Physics- and AI-based Scanning Electron Microscopy

András E. Vladár, Hyeokmin Choe, Pushkar Sathe, and Peter Bajcsy
National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD 20899
andras@nist.gov

The tight integration of the physics of electron–matter interactions with artificial intelligence (AI) will revolutionize the scanning electron microscope (SEM) and enable the design and efficient use of new instruments that optimize image acquisition and analysis, as well as the speed at which key, actionable information is obtained. Many of the required building blocks, methods, and solutions are already available, so the time is now to establish this new technology comprehensively.

To determine the optimal image acquisition parameters, the physics-based SEM relies on highly accurate yet computationally intensive forward Monte Carlo simulations and models of signal generation as a function of beam landing energy, incident angle, sample geometry, material composition, and the detectors' energy- and trajectory-detection efficiencies.

Integrating AI into the SEM for image formation and enhancement, with optimized, pixel-level noise management, denoising, and super-resolution using convolutional neural networks, can deliver unprecedented quality in low-dose imaging and for sub-10-nanometer-scale sample features that inherently generate very small, noisy signals, even during high-speed measurements, especially when combined with sparse image acquisition and physics-based inpainting.

AI, combined with the physics of signal generation, is indispensable for solving inverse problems and excels at 3D reconstruction from multi-view or multi-energy SEM images. Deep learning models can effectively learn inverse mappings that are analytically intractable. AI enables real-time optimization of beam energy, current, scanning, and dwell time to automate region-of-interest discovery while balancing resolution, dose, and throughput. Together, these capabilities make SEM an active scientific instrument rather than a passive image-taking device.

To effectively use AI in SEM, large, relevant image sets are needed for training, testing, and validation. These images can be generated using Monte Carlo (MC) or analog simulators, enabling 100% repeatability while producing image sets that vary in noise, focus, stigma, vibration, drift, etc. NIST has recently developed a new 3D analog simulation method that can generate images orders of magnitude faster than rigorous MC. Figure 1 shows an example. Public-domain SW (Blender) is used to define the 3D structure. The accuracy of these images can be enhanced using some MC-calculated inputs.

Results of AI-SEM integration, sparse scanning, and methods for generating MC- and analog-simulation SEM image sets for AI will be presented.

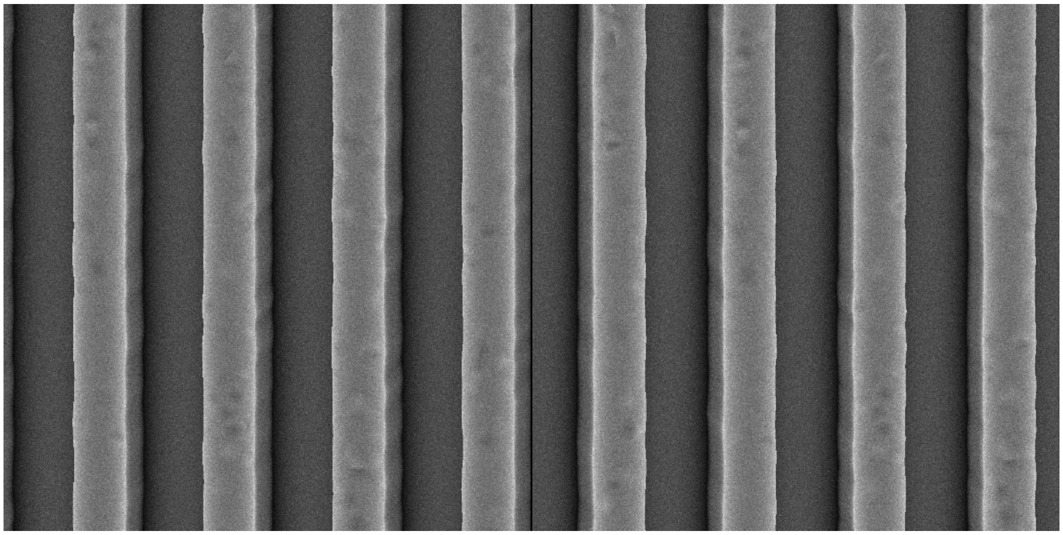

Figure 1. 3D SEM images of amorphous Si integrated-circuit lines with -10- and +10-degree tilt, generated by the NIST analog simulation method. The pitch and 3D structure (top and bottom widths, height, corner rounding, edge roughness, and surface roughness) of the lines, as well as the incident angle of the primary electron beam, can be easily varied. With these “seed” images, sets of images varying in noise, blur, stigma, etc., can be generated in a matter of minutes for AI purposes.