THE OECD-NEA THERMODYNAMICS OF ADVANCED FUELS – INTERNATIONAL DATABASE (TAF-ID) PROJECT

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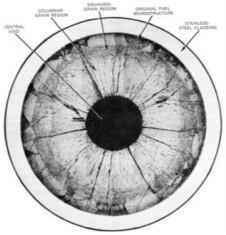
CONTEXT AND AIM OF THE TAF-ID PROJECT

AIM

- To develop a **thermodynamic database** as a **computational tool** to perform thermodynamic calculations on advanced fuel materials using the Calphad method
  ➡ **Phase diagrams + Thermodynamic properties of the phases**
- To **exchange** on the models, review of experimental data, softwares, assessments ….

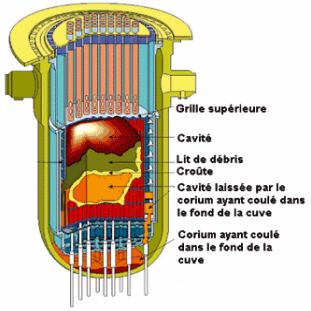
CONTEXT ➡ Fuel materials for Generation 2,3 & 4 reactors

- **Fuels**
  - UO_2, $(U,Pu,Am,Np)O_2$, $(U,Th)O_2$, (U,Pu,Zr,Am,Np), UN, (U,Pu)C
- **Fission products**
  - Ba, Sr, Mo, Zr, Lanthanides (Ce, La, Nd, Gd), metallic FPs (Pd, Ru, Rh, Te), Volatile (Cs, I, Te)
- **Structural materials**
  - Fe-Cr-Ni, Zr alloys, Fe-Cr-Al-Y, Concrete (SiO_2-CaO-Fe_xO_y-Al_2O_3-MgO), SiC, B_4C



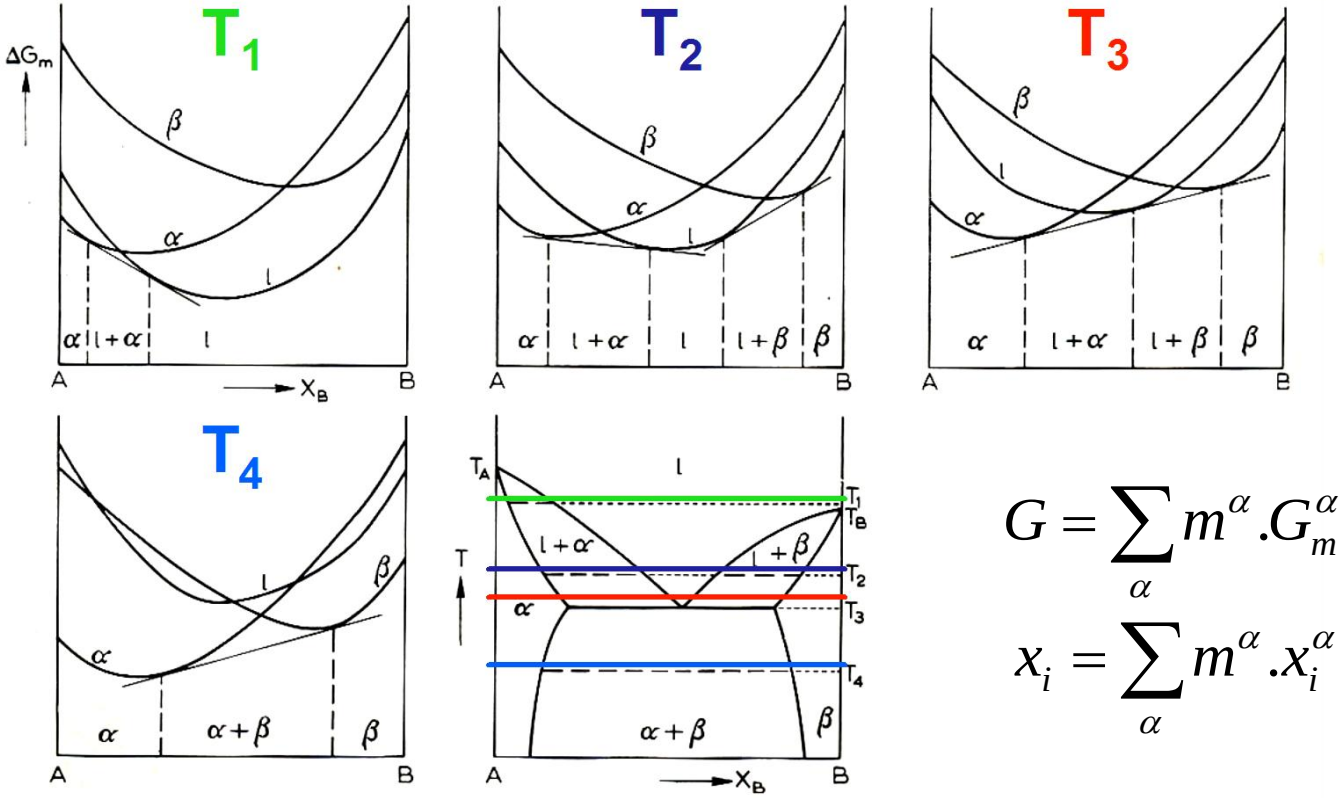
APPLICATIONS

- **Fuel behaviour at high temperature under normal and off-normal conditions**
  - Influence of the **Minor Actinides** on the fuel thermodynamic properties
  - **Fission product** « chemistry »
  - **Solid/liquid** phase transition
  - **Vaporization**
- **Fuel / cladding chemical interaction at high temperature**
- **Fuel fabrication**



CALPHAD METHOD

The thermodynamic equilibrium is calculated by minimizing the Gibbs energy of the system



$$G = \sum_{\alpha} m^{\alpha} . G_m^{\alpha}$$

$$x_i = \sum_{\alpha} m^{\alpha} . x_i^{\alpha}$$

$$\min(G) = \min\left(\sum_{\alpha} m^{\alpha} G_m^{\alpha}(T, p, x_i^{\alpha} \text{ or } y_k^{(l,\alpha)}) \right)$$

TAF-ID PROJECT

2013-2016: Thermodynamics of Advanced Fuels – International Database

➡ **The aim is to make available a comprehensive, internationally recognised and quality-assured thermodynamic database for advanced fuels**

- Coordinated by S. Massara from OECD/NEA➡ http://www.oecd-nea.org/science/taf-id

		Programme Review Group	
Country	**Signatory**	**Representative**	**Alternate Member**
Canada	CNL, RMCC, UOIT	M. Piro	E.C. Corcoran
France	CEA	C. Guéneau (Chair)	J.-C. Dumas
Japan	JAEA, CRIEPI	M. Kurata	T. Ogata
The Netherlands	NRG	R. Hania	G.-J. de Haas
Rep. Of Korea	KAERI	B.-O. Lee	J.-H. Kim
USA	DOE	T. Besmann (Vice-Ch)	P. Turchi

- The TAF-ID database is being built by **merging existing databases**
- N. Dupin (consultant) is responsible for the maintenance and documentation of the database

EXISTING DATABASES

Country	Software	Chemical system	Model
Canada AECL RMC UOIT	*FACTSAGE*	Fuel UO_2 + Np, Pu + Coolant H_2O FPs: (Kr), Rb, Sr, Y, Zr, Mo, Tc, Ru, Rh, Pd Te, I, Xe, Cs, Ba, La, Ce, Pr, Nd	302 comp. 17 solutions
France CEA	*Thermo-Calc*	Fuel UO_2, MOX+Am,Np,(U,Pu,Zr), (U,Pu)C, (U,Pu)N FPs: Ag, Ba, Cs, I, La, Mo, Nb, Ru, Sr, Te Materials: Concrete, B-C, Fe-Cr-Ni, SiC,Ta, W, V	Solutions 561 binaries 30 ternaries
Japan JAEA, CRIEPI	*Thermo-Calc*	Metallic fuel: Am-Cd-Ce-Fe-Gd-La-Nd-Np-Pr-Pu-U-Y-Zr Oxide fuel: Pu-Zr-O, Fe-B-C-O	Solutions
Netherlands NRG	*FACTSAGE*	Fuel: (U, Pu, Am, Np, Th)-(C, N, O) FPs: Ag, Ba, Br, Ce, Cs, Eu, I, La, Mo, Nb, Nd, Pd, Rb, Ru, Sb, Sn, Sr, Te, Y, Zr Materials: Fe, Ni, Si, Ti, Ta, W, Zn + Na, H, Pb	727 comp.
USA ORNL LLNL	*FACTSAGE* *Thermo-Calc*	UO_2 + RE: Pu-U-Gd-Ce-La-O Metallic fuel: Am-Pu, Mo-Pu,Mo-U,Nb-U,Nb-Zr,Pu-U,Ti-U,U-Zr Materials: Be-Cu-Fe-Nb-Ta-Ti-Zr	C1 solution solutions

➡ Different databases with different models.

➡ FACTSAGE and Thermo-Calc softwares are used.

THERMOCHEMICAL MODELS

- **The models are different from one database to another**

- **Models with stoichiometric phases and a few solid solutions**

  TBASE+RMC+UOIT: many compounds are described

  ➡ Associate model for oxide solid solutions (A,AO_2,AO_3 …)

  ➡ The phase diagrams can not be calculated

  A solution model for (Mo,Pd,Rh,Ru,Tc)

- **Model for MOX solid solution with Lanthanides**

  ORNL: to calculate oxygen potential versus burnup

  ➡ Ionic three sublattice model for MOX : Compatible with CEA database

  ➡ The phase diagrams can not be calculated

- **Models with a full description of non stoichiometric phases** (solid & liquid)

  JAEA+CEA+LLNL ➡ The phase diagrams can be calculated

In case of no phase diagram data, the G functions of the compounds will be introduced.

The aims of our project are:
- to merge these different databases,
- to **agree on thermodynamic descriptions** for binary and ternary sub-systems
- to **propose experiments** to improve the descriptions

in order to provide a **consistent database**

ORGANIZATION

- Every year, the PRG agrees on the list of chemical systems (binary and ternary systems) to be introduced in the TAF-ID Database:

  - Models published in the literature;
  - Models coming from a partner of the TAF-ID project
  - New models developed from exp. data by N. Dupin.

- A documentation is developed in HTML format by N. Dupin.

- In case of several existing models on a system, a comparison is done. The group decides which model is introduced in the TAF-ID database.

- 2 or 3 meetings / year

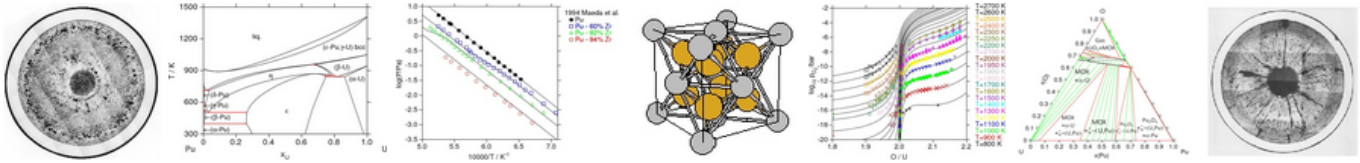
- Exchanges on models and experimental data.

- A code is being developed to convert the database in both Thermo-Calc and FACTSAGE formats

TAF-ID DATABASE (VERSION 5 – JANUARY 2015)

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:

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Rep. of Korea	KAERI	B.-O. Lee	J.-H. Kim
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.*

Current version: V5 2015 January 27th

TAF-ID DATABASE (VERSION 5 – JANUARY 2015)

ELEMENTS ➡ 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

BINARY SYSTEMS

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

In red*: 72 assessed within our project
In blue: 116 coming from the literature

TERNARY SYSTEMS

Al-Ca-O Al-Cr-O Al-Fe-O Al-Mg-O
Al-O-Si Al-O-U Al-O-Zr
Am-O-Pu
B-C-Fe B-C-U B-C-Zr B-Fe-Zr B-Pu-U
C-Mo-Re C-Mo-Si C-Mo-Ti C-Mo-U C-N-Ti C-N-U
C-O-Pu C-O-U C-Pu-U C-Pu-W C-Re-U C-Re-W
C-Si-Ti C-Si-U C-U-W C-U-Zr
Ca-Fe-O Ca-Mg-O Ca-O-Si Ca-O-U Ca-O-Zr
Cr-Fe-O Cr-Fe-Zr
Cs-Mo-O Cs-O-U Cs-O-Zr
Fe-O-Si Fe-O-U Fe-O-Zr Fe-U-Zr
Gd-O-U
La-O-U
Mg-O-Si Mg-O-U Mg-O-Zr
Mo-O-U Mo-Pd-Rh Mo-Pd-Ru Mo-Rh-Ru
Nb-O-U
Nd-O-U
Ni-O-Si
O-Pu-U O-Pu-Zr O-Si-U O-Si-Zr O-U-Zr
Pd-Rh-Ru
Pu-U-Zr

PROGRAM OF WORK 2015

Materials	Assessed systems
FP Grey phases in Oxide fuels ➡ Mo-Ba-Zr-Sr-O-U-Pu	Ba-Zr, Ba-Sr, Ba-U, Ba-Pu
FP Grey phases in Oxide fuels ➡ Mo-Ba-Zr-Sr-O-U-Pu	Sr-Zr, Sr-U, Sr-Pu
FP Grey phases in Oxide fuels ➡ Mo-Ba-Zr-Sr-O-U-Pu	Ba-O-Zr
FP Grey phases in Oxide fuels ➡ Mo-Ba-Zr-Sr-O-U-Pu	Sr-Zr-O
FP Grey phases in Oxide fuels ➡ Mo-Ba-Zr-Sr-O-U-Pu	Ba-O-U
FP Grey phases in Oxide fuels ➡ Mo-Ba-Zr-Sr-O-U-Pu	Sr-O-U
FP Grey phases in Oxide fuels ➡ Mo-Ba-Zr-Sr-O-U-Pu	Ba-Pu-O, Sr-Pu-O
FP Grey phases in Oxide fuels ➡ Mo-Ba-Zr-Sr-O-U-Pu	Ba-Mo-O, Sr-Mo-O
FPs phases in Oxide fuels	Cs-U, Sr-U
Corium in LWRs ➡ Steel/B4C interaction	Cr-B, Ni-B
Metallic fuels / FPs / Steel clad ➡ (Cr,Fe)-(Nd,Pd)-(U,Pu,Zr)	Cr-Pd, Fe-Pd, Pd-Zr
Metallic fuels / FPs / Steel clad ➡ (Cr,Fe)-(Nd,Pd)-(U,Pu,Zr)	Nd-Pd, Nd-Pu, Nd-Zr

CRYSTALLOGRAPHIC DATA

TAF-ID : Thermodynamics of Advanced Fuels - International Database

Home | Introduction | Models | Phases | Systems

Phases described by
- usual name: ε-Pu...
- database name: BCC_A2...
- prototype: W...
- StrukturBericht: *A2*...

Table

BETA_RHOMBO_B	B	*hR*105		(B)
BETA_SIALON	β-Si_3N_4	*hP*14		$(Si^{4+})_3$ $(N^{3-})_3$ (N^{3-})
BF_CASI	BCr	*oC*8	*Bf*	(Ca) (Si)
BH_MC_SHP	WC	*hP*2	B_h	(Mo, Re, W) (C)
MoC, WC				
C1_MO2	CaF_2	*cF*12	*C*1	$(Al^{3+}, Am^{3+}, Am^{4+}, Ca^{2+}, Np^{3+}, Np^{4+}, Pu^{3+}, Pu^{4+}, Th^{4+}, U^{3+}, U^{4+}, U^{5+}, Zr^{2+}, Zr^{4+})$ $(O^{2-}, ∅)_2$ $(O^{2-}, ∅)$
UO_2, PuO_2, ZrO_2, AmO_2, NpO_2				
C2_MTE2	FeS_2	*cP*12	*C*2	(Rh,Ru,∅) $(Te)_2$
Pyrite				
C4_RUTILE	TiO_2	*tP*6	*C*4	(Ru^{4+}, Ti^{4+}) $(O^{2-})_2$
C4_TI2N	TiO_2	*tP*6	*C*4	$(Ti)_2$ (C, N)
Described independently of TiO_2				
C6_B81	NiAs	*hP*4	$B8_1$	(Pd,Rh) (Pd,Rh,∅) $(Te)_2$
Identical model for CdI_2				
C6_B81_2	CdI_2	*hP*3	*C*6	(Pd,Rh
Identical model for NiAs				
C11B_AGM2	$MoSi_2$	*tI*6	$C11_b$	(Ag) (T
C11B_MOSI2	$MoSi_2$	*tI*6	$C11_b$	(Mo, R
C12_CASI2	$CaSi_2$	*hR*18	*C*12	(Ca) (S
C14_LAVES	$MgZn_2$	*hP*12	*C*14	(Cr, Fe
C15_LAVES	$MgCu_2$	*cF*8	*C*15	(Al, Cr
C16_THETA	$CuAl_2$	*tI*12	*C*16	(Ta, Z
C23_CA2SI	Co_2Si	*oP*12	*C*23	$(Ca)_2$ (

TAF-ID : Thermodynamics of Advanced Fuels - International Database

Home | Introduction | Models | Phases | Systems

Usual name

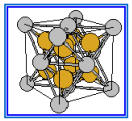
ZrO_2-γ, PuO_2, UO_2, AmO_2, NpO_2, ThO_2

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

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

Assessed systems where the phase is stable

Am-O Ce-O Np-O O-Pu O-Th O-U O-Zr Am-O-Pu C-O-Pu C-O-U Nd-O-U O-Pu-U O-Pu-Zr

A single sublattice model for all the phases with the same crystalline structure

Al-Zr

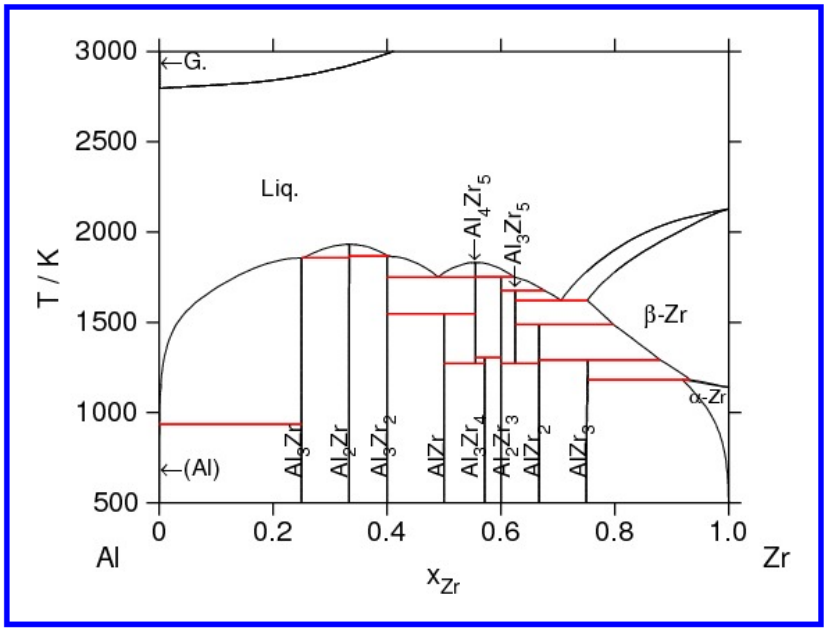
The source of the description is clearly mentioned.

TAF-ID : Thermodynamics of Advanced Fuels - International Database

Home | Introduction | Models | Phases | Systems | TDB

Binary system Al-Zr

Al-O-Zr Al Zr Binary systems Ternary systems Periodic table



Source of the description

T. Wang, Z. Jin, J.-C. Zhao, *J. phase equilibria*, **22** (5), 544-551, 2001.

Comments

The Al_2Zr and $AlZr_3$ descriptions are slightly modified in order to model them as the phases having the same prototype. The $L1_2$ phase corresponding to the $AlZr_3$ phase is rejected by default but restored by default when using the BINARY module of ThermoCalc.

File to calculate the phase diagram

Al-Zr.TCM

Cr-Fe-Zr

The source of the description is clearly mentioned.

TAF-ID : Thermodynamics of Advanced Fuels - International Database

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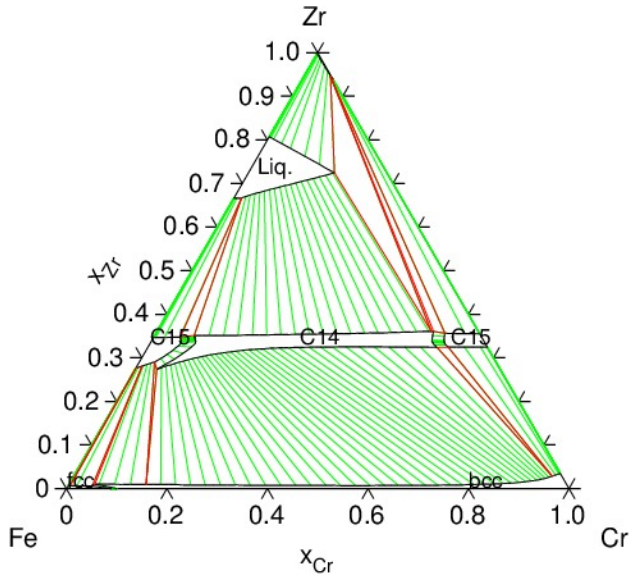
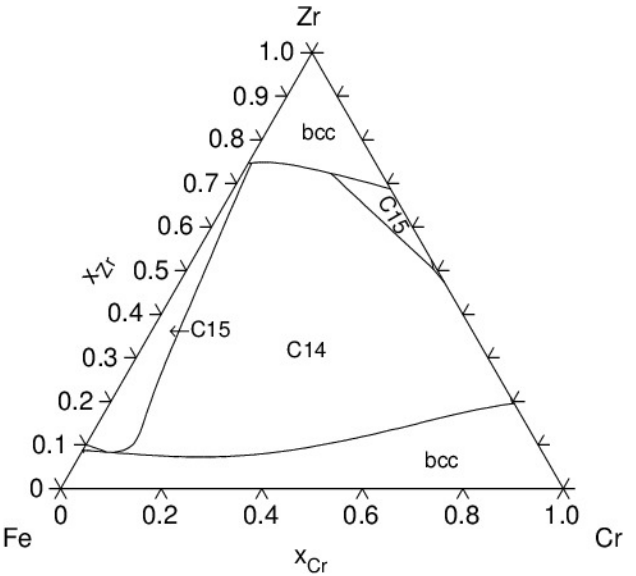
Ternary system Cr-Fe-Zr

Cr-Fe Cr-Zr Fe-Zr Cr Fe Zr Binary systems Ternary systems Periodic table

Isothermal section at 1500 K



Projection of the monovariant lines of the liquidus



Source of the description

N. Dupin, TAF-ID, 2014 october

Comments

The description recently published by Yang *et al.* was not used because of different descriptions for the Fe-Zr and Cr-Zr subsystems. The early description by Barberis *et al.* was using a Cr-Zr description with an overestimated enthalpy of formation for the Laves phases.

Cr-Fe-Zr

TAF-ID : Thermodynamics of Advanced Fuels - International Database

Home | Introduction | Models | Phases | Systems | TDB

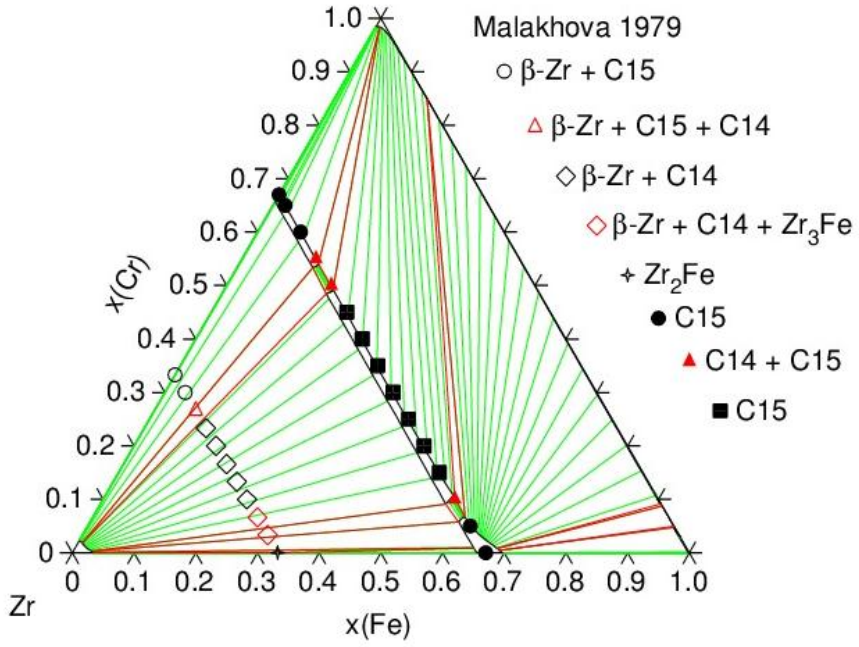
Ternary system Cr-Fe-Zr

Cr-Fe Cr-Zr Fe-Zr Cr Fe Zr Binary systems Ternary systems Periodic table

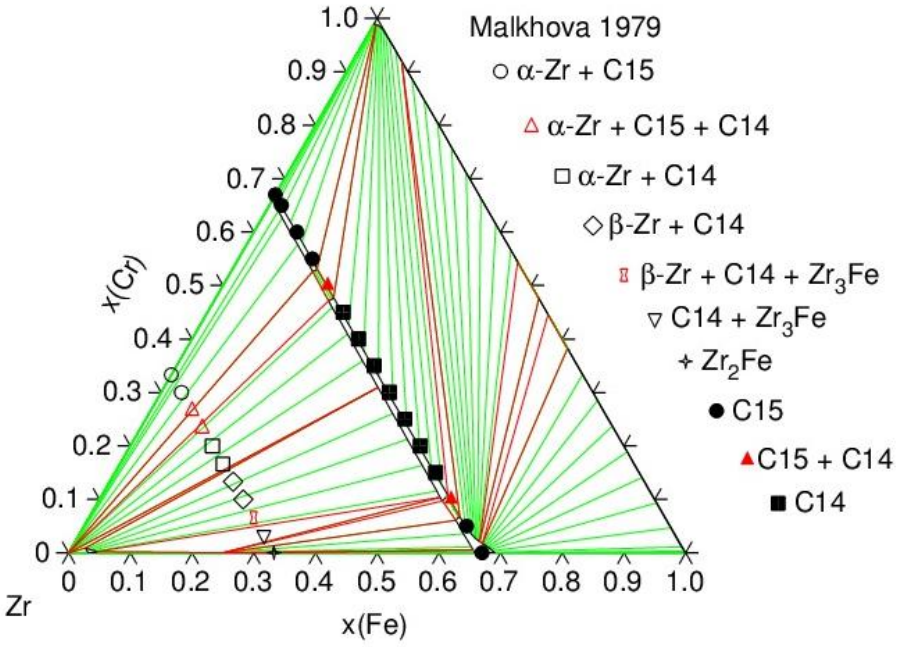
Comparison with experiments

Phase diagram

T = 1148 K



T = 1073 K



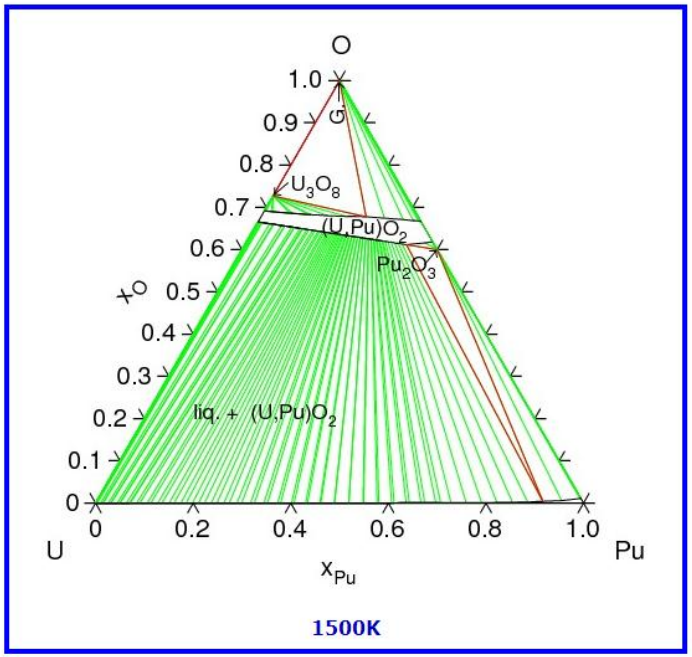
O-PU-U

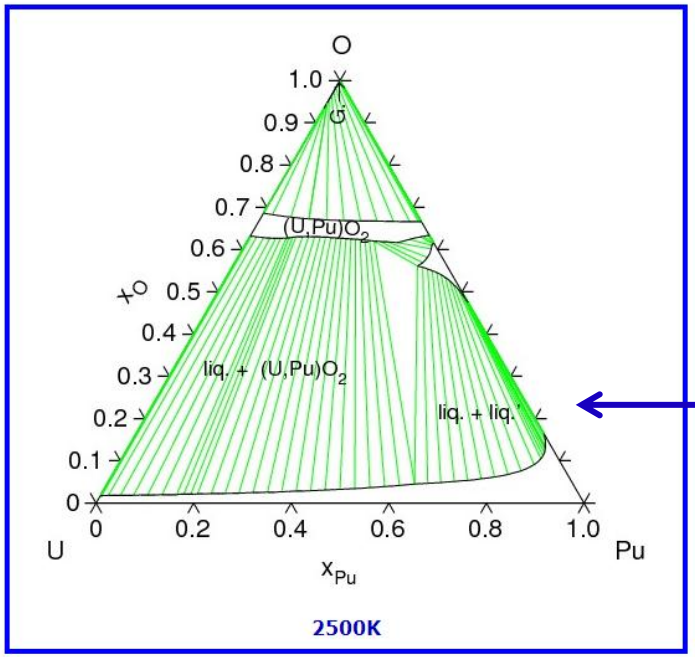
TAF-ID : Thermodynamics of Advanced Fuels - International Database

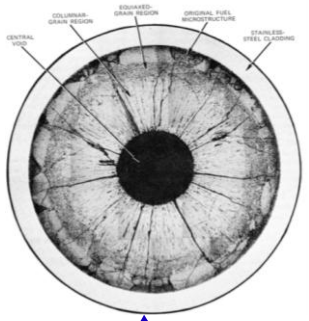
Home | Introduction | Models | Phases | Systems

Ternary system O-Pu-U

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







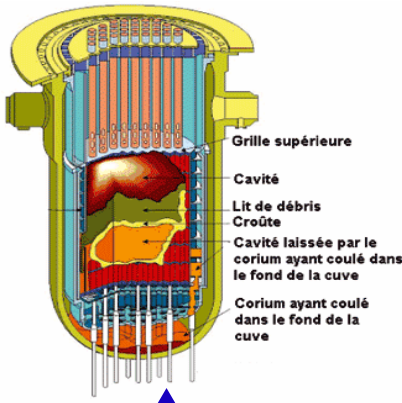
MOX fuel in SFR

-Interaction with steel clad
- Fission product chemistry

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

O-U-ZR



Corium (U,Zr,O) forming from UO_2/Zr interaction

TAF-ID : Thermodynamics of Advanced Fuels - International Database

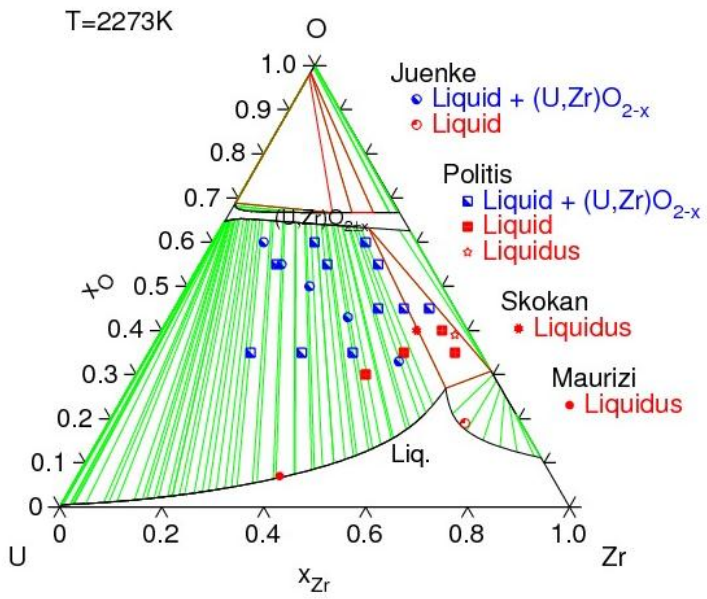
Home | Introduction | Models | Phases | Systems

Ternary system O-U-Zr

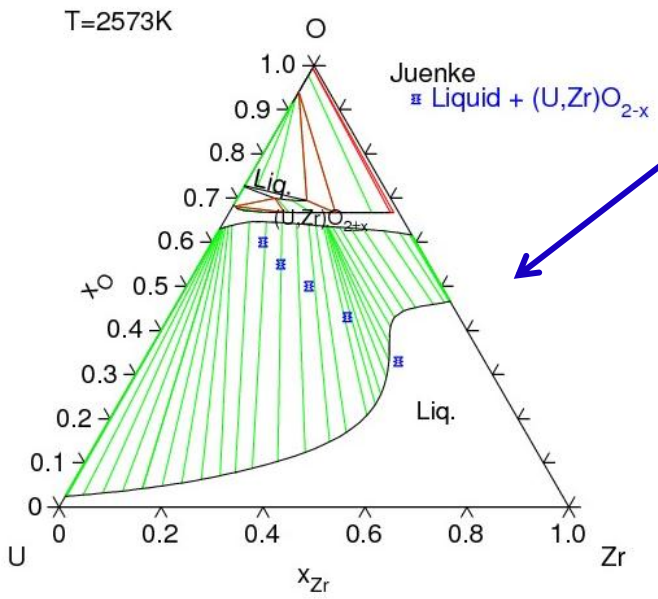
O-U O-Zr U-Zr O U Zr Binary systems Ternary system

Comparison with experiments

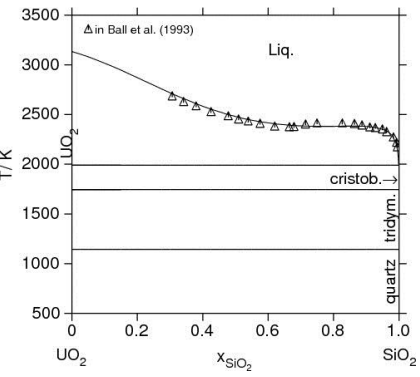
Isothermal section at 2273K

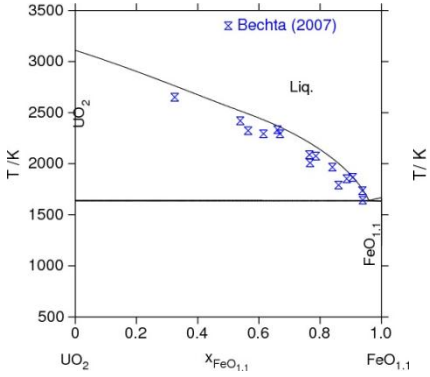


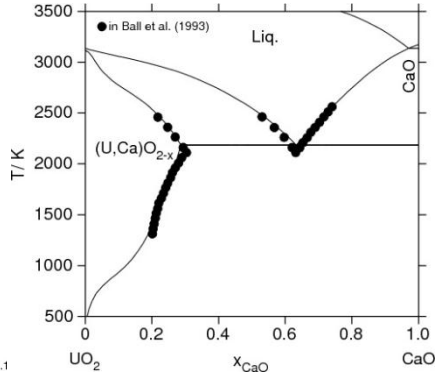
Isothermal section at 2573K

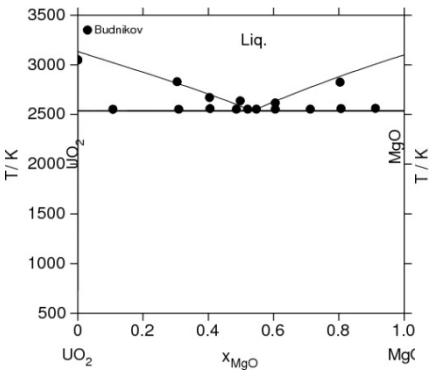


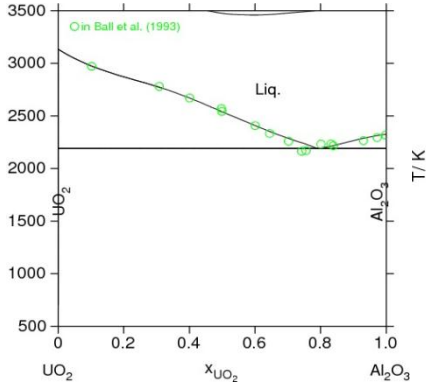
UO2-CONCRETE AND ZRO2-CONCRETE INTERACTION

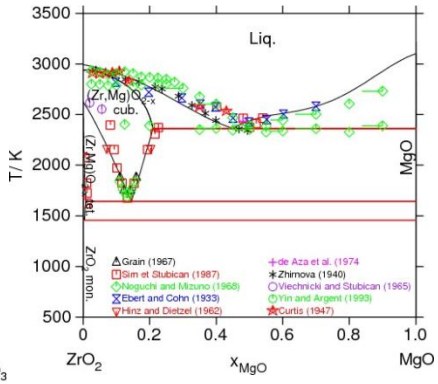


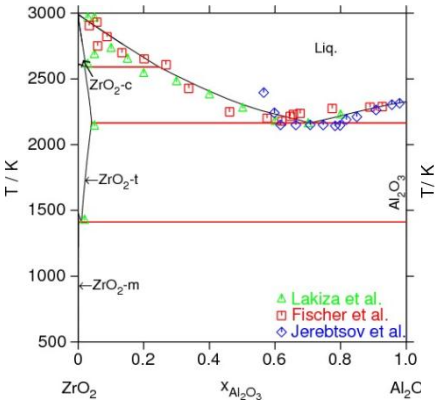


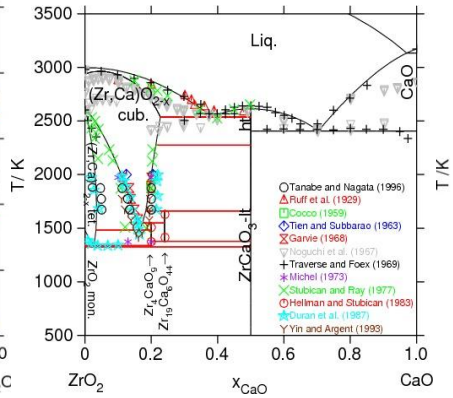


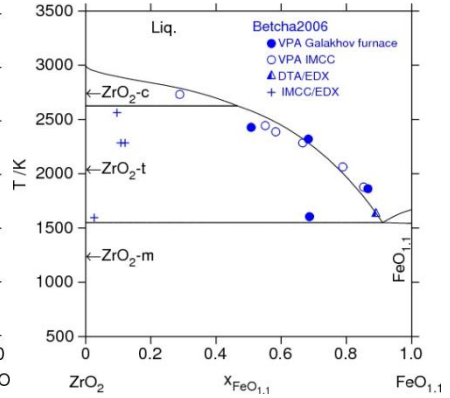


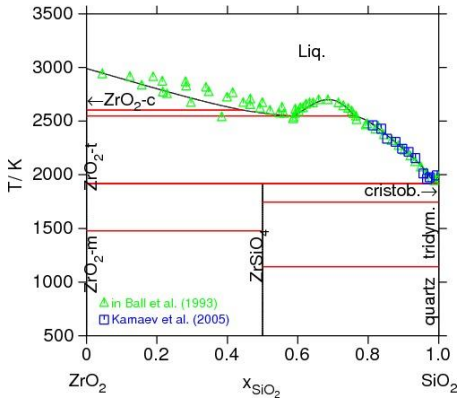


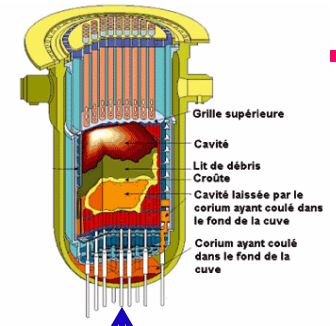












Corium (U,Zr,O,Fe) forming from UO_2/Zr/Fe interaction

$UO_2 + ZrO_2$ + concrete

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Nuclear science > Projects > TAF-ID

TAF-ID

- Thermodynamic data
- Tools for thermodynamic calculations
- Project Organisation
- The TAF-ID Versions
- Project Signatories
- Relevant links
- Contact

Thermodynamics of Advanced Fuels – International Database (TAF-ID) Project

TAF-ID public version

The TAF-ID public version contains only data already published in the literature. Currently, the following systems are available in the public version:

- Oxide-Carbide fuel (U-Pu-O-C, released December 2014);
- Metal fuel (U-Pu-Zr, released December 2014).

This version is accessible free of charge to all NEA member countries upon request to the NEA and signature of a Non-Disclosure Agreement (NDA).

- To send to the NEA a signed copy of the Non-Disclosure Agreement (NDA) please click here;
- If you already submitted a signed copy of the NDA and you received a confirmation e-mail, please directly enter the restricted access zone (password protected | reminder) and proceed to downloading.

Contact

For more information on the TAF-ID public version, please contact: taf-id@oecd-nea.org

For more information on TAF-ID, please contact: simone.massara@oecd.org

Last reviewed: 8 January 2015

TAF-ID working areas

- Programme review group
- TAF-ID working version
- TAF-ID public version

SUMMARY

- The Working Version 5 of TAF-ID database is available for the participants of the TAF-ID project
- A public version restricted to only published work is available for all the member countries of OECD/NEA since december 2014
  - ➡ https://www.oecd-nea.org/science/taf-id/taf-id-public/
- The TAF-ID database will be available in Thermo-Calc and FACTSAGE formats
  - A software to convert the databases from both codes is being developed
- Brazil and UK shall join the project in 2016
- The TAF-ID project will be extended to 2017

PROGRAM OF WORK 2014

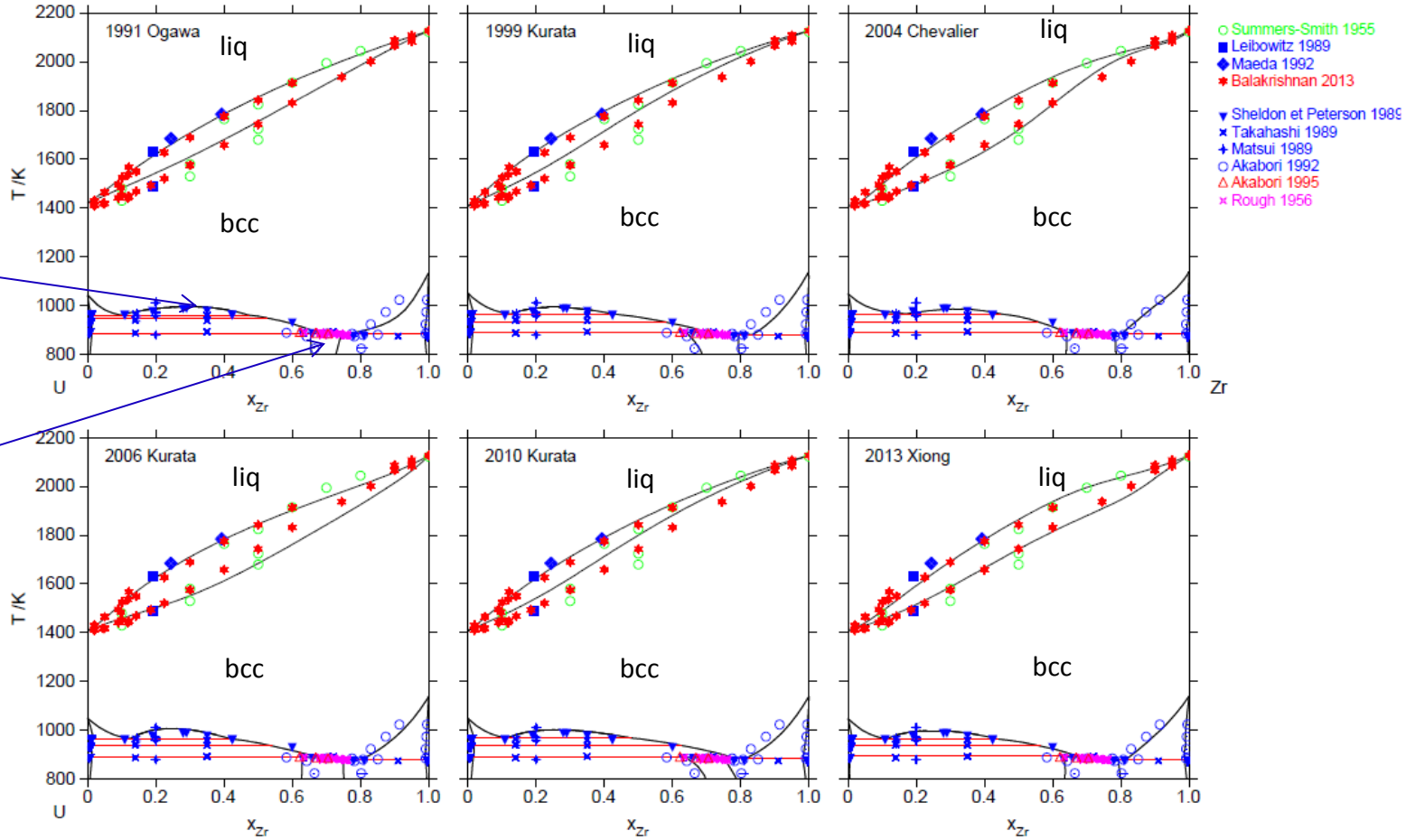
Materials	Systems
FPs oxide phases in oxide fuels	U-Nd-O
FPs oxide phases in oxide fuels	U-Nb-O
FPs oxide phases in oxide fuels	U-Mo-O
FPs oxide phases in oxide fuels	Cs-Mo-O
FPs oxide phases in oxide fuels	Cs-U-O, Cs-Zr-O
FPs metallic phases in oxide fuels	Rh-Te, Pd-Rh-Ru
FPs metallic phases in oxide fuels	Other ternaries in Rh-Ru-Pd-Mo-Tc
Corium in LWRs	Ag-O
Corium in LWRs	Ni-U, Fe-U-Zr
Corium in LWRs	B-O
Corium in LWRs	B-Zr
Corium in LWRs	B-C-U, B-C-Zr, Fe-B-Zr
Corium in LWRs	Cr-Fe-Zr
FPs in Metallic fuels	Pd-Zr
FPs in Metallic fuels	Ce-Fe
FPs in Metallic fuels	Ce-Cr
FPs in Metallic fuels	Nd-Fe, Nd-Cr
Database + documentation for the Public Version	U-Pu-O-C
Database + documentation for the Public Version	U-Pu-Zr
Carbide fuels	U-C-N

COMPARISON OF EXISTING DESCRIPTIONS
EXAMPLE: U-ZR SYSTEM (1)

- U-Zr is a key system to describe metallic fuels (U-Pu-Zr system) and chemical interaction between UO_2/Zr during severe accident (U-Zr-O system)
- 6 different assessments: Ogawa 1991, Kurata 1999, Chevalier 2004, Kurata 2006, Kurata 2010, Xiong 2013

Miscibility Gap in bcc

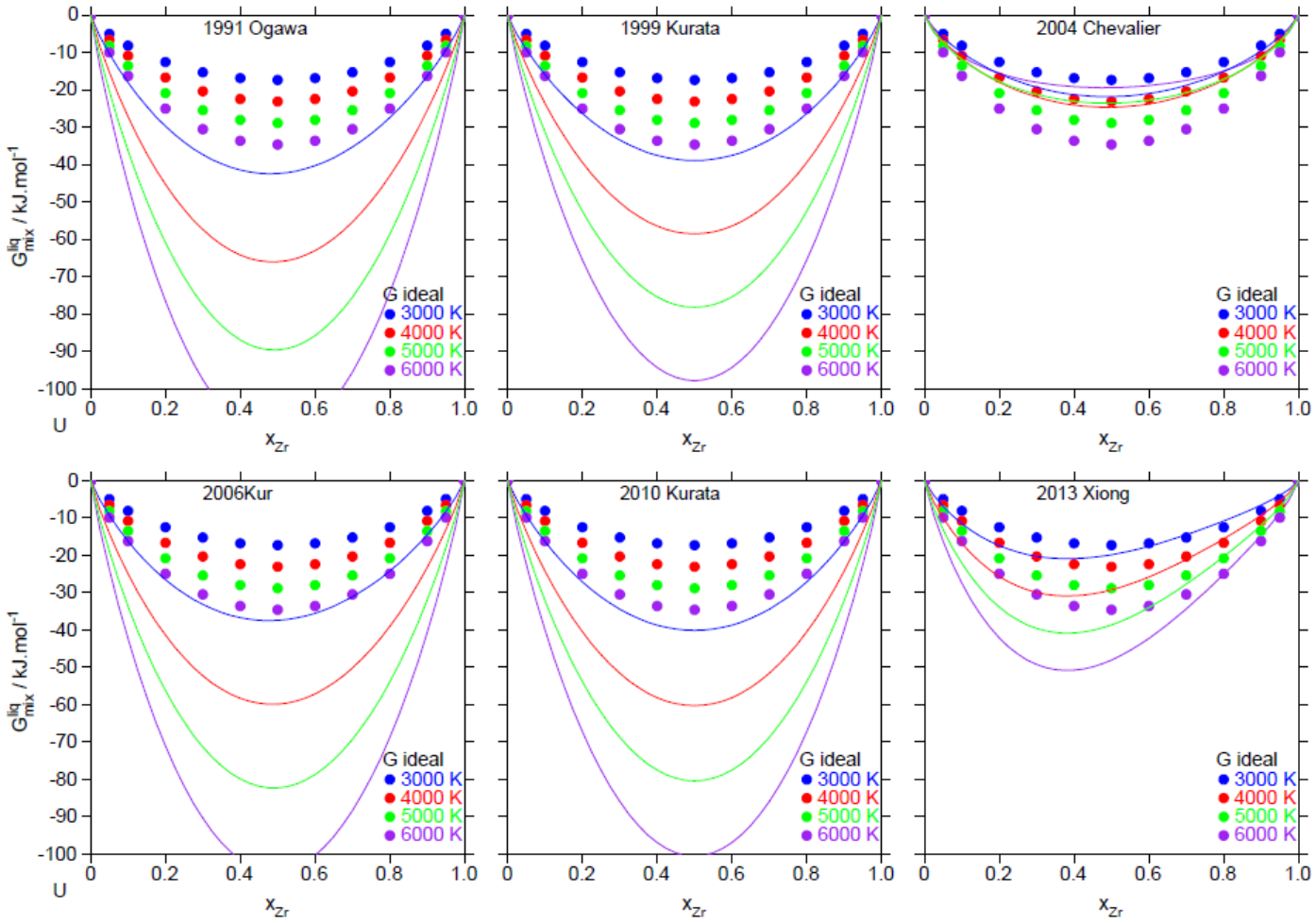
Delta-UZr_2



- The phase equilibria are not well established in the region close to delta-UZr_2 phase
- According to the liq/bcc phase boundaries, an ideal mixing is expected in the liquid.

COMPARISON OF EXISTING DESCRIPTIONS
EXAMPLE: U-ZR SYSTEM (2)

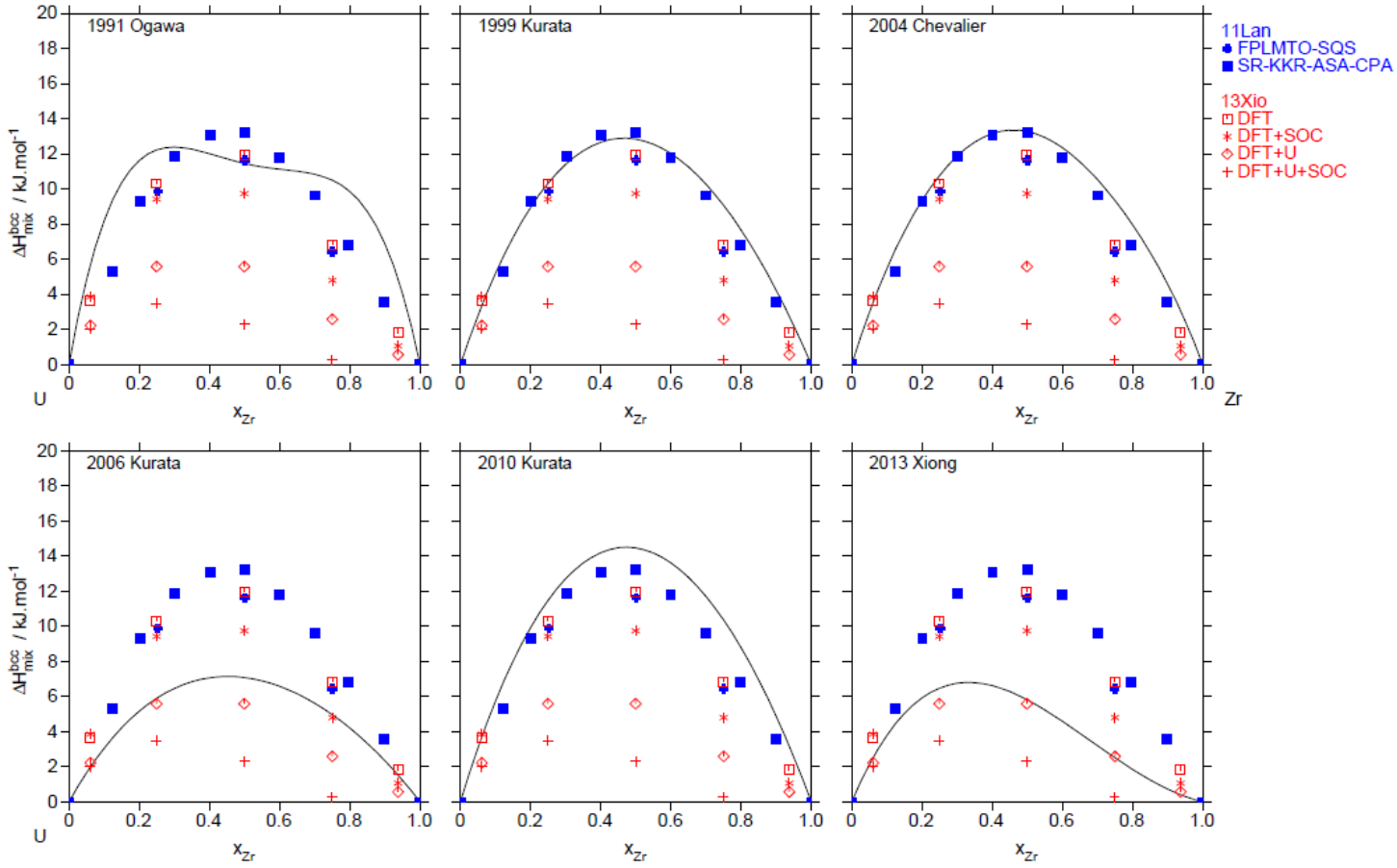
Mixing in the liquid phase at high temperature



➡ Different extrapolations at high T whereas an ideal behaviour is expected

COMPARISON OF EXISTING DESCRIPTIONS
EXAMPLE: U-ZR SYSTEM (3)

Mixing enthalpy in the bcc phase



➡ Two different datasets for mixing enthalpy in bcc solid solution from ab-initio