Workflow for digital twin creation for secondary aluminium alloy in automotive parts

Eugen Gazenbiller[1], Lukas C. Jarren[1], Markus Apel[2], Janin Eiken[2], Franz Roters[3], Sharan Roongta[3], Daniel Höche[1], Mikhail Zheludkevich[1]

1. Introduction

The utilization of secondary aluminium, derived from post-consumer scrap, plays a pivotal role in the sustainable practices of the industrial sector. While recycled aluminium is instrumental in the production of various automotive and engineering components, challenges arise as impurity elements accumulate during the recycling process. [1] The presence of iron, even in small amounts, impacts the characteristics of aluminium alloys, influencing factors such as strength, ductility, fracture toughness and corrosion properties. The effects are governed by the alloy microstructure, especially by the presence of additional secondary particles like β-AlFeSi, which are reported to be harmful for mechanical and corrosive properties. [2,3] The aim of the project is the development of a digital workflow, which facilitates the prediction of mechanical and corrosive properties from the impurity content in the utilized aluminium scrap. The approach will enable fast assessment of scrap quality and suitability for specific car components.

2. Schematic workflow structure

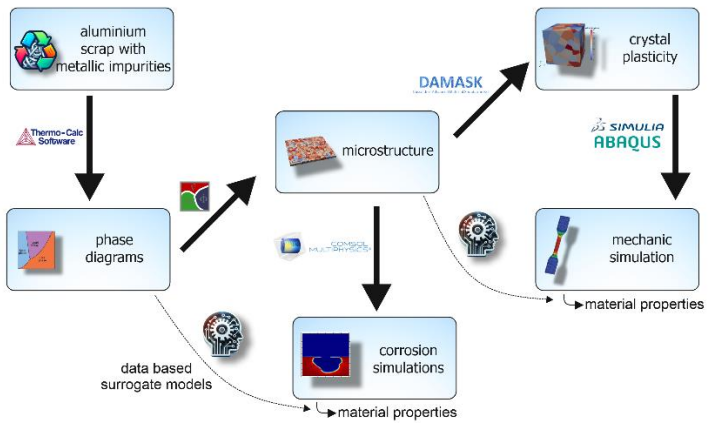

Figure 1: Schematic workflow for digital twin creating including utilized software packages.

The workflow utilizes a combination of free and commercial software packages (Fig. 1) to simulate the formation of the secondary alloy microstructure and its effects on the final mechanical and corrosive properties. [4,5] The approach combines phase field models with regular FEM models and Machine Learning techniques for surrogate model creation. Each of the steps requires dedicated data transfer between the generated and required formats to ensure a flawless transition between the

[1] Helmholtz-Zentrum Hereon, Max-Planck-Str. 1, 21502 Geesthacht *(eugen.gazenbiller@hereon.de)*
[2] Access e.V. Intzestr. 5, 52072 Aachen
[3] MPIE GmbH, Max-Planck-Str. 1, 40237 Düsseldorf

simulation steps. An important step between all steps is the experimental validation of the obtained results.

3. First selected results

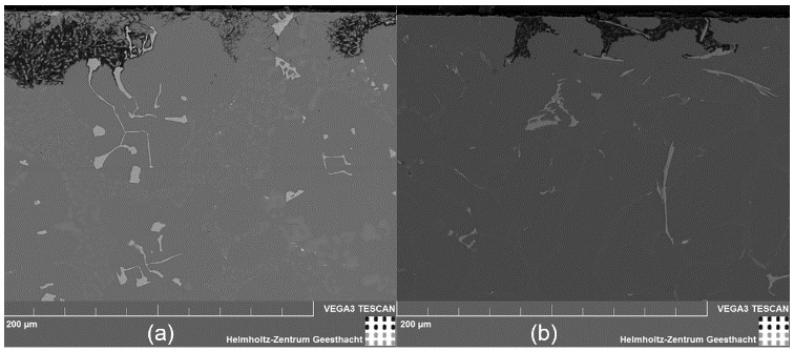

Figure 2: SEM of cross-section after potentiodynamic experiment of artificially impurified AlSi7Mg0.3 with (a) 1.0% Fe, 0.6% Cu, 0.6% Mn and (b) 0.5% Fe, 0.05% Cu, 0.2% Mn

In this work, the workflow will be demonstrated on the example of a AA6063-based secondary alloy with Fe and Cu impurities. The impurity content was artificially adjusted and the effects on the microstructure and corrosion characteristics were analyzed. The corrosion characteristics of AA6063 are highly dependent on the amount and kind of intermetallic particles. Due to reported cathodic potential of both AlFeSi phases compared to Al-matrix, the formation of microgalvanic cells leads to elevated localized corrosion tendency. Moreover, Mg+Si-containing phases are anodic and dissolve preferentially, whereas Mg is removed via dealloying, and Si-remnants can act as a cathode afterwards.[3] This interplay between the electrochemically active phases leads to complicated corrosion mechanisms, as can be seen in SEM cross-sections in Fig. 2. The different intermetallic phases and resulting geometries due to intergranular and trenching corrosion indicate impurity-dependent mechanisms. First solidification simulations (Fig. 3) based on thermodynamic data revealed that the occurrence of the β-AlFeSi phase can be prevented by adding Mn to the melt.

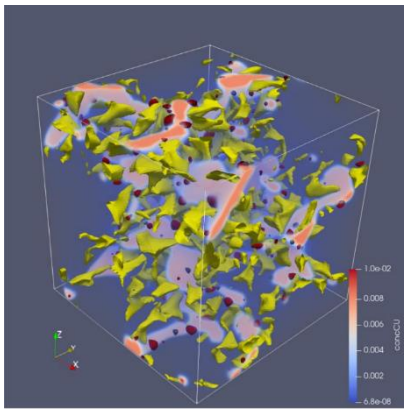

Figure 3: Exemplified result of a MICRESS simulation.

4. Conclusions

The first part of the project lead to promising results which reveal the occurrence of Fe-containing phases in impurified alloy. The precipitation of detrimental β-AlFeSi phases can was simulated via MICRESS software and validated experimentally. The next steps will involve the calculation of the mechanical properties with DAMASK package and FEM corrosion simulations based on the calculated microstructures. The proposed digital workflow is a valuable tool for transformation towards accelerated material design with sustainable recycled alloys.

5. References

[1] Raabe, D., et al. *Progress in Materials Science* 128, 100947 (2022). [10.1016/j.pmatsci.2022.100947]

[2] Khan, M.H., et al. *Intermetallics* 132, 107132 (2021). [10.1016/j.intermet.2021.107132]

[3] Kairy, S.K. and Birbilis, N., *Corrosion* 76(5), 464–475 (2020). [10.5006/3457]

[4] Eiken, J., et al. *Phys. Rev. E* 73, 066122 (2006). [10.1103/PhysRevE.73.066122]

[5] Roters, F., et al. (2019). *Computational Materials Science* 158, 420–478 (2019). [1016/j.commatsci.2018.04.030]