Constitution of Calphad multicomponent databases

Nathalie Dupin

Calcul Thermodynamique

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Walt Disney World . Orlando, Florida, USA

Calphad assessments

- binary or ternary systems
- widely available in publications
- full description based on
  - experimental information
  - ab initio results
- not always compatible between them
- basis of multiconstituent databases

Multiconstituent databases

- many constituents, many phases
- commercial databases or industrial property
- reduced composition area of validity
- simulation of industrial alloys/processes
- developpment of new grades

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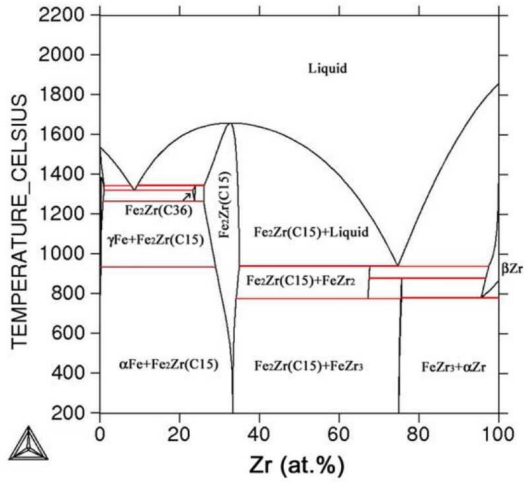
C. Toffolon-Masclet *et al.*
JAI101122



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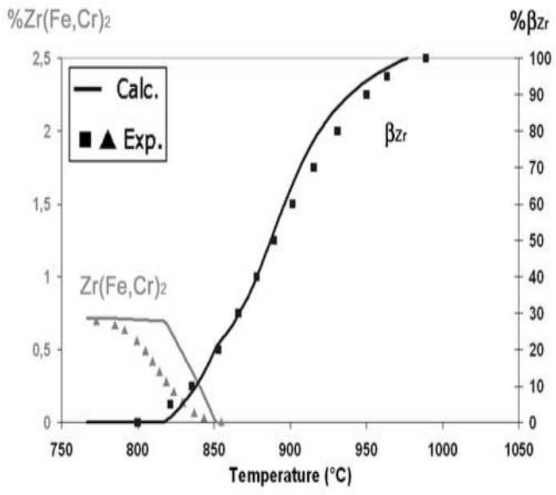

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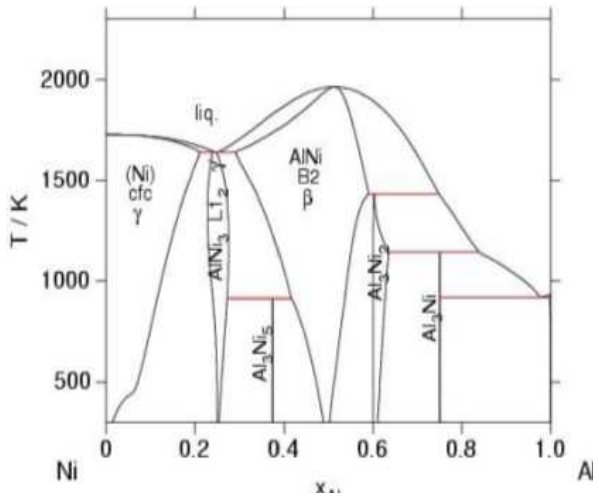
J. Bratberg *et al.*
Superalloys 2012



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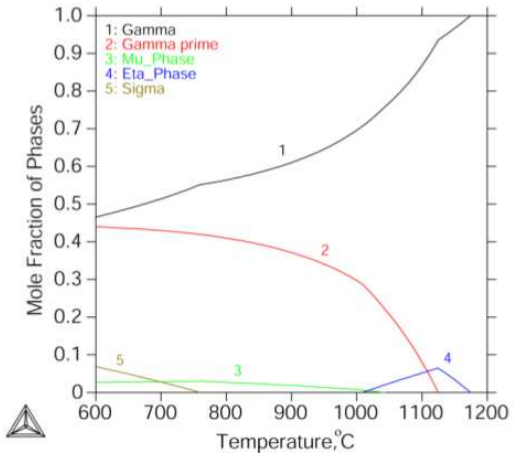

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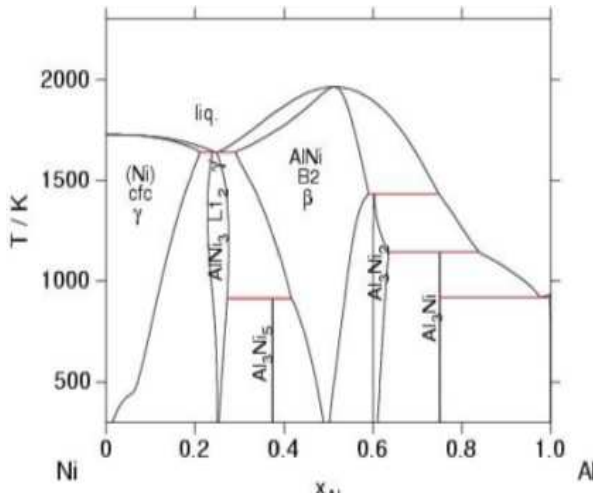

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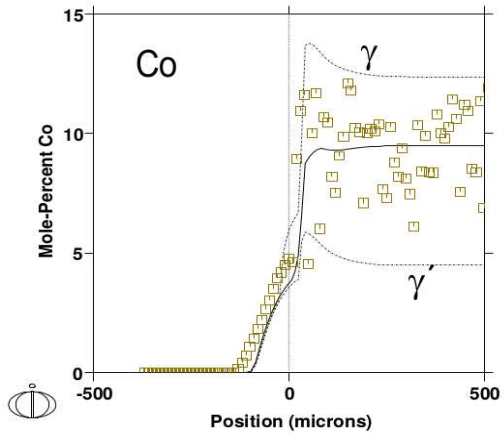

Calphad assessments

www.oecd-nea.org/science/taf-id

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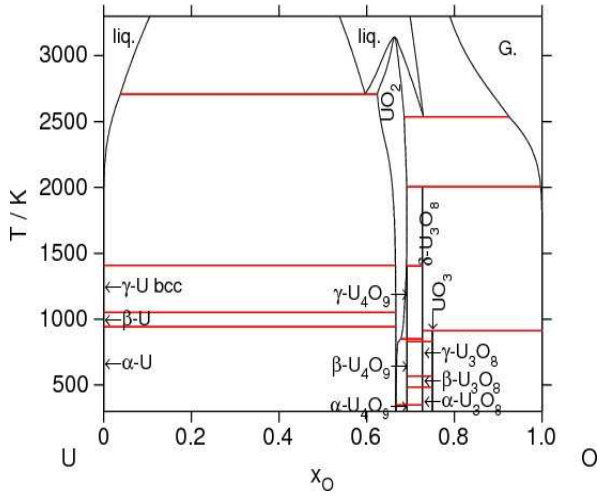

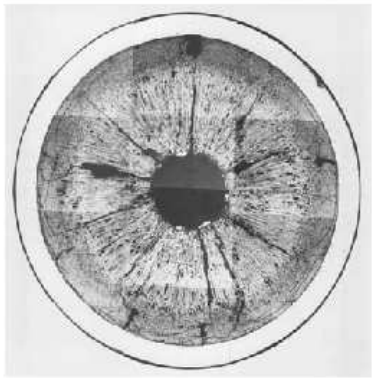

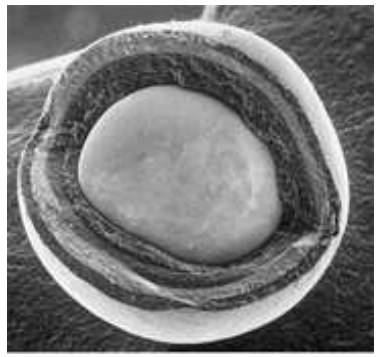

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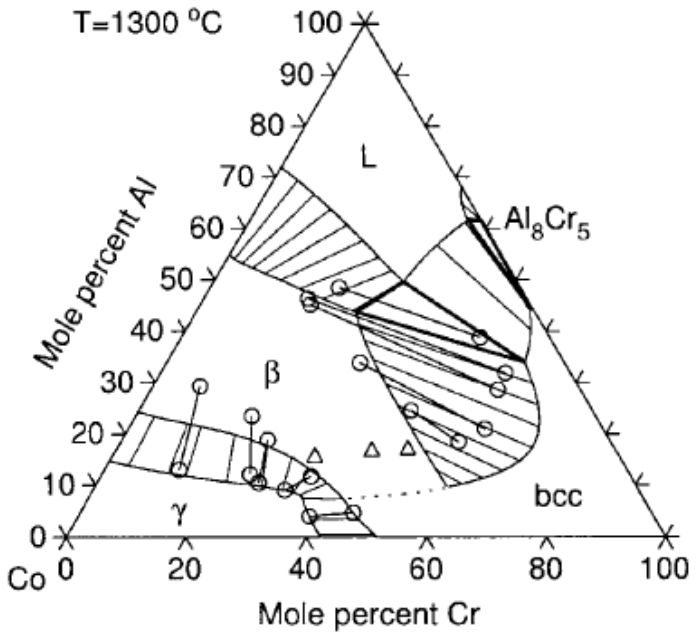
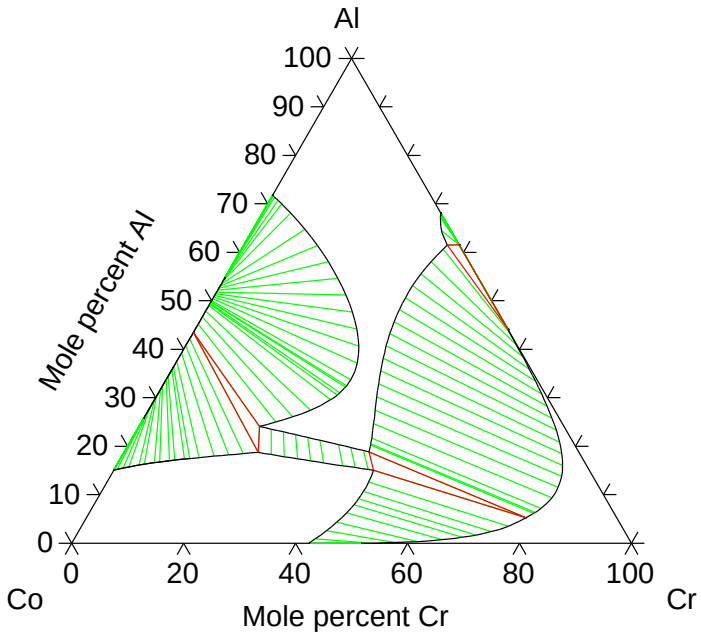
A multicomponent database is not a collection of binaries

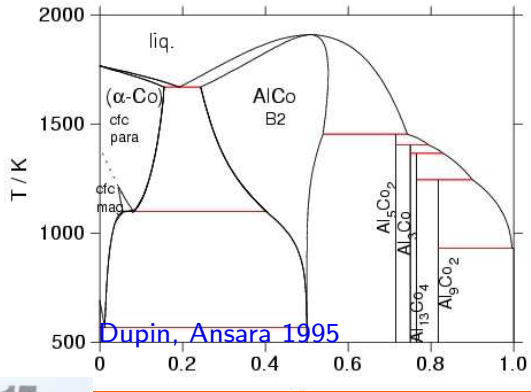
T. Gómes-Acebo et al. JPEDAV (2004) 25:237-251

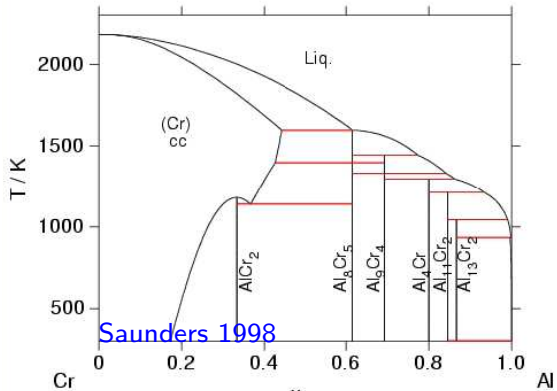




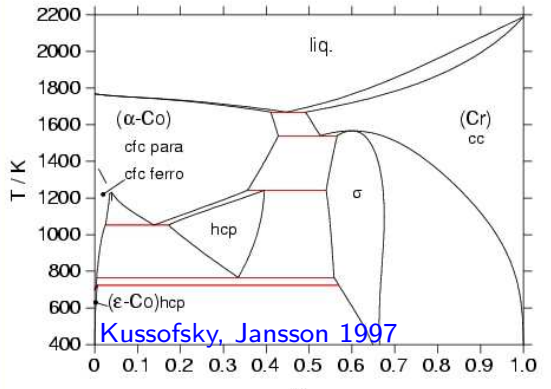
exp.: Ishikawa et al. *Ber.Bun/Phys.Chem.* **102** 1206 (1998)

TCNI β and bcc : (Al,Co,Cr,Va)(Al,Co,Cr,Va)





β: (Al,Co)(Co,Va)



Constitution of a multicomponent database

- Definition of the elements and phases of interest
- Choice of the models
  - Modification of existing assessments
- Assessment of missing constituting systems
- Metastable inputs based on ternary knowledge/guess
- Validation

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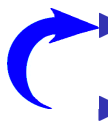

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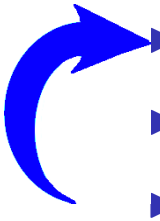

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...

- Feedback of users
- New project
  - revision of some phases
  - wider validity range
  - more elements

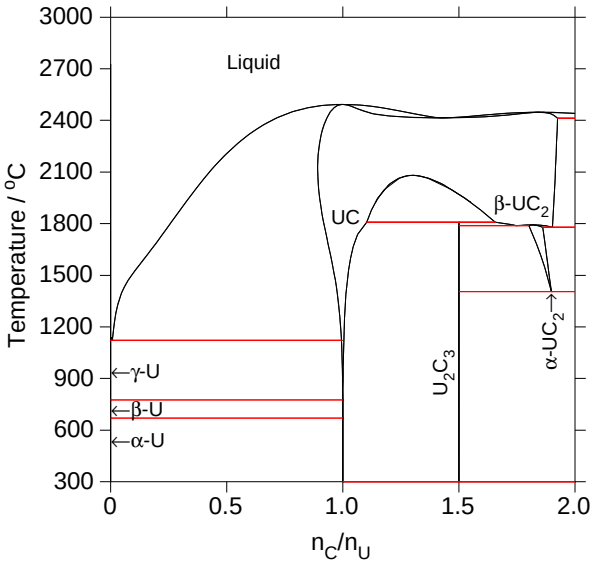
Choice of models

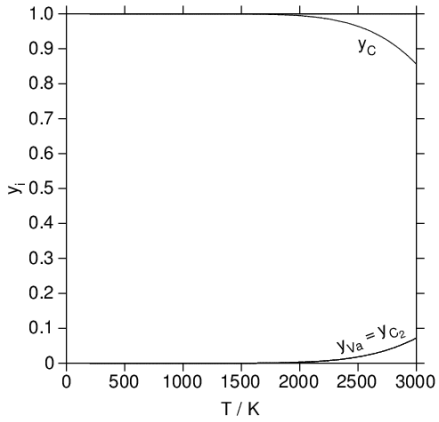
- Same crystallographic structure $\Rightarrow$ same model
  - not always that obvious
- Crystallographic analysis allows description of
  - ordering relationship
  - thermodynamics
  - phase diagram
- Good models "work" in all systems.
- FP results help.

Defects: phase diagram and thermodynamics

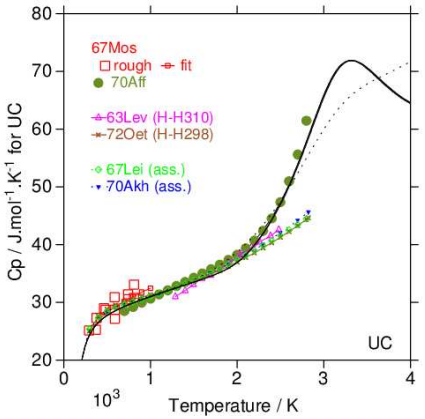
(U)(C,□,C_2)

C. Guéneau *et al.* JNM 419 (2011) 145-167

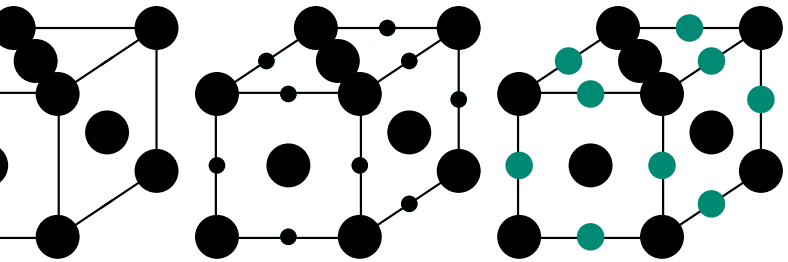




vs temperature for x_C=0.5

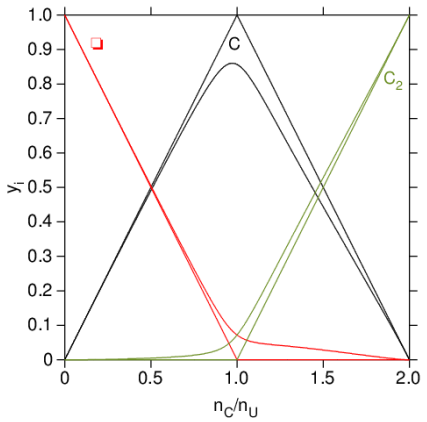


(U)(C_2,C_2,□) at x_C=0.5

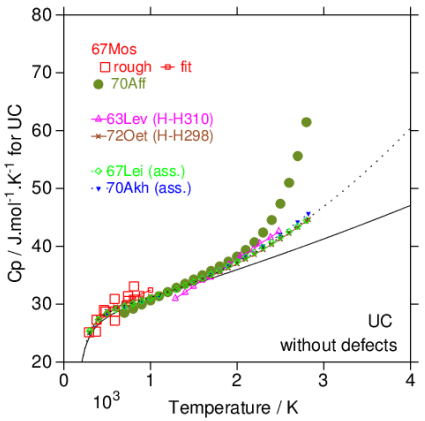


A1 B1

Cu NaCl KCN

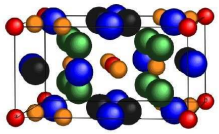


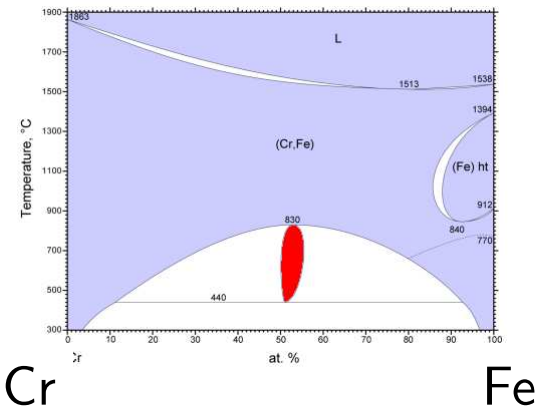
vs composition at 1500 and 3000K



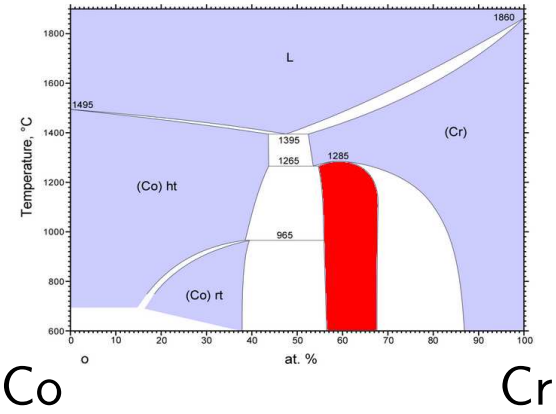
(U)(C)

Good models

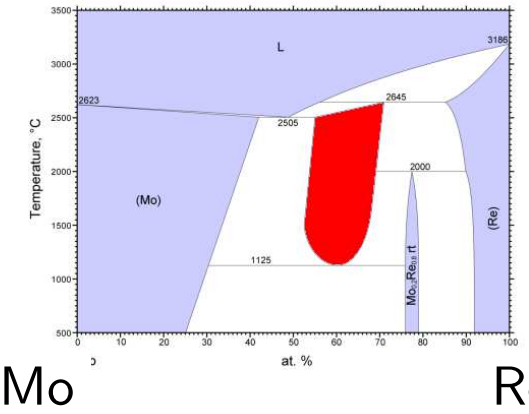




Cr Fe

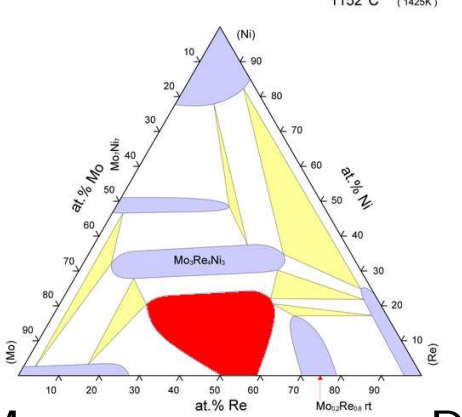


Co Cr



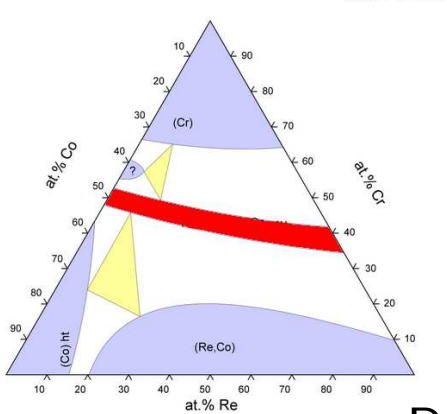
Mo Re

Ni



Mo Re

Cr



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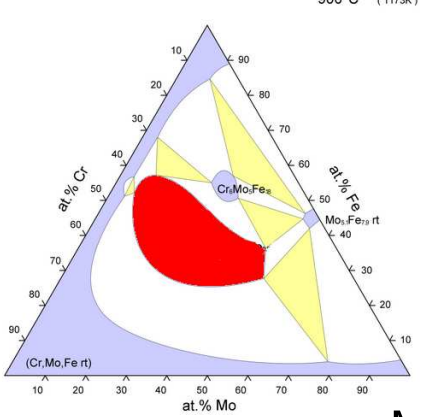


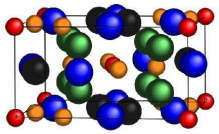
Cr Mo

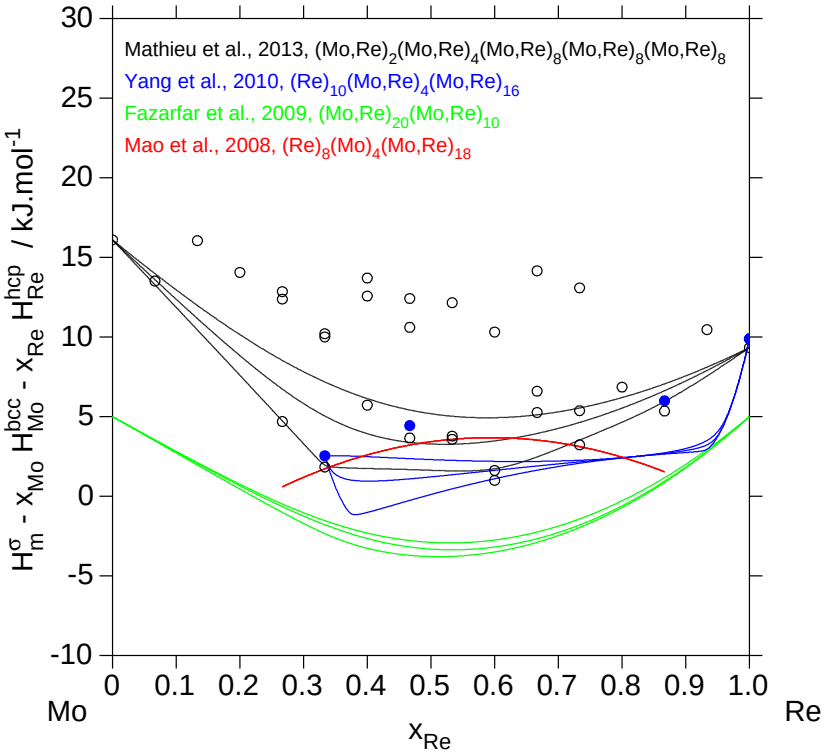
The σ phase presents different ordering degrees, different topology.
A good model should describe this in all the systems considered.

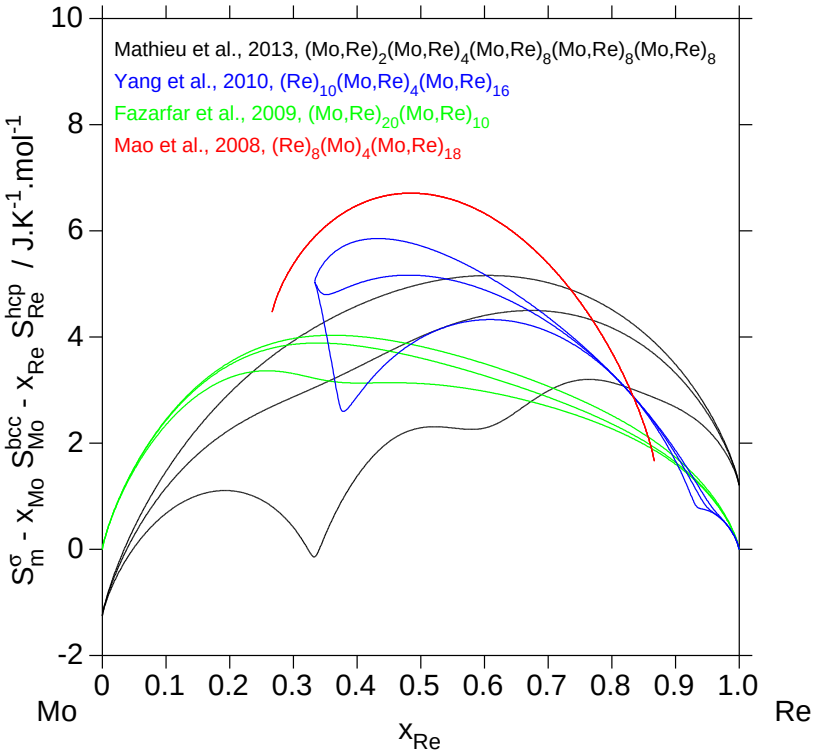
http://www1.asminternational.org/AsmEnterprise/APD access warmly acknowledged

Good models

R. Mathieu *et al.* Calphad 43 (2013) 18-31







A good model should be able to separate $S^{conf.}$ from $S^{vib.}$.

Good models

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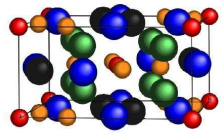
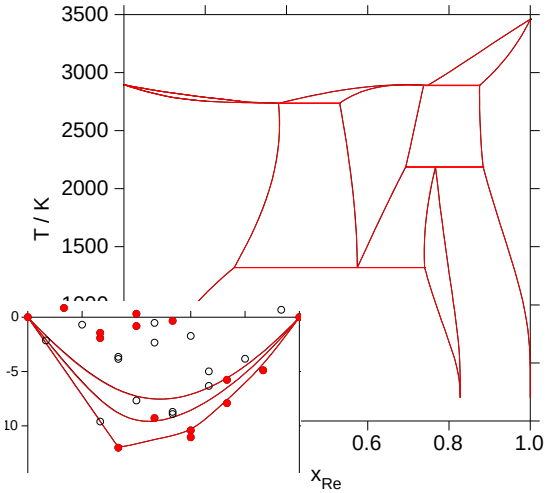
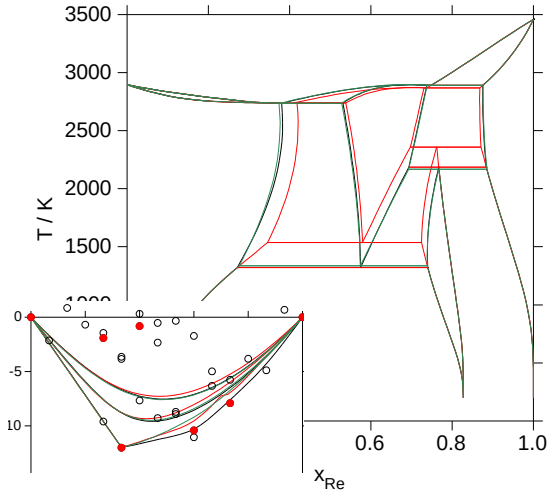
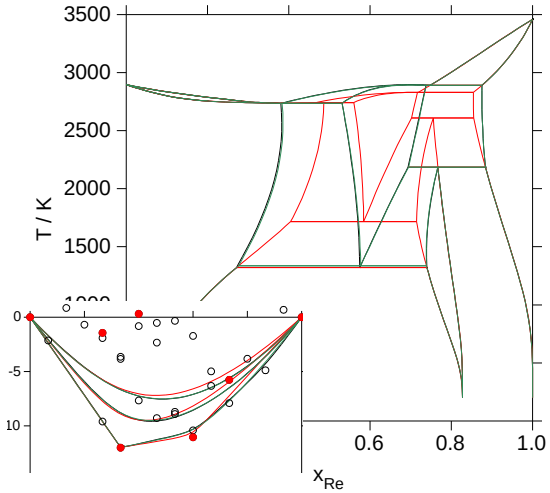




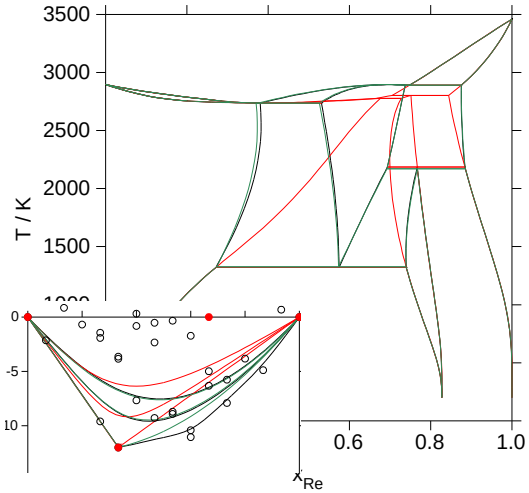
→4SL: $(A,B)_{10}(A,B)_4(A,B)_8(A,B)_8$
L(SIGMA,MO,RE:*:*:*;0)=0



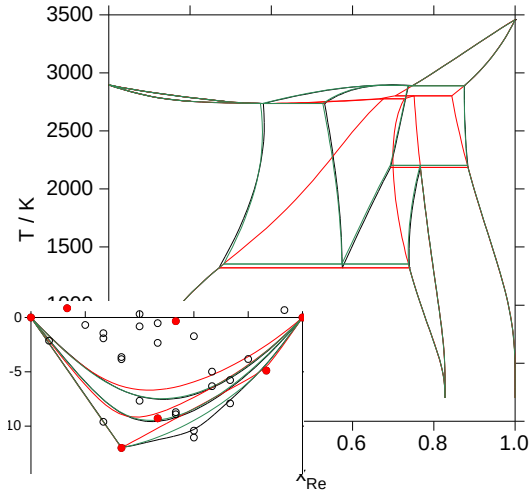
→3SL-23: $(A,B)_{10}(A,B)_{12}(A,B)_8$
L(SIGMA,MO,RE:*:*;0)=0
L(SIGMA,*:MO,RE:*;0)=-45800+7.8*T



→3SL-25: $(A,B)_{10}(A,B)_{12}(A,B)_8$
L(SIGMA,MO,RE:*:*;0)=0
L(SIGMA,*:MO,RE:*;0)=-67750+2.8*T



→2SL: $(A,B)_{10}(A,B)_{20}$
L(SIGMA,MO,RE:*;0)=0
L(SIGMA,*:MO,RE;0)=-242810+11.4*T

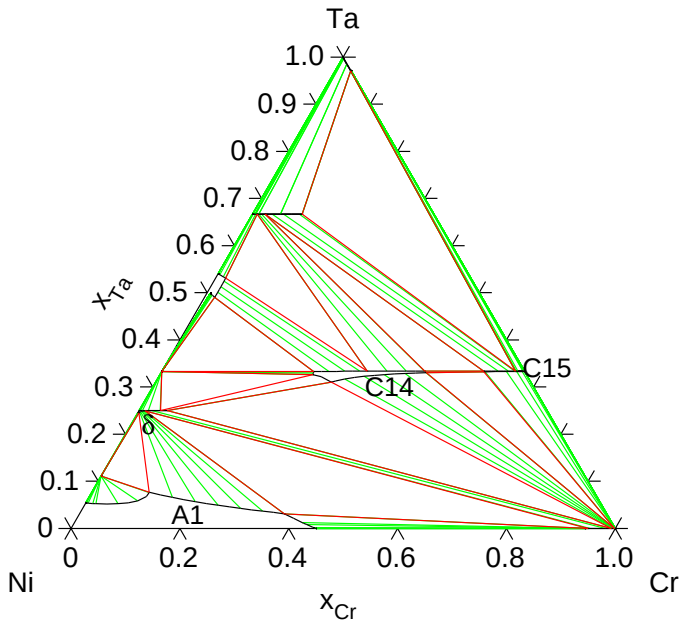


→3SL-35: $(A,B)_{10}(A,B)_4(A,B)_{16}$
L(SIGMA,MO,RE:*:*;0)=0
L(SIGMA,*:*:MO,RE;0)=-130000-1.1*T

A good model should be able to separate H and S contributions.

Recommended 3SL : $(A,B)_{10}(A,B)_{12}(A,B)_8$ rather than classical $(A,B)_{10}(A,B)_4(A,B)_{16}$

Assessment of metastable states



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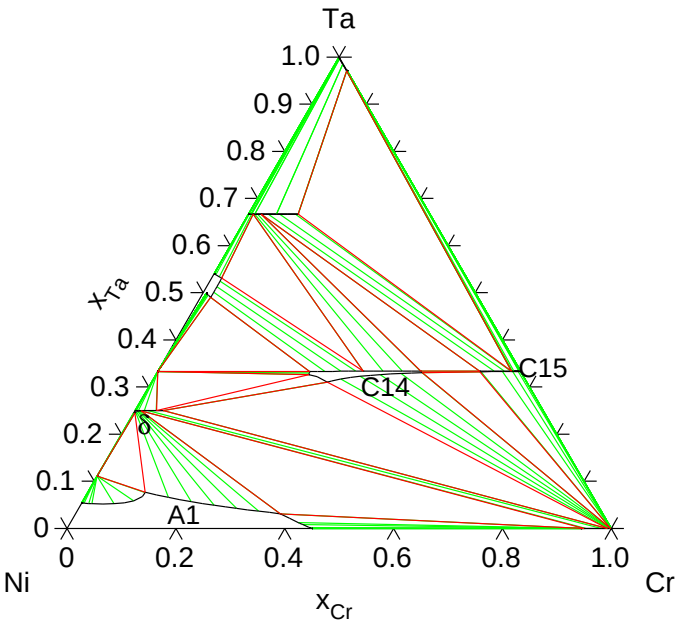

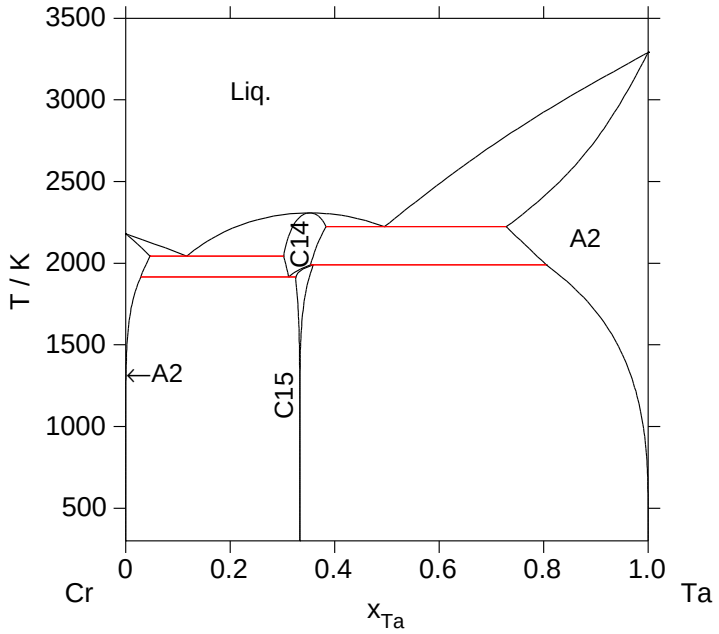

In order to describe the fcc phase in the ternary Cr-Ni-Ta, it has to be described in the binary Cr-Ta where it is not stable. It has to be identical whatever system implying Cr-Ta system. Nowadays, FP results help in such assessment.

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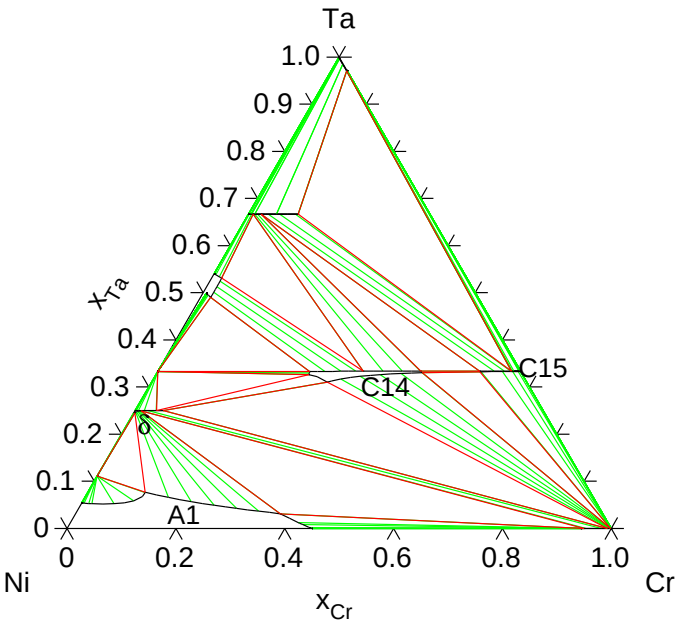

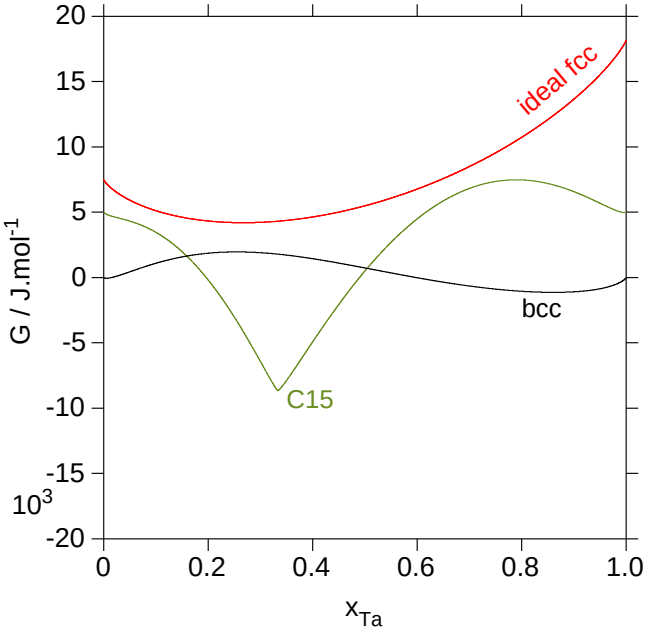

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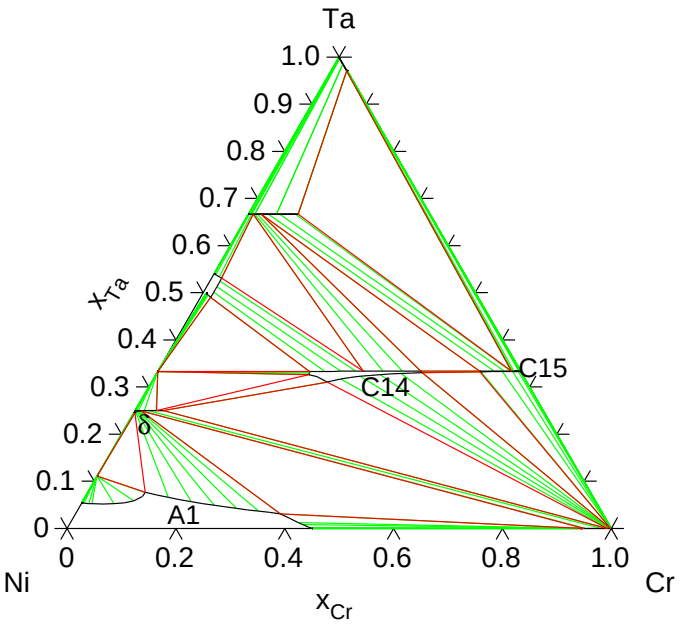

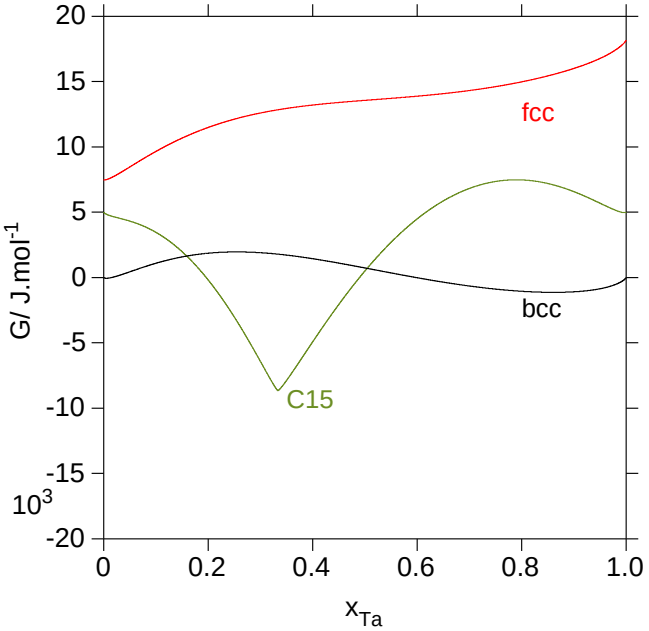

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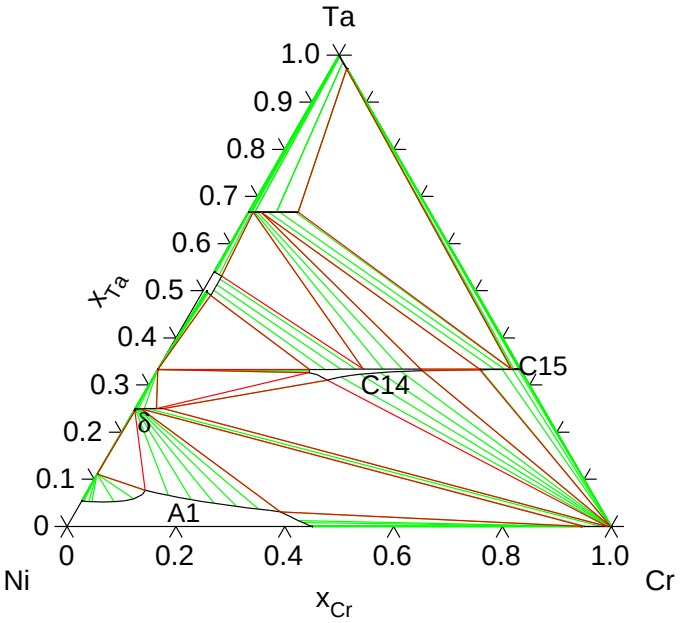
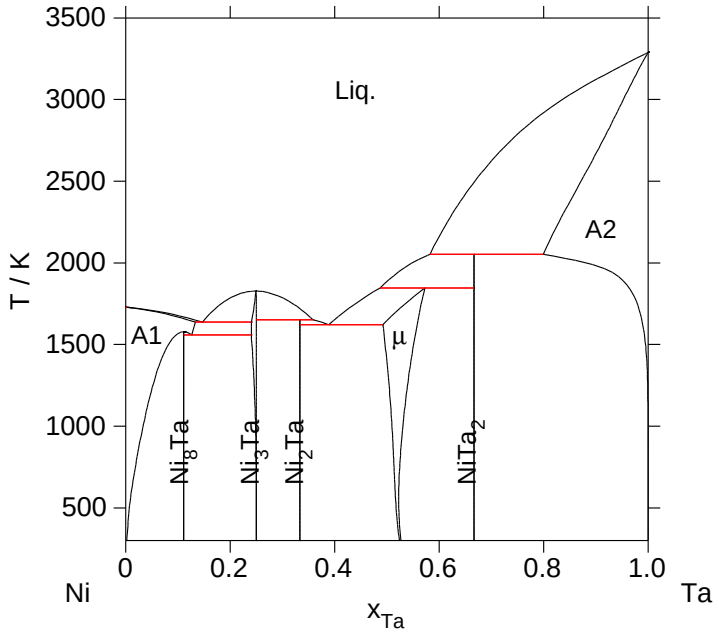
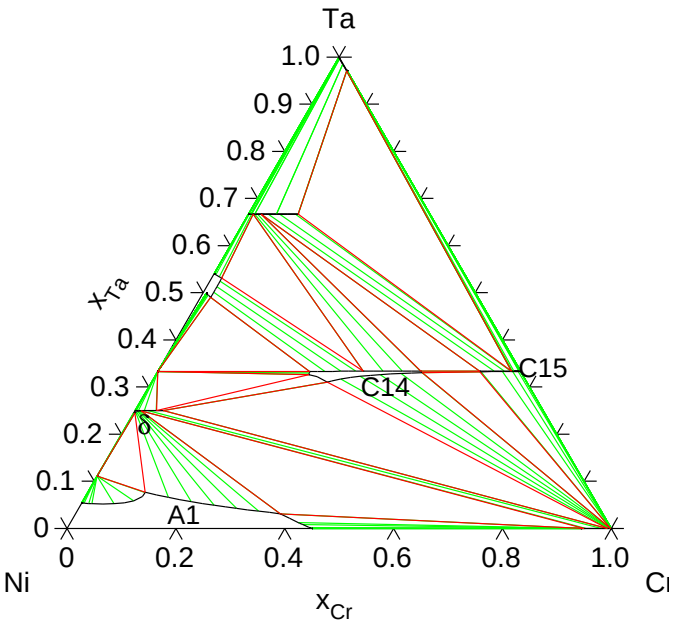
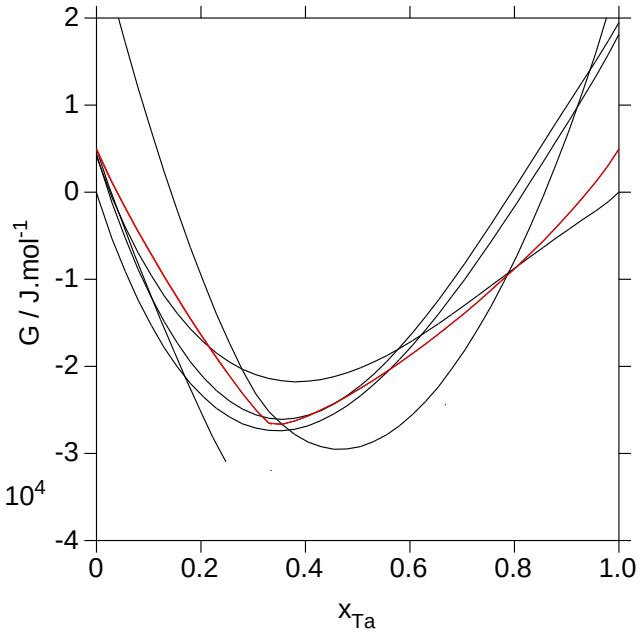




In order to describe the C14 stability in the ternary Cr-Ni-Ta, the binary metastable C14 phase in Ni-Ta has to be described. It has to be identical whatever system implying the Ni-Ta system. Care should be given to keep the phase metastable in the binary.

Assessment of metastable states



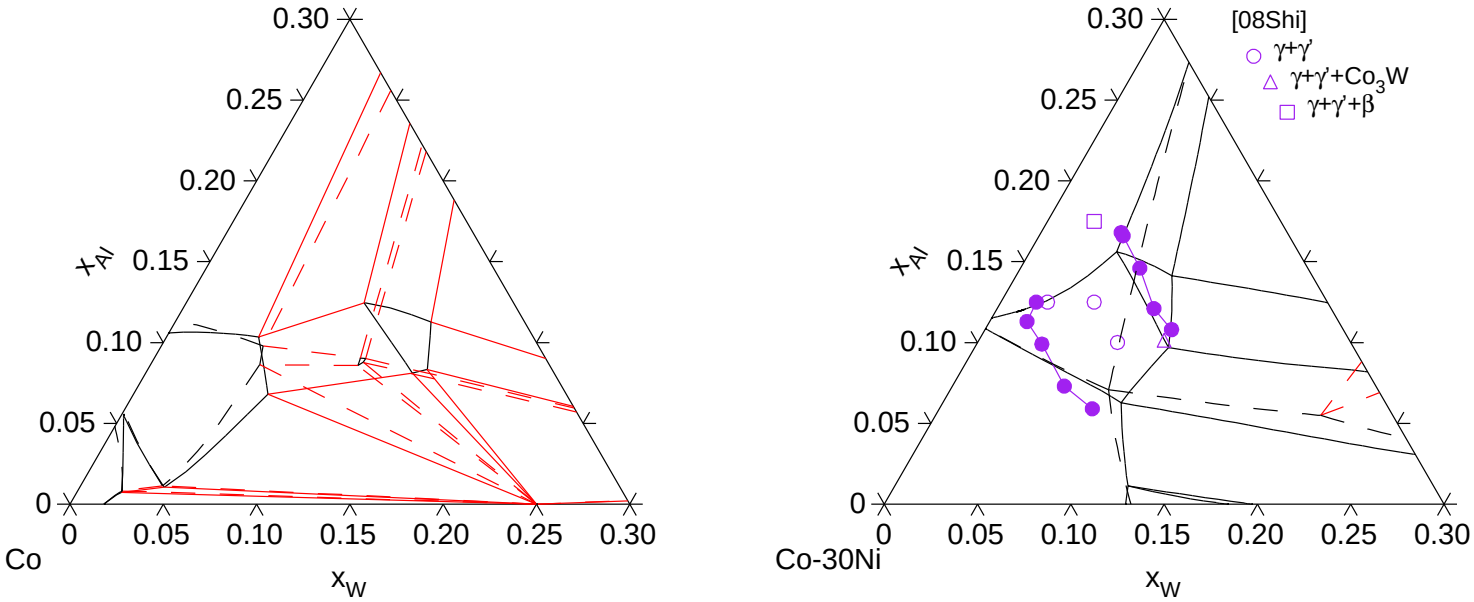


In order to describe the C14 stability in the ternary Cr-Ni-Ta, the binary metastable C14 phase in Ni-Ta has to be described. It has to be identical whatever system implying the Ni-Ta system. Care should be given to keep the phase metastable in the binary.

Always under improvement

The stability of the γ' phase in the ternary Al-Co-W was reported for the first time about 10 years ago. The experimental knowledge of the γ' phase extension from this area has rapidly improved as well as its description.

J. Bratberg *et al.* Superalloys 2012



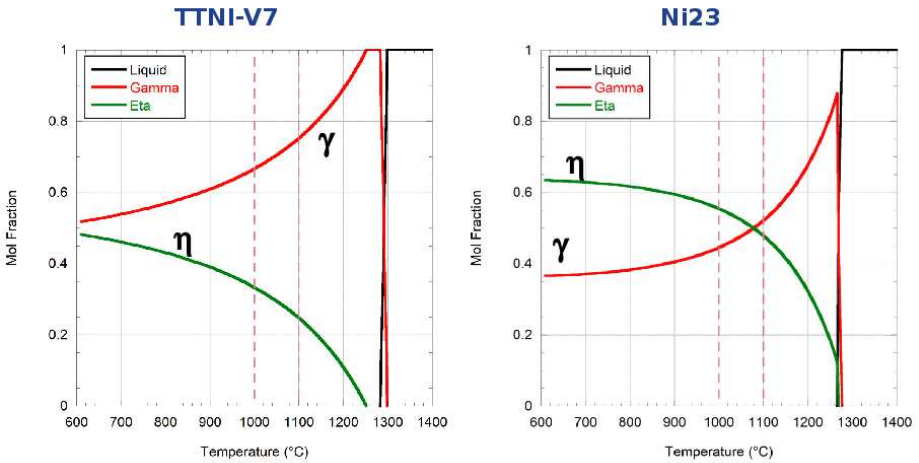
Full lines TCNI5 (2011), dashed lines TCNI4 (2008)

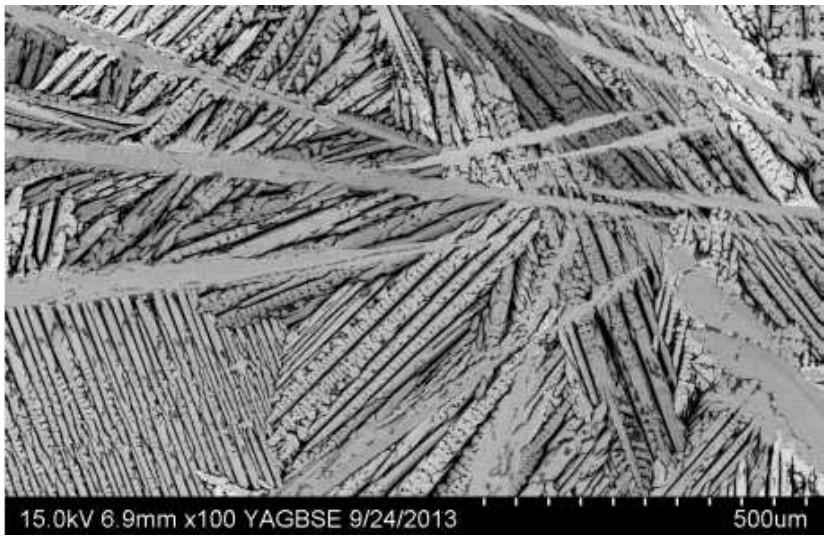
[08Shi] Shinagawa et al. *Mat. Tr.* **49** 1474 (2008)

Always under improvement

Ni-5Ta-12.9Ti (at.%)

GE property: Raghav Adharapurapu, Rich DiDomizio, Ian Spinelli





- TTNI-V7
  γ primary phase,
  η formed in solid state
- NI23 (TCNI5)
  γ primary phase,
  η from the liquid

- experimentally
  η primary phase

- as cast and equilibrated states experimental study will help a new assessment

To constitute multicomponent databases

- Good models are mandatory
- FP results help
- Experimental knowledge is key

Thanks

Presented during the TMS annual Meeting: Hume-Rothery Award Symposium: Multicomponent Alloy Metallurgy, the Bridge from Materials Science to Materials Engineering,
Orlando, FL, March 16-19, 2015
dedicated to W.J. Boettinger

The view 18 of the present version has been slightly amended since after a question formulated by Ursula Kattner during the lecture.