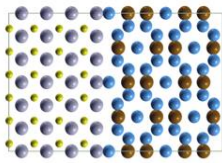
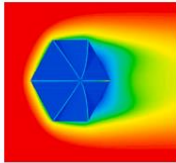




<p>IC-MPPE / Integrated Computational Materials Process and Product Engineering</p> <p>Programme: COMET – Competence Centers for Excellent Technologies</p> <p>Programme line: COMET-Centre (K2)</p> <p>Type of project: Multi-firm project</p> <p>Project: Model based smart-planning of processes across the hot-dip galvanizing process chain (GalvaSMART), 2017-2021</p>	<p>Atomic scale DFT modelling</p> 	<p>material growth model</p> 	<p>CFD process model</p> 
	<p>nm μm mm m Length scale</p> 		

INTEGRATED MATERIAL AND PROCESS SIMULATION OF ZINC BATH PHENOMENA IN HOT-DIP GALVANIZING

MULTI-SCALE MATERIAL AND PROCESS MODELLING OF DROSS FORMATION IN THE ZINC BATH AND ON THE BATH EQUIPMENT

Corrosion causes annual losses of up to approx. 3.4% of the global gross domestic product (GDP). The application of a suitable corrosion protection reduces costs and saves the environment. Many products are therefore protected against corrosion. For example, steel strips are coated with zinc-based corrosion protection layers to protect the products made from them, e.g. deep-drawn car body parts.

The continuous coating of steel strips in hot-dip galvanizing zinc baths is the main technology for corrosion protection of steel strips. Although widely used and long established, the hot-dip galvanizing process is confronted with new challenges regarding the coating quality and appearance. Novel coating alloys lead to unwanted chemical reactions in the

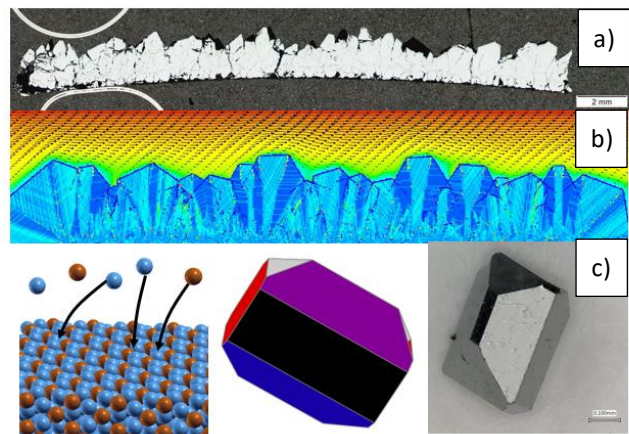


Fig.1: Comparison between real and virtual world: (a) real dross particles grown on a roll, (b) simulation of dross particles growing on a roll, (c) atomistic modelling of dross crystals to predict preferred habitus planes and comparison with a real dross particle grown in the melt.

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liquid zinc bath and on the bath equipment in the form of intermetallic dross particles, as shown in Fig.1. These particles cause surface defects of the coating on the steel strip and costly maintenance time in the production line.

In order to understand these phenomena and develop suitable solutions for the industry partners, multi-scale material and process models of the dross formation were designed. The main part for the practical analysis is the macroscale thermo-chemical fluid flow simulation which contains a virtual model of the zinc bath in the hot-dip galvanizing process. Operational process parameters are translated in this macroscale model to flow, temperature and concentration fields within the zinc bath. This information is coupled with developed thermo-dynamic and reaction-kinetic models to illustrate the local conditions in the zinc bath to the operators (see Fig.2).

The macroscale process model is linked to a microscale crystal growth model, which is able to describe the mass transfer between the liquid zinc and the crystal surface and to calculate the faceted growth of the dross particles. In order to acquire the model parameters atomic scale Density Functional Theory (DFT) modelling was conducted to predict the surface energies and the dross particle shape (see Fig.1).

Impact and effects

The results of the multi-scale material and process modelling will enable the industrial partners to better understand the hot dip galvanizing process and to derive optimized process parameters in order to reduce maintenance times and improve coating quality. High quality steel sheets can be sold at a price range up to 25% higher than steel sheets with standard surface quality. Current estimates show a potential added value to the industry due to improved coating quality of well over ~100 million dollars worldwide.

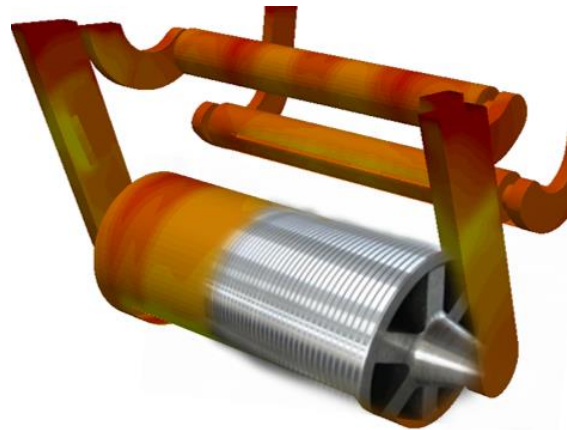


Fig.1: Image assembly from real and simulation images of the bath equipment: Dross formation rate on the bath equipment (sink roll) computed with the process model based on real operating conditions. Red colour indicates higher and yellow colour lower growth rates.

Project coordination (Story)

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