Three-Dimensional Percolation Properties Simulation of a Marine Coating Based on Its Real Structure Obtained From Ptychographic X-Ray Tomography

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Abstract

Artificially structured coatings are widely employed to minimize materials deterioration and corrosion, the annual direct cost of which is over 3% of the gross domestic product (GDP) for industrial countries. Manufacturing higher performance anticorrosive coatings is one of the most efficient approaches to reduce this loss. The recently BP-sponsored £100 million project aiming at developing advanced anticorrosive coatings is a living example showing the importance. However, three-dimensional (3D) structure of coatings, which determines their performance, has not been investigated in detail. Here we present quantitative nano-scale analysis of the 3D spatial structure of an anticorrosive aluminium epoxy barrier marine coating obtained by ptychographic X-ray computed tomography (PXCT) [1-3] and Serial-Block Face Scanning Electron Microscopy (SBFSEM) [1, 4]. From the analysis, orientations, lengths and volumes of individual objects in the coating film were revealed. We then use COMSOL Multiphysics® simulation to do finite element simulations on the acquired real 3D structures to demonstrate how percolation through this actual 3D structure impedes ion diffusion in the composite materials (see Figures 1 and 2). We found the aluminium flakes align within 15o of the coating surface in the material, causing the perpendicular diffusion resistance of the coating to be substantially higher than the pure epoxy, normally over twice of the pure epoxy's [1]. The work demonstrated an approach for validating mechanistic assumptions of materials and potentially provides a practical method to engineer the efficacy of anti-corrosion coatings by modelling electrochemical process in the materials based on the actual 3D structures of the materials themselves.
(This abstract is based on the content from reference [1].)

Reference

[1] Chen, B. et al. Three-Dimensional Structure Analysis and Percolation Properties of a Barrier Marine Coating. Sci. Rep. 3, 1177 (2013).
[2] Dierolf, M. et al. Ptychographic X-ray computed tomography at the nanoscale. Nature 467, 436–439 (2010).
[3] Guizar-Sicairos, M. et al. Phase tomography from x-ray coherent diffractive imaging projections. Opt. Express 19, 21345–21357 (2011).
[4] Denk, W. & Horstmann, H. Serial block-face scanning electron microscopy to reconstruct three-dimensional tissue nanostructure. PLoS Biol. 2, e329 (2004).

Figures used in the abstract

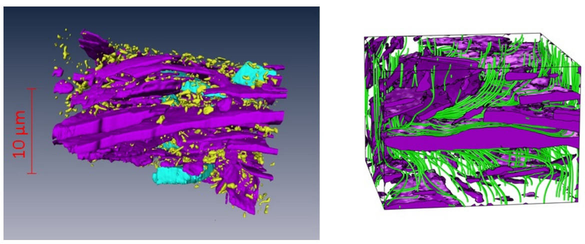

Figure 1: Figure 1. Left, 3D Rendering of spatial structure of the anticorrosive aluminium epoxy barrier marine coating sample obtained by ptychographic X-ray computed tomography (PXCT); Right, Simulated ion flow along the direction perpendicular to the coating surface presented as streamlines in green within the real structure (done by COMSOL).

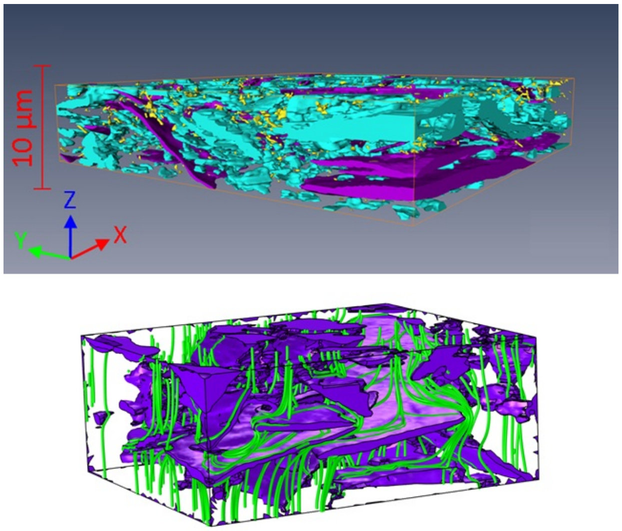

Figure 2: Figure 2. Upper, 3D Rendering of spatial structure of the anticorrosive aluminium marine coating sample obtained by Serial-Block Face Scanning Electron Microscopy (SBFSEM); Lower, Simulated ion flow along the direction perpendicular to the coating surface presented as streamlines in green within the real 3D structure (done by COMSOL).