Doing More with Less: Artificial Intelligence Guided Analytics for Electron Microscopy Applications

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Scanning transmission electron microscopy (STEM) is an important tool in the study of microstructures and ultimately a wide range of material and chemical systems. Quantitatively describing these microstructures with advanced artificial intelligence (AI) techniques has recently become an emerging and impactful area of research in the materials domain [1]. Sophisticated new models and algorithms are being developed to automate the task of image characterization, bypassing the need for expensive manual analysis and enabling the discovery of new and unexpected features within an image. However, typical AI workflows use large libraries of labeled data to train specialized networks toward specific tasks, e.g., segmentation of a specific material class. One serious challenge for AI in this area is the lack of high-quality, well curated training data. Additionally, the need to instantly adapt to changing imaging conditions, length scales, detectors, aberrations, and materials systems is a top priority for materials characterization and a challenge for specialized AI.

We explore the topic of few-shot or low-shot learning (FSL) techniques in the context of creating adaptable AI designed for flexibility in both analytics and data acquisition. FSL, as the name suggests, uses little to no data in training and nearly eliminates the laborious task of data annotation. We have observed success with FSL for flexible segmentation of STEM image data, leading to powerful data-driven opportunities for microstructural characterization for materials discovery and design [2,3,4]. We will discuss the potential for FSL techniques to draw upon multiple imaging and spectroscopic data streams simultaneously, in a multimodal framework shown in Figure 1, for improved interpretability and enhanced latent signature detection [5].



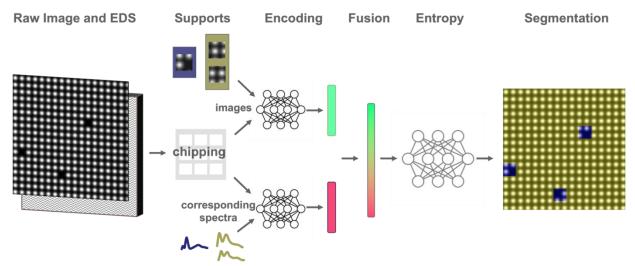


Figure 1. Framework for electron microscopy image segmentation using a chipping scheme as in [4] with extensions for multimodal data. The image is chipped into smaller pieces and chips, along with supports, are encoded. Corresponding data, shown here as energy-dispersive X-ray spectroscopy (EDS) spectra, are encoded separately. Encoded sources are fused before an entropy step resulting in chip level classification.

References:

- [1] JM Ede, Mach. Learn.: Sci. Technol. 2 (2021), p. 011004.
- [2] C Doty et al., Computational Materials Science 203 (2022), p. 111121.
- [3] M Olszta et al., Microscopy and Microanalysis 27(S1) (2021), p. 2986.
- [4] S Akers et al., npj Computational Materials 7(1) (2021), p.1.
- [5] This research was supported by the Energy Storage Materials Initiative/Investment (ESMI), under the Laboratory Directed Research and Development (LDRD) Program at Pacific Northwest National Laboratory (PNNL). Some code development was supported by the Chemical Dynamics Initiative/Investment (CDi), under the LDRD Program at PNNL. PNNL is a multi-program national laboratory operated for the U.S. Department of Energy (DOE) by Battelle Memorial Institute under Contract No. DE-AC05-76RL01830.