Design of Diffusion Coatings Developed via Pack Cementation

A. Naji, M.C. Galetz, M. Schütze
e-mail: naji@dechema.de

Funded by: BMWi via AiF
Period: 01.03.2012 - 28.02.2015

Gefördert durch: Bundesministerium für Wirtschaft und Energie aufgrund eines Beschlusses des Deutschen Bundestages

Concept and Goal of the Coating Design

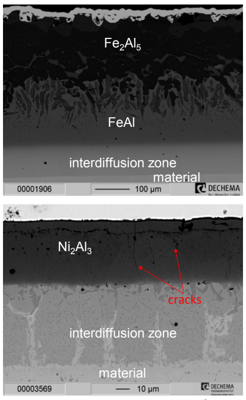

Figure 1: Cross sections of an Al coated austenitic steel and Ni-base alloy with brittle phases and cracks.

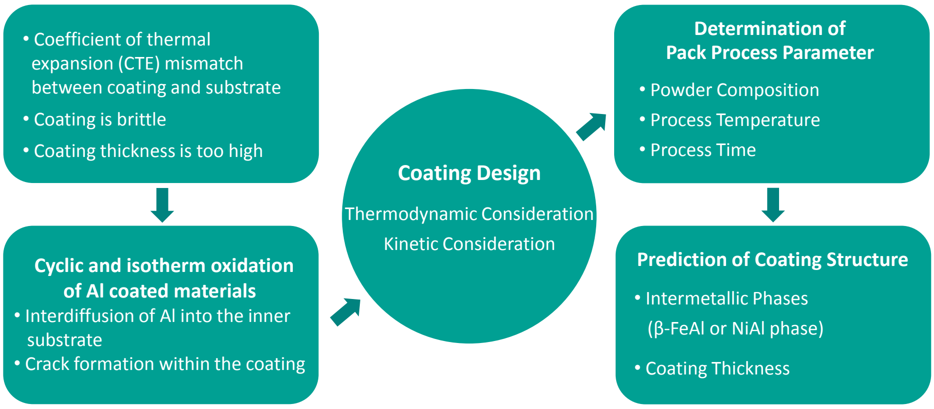

Figure 2: Illustration of the coating design procedure.

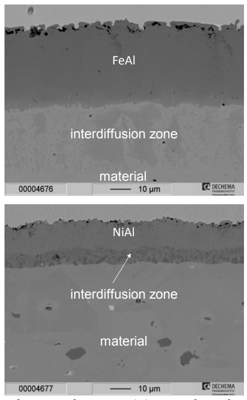

Figure 3: Cross sections of an Al coated austenitic steel and Ni-base alloy with the desired β-phases without cracks.

Approach of the Coating Design

Thermodynamic Consideration

Pack Cementation Process

- Gaseous diffusion step (Al chlorides diffuse from powder pack to the substrate surface)
- Solid state diffusion step (Al chlorides dissociate on the substrate surface and Al diffuses into the substrate)
- Solid state diffusion is assumed to be the rate limiting step

Step 1:
Calculation of the Al activity within the intermetallic phase, that can occur due to the coating process (β-FeAl, β-NiAl, Fe_2Al_5, Ni_2Al_3).

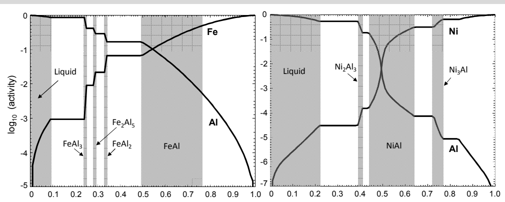

Figure 4: Via FactSage calculated Al, Fe and Ni activities within the Fe-Al and Ni-Al systems at 1000°C.

Step 2:
Calculation of the Al activity within the pack in dependence of the process temperature and the pack powder composition (diffusion element, activator NH_4Cl and filler Al_2O_3.

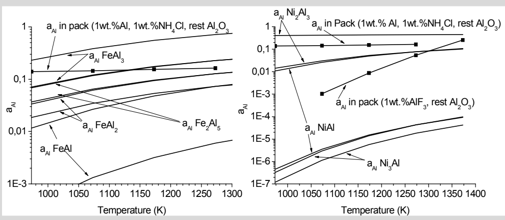

Figure 5: Comparison of the Al activity within the Ni-Al system and the Al activity within the pack.

Kinetic Consideration

- Kinetic considerations are based on Fick's first law
- Linearization of the concentration gradient between the pack/coating and coating/substrate interfaces (Figure 6) leads to an analytical, instead of a numerical solution of the differential equation.

Fick's first law

$$j = -D \frac{\partial a}{\partial x}$$

resulting coating thickness

$$x^2 = 2\frac{D}{q}\Delta a\, t$$

x: resulting coating thickness
Δx: distance
D: diffusion coefficient of Al in the intermetallic phase
q: constant
Δa: Al activity difference between the pack and the substrate
t: process time.

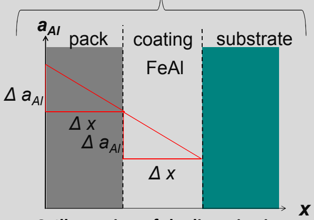

Figure 6: Illustration of the linearization of the Al activity differences.

Step 1: coating of the material at three different process temperatures

Step 2: determination of the diffusion coefficient *D* of Al in β-FeAl or β-NiAl via Matano analysis at these temperatures

Step 3: determination of the pre-factor of D_0 and the activation energy E_A for Al diffusion in the intermetallic phase by plotting $lnD(T)$ vs. 1/T

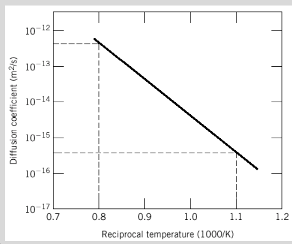

Figure 7: Plotting of the diffusion coefficient vs. Temperature.

Application of the coating design model

Development of a β-FeAl coating on a material/diffusion element couple

1. Thermodynamic calculation of the appropriate pack powder mixture and process temperature in order to achieve a β-FeAl coating.
2. Three test coating procedures at different process temperatures
3. Determination of the diffusion coefficient *D* of Al in β-FeAl via Matano analysis
4. Determination of D_0 and the activation energy E_A for Al diffusion in β-FeAl by plotting $lnD(T)$ vs. 1/T
5. Prediction of the coating properties for all other process parameters for every alloy and coating

Table 1: Comparison of predicted and measured coating thicknesses.

		AISI 321		AISI 314		Alloy 800	
pack composition	*T*	predicted coating thickness	measured coating thickness	predicted coating thickness	measured coating thickness	predicted coating thickness	measured coating thickness
1wt.% Al,	800°C	12 µm	11 µm	9 µm	8.5 µm	3.9 µm	3.5 µm
1wt.% NH_4Cl,	900°C	25.3 µm	24 µm	23µm	22 µm	19.9 µm	18.5 µm
98wt.% Al_2O_3	1000°C	50 µm	50 µm	51 µm	51 µm	54 µm	54 µm

Project Partners

- O. Pasdag, Zentrum für Brennstoffzellen Technik GmbH, Duisburg
- A. Lüderitz, Institut für Fügetechnik und Werkstoffprüfung GmbH, Jena

Acknowledgement

This work is financially supported by the German Ministry of Economics and Technology (BMWi) via AiF under IGF-contract no. 16881 BG, which is gratefully acknowledged.