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An example of thermodynamical calculations applied to the study of the high temperature behaviour of Co-base superalloys strengthened by tantalum carbides



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Cobalt-base superalloys are currently used as bulk materials for parts of aeronautic turbines. These latter support mechanical and thermal constraints. As the lifetime of these parts is limited, the aim of this work is to elaborate new alloys with higher solidus temperature and mechanical resistance. The best way to speed up development of new materials is thanks to thermodynamic simulations (Thermo-Calc), which will propose solutions to choose the microstructure and the alloy elaboration process.

Database constitution

The following tables summarize the binary and ternary systems added to SSOL SGTE solutions database to build our own database :

Co-C	Ni-C	Cr-C	Ta-C	Co-Ni	Co-Ni-Cr	Co-Cr-Ta	Co-Ta-C	Co-Ni-Ta	Co-Cr-C
ssol (SGTE)	ssol (SGTE)	ssol (SGTE)	(1)	ssol (SGTE)	ssol (SGTE)	not added	(5)	not added	ssol (SGTE)
Co-Ta	Ni-Ta	Cr-Ta	Co-Cr	Ni-Cr	Co-Ni-C	Ni-Cr-C	Ni-Cr-Ta	Ni-Ta-C	Cr-Ta-C
(2)	(3)	(4)	ssol (SGTE)	ssol (SGTE)	ssol (SGTE)	ssol (SGTE)	(6)	not added	not added

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Prediction of phases equilibrium versus temperature and composition: Influence of C content on the Alloy 1 **Co-base superalloy microstructure.** 1500

In the cobalt-base superalloys reinforced by TaC, the best mechanical properties are related with :

- a high solidus temperature

- the absence of chromium carbides

As a consequence, the optimum carbon content predicted by the phase diagram (on the right) is 0.38%w

The microstructures obtained (alloys 1 & 2) are in good agreement with the phase diagram heating and aged for 100 hrs at 1200°C calculation.

Alloys compositions						
wt %	Co	Ni	Cr	Та	С	
Alloy 1	bal	8.7	28.4	5.8	0.37	
Alloy 2	bal	8.7	28.4	5.8	0.80	
Alloy 3	bal	8.7	28.4	3	0.19	
Alloy 4	bal	8.7	28.4	4	0.25	
Alloy 5	bal	8.7	28.4	5	0.33	
Alloy 6	bal	8.7	28.4	7	0.44	

These alloys were synthesized by induction



Use of isothermal sections to select particularly high refractory materials



	Solidus	Experimental	ΔT
	temperature °C	(DTA) melting	°C
	(Thermo-Calc)	temperature°C	
Alloy 3	1290	1348	58
Alloy 4	1289	1336	47
Alloy 5	1288	1337	49
Alloy 1	1287	1338	51
Alloy 6	1286	1338	52

The comparison between the melting temperature predicted by Thermo-Calc with those determined by Differential Thermal Analysis shows a constant difference of about 50°C.

The absolute melting temperature can not be reached by Thermo-Calc calculations. Nevertheless, these results obtained thanks to this software allow the alloys classification according to their solidus temperature.

The solid domain predicted by Thermo-Calc is precise enough to elaborate alloys with the desired microstructure (TaC precipitated in the matrix).

Evaluation of local melting temperature : Case of the skin of Co base alloy during air oxidation at 1300°C Alloy 1 oxidized for 100 hrs at 1300°C



Alloy	compositio	n	versus	surface
distance	obtained	by	Electron	Probe
Microar	nalvsis.			

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	d (µm)	Co	Ni	Cr	Та	C*	
	0	bal	11.40	12.97	0	0	
	100	bal	11.20	17.33	0.69	0.13	
	200	bal	10.07	19.89	1.05	0.25	
	300	bal	9.65	23.77	5.80	0.37	
	400	bal	9 42	26 59	5.80	0.37	1

* : By hypothesis, carbon content decreases linearly from the bulk to the oxide scale

Prediction of an eventual solidus temperature diminution near the metaloxide interface due to a variation of the alloy composition.

Conclusions

In our research fields, thermodynamic simulations allow:

the prediction of the equilibrium phases

- to better select the chemical composition in order to obtained the desired phases (natures and quantities) - to prevent the risk of apparition of undesirable phases

(σ phase, TCP phases....)

the selection of highest refractory materials

- to select an alloy with the solidus temperature as far as possible of the working temperature.

the evaluation of local melting temperature

- to predict a possible minimizing of surface mechanical properties induced by the oxidation phenomena.