Geometric Models for Microstructures of Active Protective Coatings

Jelena Zaninović[1,2], Michael Godehardt[1], Christian Jung[2], Peter Klein[1], Natalia Konchakova[3], Katja Schladitz[1], Peter Visser[4]

[1]Fraunhofer Institute for Industrial Mathematics, Fraunhofer-Platz 1, 67663 Kaiserslautern, Germany

[2]Department of Mathematics, University of Kaiserslautern-Landau (RPTU), Gottlieb-Daimler-Straße 48, 67663 Kaiserslautern, Germany

[3]Helmholtz-Zentrum Hereon, Mac-Planck-Straße 1, 21502 Geesthacht, Germany

[4]AkzoNobel, Rijksstraatweg 31, 2171 AJ Sassenheim, The Netherlands

Abstract

Corrosion is a persistent challenge in aerospace engineering, hence corrosion control remains a principal part of the design process of aircraft. Active protective coatings containing sparingly soluble inhibitor particles offer long term protection against corrosion. The inhibitor particles dissolve in contact with water, releasing ions that passivate the surface damage. This process is called leaching and it is the key mechanism behind active protective coatings. The microstructure of the coatings, i.e. the loading size, shape, and placement of the inhibitors, pigments and extenders, strongly influences the leaching kinetics. However, our understanding of the relation between the microstructure and leaching kinetics is not yet sufficiently deep to successfully simulate and optimize the leaching process on the microscale.

One of the aims of project VIPCOAT was to fill this knowledge gap and facilitate development of new coatings. Coating samples were imaged non-destructively in 3D by nano- and microcomputed tomography using synchrotron radiation. The resulting volume images were processed and analyzed to extract geometric properties of the inhibitor particles that are relevant to leaching, such as particle size and shape distribution. We used the insights gained from observing the microstructure to construct stochastic geometric models of active protective coatings. Two models were created: a complex polyhedral model [1], matching size and shape distributions of the inhibitor particles very tightly, and a much rougher model using cuboidal shapes exclusively. The latter is intended for real-time use via the VIPCOAT Open Innovation Platform, offering more interactivity. Furthermore, we studied and compared the percolation behavior of the two models to our in-situ observations to validate and further improve the accuracy of their output.

Today, considerable effort is invested in designing environmentally friendly, high-performing active protective coatings. This work requires extensive testing, which is expensive and time consuming. In the long run, simulations with our geometric and leaching models will support research and significantly decrease the effort needed to develop sustainable active protective coatings.

Figure 1: From left to right: an observation of a lithium sulfate particle system, the polyhedral model, the simplified cuboid model. The observation is the result of a SR-nano-CT imaging campaign at the PETRA III beamline P05 at DESY.

Acknowledgement: VIPCOAT: H2020-NMBP-TO-IND-2020, GA 952903.

References

1. K. Schladitz, C. Jung, S. Flenner, M. Godehardt, B. Grevelhörster, I. Greving, P. Klein, N. Konchakova, C. Redenbach, P. Visser, J. Zaninović, Geometric modelling of corrosion inhibitor pigments in active protective coatings based on SR-nano-CT images, Progress in Organic Coatings, Volume 197 (2024), doi:10.1016/j.porgcoat.2024.108762

2. P. Visser, H. Terryn, J.M.C. Mol, Aerospace Coatings. In: A. Hughes, J.M.C. Mol, M. Zheludkevich, R. Buchheit (Eds.), Active Protective Coatings: New-Generation Coatings for Metals, Springer Netherlands, Dordrecht, 2016, pp. 315–372. doi:10.1007/978-94-017-7540-3_12

3. E. Bonetti, A modelling approach to study the microstructure and leaching behaviour of active protective coatings, PhD thesis, University of Manchester (2021)