Three-dimensional Percolation Properties Simulation of a Marine Coating Based on Its Real Structure Obtained from Ptychographic X-ray Tomography

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Materials science is three-dimensional (3D) science. Observing 3D spatial structures of materials, especially synthetic materials, are crucial for the future industrial product design and manufacture.

Here, we present 3D spatial structure of a barrier aluminium marine coating obtained from ptychographic X-ray computed tomography (PXCT) [1, 2]. The outstanding anti-corrosive property of this coating is mainly generated by the aluminium flake pigments whose shape and spatial arrangement determine the product barrier properties by affecting the transporting rate of corrosive substances through coating films. Those information cannot be fully obtained without 3D spatial structures.

Ptychographic X-Ray Computed Tomography (PXCT)

is a scanning coherent X-ray diffractive imaging method, namely X-ray ptychography [3], combined with conventional X-ray tomography. Figure 1 displays the real experimental set-up of the method.

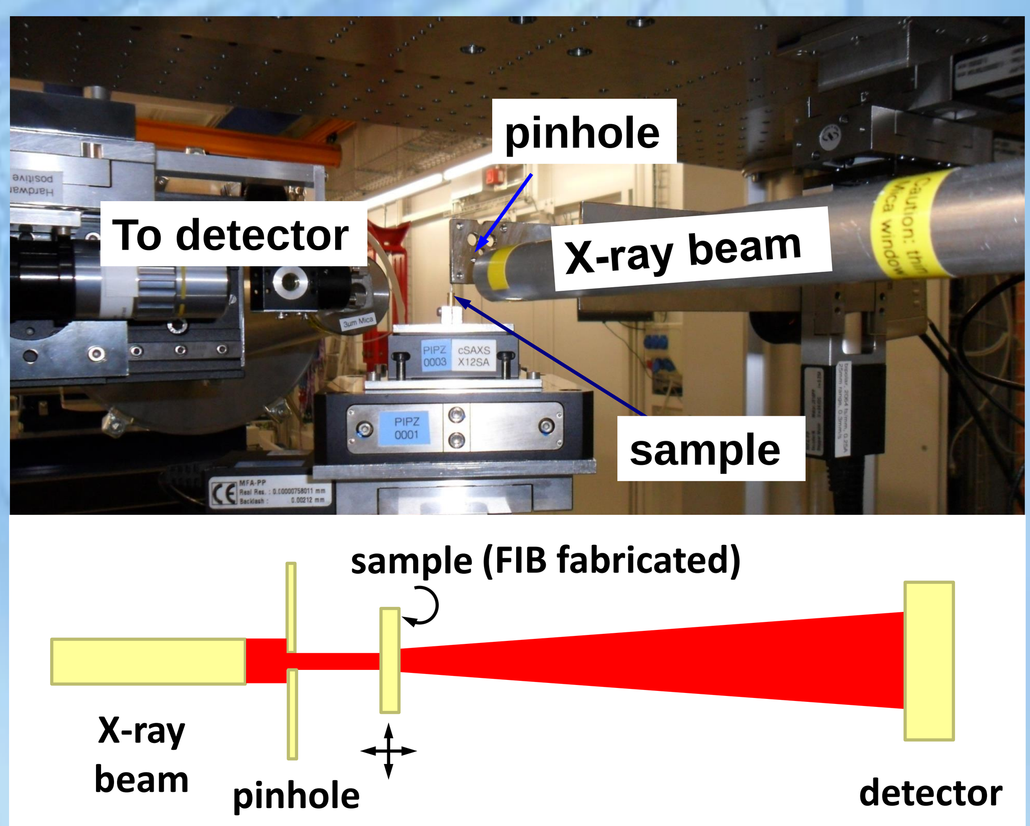

Figure 1. Set-up of ptychographic X-ray computed tomography. Upper photo is the on-site experimental set-up, lower diagram is a schematic expression.

Tomographic projection at each rotation angle is reconstructed from multiple X-ray diffraction patterns by ptychography using a phase-retrieval algorithm. Generated Phase contrast projections are then reconstructed into 3D images by a revised filtered back-projection algorithm. Figure 2 shows result from the PXCT.

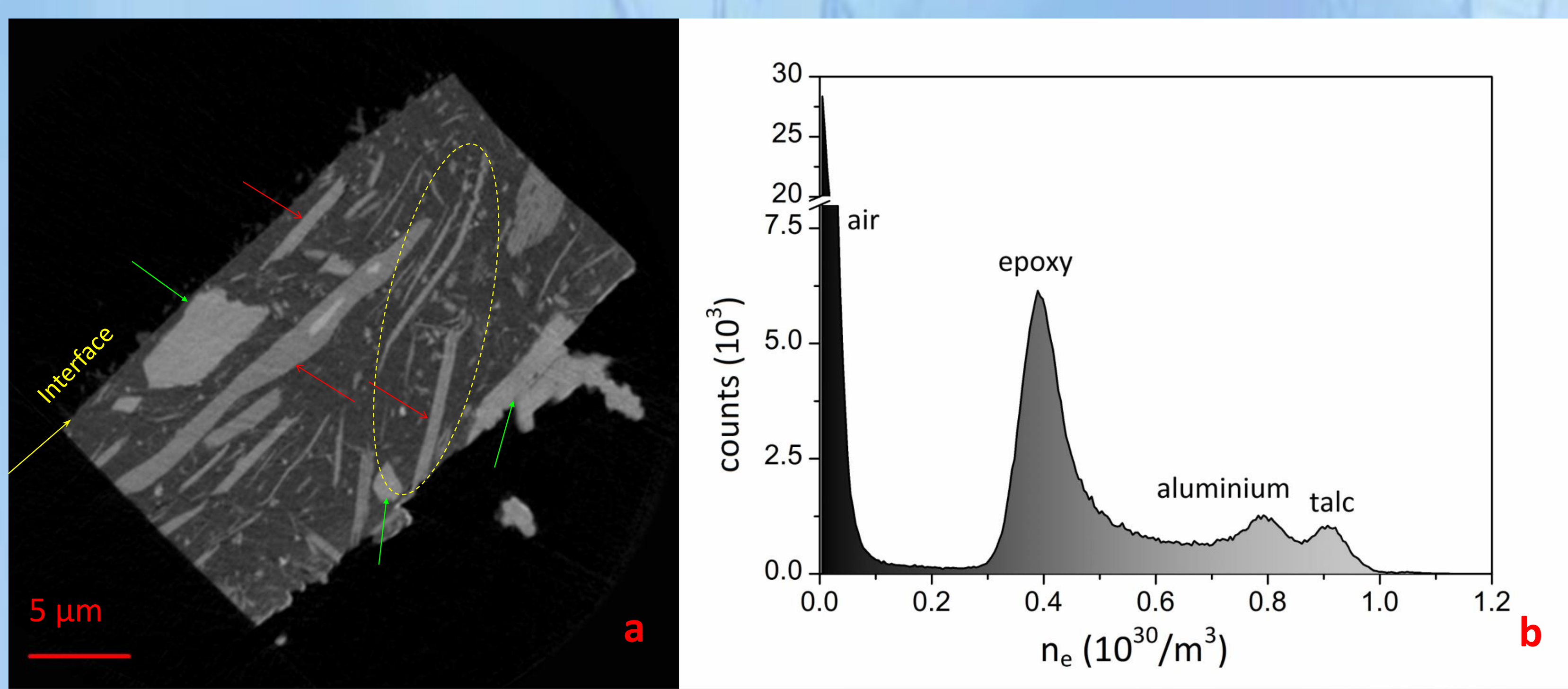

Figure 2. PXCT results of the aluminium marine coating. (a) One of tomogram slices of the reconstructed 3D volume. Arrows point to some of the identified aluminium flakes in red and talc fragments in green. (b) Histogram of electron density distribution of the tomogram slice in figure 2a, which enables accurate composite identification.

Figure 2 shows clearly that the four components of this complex industrial coating, aluminium flakes, talc, iron oxide particles and epoxy resin (matrix material), can be quantitatively identified through the electron density map given out by PXCT measurement.

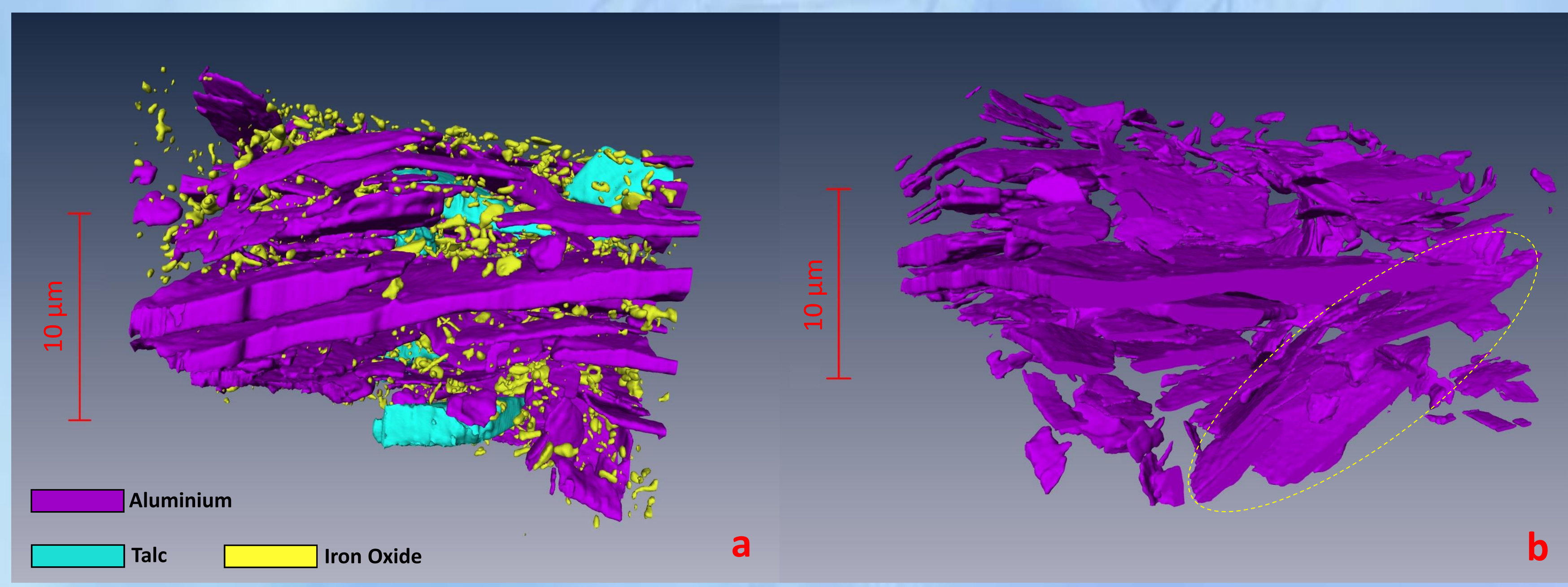

Figure 3. 3D Rendering of spatial structure of the sample from 2 different viewpoints. (a) Rendering of 3D spatial structure image of the sample. (b) 3D spatial arrangement image of just the aluminium flakes in the material.

The orientations, lengths, volumes and etc. of individual objects in the materials can be quantitatively obtained from morphometric analysis after 3D image segmentation, whose result was rendered in figure 3. From the analysis, we found that the aluminium flakes arrange nearly parallel to the coating film surface, mostly within 15° deviation, as shown in figure 4a. Through 3D finite element simulation of the percolation properties of the coating based on its segmented real structure, the perpendicular diffusion resistance of the coating was revealed to be substantially higher than the pure epoxy. See details of the analysis and simulation in reference [1].

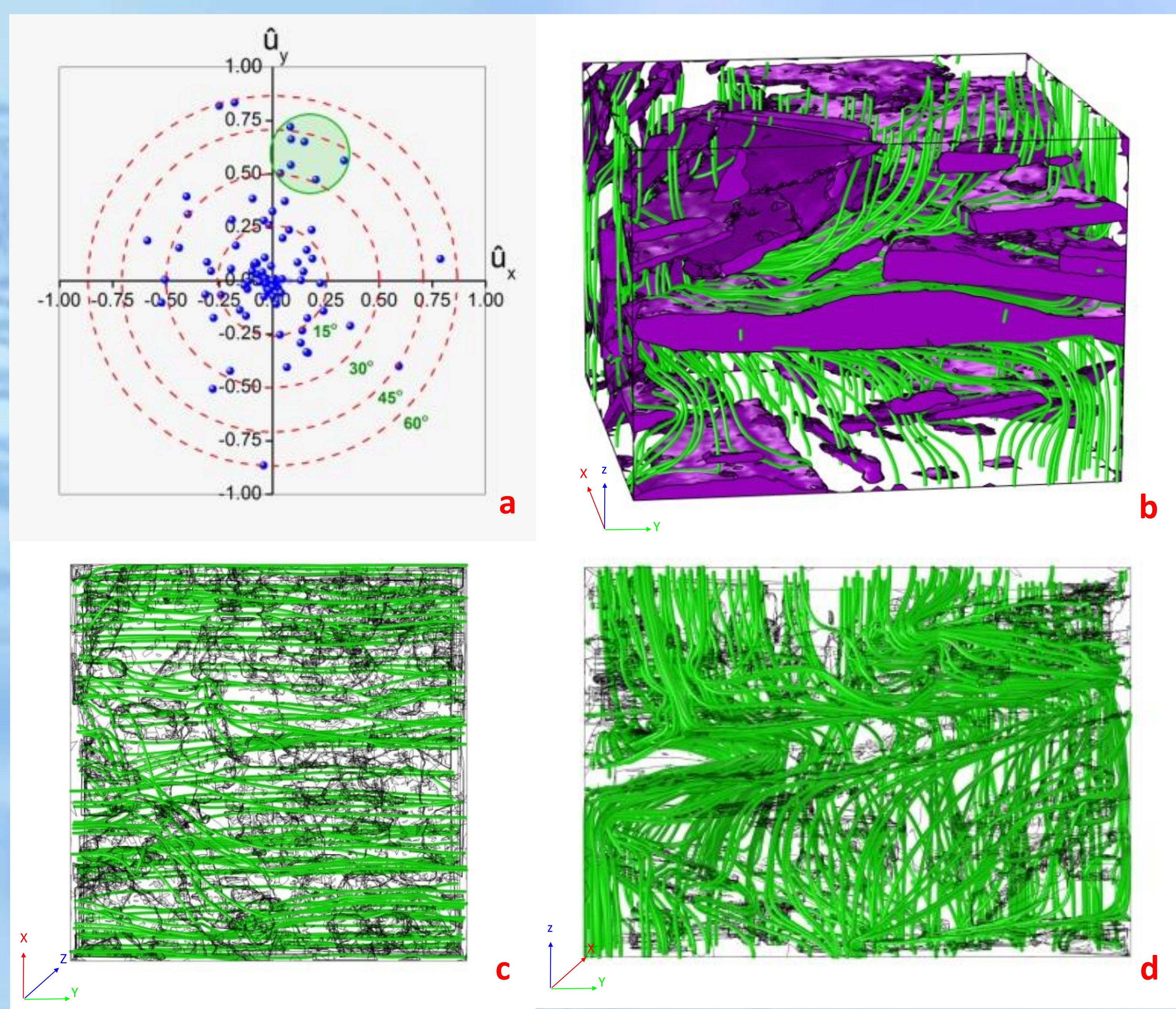

Figure 4. Quantitative analysis and simulation results. (a) Quantitative orientation analysis of the aluminium flakes in the material. (b) Simulated ion flow along the direction perpendicular to the coating surface presented as streamlines in green within the real structure. (c & d) Simulated flow (only) along the directions parallel and perpendicular to the coating surface.

References: [1] B. Chen *et al.*, Scientific Reports. 2013; 3: 1177.
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