Application of DICTRA in development of MCrAlX coatings

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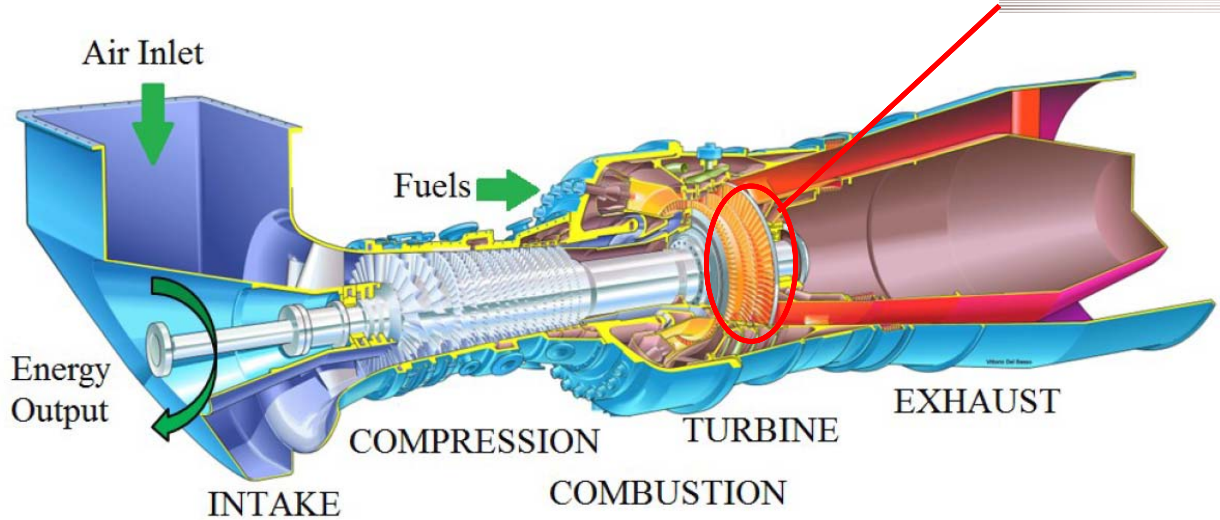
KME – konsortium materialteknik för termiska energiprocesser

OUTLINE

- Background
- Oxidation-Interdiffusion Modelling
  - Model description
  - Coating design
  - β-layer formation
- Conclusions

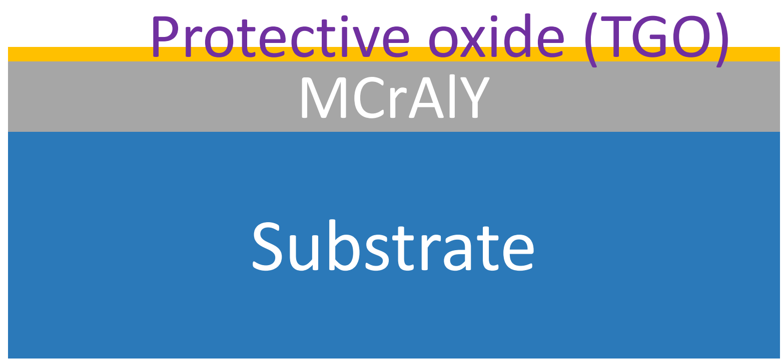
High temperature protection

- Oxidation and corrosion protection:
  e.g. MCrAlY, diffusion coatings
- Temperature reduction: TBC systems



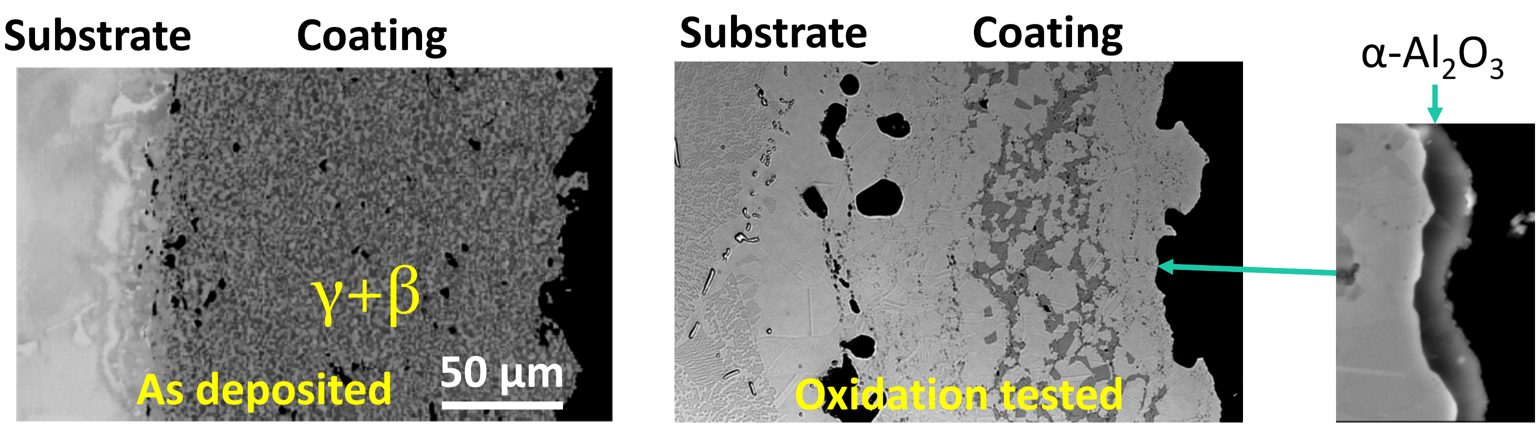
MCrAlY coatings

- Ni and/or Co base alloy with protective scale formers Cr and Al as well as minor additions, e.g. Y, Si, Ru.
- Oxidation resistance relies on a dense, continuous scale of Al-oxide (α-alumina) formed on the coating surface
- >3.5% Al is required to maintain a continuous α-alumina layer in Cr-containing alloys

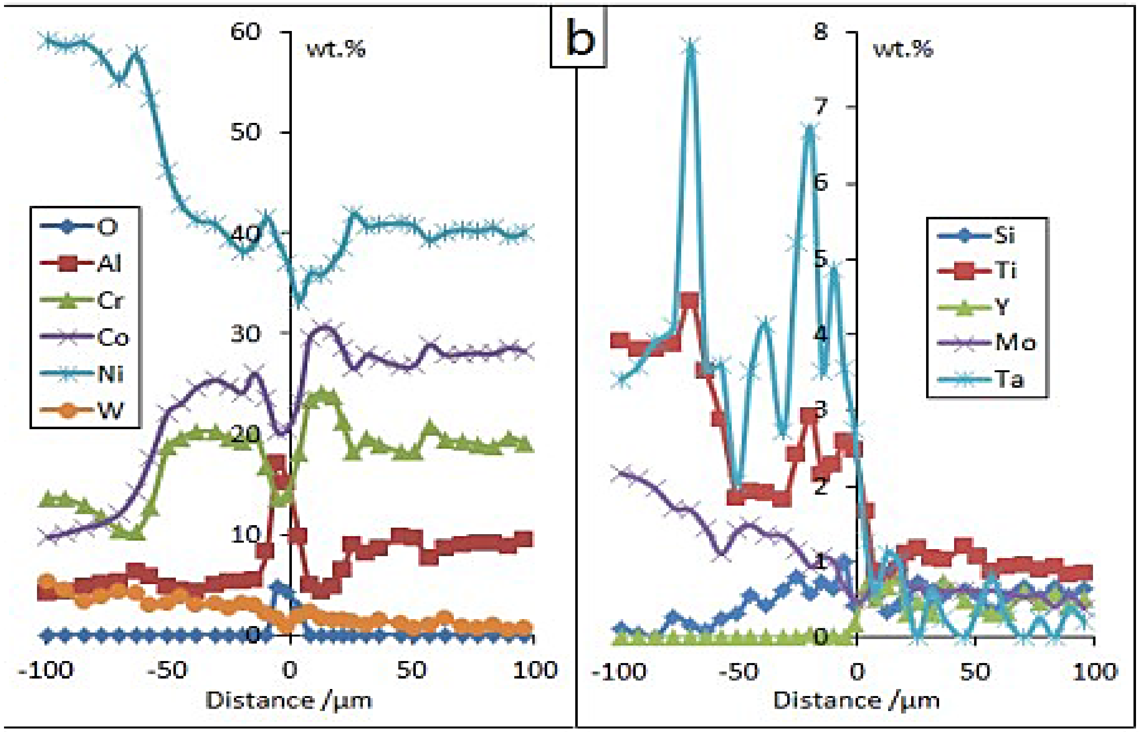


The oxidation life

- Chemical composition changes (Al-depletion) due to
  - ➢ Continued surface oxidation
  - ➢ Interdiffusion between the substrate and coating
- The oxidation life depends on resistance against Al-depletion (β-depletion)



- **Chemical composition profile** of Ni-15Cr-28Co-11Al-0.4Y-0.25Si on IN 792 after oxidation for 100 hrs @1100 °C



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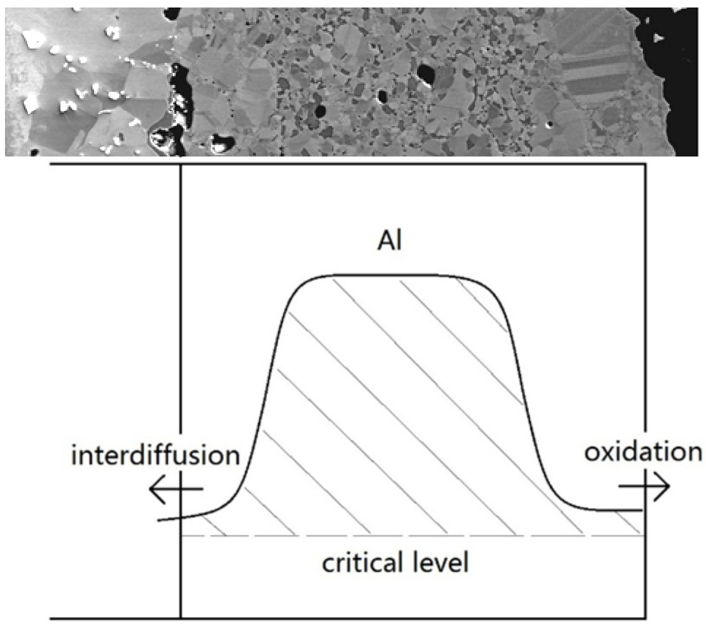
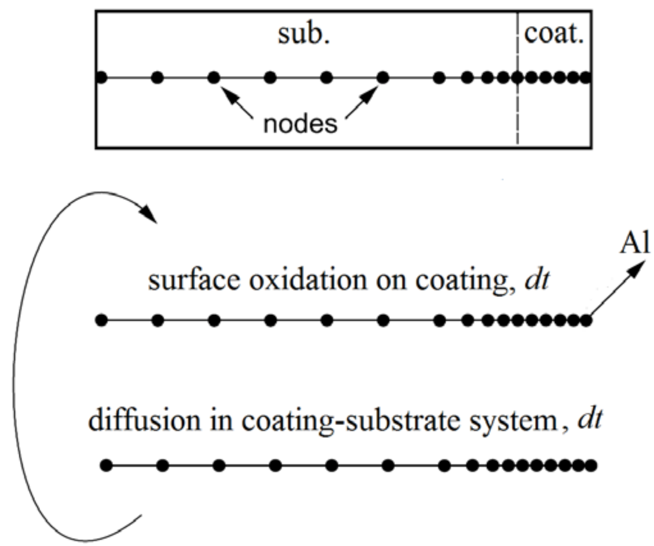
The oxidation-diffusion model

- Substrate-coating couple in 1D
- Each node presents a location in the couple with composition of the material at the point



Al consumption in coating



Oxidation and diffusion simulation

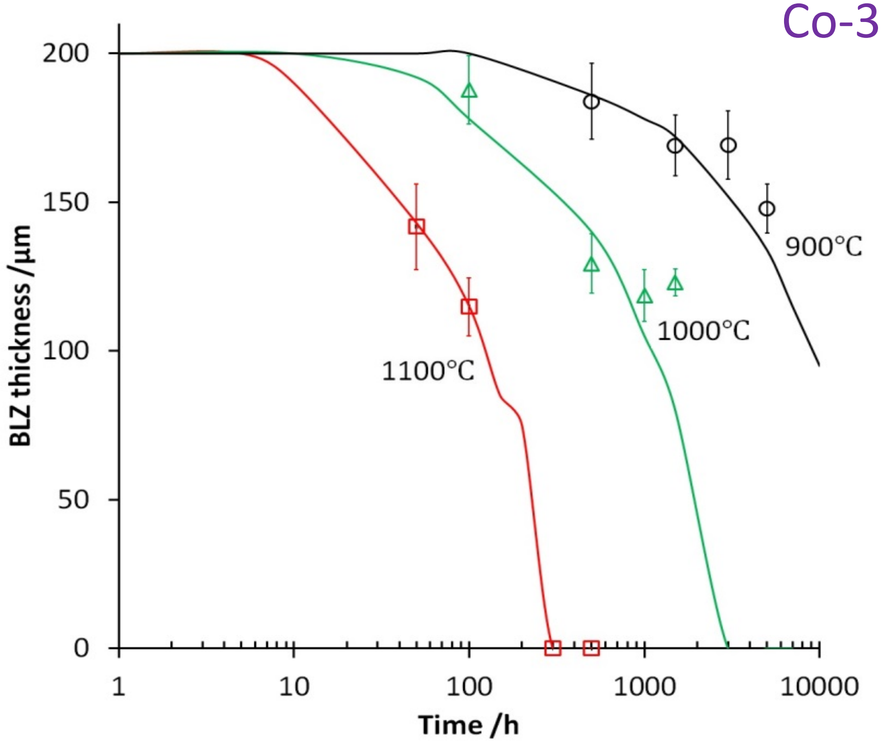
- DICTRA and databases from Thermo-Calc
  - Phases considered typically include γ, β, α, γ'
- Surface oxidation induced Al-depletion, derived from TGO thickness, h

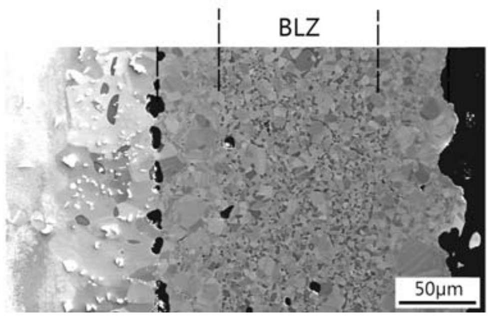
$$h = h_0 + (kt)^{1/n}$$

- Diffusion
  - ✓ Upper bound diffusion: $D^{eff} = \sum f^i D^i$
  - ✓ Lower bound diffusion: $D^{eff} = D^i + \frac{f^i}{\frac{1}{D^j - D^i} + \frac{f^j}{3D^i}}$

Simulated β-depletion

Co-30Ni-28Cr-7.5Al-X on IN 792



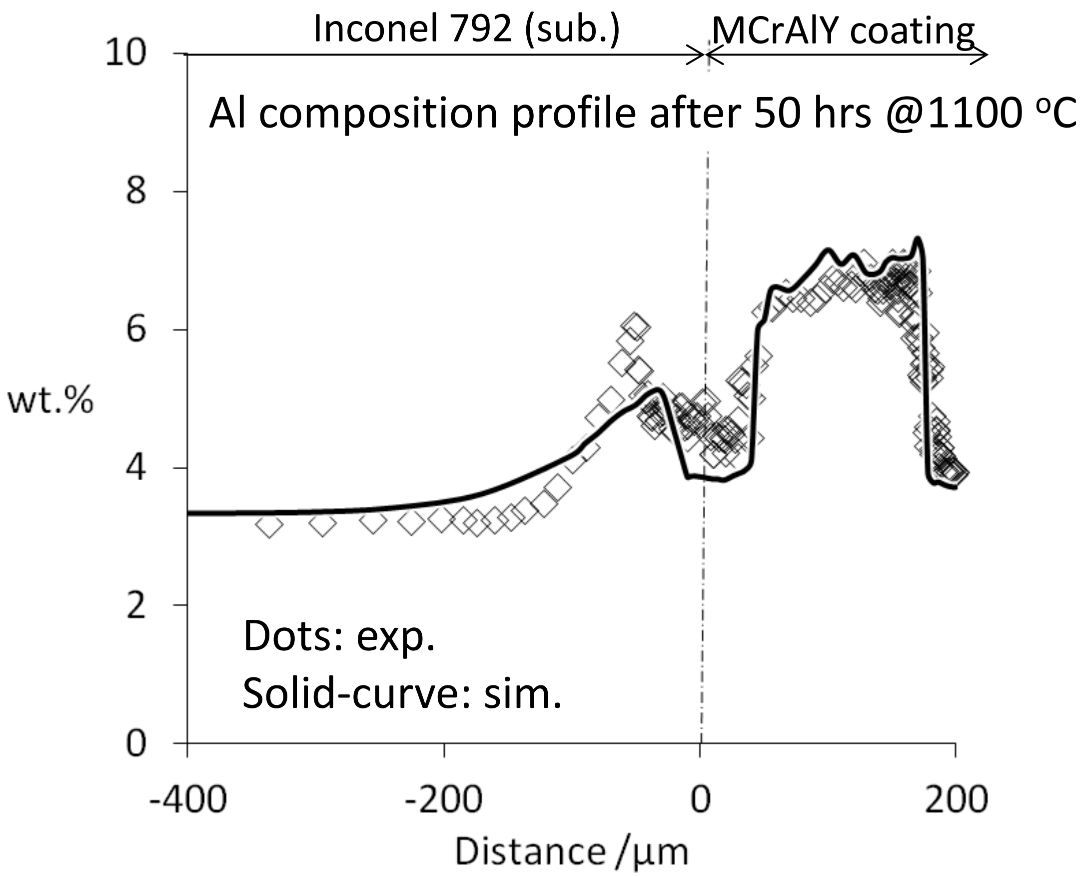


BLZ: β left zone

- Good agreement with observed microstructural change

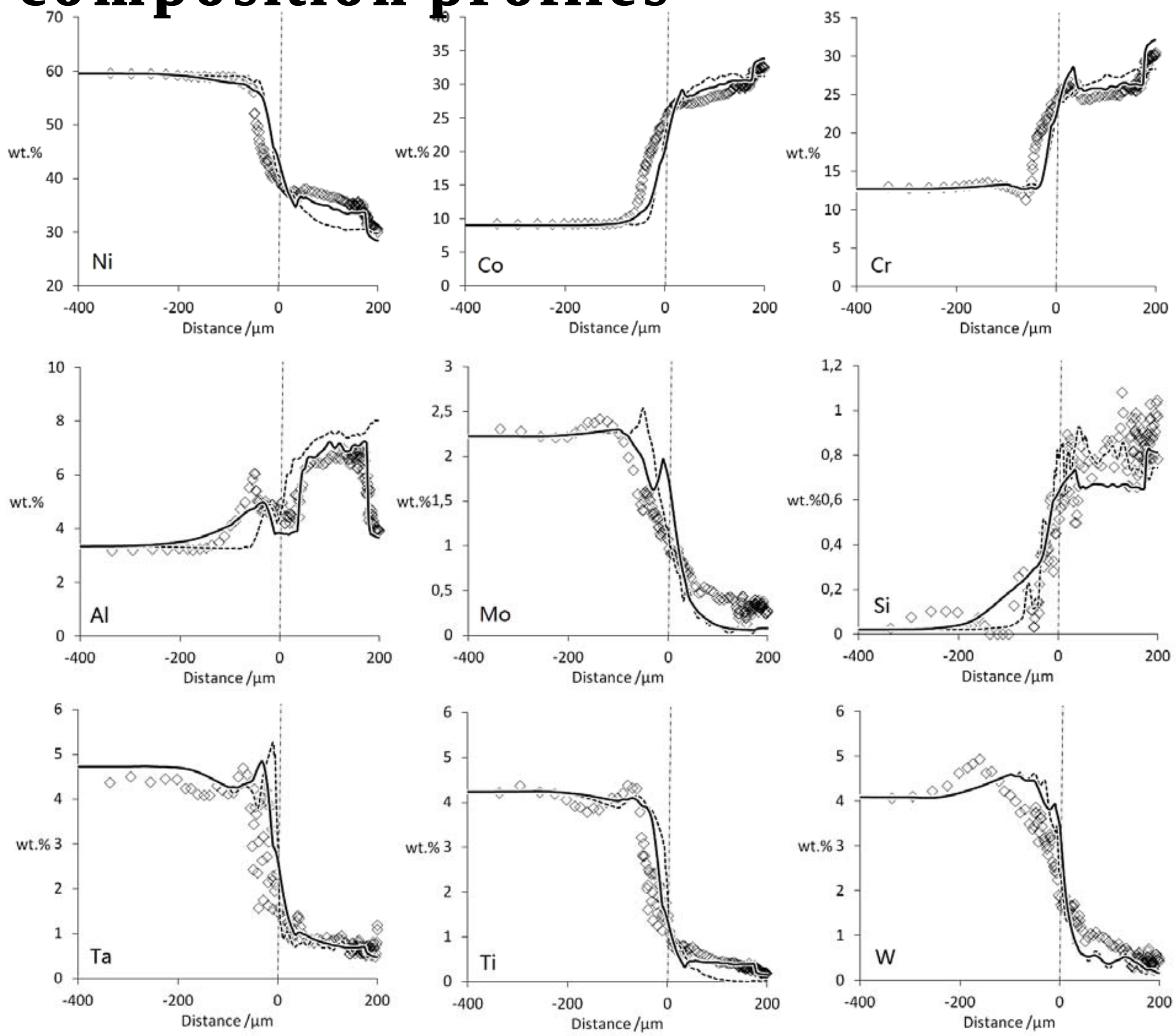
Kang et al. Surface & Coatings Technology 232 (2013) 204–215

Simulated chemical composition profiles



- Changes in chemical composition profiles were captured

Other composition profiles



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Simulation set-up

- Varied composition in coating: Cr, Co, and Al
- Varied composition in substrate: Al
- Surface oxidation, derived from TGO thickness

$$h = (kt)^{1/2} \text{ where } k = k_0 e^{-\frac{Q}{RT}}$$

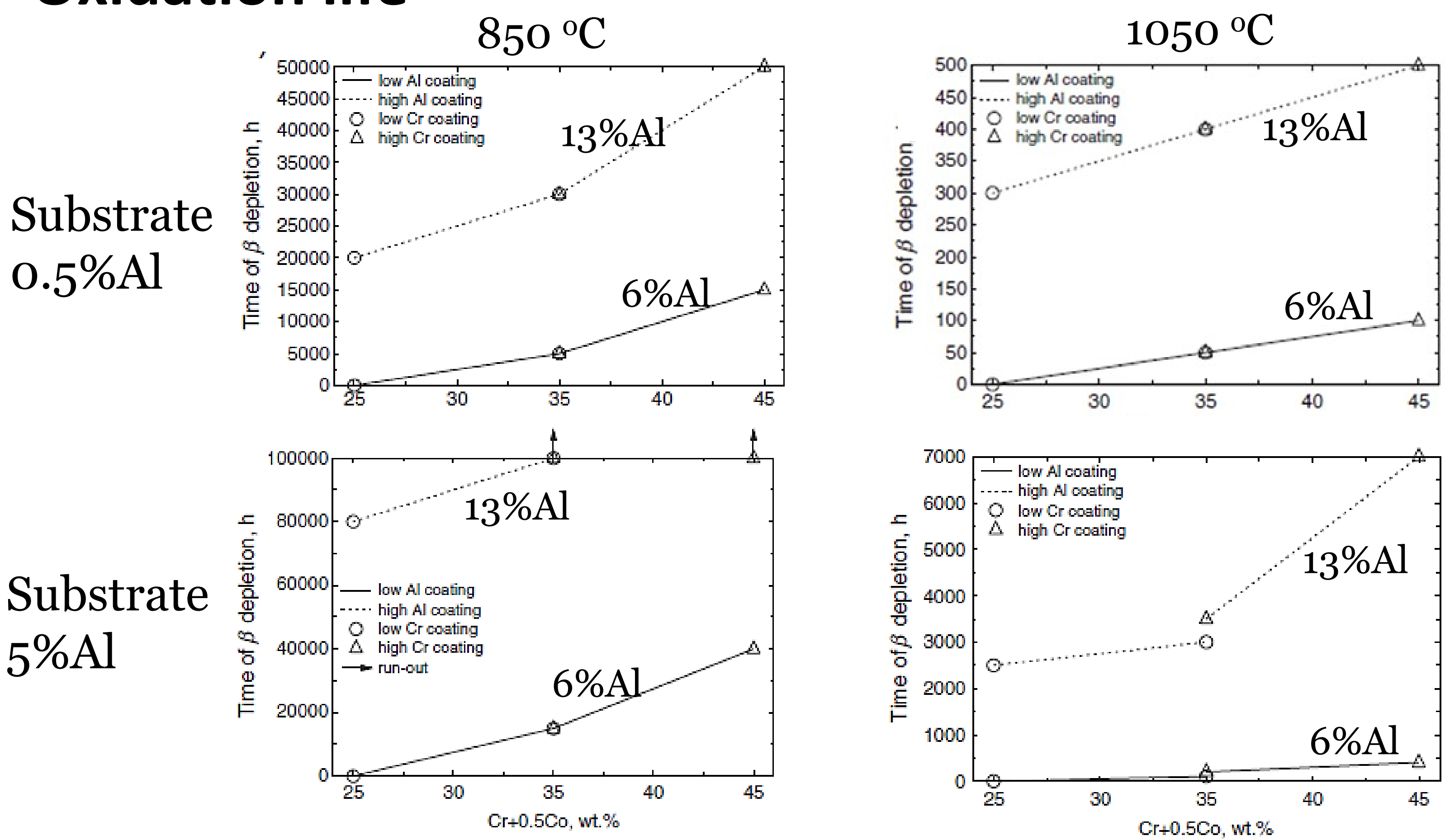
$$k_0 = 3.20 \cdot 10^4 \mu m^2/h; Q = 1.45 \cdot 10^5 \mathrm{J/mol}$$

- Oxidation Life Criterion
  - ➢ Time to complete β depletion
- Cr-equivalent

$$Cr_e = Cr + 0.5Co$$

Ericsson et al. Surface & Coatings Technology 253 (2014) 27–37

Oxidation life



- A stronger effect of increasing coating's Al on high Al substrate: 3 to 8 times for 0.5% Al substrate against 3 to 30 times for 5% Al substrate
- The influence of substrate Al is larger at higher oxidation temperature.

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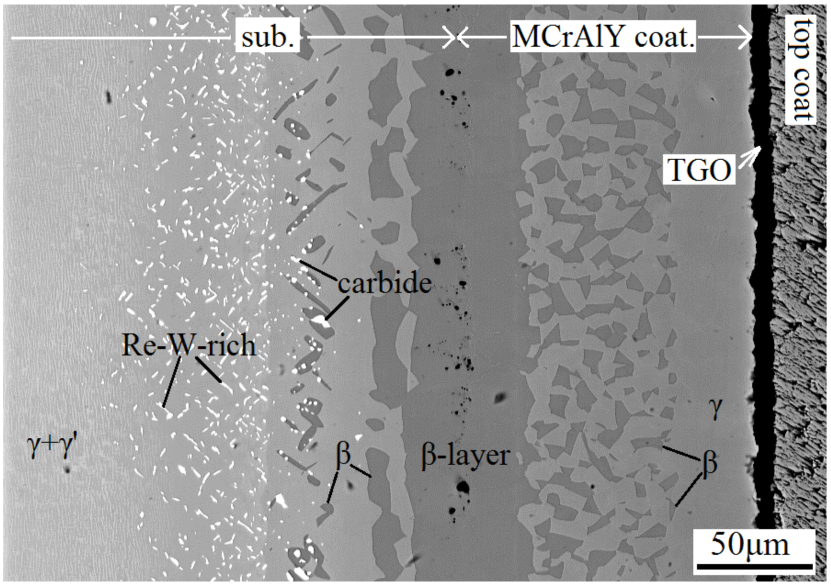
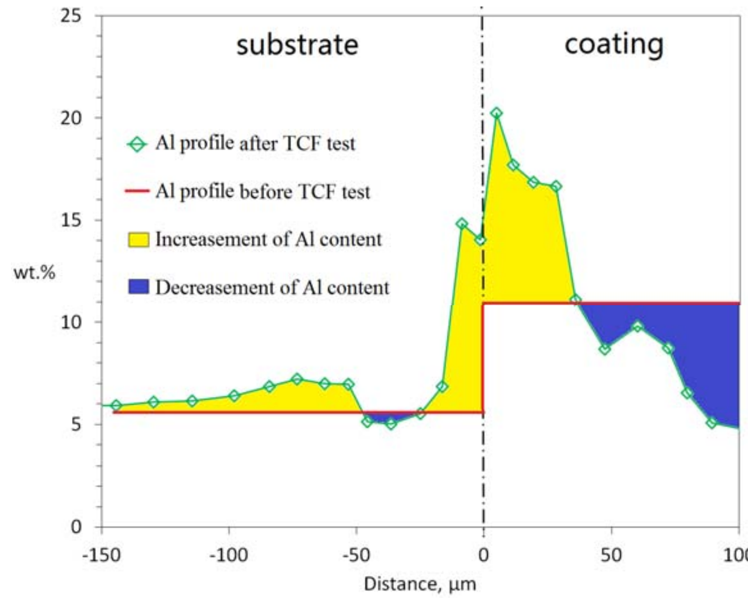
A continuous β-layer formed after TCF test

100-1100 °C for ~300 cycles



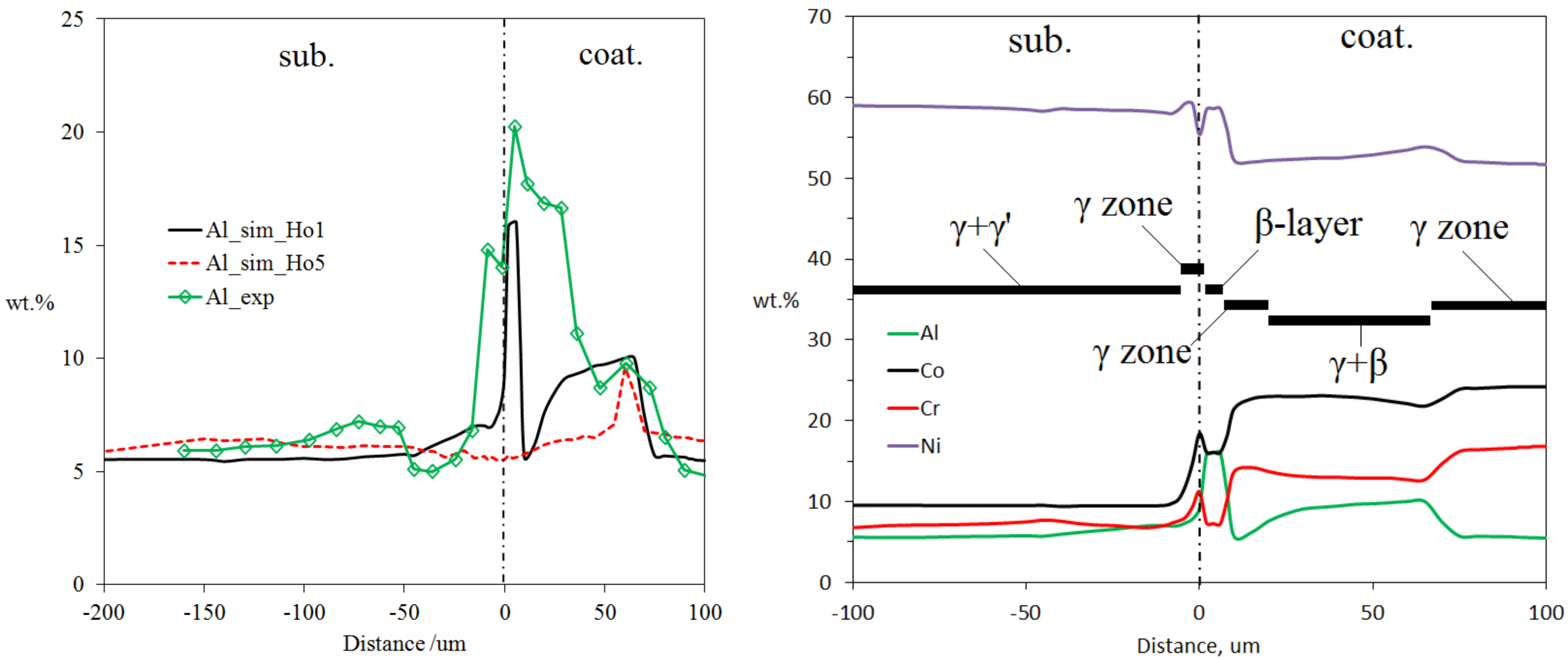


- The β-layer corresponds to Al accumulation at coating-substrate interface

	Ni	Co	Cr	Al	Y	Si	Ta	Ti	Mo	W	Re
Coat-1	50.3	22.2	14.7	11.4	0.1	0.3	1.0	-	-	-	-
CMSX-4	59.3	9.6	6.3	5.5	-	-	7.0	1.0	0.6	6.6	4.0

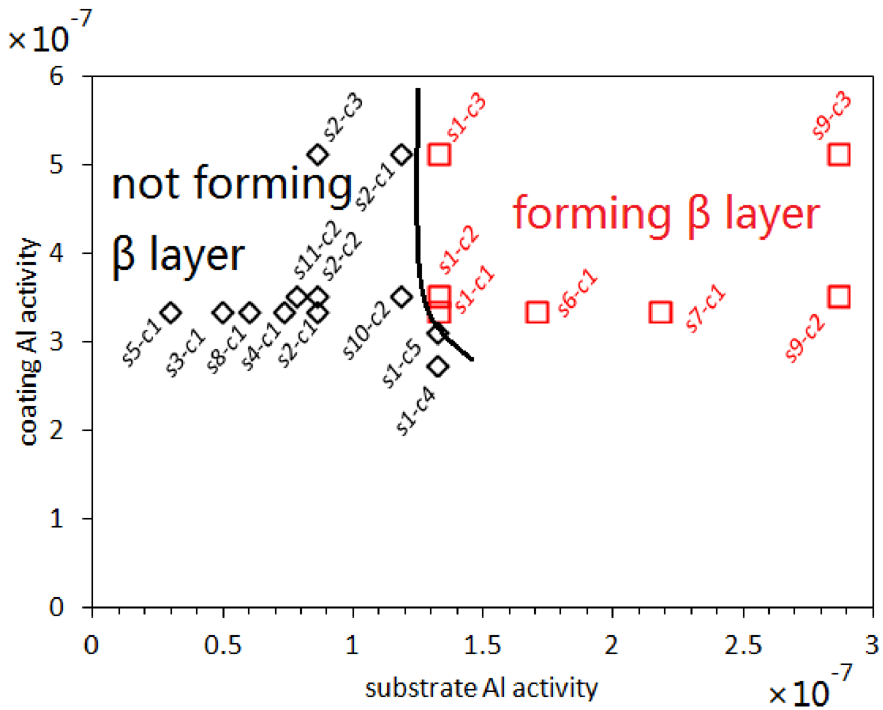
Kang et al. Journal of Thermal Spray Technology, Volume 25(1-2), 2016, 244-251

Modelling resoluts



- Simulation using the lower bound diffusion module predicts the formation of the β-layer.
- The characteristic layered microstructure were also predicted, except for the extra γ-zone between the β and γ+β zones.

Composition for the formation of β-layer



<u>c1 to c5</u>
MCrAlY coatings

<u>s1 to s11</u>
Superalloy substrates

- Critical Al-activity in the coating and substrate
- Substrate of high Al activity has a low sinking effect on Al
- Cr, Ta, Mo and Re can increase the Al-activity

Conclusions

- Interdiffusion plays an important role in the oxidation behavior of MCrAlY-superalloy systems.
- The effect of interdiffusion on oxidation life is dependent on temperature and composition of the coating and substrate.
- The simulations indicate the potential and possibility of enhancing oxidation resistance of MCrAlY-superalloy systems by matching coatings to substrate alloys.
- DICTRA is a powerful computational tool in metallic coating development ad life modelling.

Thanks you for your attention!

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