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Machine Learning-Based Reconstruction of Quantitative Compositional Maps in Complex Microstructures: Fusion of Neutron and X-ray Tomography with Raman Analysis

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The intricate and unstable nature of corrosion in iron-based materials, such as in archaeological materials, necessitates advanced non-destructive methods for compositional analysis and phase segmentation. The accurate quantitative clustering of these compounds requires a robust analytical framework capable of delineating the various phases present in the thick and irregular corrosion layers. This research presents a multimodal and multi-resolution imaging framework for accurately segmenting and quantifying the phases in corroded iron-based materials, exemplified by Roman nails unearthed from archaeological sites. We employ a workflow that first registers and fuses Neutron (NCT) and X-ray (XCT) tomograms, which are subsequently registered with high-resolution 2D optical microscopy (OM) images. These OM images were acquired on multiple physical cross-sections of these nails and annotated with chemical information obtained by Raman spectroscopy. This 2D-to-3D registration is pivotal in associating non-destructive imaging data with precise phase identification, enabling the accurate labeling of phases within the fused X-ray and neutron tomogram cross-sections (currently only at several 2D cross-sections). This is fulfilled by leveraging a U-Net based deep learning model, adapted for learning the complex relationship between low-resolution and high-resolution labels. This workflow enables discerning and generalizing the identification of these phases, thus achieving a reliable 2D segmentation (creating a composite mapping). Future work will extend these methodologies into three dimensions, aiming for a holistic 3D quantification of corrosion compounds. Such a 3D reconstruction will be reinforced using energy-dependent cross-section curves from energy-resolved time-of-flight measurements and calibration NCT-XCT tomographies from the compressed standard powder pallets of the expected corrosion products in our samples (above 9 expected compounds), ensuring the accuracy of phase differentiation in the three dimensions. The adoption of a V-Net architecture will further enable this extrapolation of the 2D segmented phases into a 3D volume, capturing the full complexity of the corroded samples. After training on several samples, this model should allow us to predict the compositional map of similar samples based on their tomography without the need for further destructive analysis. This method underscores the potential of combining multimodal imaging and deep learning in revolutionizing the analysis of corroded materials, with implications that stretch beyond laboratory applications. The proposed approach will not only enhance our understanding of the material degradation but will also serve as a precursor for our future predictive computational simulations. These simulations will model the behavior of corroded materials under various environmental conditions, aiding the conservation of artifacts and guiding materials engineering practices. Furthermore, the versatility of this framework makes it adaptable to a wide array of material science problems, by offering an approach for a 3D compositional map reconstruction of complex samples, for which to the best of our knowledge there is no existing destructive or non-destructive method.

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