Project Area C: Modelling

11 Thermodynamic modelling of ductile and oxidation resistant Cr-Mo-Si alloys

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Objectives

- Some alloys within the Cr-Mo-Si system show encouraging experimental results on oxidation resistance and mechanical performance [1]: the development of these materials should be accelerated by thermodynamic modelling. Thermodynamic assessment of the system Cr-Mo-Si will be performed by the analytical description for the Gibbs free energy functions of present phases using CALPHAD.
- The data generated will allow (i) thermodynamic calculations using FactSage to narrow down the compositional areas of alloys and (ii) serve as input data for the phase-field simulations in project **P9**.

First results

The analytical Gibbs free energy descriptions of the phases in binary systems Mo-Si, Cr-Mo and Cr-Si are transformed into the FactSage software from the references [2], [3], and [4], respectively.

Mo-Si [2]

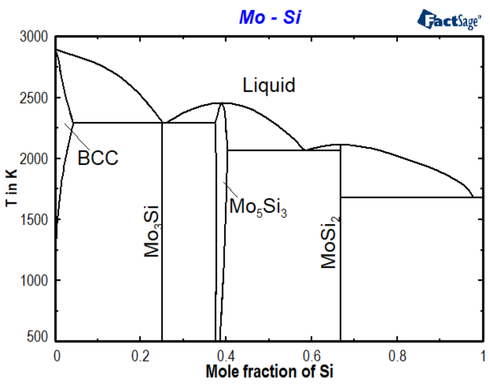
- Mo-Si consists of liquid, BCC, Mo_3Si, Mo_5Si_3, $MoSi_2$ and Si.
- Phase equilibria temperatures are well agreed with literature except for $MoSi_2 \rightarrow L$ (90 K difference).

Cr-Mo [3]

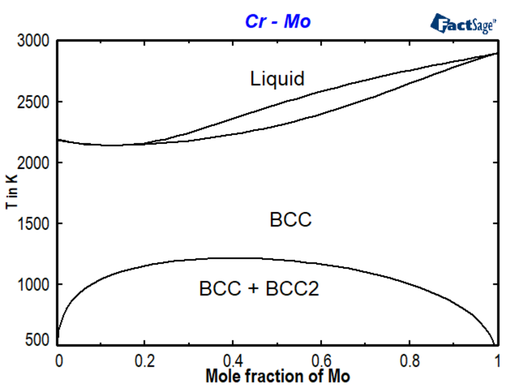
- Cr-Mo consists of liquid phase, and solid phase with miscibility gap (BCC1+BCC2).

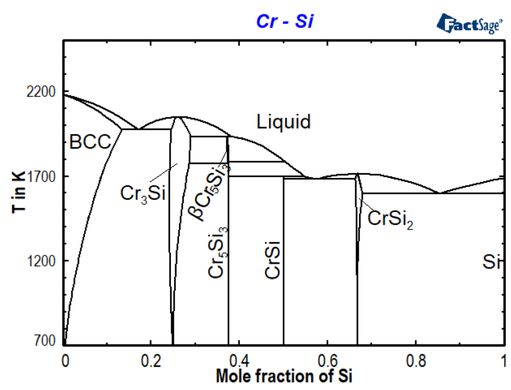
Cr-Si [4]

- Cr-Si consists of liquid, BCC, Cr_3Si, β-Cr_5Si_3, α-Cr_5Si_3, CrSi, $CrSi_2$ and Si phases.
- Phase equilibria temperatures are well fitted with literature.



Reaction	Calculated, K
L ⇔ Mo_3Si + Mo_5Si_3	2294.15
L ⇔ Si + $MoSi_2$	1680.56
L ⇔ Mo_5Si_3 + $MoSi_2$	2122.25
BCC + L ⇔ Mo_3Si	2294.94
Mo_5Si_3 ⇔ L	2448
$MoSi_2$ ⇔ L	2203





Reaction	Calculated, K
L ⇔ Cr_3Si + Cr	1972.37
L ⇔ Cr_3Si	2048.15
α-Cr_5Si_3 + L⇔ CrSi	1697.92
β-Cr_5Si_3 ⇔ α-Cr_5Si_3 + Cr_3Si	1774.21
L ⇔ CrSi + $CrSi_2$	1680.02
L ⇔ $CrSi_2$	1713.15
L + β-Cr_5Si_3 ⇔ α-Cr_5Si_3	1781.96
L ⇔ $CrSi_2$ + Si	1596.02

Work plan for P11.2

- Thermodynamic description of the ternary system Cr-Mo-Si.
- Experimental evaluation of the data by microstructural investigation of alloys in the ternary system starting with 70Cr-11.5Si-18.5Mo (at.%) as the reference.
- Microstructure and phase compositions will be characterized by XRD, electron microscopy and local chemical analyses such as EDX and WDX. Thermodynamics of phase transformation will be studied by thermal analysis and calorimetry.

Outlook for P11.3

The addition of O and a rare earth element, e.g., Hf to the Cr-Mo-Si database for the further alloy development.

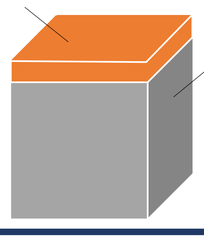
Associated Project:
(Dr. Kateryna Khanchych, KIT)

Refractory metal-based alloys with integrated coatings for applications in aviation and aerospace technology (funded by BMWK, funding code 20E2112B)

Objective: Development of novel high temperature materials within two systems (Mo-Si-B-V and Ta-Mo-Cr-Ti-Al) with integrated coatings.

Coating:
$MoSi_2$
RHEA Ta-Mo-Cr-Ti-Al
Pack cementation, magnetron sputtering

Advantages of the coated material:
- High melting point (bulk)
- Excellent heat and creep resistance (bulk)
- Good oxidation resistance (coating)
- Low density (bulk)



Substrate:
Mo-Si-B-V
RHEA Ta-Mo-Ti-(Cr, Al)
Powder metalurgy

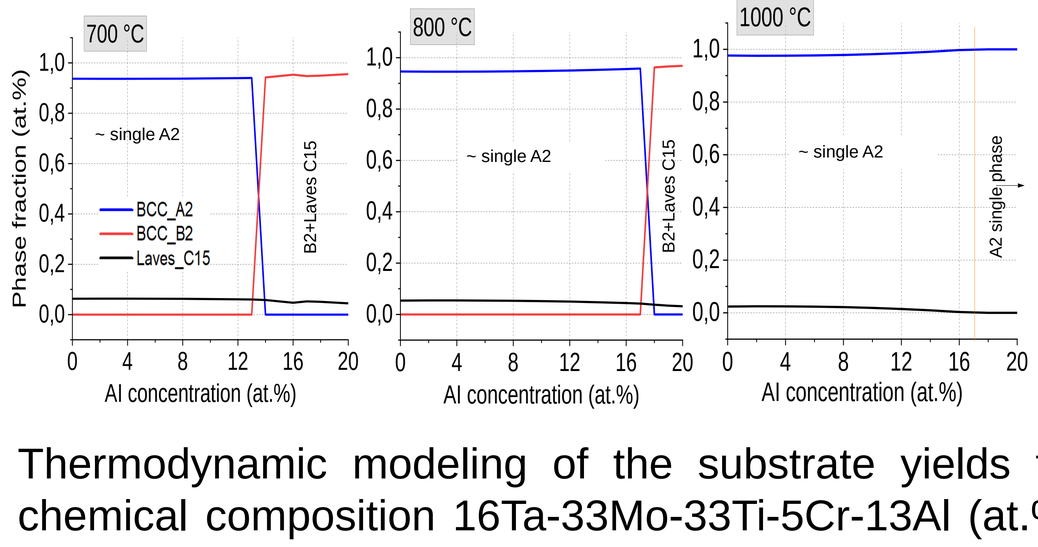
Projektträger DLR Luftfahrtforschung

Otto von Guericke Universität Magdeburg

KIT Karlsruher Institut für Technologie

Criteria to model the substrate: system Ta-Mo-Cr-Ti-Al

1. A2 phase fraction ≥ 94 % between 700°C and 1000°C
2. Cr and Al as high as possible, starting with 5 at.% Cr
3. Ta content as low as possible, Ti concentration as high as possible



Thermodynamic modeling of the substrate yields the chemical composition 16Ta-33Mo-33Ti-5Cr-13Al (at.%). Next steps: Manufacturing and experimental validation.

Interactions within GRK 2561

P5	Thermodynamic knowledge sharing of Cr-Mo-Si
P7	Meetings about thermodynamic calculations
P8	Experimental knowledge exchage about Cr-Mo-Si
P9	Interactions and thermodynamic database input for Cr-Mo-Si

References

[1] F. Hinrichs et.al., Corr. Sci. (2022), 207
[2] C. Guo et.al., Calphad (2012), 36
[3] K. Frisk et.al., Calphad (1988), 12
[4] H. Chen et.al., Calphad (2009), 33