Mo-V Mo-W
Mo-Y Mo-Zr N-Nb N-Ni N-O N-Pd° N-Pt° N-Re° N-Si N-Ta N-Ti N-V N-W N-Zr Nb-Ni+ Nb-O
Nb-Pd* Nb-Pt* Nb-Re Nb-Ru* Nb-Si Nb-Ta Nb-Ti Nb-V Nb-W Nb-Y Nb-Zr Ni-O Ni-Pd Ni-Pt
Ni-Re* Ni-Ru* Ni-Si+ Ni-Ta+ Ni-Ti Ni-V+ Ni-W+ Ni-Y Ni-Zr O-Pd O-Pt O-Re O-Ru O-Si O-Ta O-Ti
O-V O-W O-Y O-Zr Pd-Pt* Pd-Re* Pd-Ru Pd-Si Pd-Ta* Pd-Ti* Pd-V* Pd-W* Pd-Y Pd-Zr+ Pt-Re*
Pt-Ru Pt-Si+ Pt-Ta* Pt-Ti* Pt-V* Pt-W Pt-Y* Pt-Zr+ Re-Ru* Re-Si* Re-Ta* Re-Ti* Re-V* Re-W* Re-Y
Re-Zr* Ru-Si Ru-Ta* Ru-Ti* Ru-V* Ru-W* Ru-Y Ru-Zr* Si-Ta Si-Ti Si-V Si-W Si-Y Si-Zr Ta-Ti Ta-V
Ta-W Ta-Y* Ta-Zr Ti-V Ti-W Ti-Y Ti-Zr V-W V-Y V-Zr W-Y* W-Zr* Y-Zr*

ie 325 binary systems :
265 systems described in the present database,
+41 extracted from the open litterature but modified during the present work,
*62 systems assessed during the present work (NI13-NI22).
°5 systems not assessed but for which some comments are available in this documentation.

Nuclear Fuel database

TAF-ID : Thermodynamics of Advanced Fuels - International Database

To support the development of Generation 4 reactors (SFR, SCWR, GFR, LFR, MSR, VHTR) and to contribute to lifetime extension, safety improvement and safety analysis for Generation 2 & 3 systems (PWR, BWR, PHWR), there is a need to make available a comprehensive, internationally recognized, and quality-assured thermodynamic database. For this reason, a joint Project between 9 organizations representing 6 member states coordinated by the OECD-Nuclear Energy Agency (NEA) was started in 2013 with an initial 3 years period. The objective of the project titled Thermodynamics of Advanced Fuels – International database (TAF-ID) is to develop a thermodynamic database using the Calphad method to perform thermodynamic calculations on different types of fuels (oxide, metallic, nitride, carbide) including minor actinides (Am, Np), fission products (Cs, I, Ba, Sr, Mo, Zr, lanthanides, metallic fission products) and structural materials (steel, Zr alloy, B4C, SiC, concrete). Thermodynamic properties of fuels versus temperature and composition (with fission products and minor actinides) will be provided. The inclusion of structural materials will allow the prediction of fuel/cladding chemical interactions under normal and off-normal conditions. The database will be generated and regularly updated by merging existing and developing databases from the various participating organizations. The database will be available in both Thermo-Calc and FACTSAGE usable formats.



Members of the Programme Review Group:

Country	Signatory	Representative	Alternate member
Canada	AECL, RMCC, UOIT	D. Barber	E.C. Corcoran
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USA	DOE	T. Besmann (Vice-Ch.)	P. Turchi

Consultant: N. Dupin, Calcul Thermodynamique, France

Coordinator: OECD-NEA (S. Massara)

Remarks and comments on this documentation and on the thermodynamic database are welcome. We thank you to ask for the autorization in case where you would like to communicate this documentation and/or the database to any other person. The database and the documentation cannot be modified. *This documentation uses javascript. You must allow it in order to get it work properly.*

Nuclear Fuel database

TAF-ID : Thermodynamics of Advanced Fuels - International Database

Home | Introduction | Models | Phases | Systems

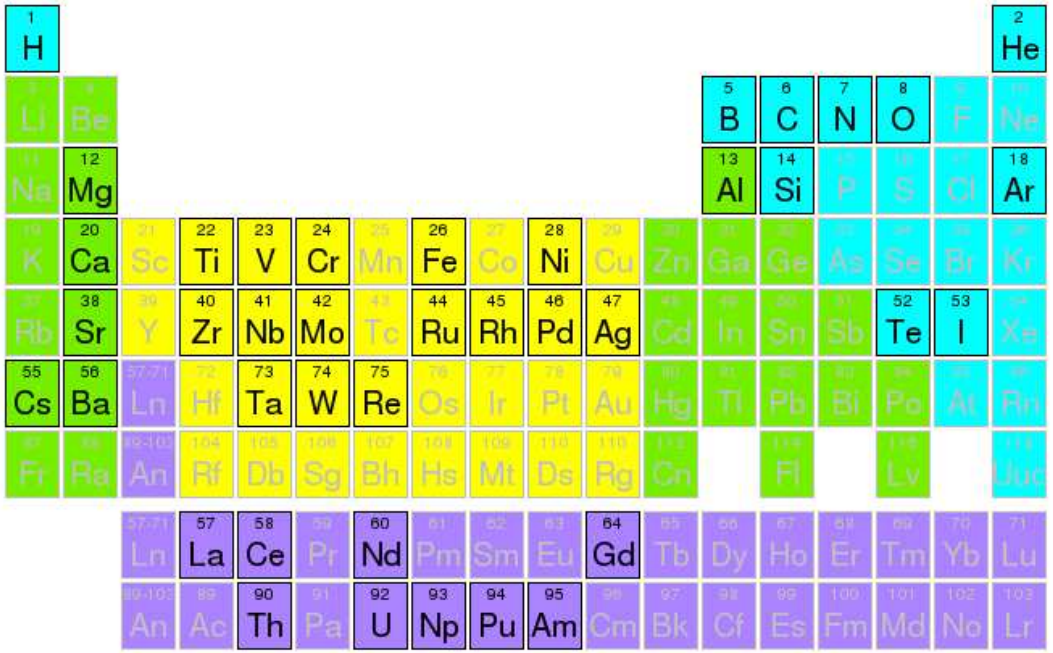
Elements

Assessed binary systems

Assessed ternary systems

Systems with **Ag**, **Al**, **Am**, **Ar**, **B**, **Ba**, **C**, **Ca**, **Ce**, **Cr**, **Cs**, **Fe**, **Gd**, **H**, **He**, **I**, **La**, **Mg**, **Mo**, **N**, **Nb**, **Nd**, **Ni**, **Np**, **O**, **Pd**, **Pu**, **Re**, **Rh**, **Ru**, **Si**, **Sr**, **Ta**, **Te**, **Th**, **Ti**, **U**, **V**, **W**, **Zr**

Periodic table



Nuclear Fuel database

TAF-ID : Thermodynamics of Advanced Fuels - International Database

Home | Introduction | Models | Phases | Systems

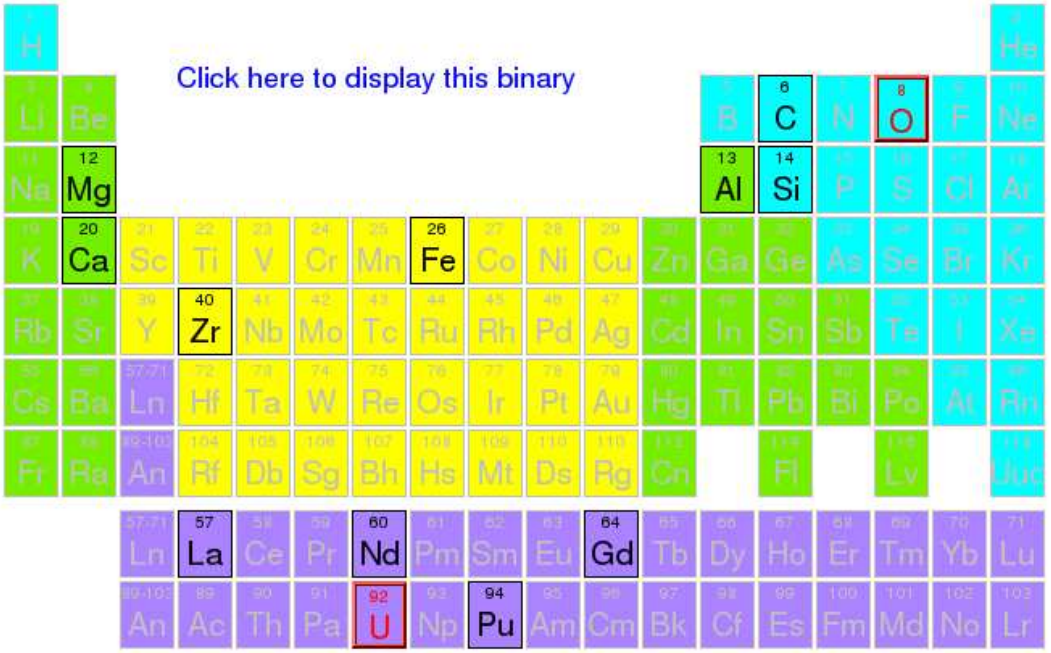
Elements

Assessed binary systems

Assessed ternary systems

Systems with **Ag**, **Al**, **Am**, **Ar**, **B**, **Ba**, **C**, **Ca**, **Ce**, **Cr**, **Cs**, **Fe**, **Gd**, **H**, **He**, **I**, **La**, **Mg**, **Mo**, **N**, **Nb**, **Nd**, **Ni**, **Np**, **O**, **Pd**, **Pu**, **Re**, **Rh**, **Ru**, **Si**, **Sr**, **Ta**, **Te**, **Th**, **Ti**, **U**, **V**, **W**, **Zr**

Periodic table



Nuclear Fuel database

TAF-ID : Thermodynamics of Advanced Fuels - International Database

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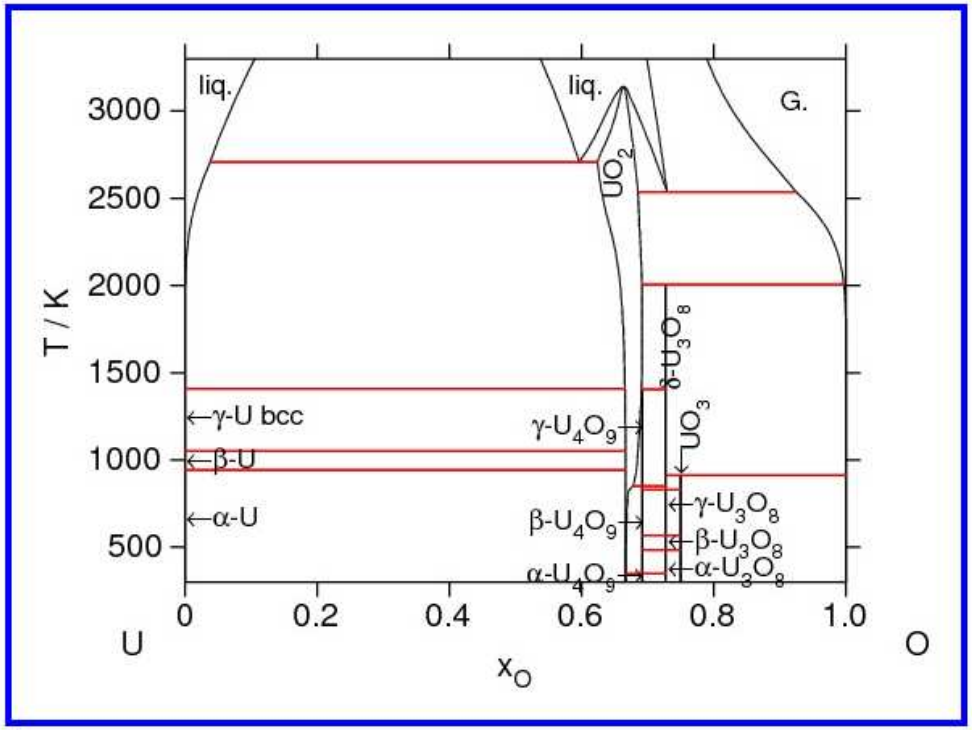
Binary system O-U

Al-O-U C-O-U Ca-O-U Fe-O-U Gd-O-U La-O-U Mg-O-U Nd-O-U O-Pu-U O-Si-U O-U-Zr O U Binary syste
Ternary systems Periodic tab



Source of the description

C. Guéneau, N. Dupin, B. Sundman, C. Martial, J.C. Dumas, S. Gossé, S. Chatain, F. De Bruycker, D. Manara, R. Konings, Thermodynamic modelling of advanced oxide and carbide nuclear fuels: Description of U-Pu-O-C systems, *J. Nuclear Materials*, **419** (2011) 145-167

Comments

The previous description has been modified in order to take into account the higher liquidus temperature recently measured. The model of the UO_2 phase has moreover been modified in order to better account the main defects of the structure.

Comparison with experiments

Bibliography

Divers files

Nuclear Fuel database

TAF-ID : Thermodynamics of Advanced Fuels - International Database

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Usual name

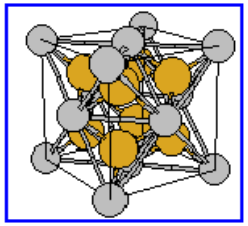
ZrO_2-γ, PuO_2, UO_2, AmO_2, NpO_2, ThO_2

Name in the database

C1_MO2

Crystallography

Prototype CaF_2 ***StrukturBericht*** *C1* ***Pearson*** *cF12* ***Space Group*** *Fm-3m*



Characteristics of the different sites for the prototype

Occupation	Multiplicity	Wickoff	Symmetry
F	8	c	-43m
Ca	4	a	m-3m

Thermodynamic model

(Al^{3+}, Am^{3+}, Am^{4+}, Ca^{2+}, Ce^{3+}, Ce^{4+}, Gd^{3+}, La^{3+}, Mg^{2+}, Nd^{3+}, Np^{3+}, Np^{4+}, Pu^{3+}, Pu^{4+}, Th^{4+}, U^{3+}, U^{4+}, U^{5+}, Zr^{2+}, Zr^{4+}) (O^{2-}, ∅)$_2$ (O^{2-}, ∅)

Assessed systems where the phase is stable

Am-O Ce-O Np-O O-Pu O-Th O-U O-Zr Al-O-U Al-O-Zr Am-O-Pu C-O-Pu C-O-U Ca-O-U Ca-O-Zr Fe-O-U Fe-O-Zr Gd-O-U La-O-U Mg-O-U Mg-O-Zr Nd-O-U O-Pu-U O-Pu-Zr O-Si-U O-Si-Zr O-U-Zr

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Nuclear Fuel database

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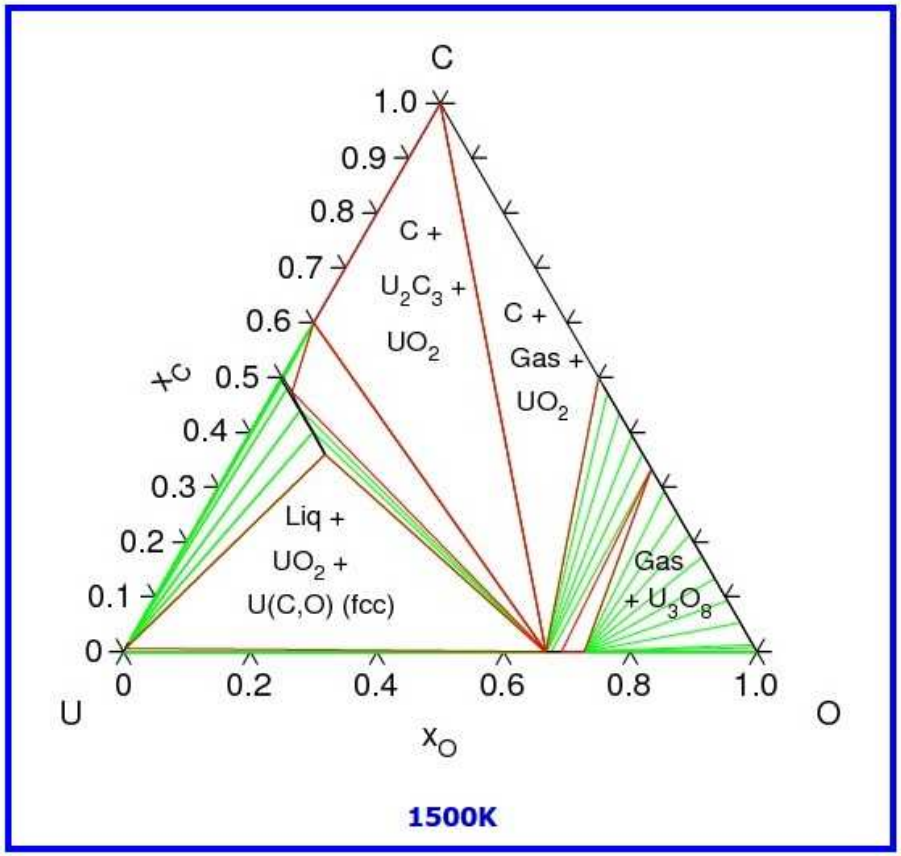
Ternary system C-O-U

C-O C-U O-U C O U Binary systems Ternary systems Periodic table



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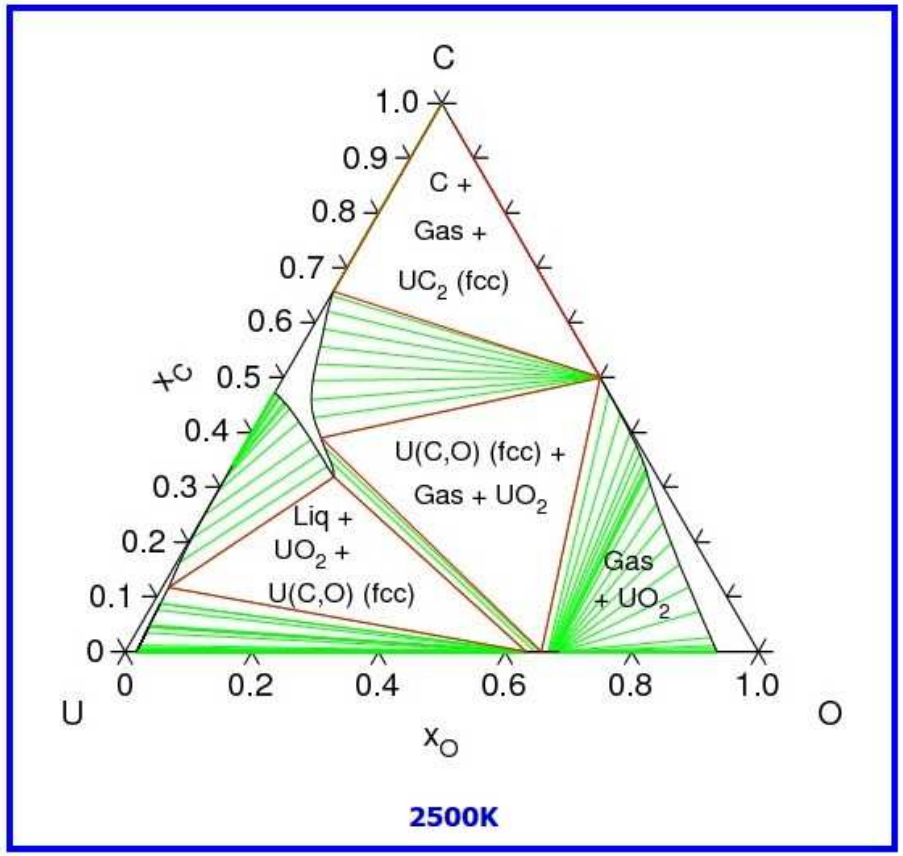

2500K

Nuclear Fuel database

TAF-ID : Thermodynamics of Advanced Fuels - International Database

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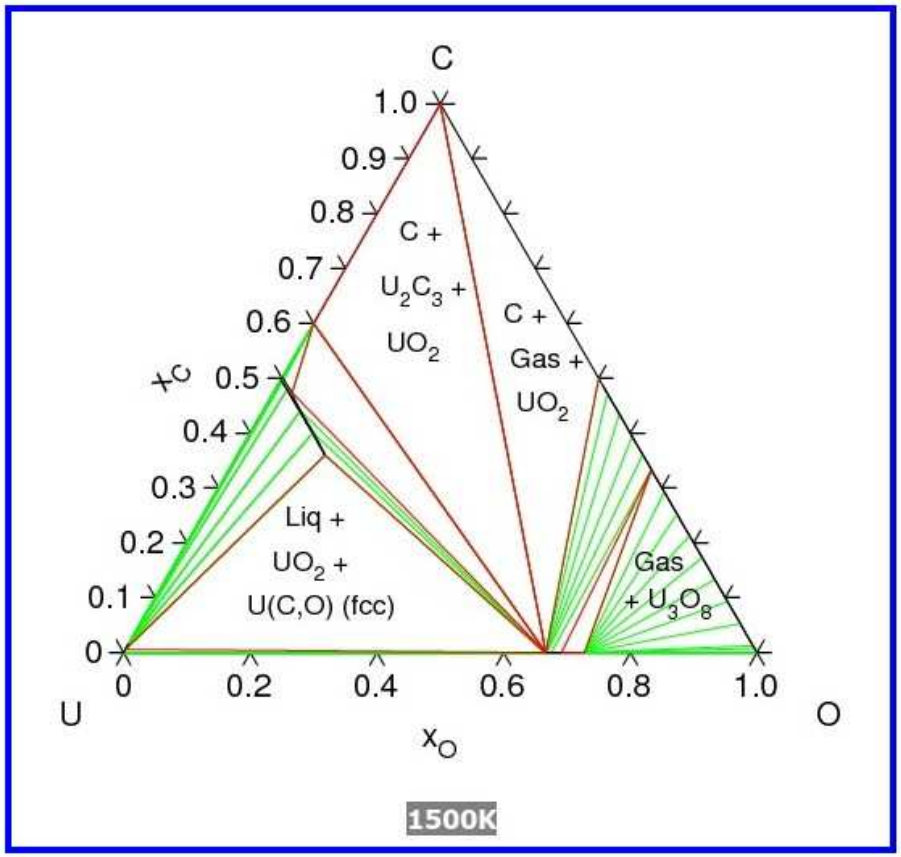

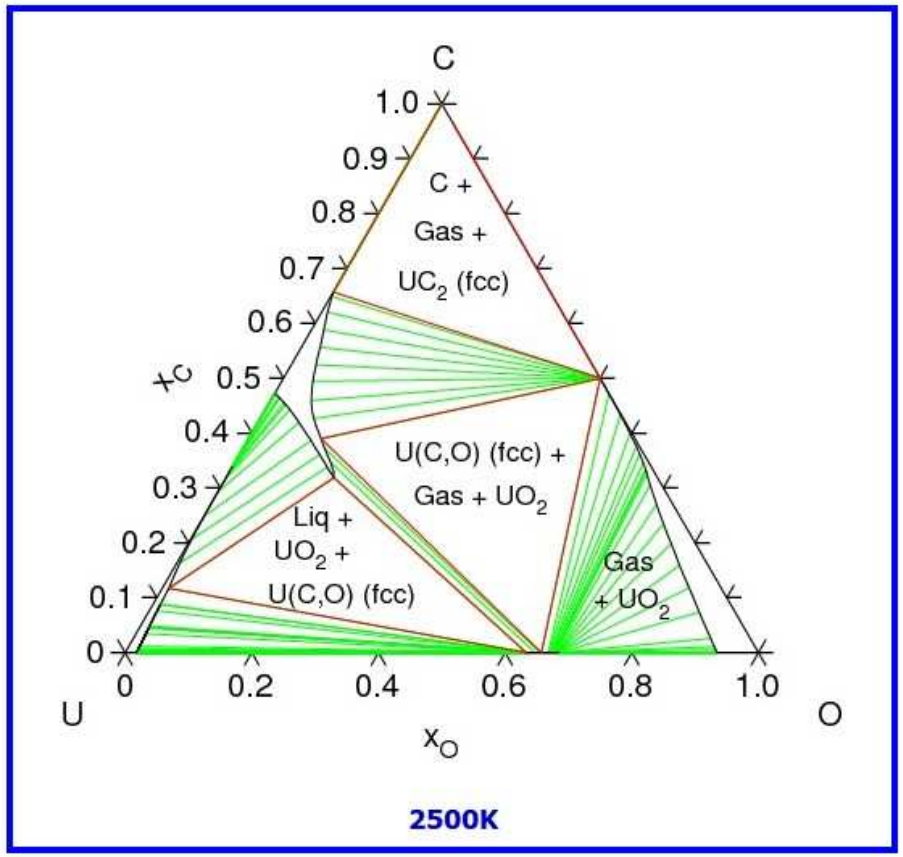

Source of the description

C. Guéneau, N. Dupin, B. Sundman, C. Martial, J.C. Dumas, S. Gossé, S. Chatain, F. De Bruycker, D. Manara, R. Konings,

Nuclear Fuel database

```
s_lab n
add .06 .75 N C +
.3
add .08 .65 N U^DO2$C^DO3$ +
.3
add .14 .55 N  UO^DO2$
.3
add .3 .6 N C +
.3
add .35 .52 N Gas +
.3
add .4 .44 N UO^DO2$
.3
add .14 .23 N Liq +
.3
add .16 .15 N UO^DO2$ +
.3
add .16 .07 N U(C,O) (fcc)
.3
add .73 .15 N Gas
.3
add .75 .08 N + U^DO3$O^DO8$
.3
s_p_o n n n ,,,,,,,,
s_cor t C
s_cor l_r O
s_cor l_l U
s_a-te x n x^DOO$
--(DOS)---  C-O-U_1500.TCM   Top L29    (Fundamental)------------------------------
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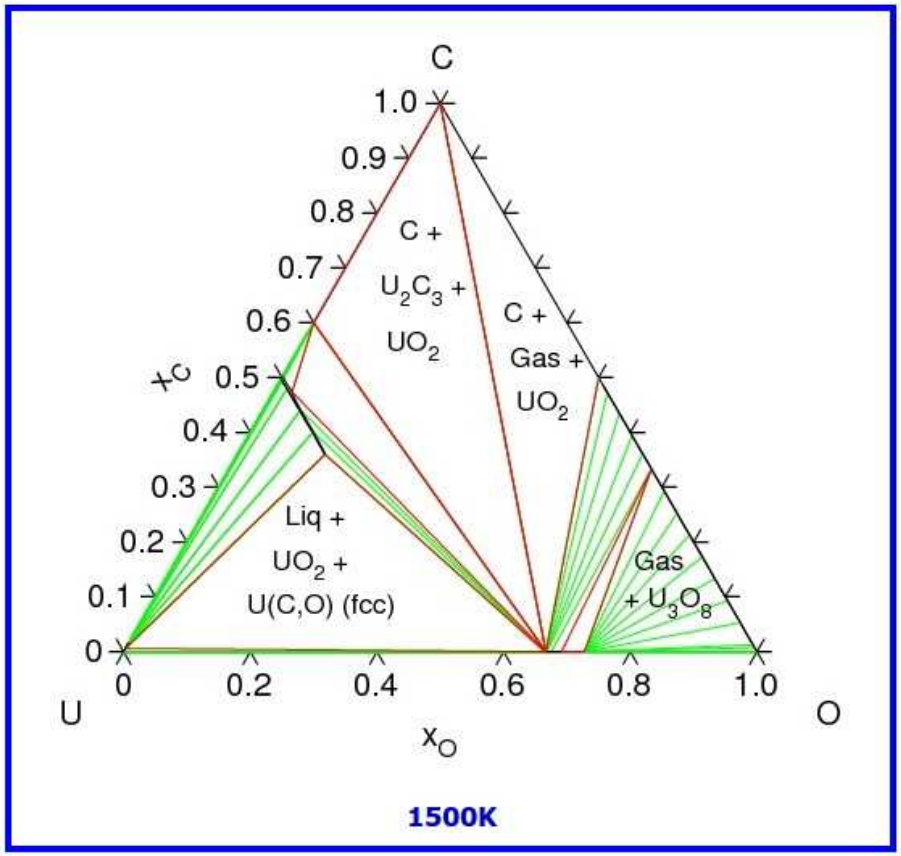
Nuclear Fuel database

TAF-ID : Thermodynamics of Advanced Fuels - International Database

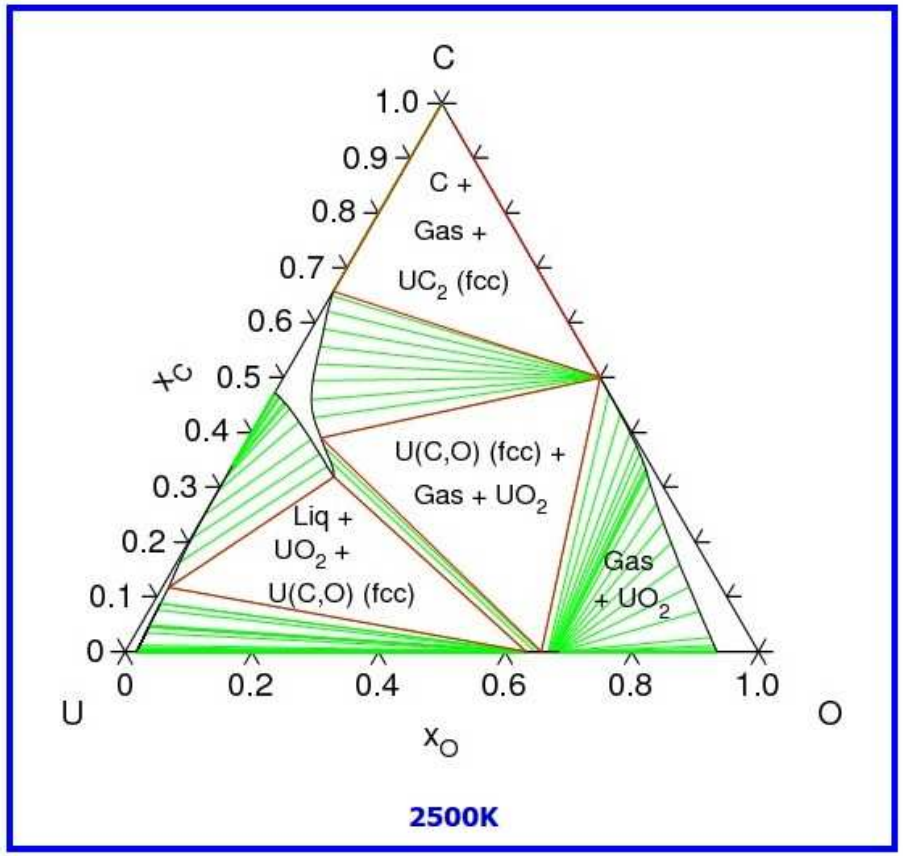
Home | Introduction | Models | Phases | Systems

Ternary system C-O-U

C-O C-U O-U C O U Binary systems Ternary systems Periodic table



1500K

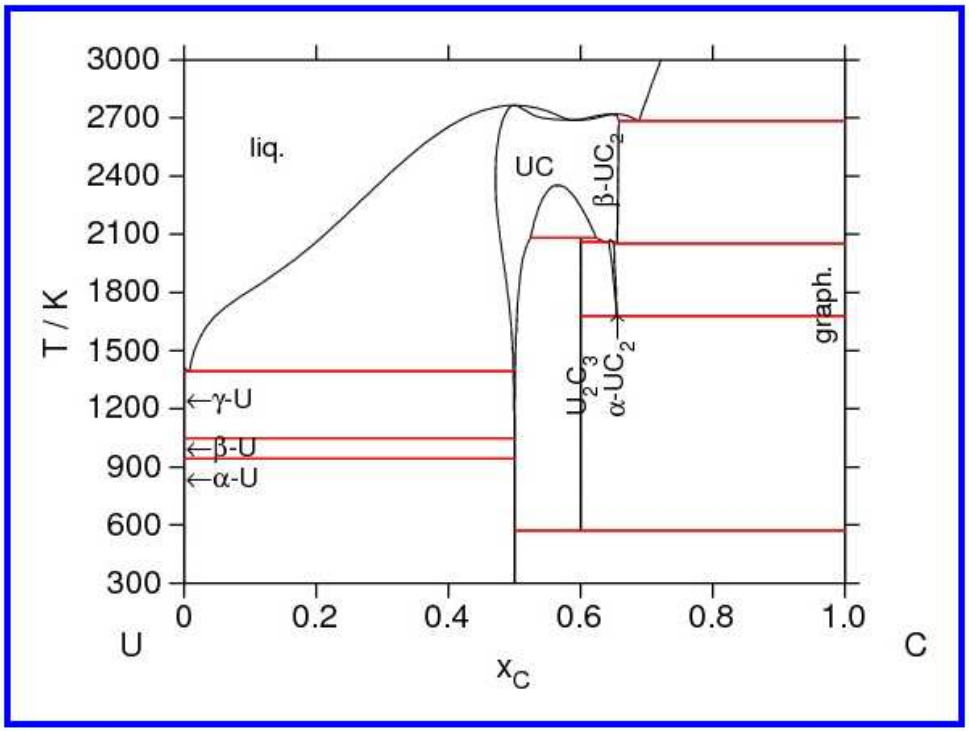


2500K

Nuclear Fuel database

TAF-ID : Thermodynamics of Advanced Fuels - International Database

Binary system C-U



Source of the description

C. Guéneau, N. Dupin, B. Sundman, C. Martial, J.C. Dumas, S. Gossé, S. Chatain, F. De Bruycker, D. Manara, R. Konings, Thermodynamic modelling of advanced oxide and carbide nuclear fuels: Description of U-Pu-O-C systems, *J. Nuclear Materials*, **419** (2011) 145-167

Comments

The use of the previous desription by Chevalier and Fischer Chevalier et Fischer having shown many problems, a deep revision of this system was run.

A detailed report on this work available clicking the present link.

Bibliography

Comparison with experiments

Divers files

Nuclear Fuel database

TAF-ID : Thermodynamics of Advanced Fuels - International Database

Home | Introduction | Models | Phases | Systems

Binary system C-U

C-Mo-U C-O-U C-Pu-U C-Re-U C-Si-U C-U-W C-U-Zr C U Binary systems Ternary systems Periodic table

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Main page for the system C-U **Divers files** **Comparison with experiments**

Other links C-Mo-U C-O-U C-Pu-U C-Re-U C-Si-U C-U-W C-U-Zr C U Binary systems Ternary systems Periodic table

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Nuclear Fuel database

TAF-ID : Thermodynamics of Advanced Fuels - International Database

Home | Introduction | Models | Phases | Systems

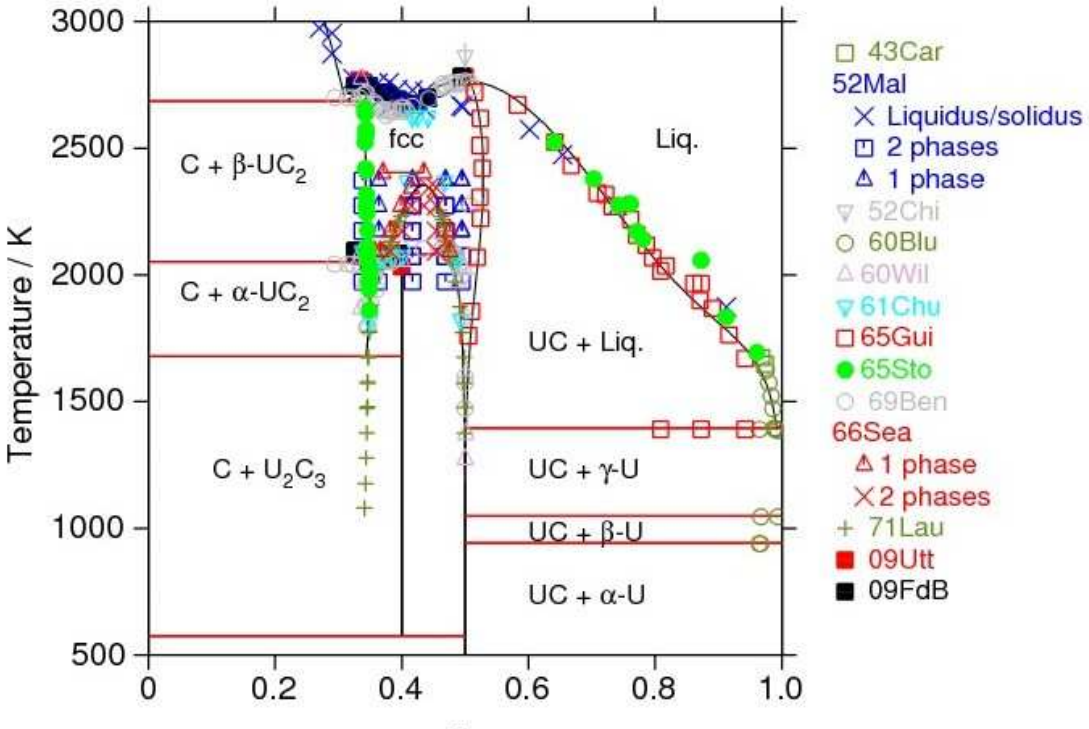
Binary system C-U

C-Mo-U C-O-U C-Pu-U C-Re-U C-Si-U C-U-W C-U-Zr C U Binary systems Ternary systems Periodic table

Comparison with experiments

Phase diagram

Compared to experiments



Nuclear Fuel database

TAF-ID : Thermodynamics of Advanced Fuels - International Database

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Binary system C-U

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Divers files

Phase diagram

C-U_dat.exp C-U_franck.exp C-U_diag_01Che.exp C-U_doc.TCM C-U_diag.TCM C-U_diag-U2C3.TCM C-U_franck.TCM C-U_franck-met.TCM

G and H of formation

C-U_gmr.TCM C-U_H298.TCM

Enthalpy increment

HUC.exp HUC2-bct.exp HUC2-193.exp HU2C3.exp HUC-che0.exp HU2C3-che0.exp HUC2-che0.exp HUCst.exp
C-U_HUC.TCM C-U_HUCstoi.TCM C-U_HUC2.TCM C-U_HU2C3.TCM C-U_fig6.TCM

Heat capacity

C_Cp.TCM U_Cp.TCM C_Cp.exp U_Cp.exp C-U_Cp.TCM C-U_Cp_U2C3.TCM C-U_Cp_UC2_01Che.exp C-U_Cp_UC2.TCM C-U_Cp_UC.TCM
C-U_Cp_UCstoi.TCM

Site occupancies of UC

C-U_yfcc.TCM C-U_yfcc_UC.TCM

Partial pressures and activities

C-U_pU-T.TCM C-U_pU-x.TCM C-U_pU_C.TCM C-U_pU_UC2.TCM C-U_pU_UC.TCM C-U_pU_U.TCM C-U_act.TCM C-U_actC.TCM

Nuclear Fuel database

```
$                                                    Phase diagram

$                                          liquidus Guinet

e_sy f TC=T-273.15;

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ch_st p fcc_b=f 0
s_c p=1E5 n(u)=1 n(c)=@1
expe TC=@2:10
$ C/U T-C
TABLE_VAL
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 9.0692e-02 1.4894e+03
 1.2298e-01 1.5942e+03
 1.4813e-01 1.6249e+03
 1.4592e-01 1.6928e+03
 1.6138e-01 1.6928e+03
 2.3625e-01 1.7419e+03
 2.2416e-01 1.7635e+03
 2.5549e-01 1.7943e+03
 2.7159e-01 1.8436e+03
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 3.1312e-01 1.9453e+03
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 5.5833e-01 2.2500e+03
 7.1489e-01 2.3977e+03
TABLE_END

$                                             solidus UC Guinet
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ch_st p fcc_b=e 1
s_c p=1E5 n(u)=1 T=@3
expe n(c)=@1:.001
s_s_v y(fcc_b,c#2)=.99
s_s_v y(fcc_b,c2#2)=0
s_s_v y(fcc_b,va#2)=.1
s_s_v y(liq,u)=.8
s_s_v y(liq,c)=.2
$ C/U T-C T-K
TABLE_VAL
 9.4130e-01     2446.4  2719.6
 9.0905e-01     2344.7  2617.9
```

Nuclear Fuel database

```
$ *** OUTPUT FROM THERMO-OPTIMIZER MODULE PARROT ***
$ Date 2010. 5. 6
$ This output should be possible to use as input to the COMPILE command.
$
$ Note that the following problems remain:
$ 1. Long lines not handeled gracefully
$ 2. Tables for experiments not used
$ 3. Some functions may have to be moved to an equilibria

 DEFINE_COMPONENTS C U
 ENTER_SYMBOL FUNCTION TC=T-273.15 ;
 ENTER_SYMBOL FUNCTION CP=HM.T ;
 ENTER_SYMBOL FUNCTION PUATM=Y(GAS,U)*P/101325 ;
 ENTER_SYMBOL FUNCTION HH298=HM-H298 ;
 ENTER_SYMBOL FUNCTION HH310=HM-H310 ;
 ENTER_SYMBOL FUNCTION HHU2C3=HM-HU2C3 ;
 ENTER_SYMBOL FUNCTION HHUC=HM-HUC ;
 $ -----------
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 CHANGE_STATUS COMPONENT VA C U =ENTERED
 CHANGE_STATUS PHASE LIQUID=ENTERED 0
 CHANGE_STATUS PHASE FCC_B1#1=FIXED 0
 SET_CONDITION  P=100000 N(U)=1 N(C)=6.1653E-2
 EXPERIMENT TC=1396.9:10
 SET_START_VAL T=1710.4  NP(LIQUID)=1.0617  Y(LIQUID,C)=5.8073E-2
 SET_START_VAL Y(LIQUID,U)=0.94193 Y(FCC_B1#1,C#2)=0.97147
 SET_START_VAL Y(FCC_B1#1,C2#2)=1.4766E-5 Y(FCC_B1#1,VA#2)=2.8515E-2
 $ -----------
 CREATE_NEW_EQUIL 2, 0
 CHANGE_STATUS COMPONENT VA C U =ENTERED
 CHANGE_STATUS PHASE LIQUID=ENTERED 0
 CHANGE_STATUS PHASE FCC_B1#1=FIXED 0
 SET_CONDITION  P=100000 N(U)=1 N(C)=9.0692E-2
 EXPERIMENT TC=1489.4:10
 SET_START_VAL T=1773.1  NP(LIQUID)=1.0907  Y(LIQUID,C)=8.3151E-2
 SET_START_VAL Y(LIQUID,U)=0.91685 Y(FCC_B1#1,C#2)=0.96376
 SET_START_VAL Y(FCC_B1#1,C2#2)=2.5197E-5 Y(FCC_B1#1,VA#2)=3.6214E-2
 $ -----------
 CREATE_NEW_EQUIL 3, 0
 CHANGE_STATUS COMPONENT VA C U =ENTERED
 CHANGE_STATUS PHASE LIQUID=ENTERED 0
 CHANGE_STATUS PHASE FCC_B1#1=FIXED 0
 SET_CONDITION  P=100000 N(U)=1 N(C)=0.12298
 EXPERIMENT TC=1594.2:10
 SET_START_VAL T=1831.4  NP(LIQUID)=1.123  Y(LIQUID,C)=0.10951
 SET_START_VAL Y(LIQUID,U)=0.89049 Y(FCC_B1#1,C#2)=0.95569
 SET_START_VAL Y(FCC_B1#1,C2#2)=4.0488E-5 Y(FCC_B1#1,VA#2)=4.4272E-2
 $ -----------
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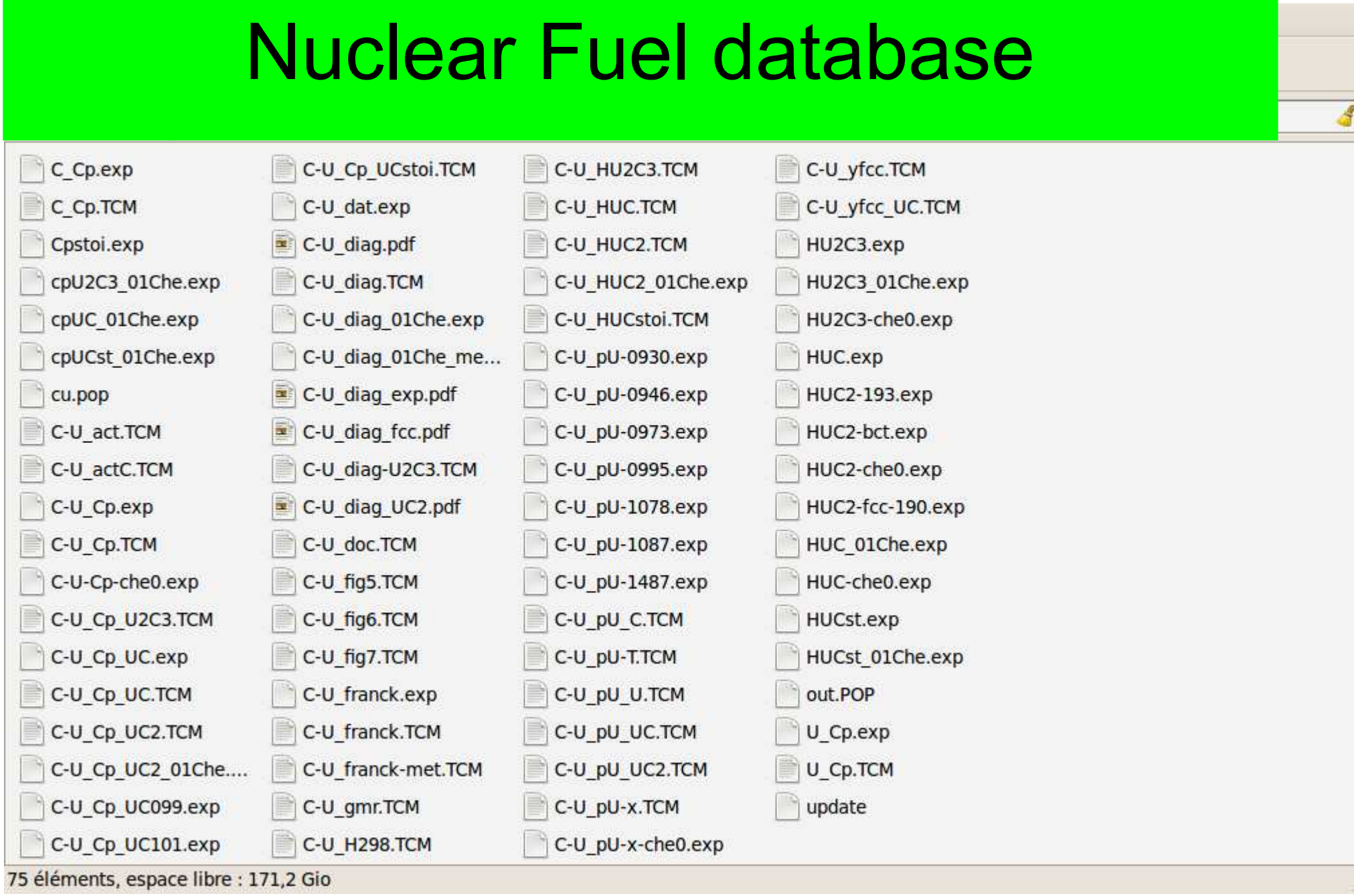
Nuclear Fuel database



Nuclear Fuel database

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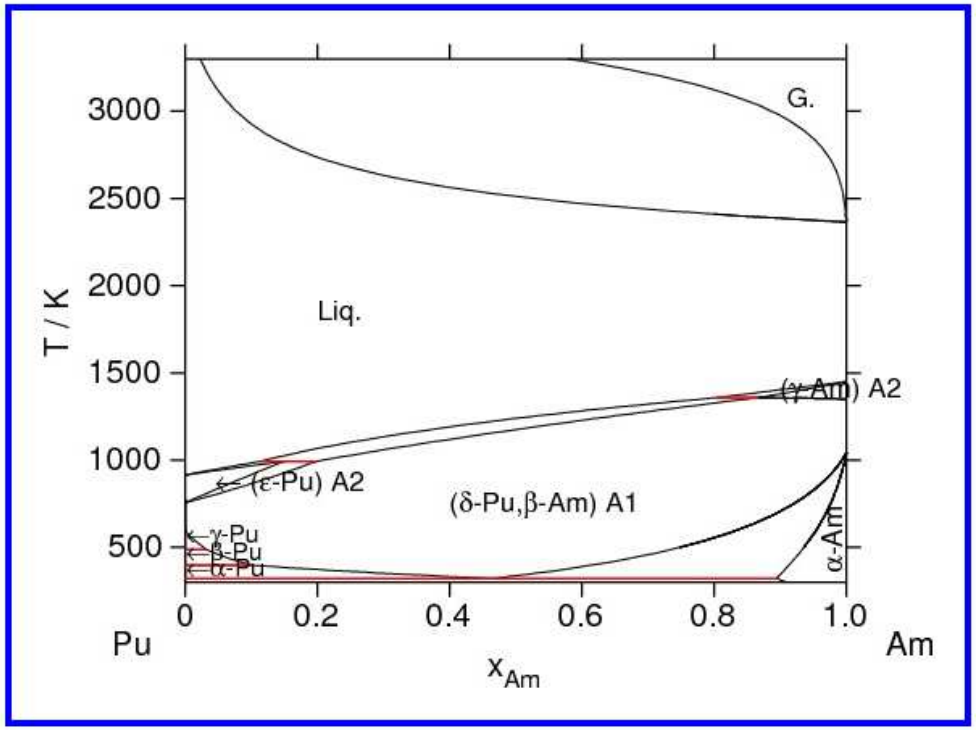
--:--- **update** Bot L109 (Fundamental)----------

Nuclear Fuel database

TAF-ID : Thermodynamics of Advanced Fuels - International Database

Binary system Am-Pu ★



Source of the description

P. Gotcu-Freis, P.Y. Colle, C. Guéneau, N. Dupin, B. Sundman, E.J.M Konings, *J. Nucl. Mater.*, **414**, 408-421 (2011)

Comments

The current description of the system Am-Pu is tentative due to the experimental uncertainty in this system. Even the equilibria involving the liquid phase are uncertain.

A report of this work is available.

A few figures.

No experimental thermodynamic data is available for this system.

This description is not in agreement with Turchi *ab initio* mixing enthalpy for the fcc and bcc phases. Turchi et al. published a Calphad description in agreement with their *ab initio* results; however this one shows excess entropy that seem overestimated. A revision of this system is desirable. A better prior experimental knowledge would be preferable.

Comparison with other descriptions

Comparison with experiments

Bibliography

Divers files

Nuclear Fuel database

TAF-ID : Thermodynamics of Advanced Fuels - International Database

Binary system Am-Pu ☆

Am-O-Pu Am Pu Binary systems Ternary systems Periodic tab

Quality of the assessment	
Phase diagram	1/3
Thermodynamic experiments	
. mixing enthalpy on whole or partial composition range	0/2
. formation or reaction enthalpies	0/1
. activity, chemical potential or partial pressure	1/1
. Cp or enthalpy increment	0/1
Thermodynamics ab initio	0/2
Crystallography	2/2
Extrapolation	1/1
Agreement with experiments	1/1
Metastability checked	0/1
Total	**5/15**

Main page for the system Am-Pu **Bibliography Divers files**

Other links Am-O-Pu Am Pu Binary systems Ternary systems Periodic table

Conclusion

- The html reporting tool I've started to developp more than 10 years ago has become an efficient tool when revising or extending a database, in particular when different people are involved.

- The feedback of the users is very positive.

- The tool allows much but the interest and quality of the information for each system is very dependent on the human effort spent.