The challenge of service life prediction related corrosion modelling

Daniel Höche [1], Eduardo Trindade [1], Mikhail L. Zheludkevich [1], Philippe Maincon [2], Ole Swang [3], Kamyab Zandi [4], Nils C. Bösch [5], Andreas Mittelbach [5], Theo Hack [6]

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13th April 2015 / Barcelona

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Complexity of modelling for service life

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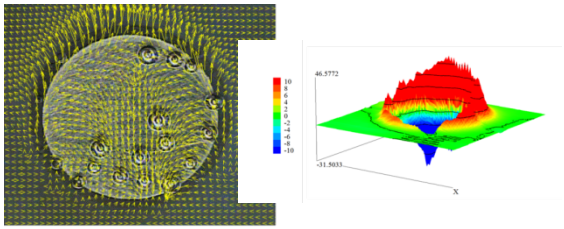
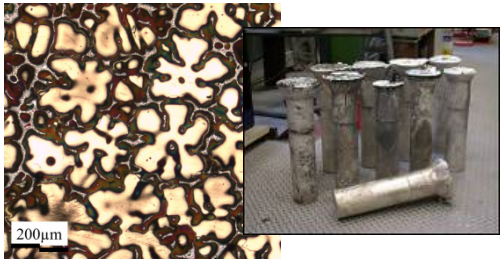
Service-Life Design (SLD)

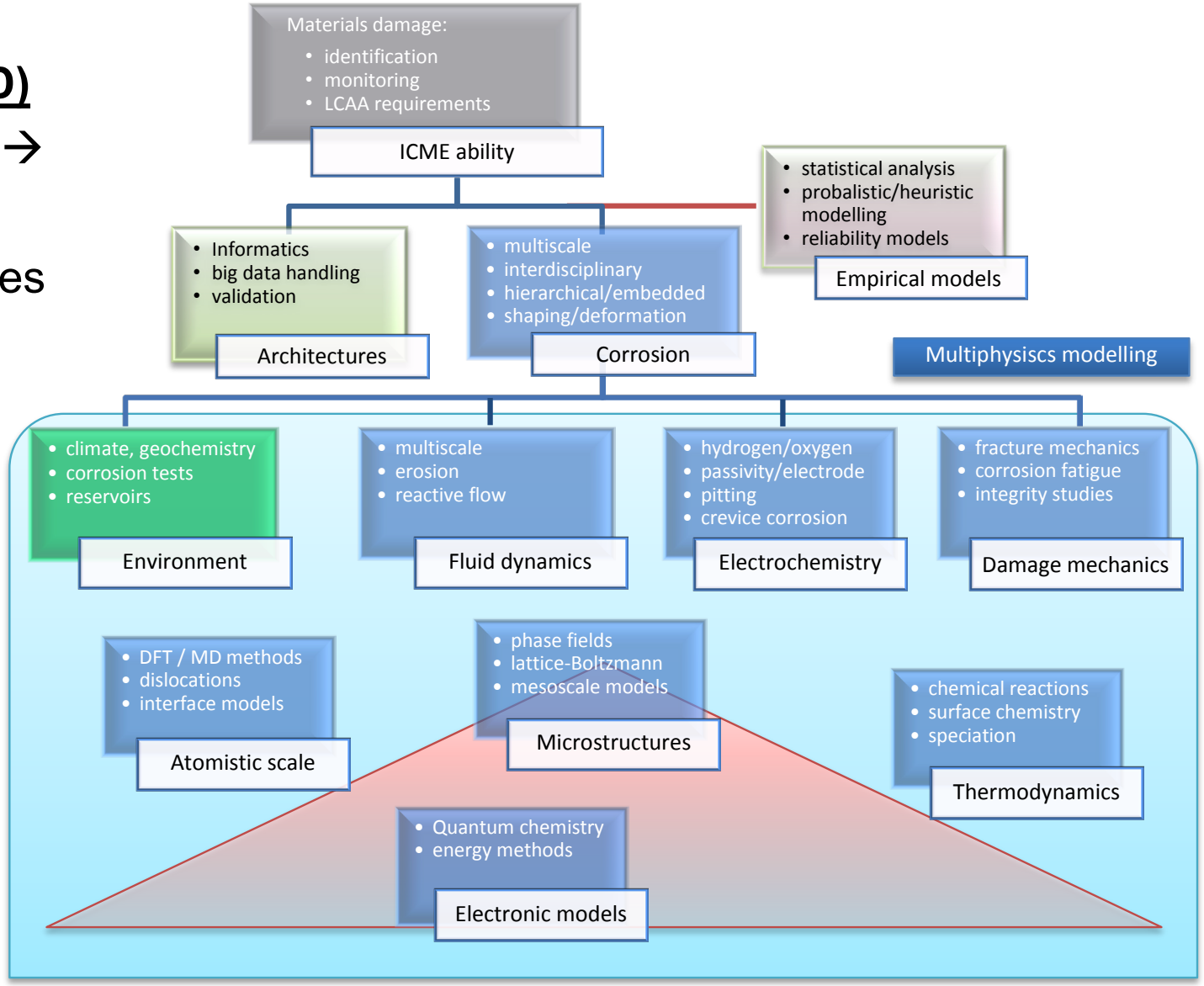
during digital Engineering → linking and coupling of materials entities and scales

Target: Processing





model input



D. Zander, D. **Höche**, J. Deconinck, T. Hack, 2015. Corrosion and its context to Service-Life, Chapter in *Handbook of Software Solutions for ICME* , August 2016.

An example – Pitting / liquid film (with flow)

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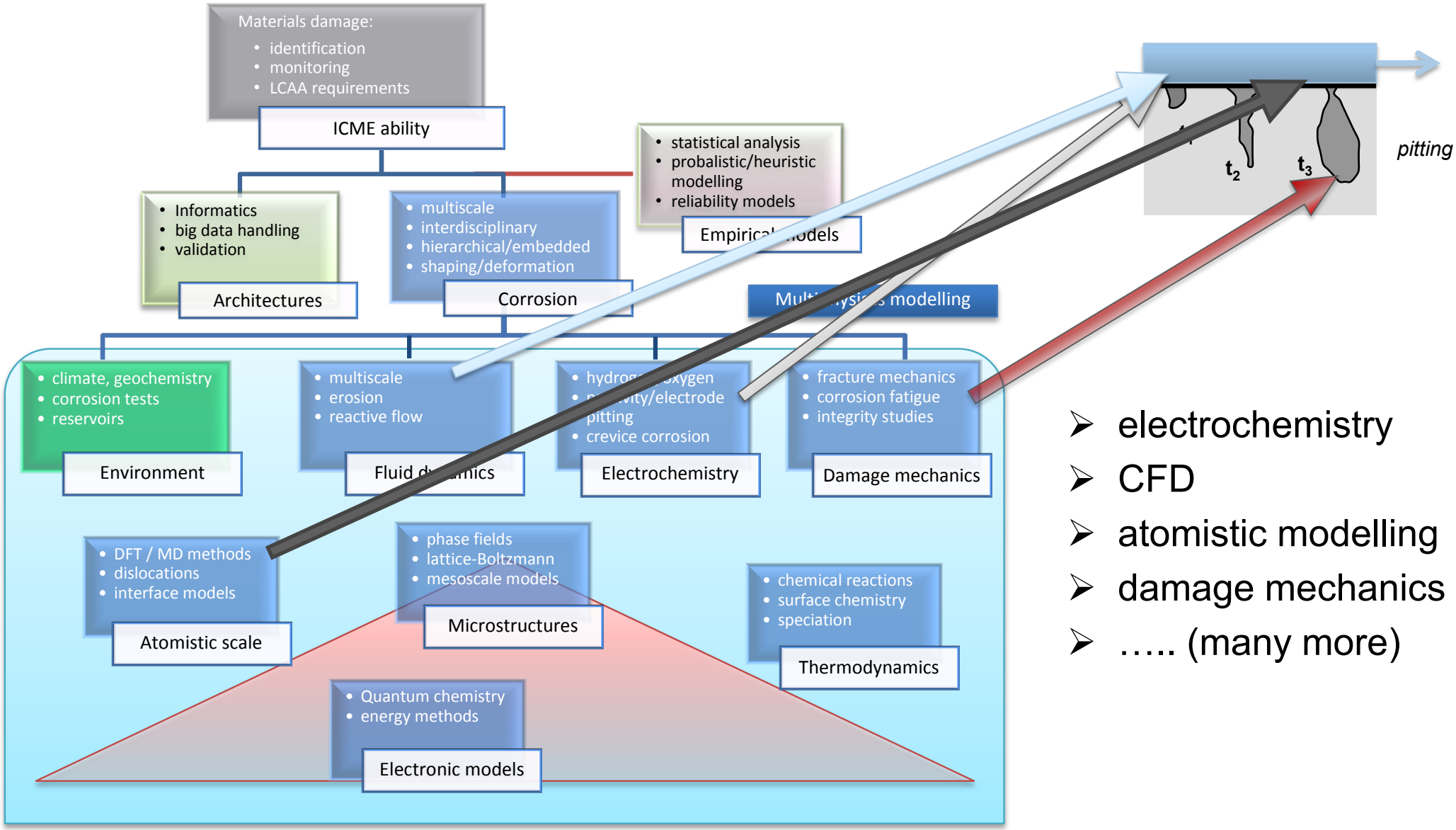

- electrochemistry
- CFD
- atomistic modelling
- damage mechanics
- ….. (many more)

Aims of current simulation action

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Idea behind → ***Corrosion meets materials simulation***

- **Assisting** engineers and scientists
  - by quantitative studies and process parameter weighting
  - by modelling corrosion properties based on equations
- **Economic** aspects - Reduction of development expenses and periods, and improved planning ability due to tailored properties
- improved **predictive power** for e.g. for engineering materials and its corrosion properties
- establishing of materials design at the PC by e.g. phase field modelling with the **target property: corrosion and degradation rate** for implants but also e.g. batteries

Challenge – service life vs. corrosion control

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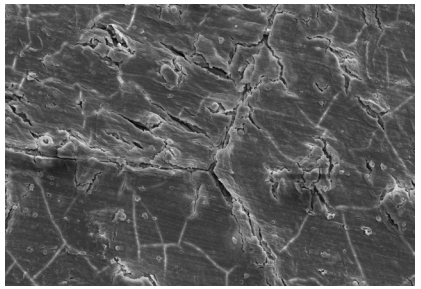
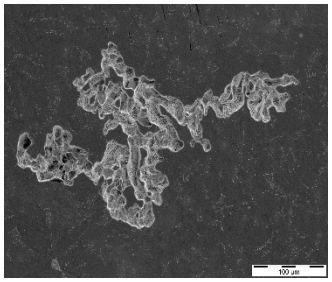
- minimizing e.g. surface engineering effort
- enhanced component failure control
- **scaling aspects**

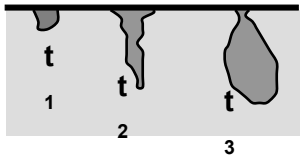
uniform corrosion – chemical conversion



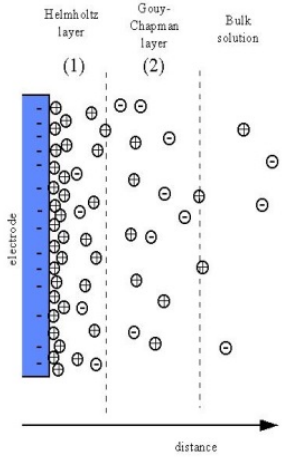
filiform corrosion



pitting

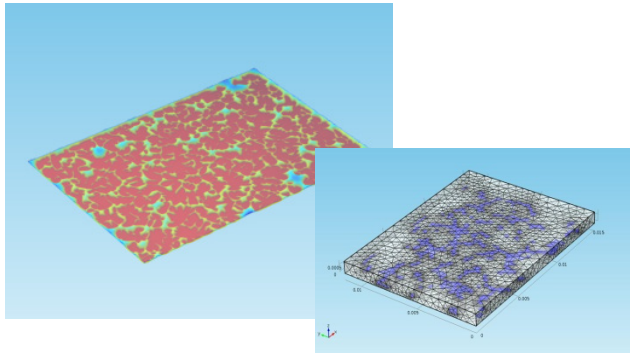


capacitive double layer (Helmholtz layer)

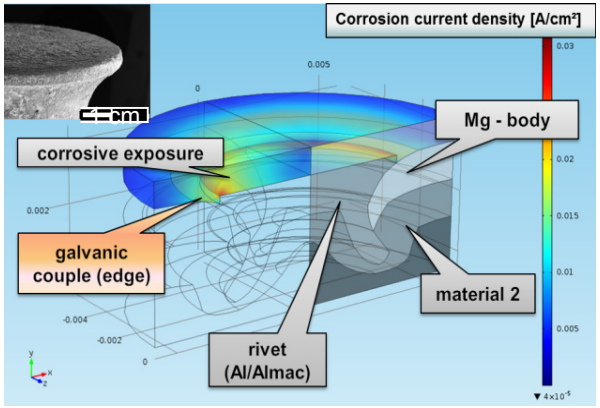


Corrosion for Science and Engineering
by K. R. Trethewey et.al 1995

microgalvanic corrosion



macrogalvanic corrosion



mesoscale

microscale

macroscale

10^{-9} 10^{-6} 10^{-3} 10^{0} m

Scaling- and methodological aspects

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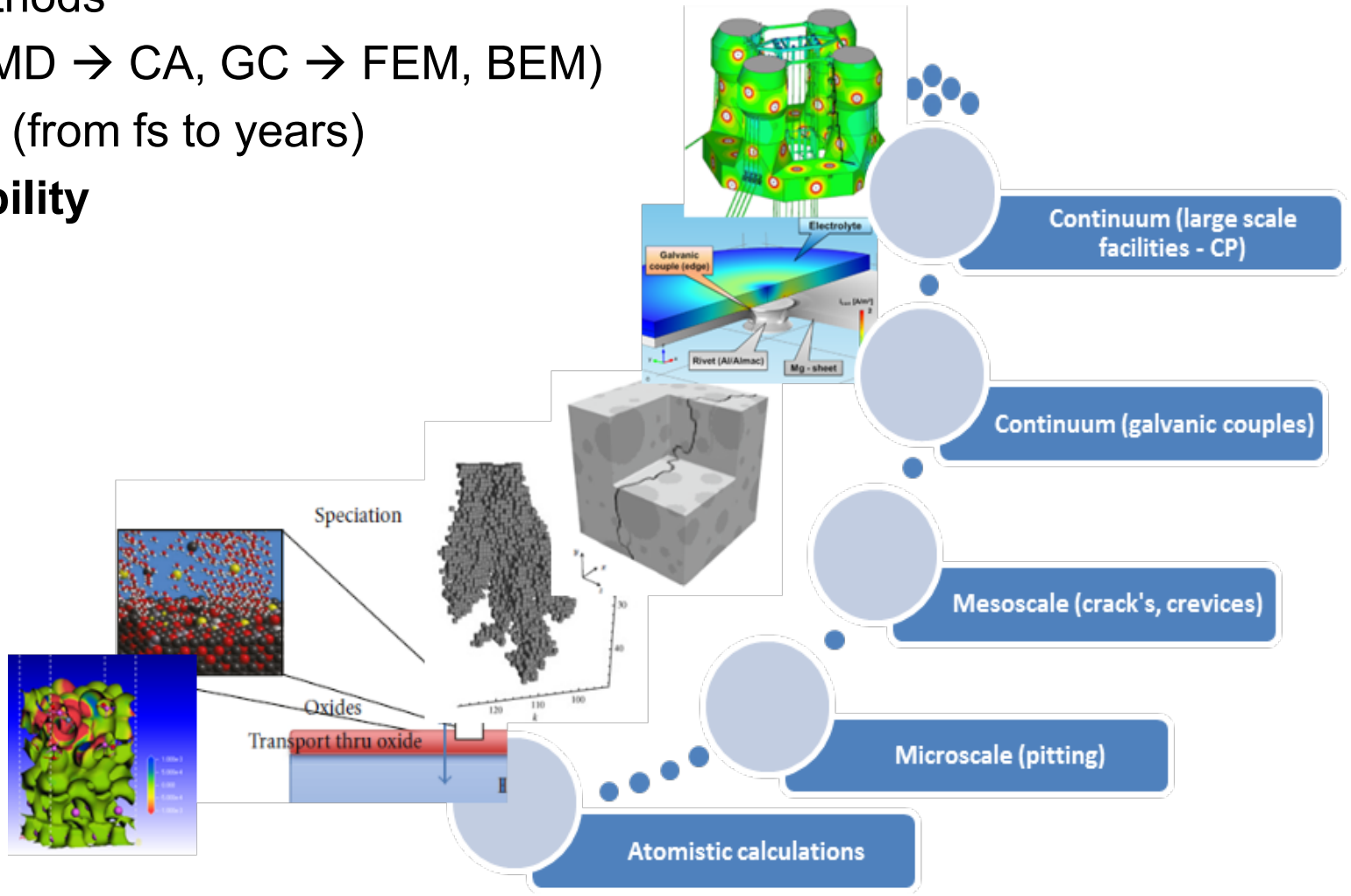
- multiple methods
  (DFT, MD → CA, GC → FEM, BEM)
- time scaling (from fs to years)
- **interoperability**



Example: Reinforced concrete service life

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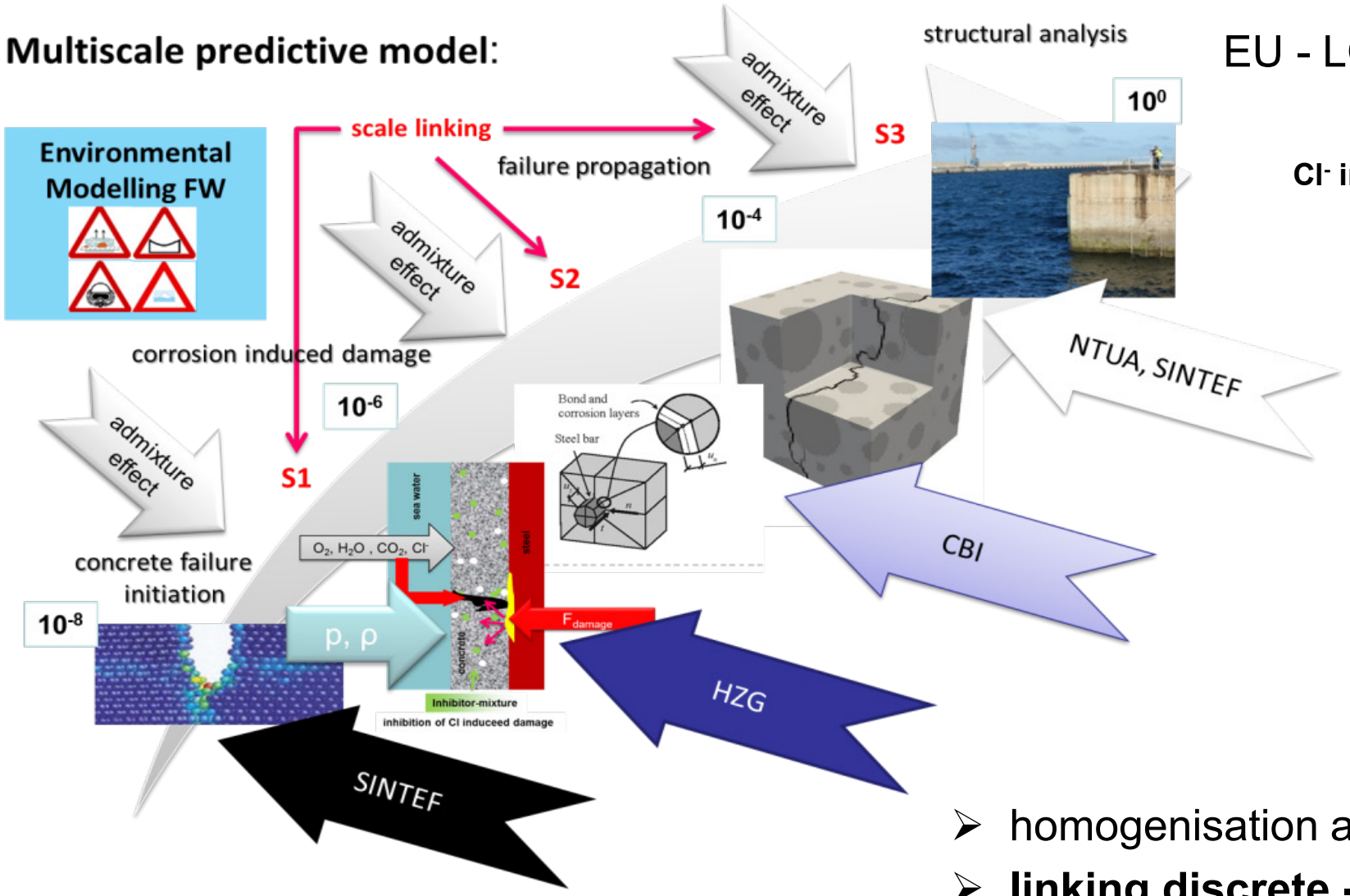

EU - LORCENIS

Cl^- ingress for 25 years

- homogenisation along the scales
- **linking discrete - continuum**

Example: Galvanic issues – Lightweight design

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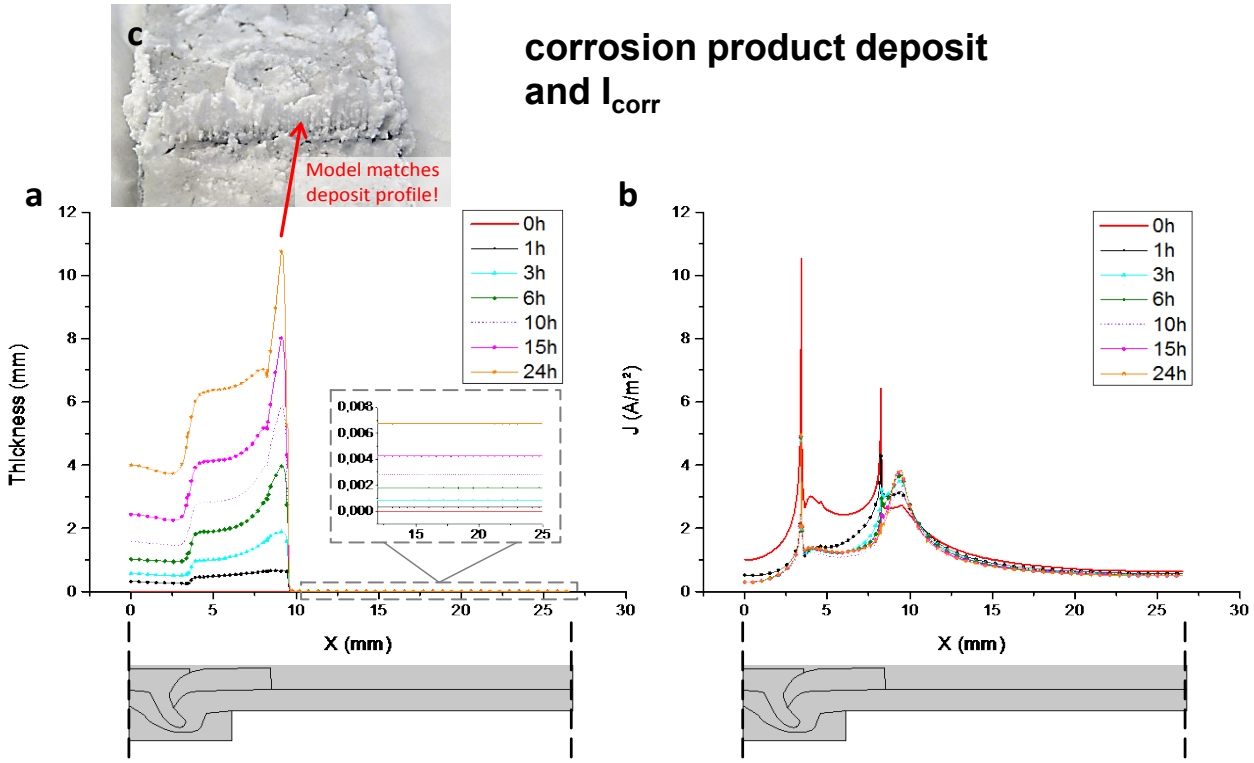
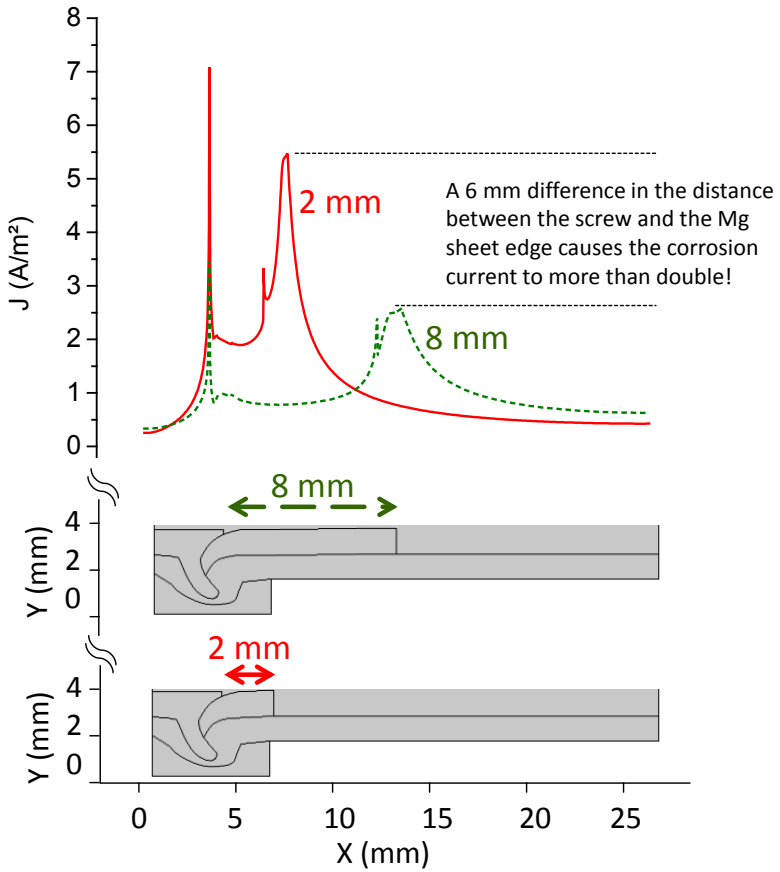


- joint design for multi material assemblies
- **big data and validation issue**

EU - ProAir

Multi-material joint layout



Example: Coatings and tests

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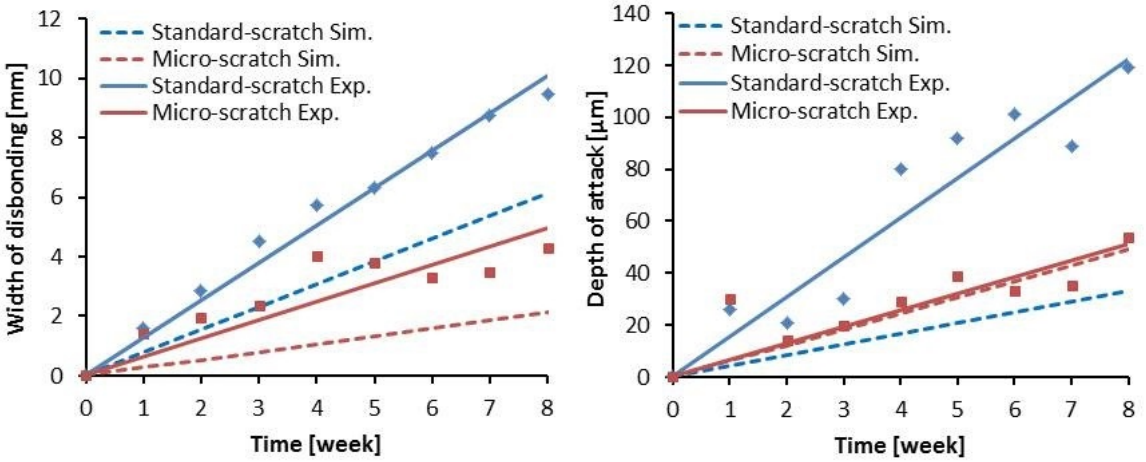
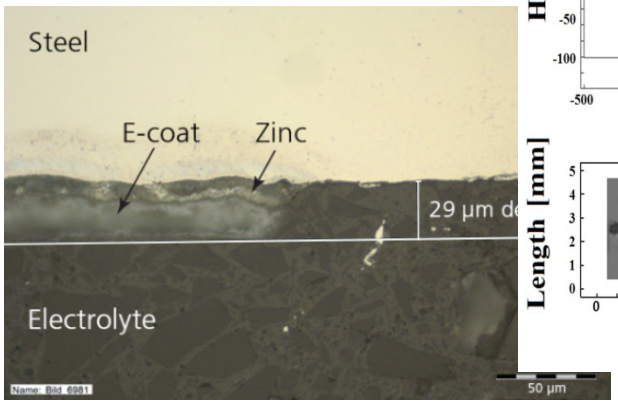
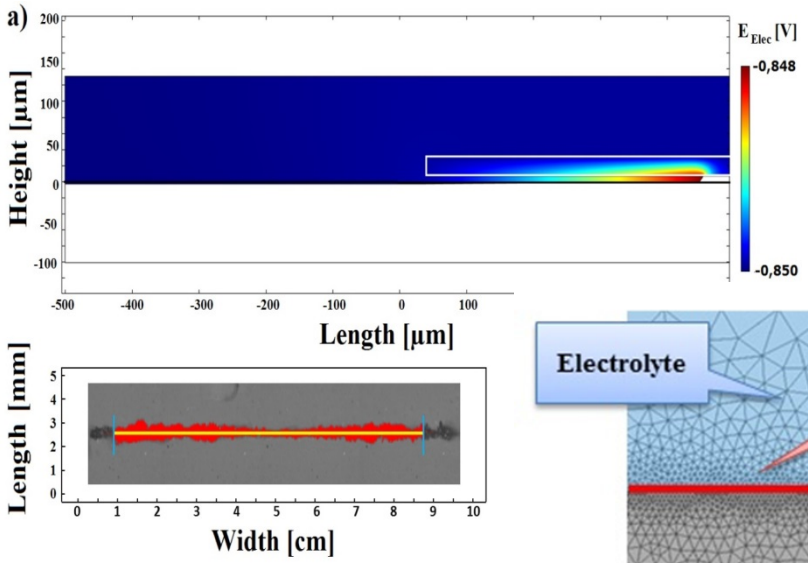
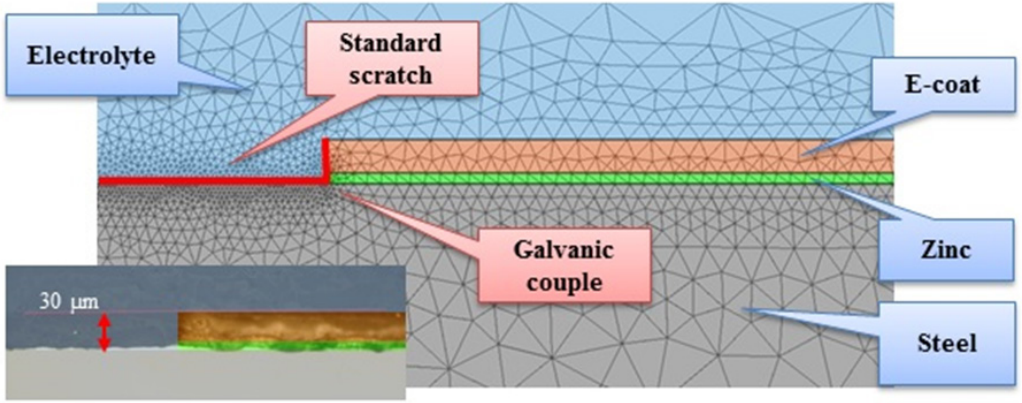
- accelerated corrosion testing (e.g. delamination in climate chamber test)
- **short developmental periods**







hot-dip galvanized steel



Source:

Example: Magnesium alloys

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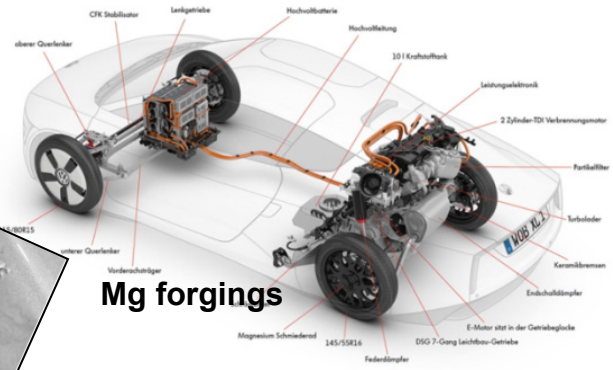
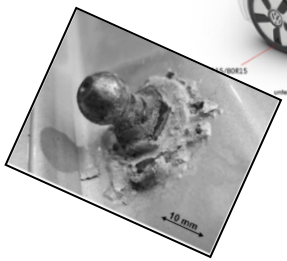
- Life cycle (service life) prediction of magnesium alloys

Transportation

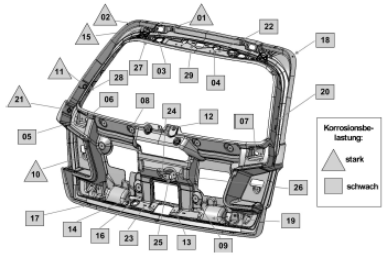
Mg sheets

Mg castings



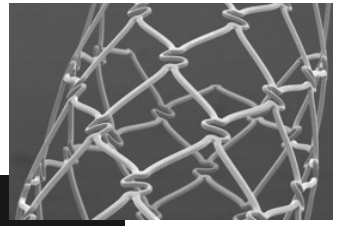


Mg forgings

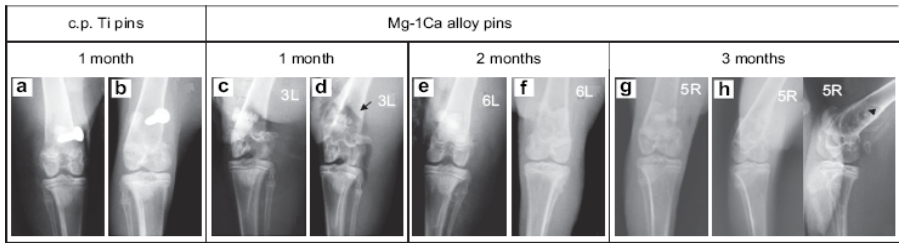


Schreckenberger et al.
Mat. und We. 41(2010) 853

Batteries

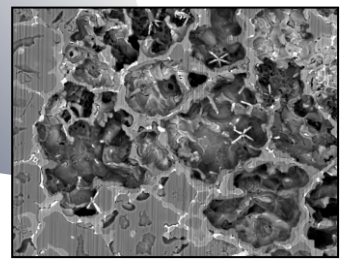


Service life



Li et al. Biomaterials 29(2008) 1329

Medicine



Aims of “predictive” materials simulation action

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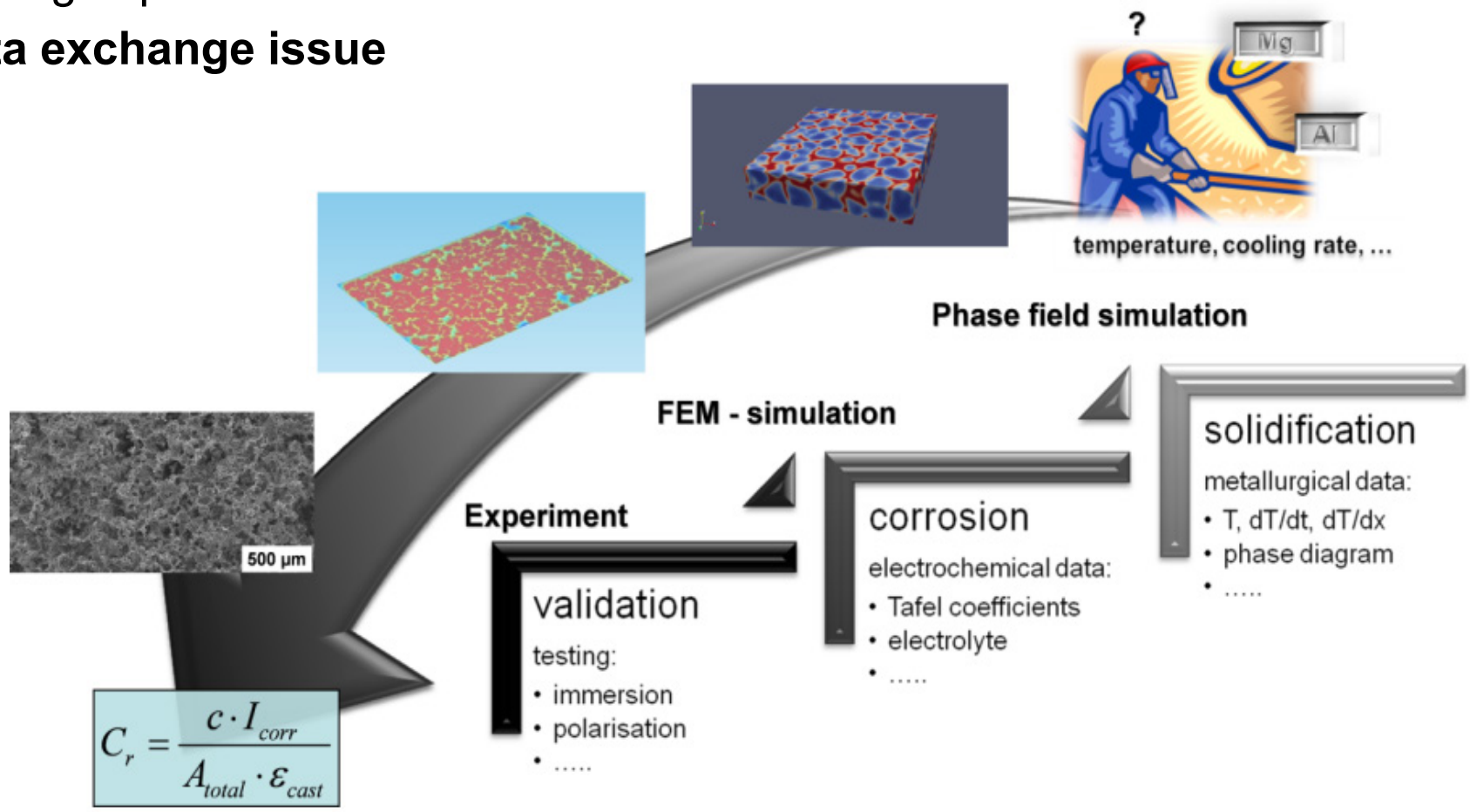
- Interdisciplinarity – microstructures meet electrochemistry
- scaling aspects
- **data exchange issue**



System Mg-Al → A multiscale problem

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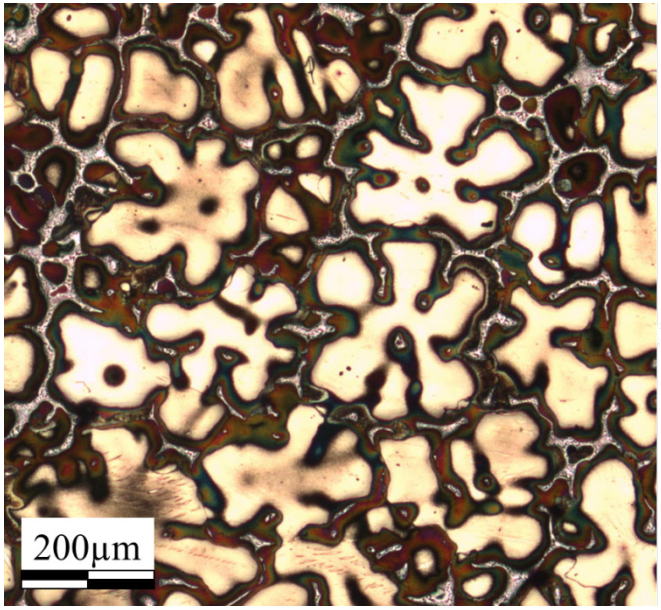
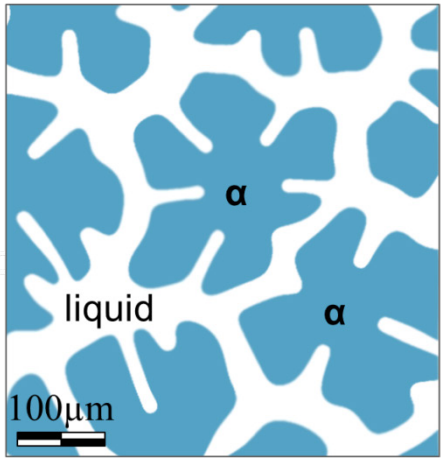
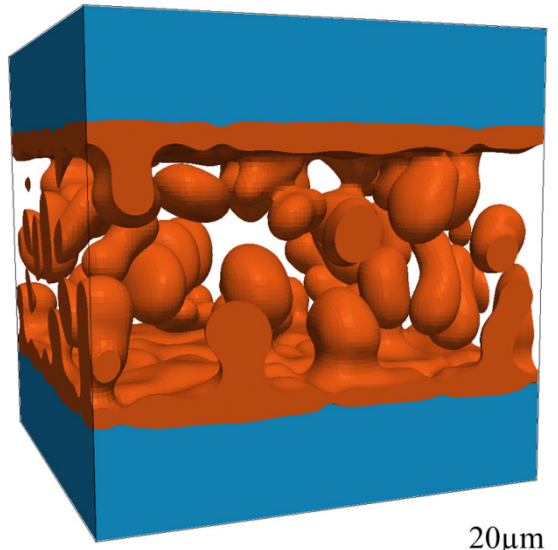
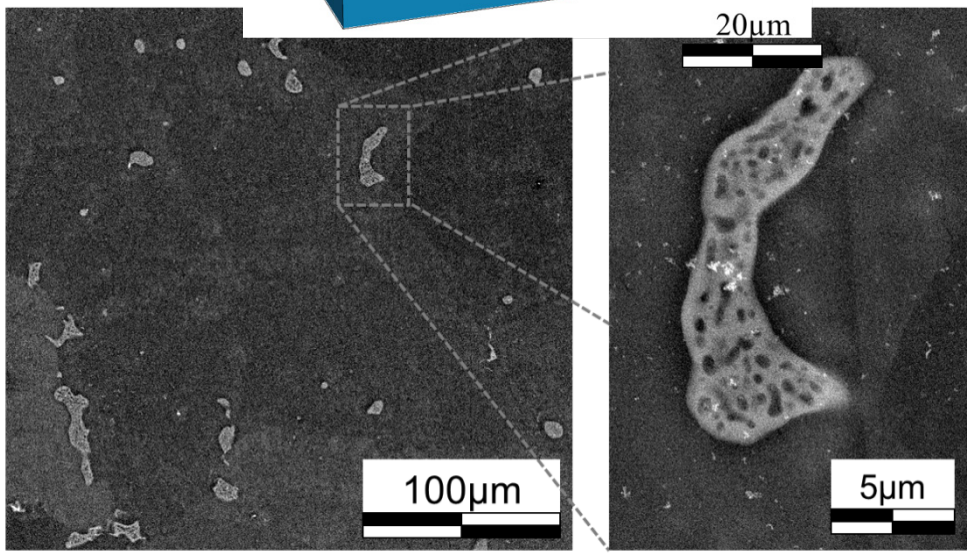






towards microstructure – corrosion coupling

ICAMS
INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION



SEM-image of Mg-5%Al microstructure and enlarged view on the eutectic region.
dark: α-phase, bright: β-phase
Se-Jong Kim, Chang Dong Yim, KIMS, Korea

Monas, A., Shchyglo, O., Kim, S. J., Yim, C. D., **Höche**, D., & Steinbach, I. (2015). Divorced Eutectic Solidification of Mg-Al Alloys. *JOM*, 1-7.

State of the art – microstructure vs. corrosion

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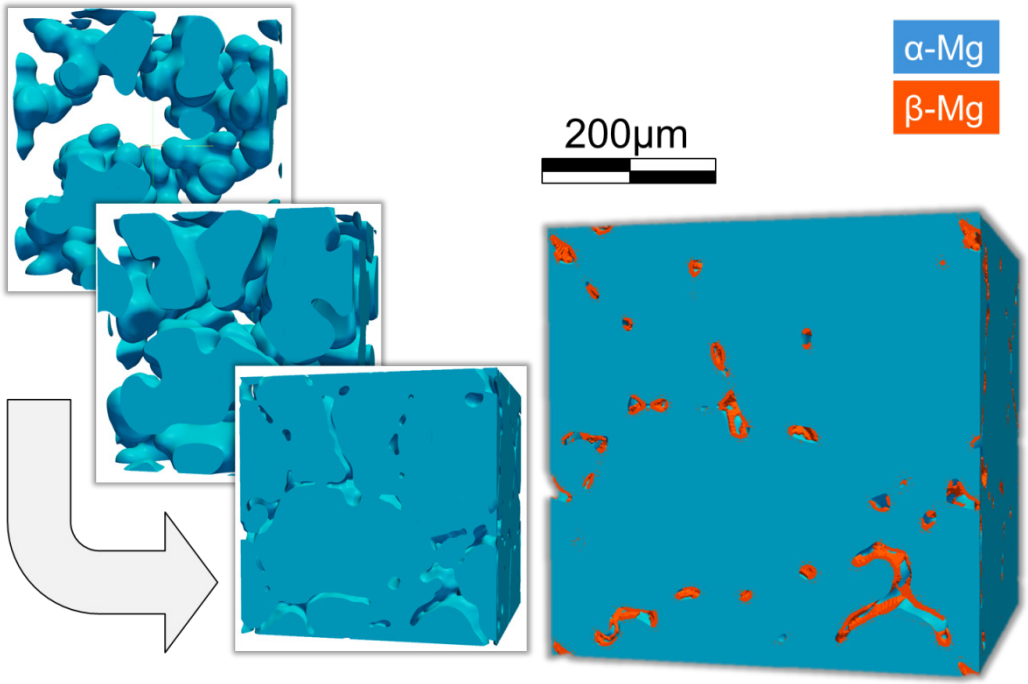

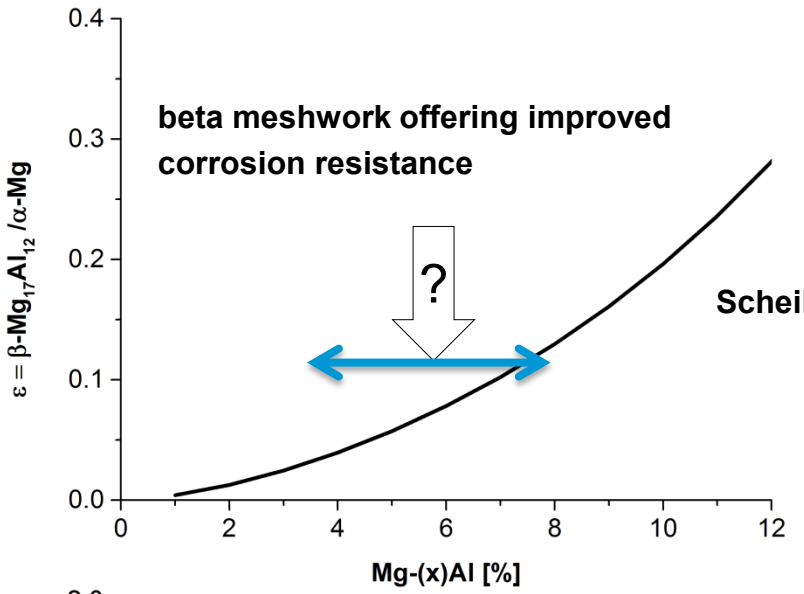

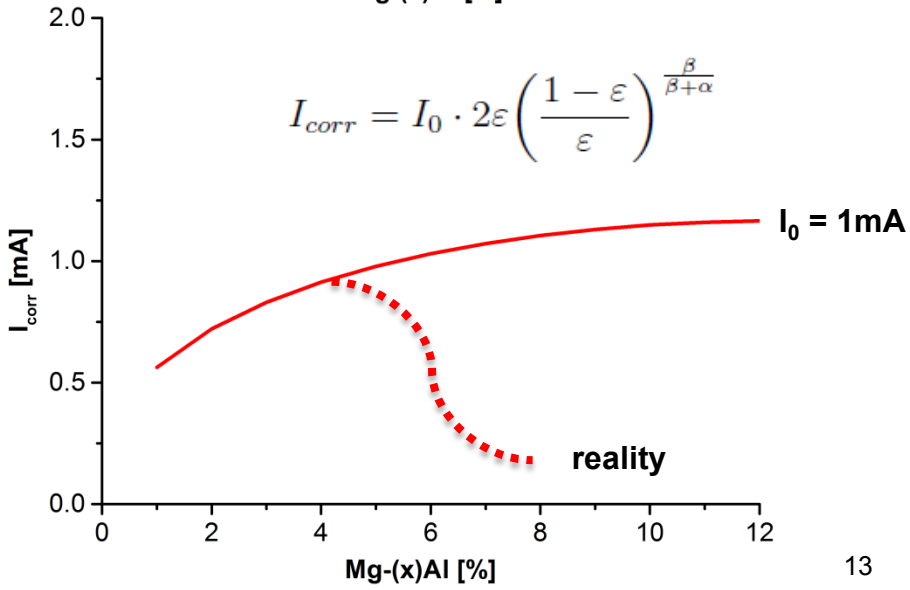

- ✓ phase field calculations simulate Mg-Al microstructure formation at different processing conditions
- ✓ primary, cooling rate sensitive **α**-phase nucleation
- ✓ secondary **β**-phase nucleation in channels
- ✓ divorced eutectic **α+β** growth

- tertiary nucleation inside residual melt-channels
- recover the transition from divorced to lamellar eutectic

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Next step – Linking to simulation of corrosion mechanisms

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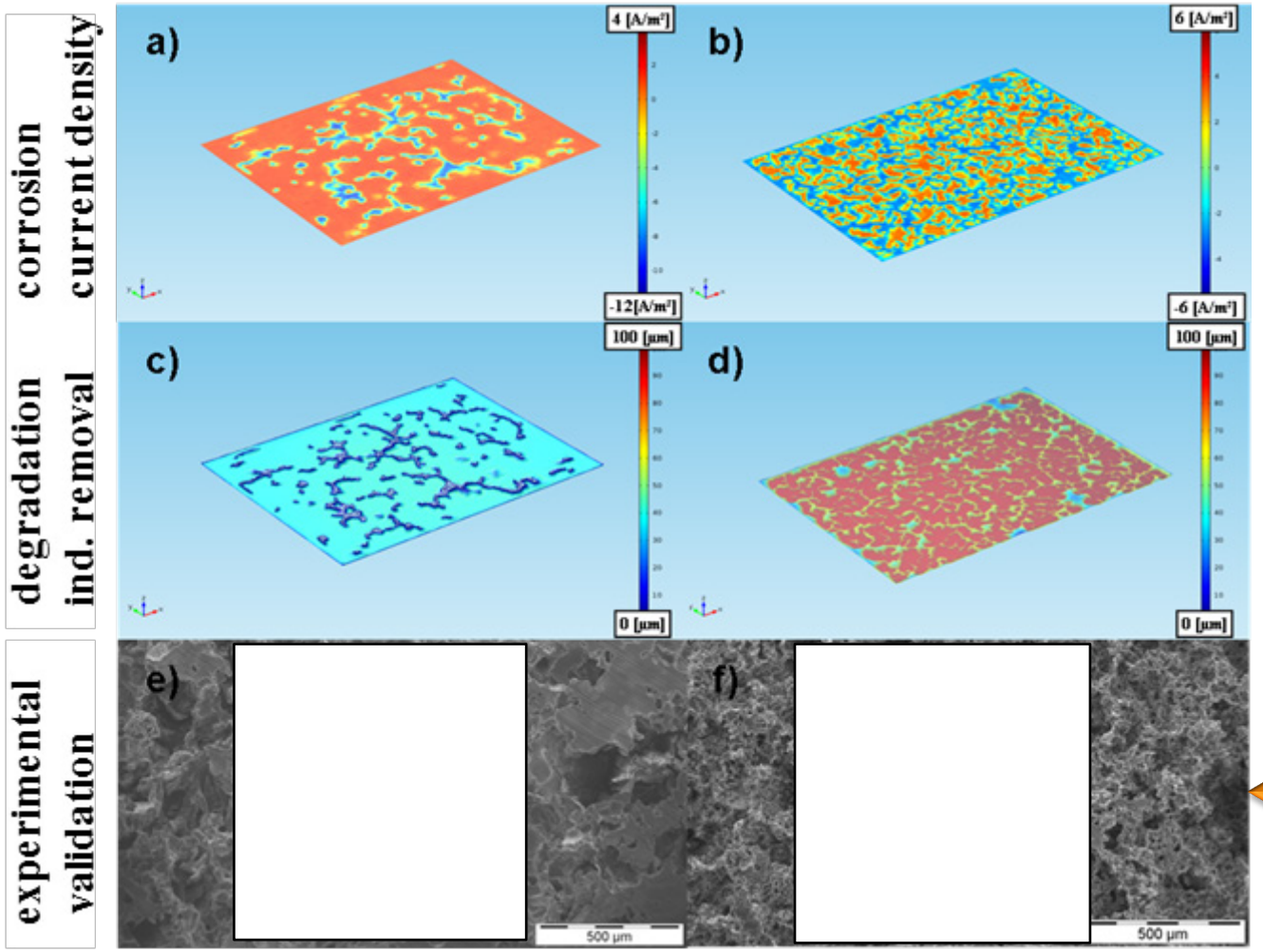

Replacement of experiments

Höche et al. CIT. 12(2013) 1951

Perspective – progress in digitalization

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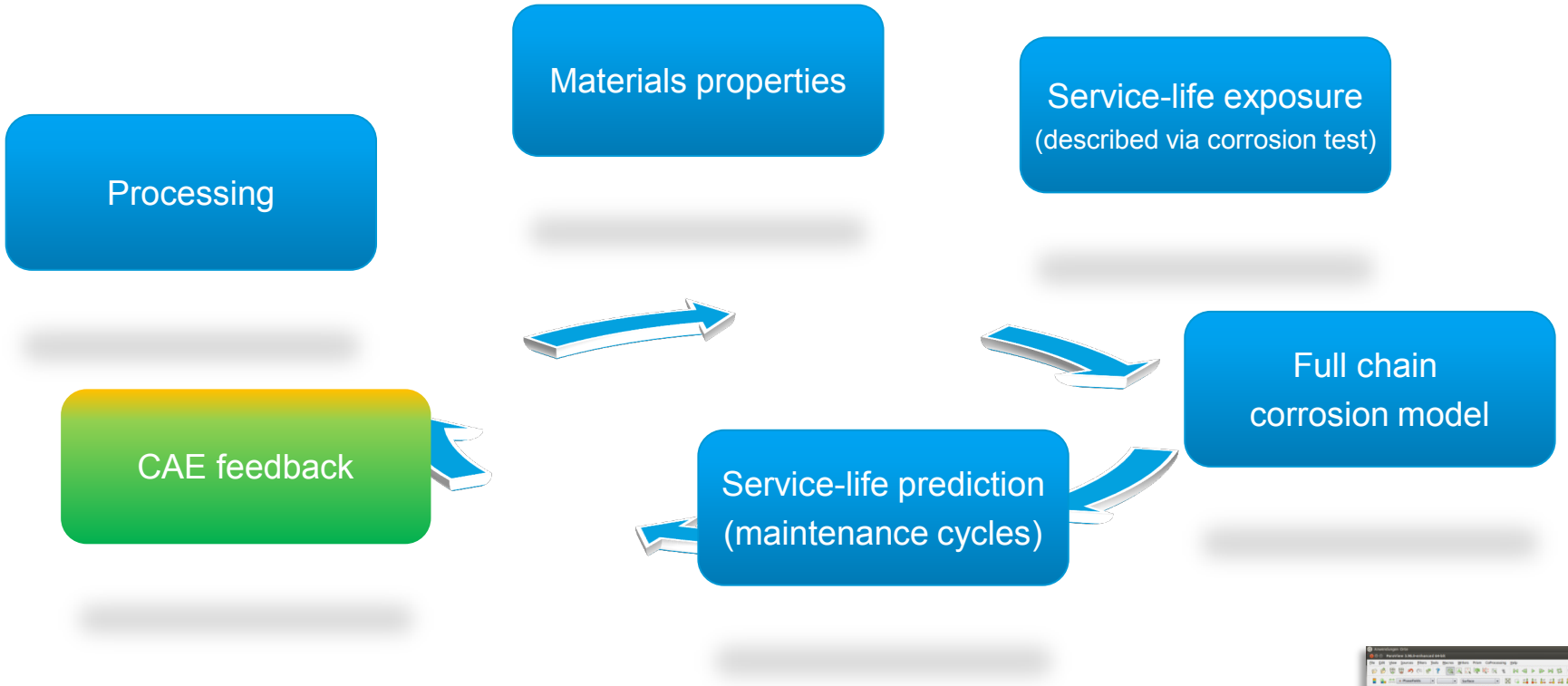
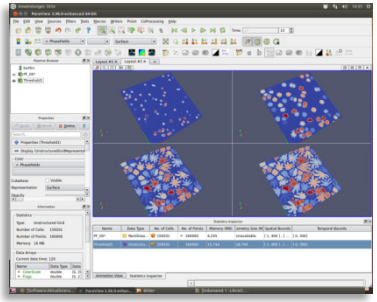
Research challange:

<u>Service-Life Design (SLD)</u> during virtual design period→



Goal: Establishment of full chain predictive modelling towards CAx considering service-life aspects



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Transfer into an ICME approach

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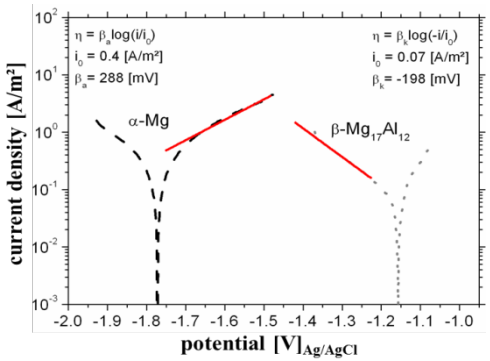
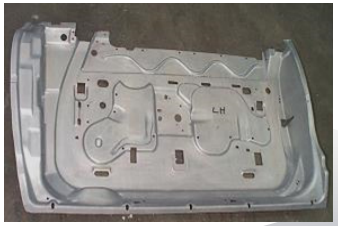
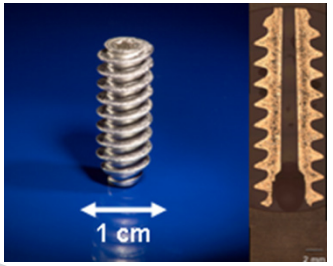
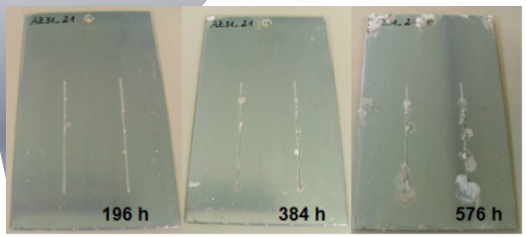
Electrochemical database

e.g. ???

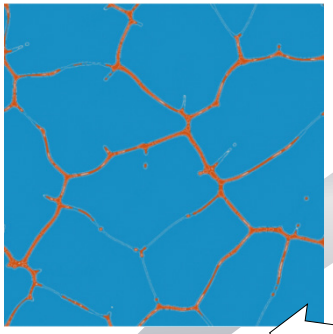




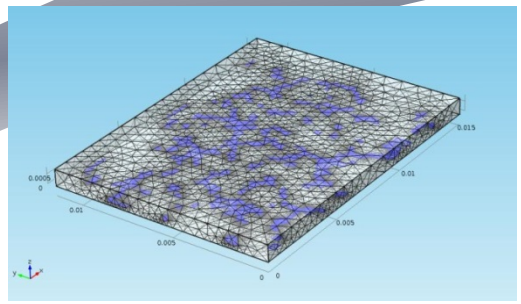




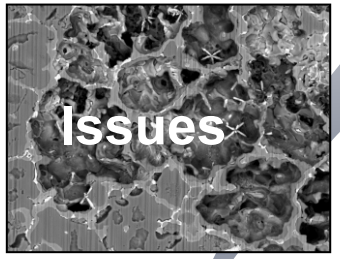
Optimized raw material for application



Thermodynamic database



Corrosion model



ICME – approach

ANY SUGGESTIONS?

Possibilities, Requirements and Limits

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Possibilities

- Establishment of a CAE like assisting tool for material development
- Determination of material parameters without expensive examinations
- Long term cost reduction and improved service life assessment

  (e.g. maintenance cycles)

Requirements

- **Integration of databases → multidisciplinary interaction and interoperability**

Limits

- Box simulation due to limited computing power – **HPC extension**
- Need of well-known environmental conditions – **validation**

  → Simulation of test conditions which describes service life – e.g. VDA

Thank you

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