Application of Thermo-Calc and DICTRA in an Industrial Setting

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Thermo-Calc/DICTRA Users Meeting
Aachen
2011-09-08/09
Outline

- Introduction
- MCrAlY Coating Development
  - Background
  - Set-Up of DICTRA Model
  - Results of Calculations
  - Experimental Validation
- Summary
Areas of Application for Thermo-Calc and DICTRA

- Heat Treatment Optimisation
- Estimation of non Conformances and Failure Analysis
- Braze Alloys and Weld Fillers Development
- Base Material Characterisation
- Base Alloy Development
- Coating-Substrate Interaction

Thermo-Calc Version S with TTNi 7 Database
DICTRA 26 with MobNi1 Database

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MCrAlY Protective Coatings

Function:
- Corrosion and oxidation protection
- Al and Cr reservoir for formation of $\text{Al}_2\text{O}_3$ and $\text{Cr}_2\text{O}_3$ protective scales
- Bond coat function for TBC

Composition (example):
- Co - 31Ni - 27Cr - 7.5Al - 0.5Y - 0.5Si

Microstructure:
- Cr and Al trapped in second phases ($\beta$ (NiAl) or $\gamma’$ (Ni$_3$Al)) in $\gamma$ Ni-matrix

Application
- Thermal spraying (VPS or LPPS)
- Bonding heat treatment
Problem Statement

Currently used system (baseline):
- Ni - Co - Cr - Al - 1.5Re - Y

Problem
- Re price extremely high

Request
- Develop coating free of Re

Approach
- variation of Cr content
- slight increase of Al concentration

Base material PWA 1483 SX
- Ni - 9Co - 12.2Cr - 1.9Mo - 3.8W - 5Ta - 3.6Al - 4.1Ti
Phase Diagrams of MCrAlY Alloys

- coating composed of $\beta$- and $\gamma$-phase above 900 °C
- near eutectic systems
- simulation of substrate-coating interaction only with single phase systems so far
Results of Ageing Trials at 1100 °C

Baseline material
- Precipitate free zone
- High $\gamma'$-content directly on interface between $\gamma$-layer and $\gamma - \gamma'$-layer

Alloy 4 (high Cr)
- Almost no precipitate free layer in coating
- Large amount of base material transforms
- Kirkendall porosity in Alloy 4 already after short times (« 300 h)

Alloy 1 (low Cr)
- Similar behaviour to baseline
- No porosity
Set-Up

- single cell problem (9 (8) species)
- double geometric grid
- element distribution via "high step" function
- effective diffusion in dispersed system with $\gamma'$ and $\beta$:

$$D_{eff}^{upper} = \left(1 + \frac{3 - 3f_{\gamma}}{f_{\gamma} - \frac{10}{3}}\right)D_{\gamma}$$

Boundary Conditions
- $T = 1100 \, ^{\circ}C$, $t_{max} = 500 - 700 \, h$
- isothermal, i.e. heating and cooling processes are not taken into account

Phase Distribution

- **Alloy 1 and baseline behave similar**
  - precipitate free zone
  - pileup of $\gamma'$ at the interface
- **Alloy 4**
  - no precipitate free zone
  - moving interface
Tracking of Kirkendall Porosity

Alloy 1 (low Cr)  baseline  Alloy 4 (high Cr)

Change of the local vacancy content at a distinct position

\[ \Delta c_{V_a} = \frac{\partial (-J_{V_a})}{\partial z} \]

Content of vacancies at a distinct position **

\[ y_{V_a} = \int_0^t \frac{\partial (-J_{V_a})}{\partial z} \, dt \]

** Höglund and Ågren: Acta mater 49 (2001) 1311-1317
Experimental Validation (Composition Profiles)

- Al profile
- Cr profile
- Ti profile

Baseline

Alloy 4 (high Cr)
Experimental Validation (Microstructure)

SEM images vs. amount of phases

Baseline

Alloy 4 (high Cr)

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Summary

- Thermo-Calc helps identifying MCrAlY coating systems

- interdiffusion between MCrAlY and substrate can be handled
  - labyrinth factors for “diffusion none” phases
  - complex material systems (9 species)
  - TCP phases and minor elements not taken into account
  - qualitative prediction of Kirkendall porosity

- experimental validation
  - shape of composition profiles met
  - no general labyrinth factor applicable
  - distribution of phases qualitatively shown

- ROI: significant reduction of experiments ➔ faster time to market (>> 9:1)
Thank you for your attention!
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