Karlsruhe Institute of Technology

Institute for Automation and Applied Informatics

Automation for Laboratories (ATLAS)

Machine Learning for High Throughput and Mechatronics (ML4HOME)

Uncertainty-aware particle segmentation for electron microscopy at varied length scales

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Abstract

Scanning Electron Microscopes (SEMs) are commonly used in materials research, but automating particle identification and morphology analysis in SEM images is challenging. In this work, we use Mask R-CNN to develop a new method for automated segmentation of particles in SEM images. We tackle measurement challenges like image blur, particle clumping, and prediction uncertainty. To handle varying length scales we create two models, separately trained for low and high magnification images. Our approach to particle segmentation surpasses traditional U-Net models when tested on various inorganic samples and achieves comparable accuracy to domain experts in a fraction of the time. These findings highlight the potential of deep learning in advancing autonomous workflows for materials characterization.

Motivation

- Electron microscopy reveals atomic-level material details.
- SEMs are commonplace for identifying particles (segmentation) [1].
- Usually, U-Net is used for segmentation [2].
- Recent studies explore Mask R-CNN's potential in biomedicine [3].
- We evaluate Mask R-CNN for SEM segmentation tasks and propose an uncertainty-aware enhancement for particle detection.

Dataset

- 90 images of 10 different compound samples.
- Low magnification: <10,000× magnification (1920×1200 px).
- High magnification: >10,000× magnification (7680×4800 px).
- Labeled by domain experts with uncertainty quantification (Fig. 1).

Neural Network

- Optimized for microscopy data with overlapping particles (Fig. 2).
- Novel uncertainty head for each detected object.

Results

- Mask R-CNN has a clear advantage over U-Net (Fig. 3 and Fig.4).
- U-Net detects particles by brightness and fails with blurry images.
- Mask R-CNN recognizes particle structure even with heavy blur.
- Strong correlation between predicted confidence and labels (Fig. 5).
- Confirmed by visual evaluation (Fig. 6).
- Mask R-CNN's ability for particle size estimation is assessed against human experts (Fig. 7).
- Previously unseen $LiCoO_2$ power is evaluated.
- Domain experts show substantial variation.
- Mask R-CNN labels images remarkably faster than humans.
- Mask R-CNN results align with the expected $LiCoO_2$ powder size.

Conclusion

- Mask R-CNN excels in handling blurry and overlapping instances.
- ML models provide significantly faster image interpretation and enhanced consistency compared to domain experts.

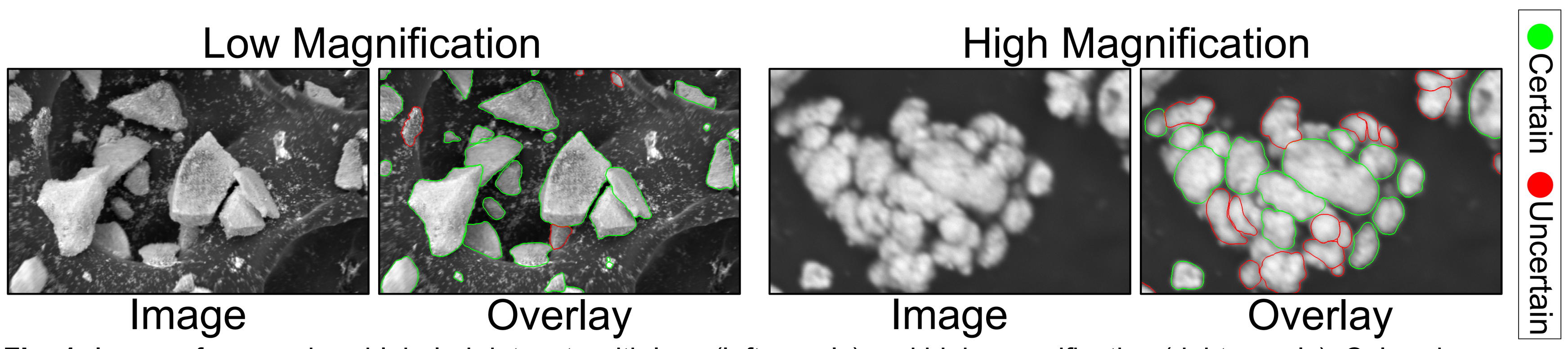

Fig. 1: Images from our hand-labeled datasets with low- (left panels) and high-magnification (right panels). Colored curves represent particle boundaries outlined by domain experts, with green indicating high-confidence labels and red denoting low confidence.

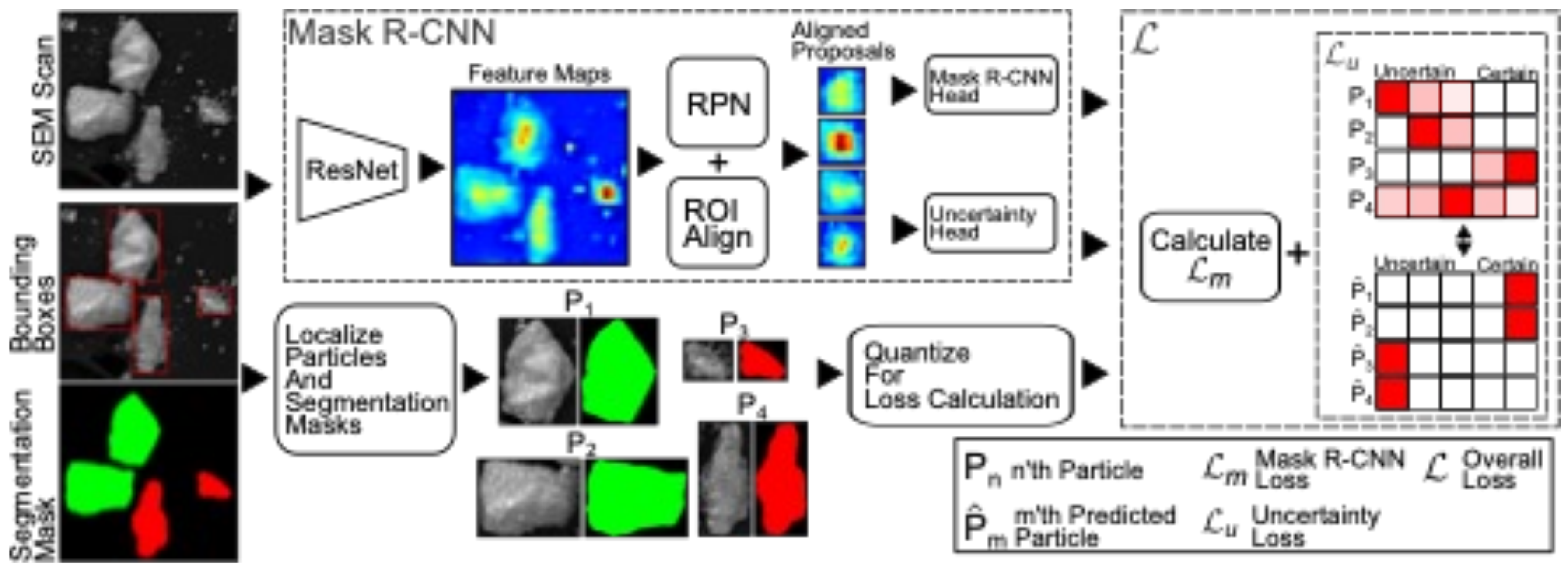

Fig. 2: Mask R-CNN uses a ResNet-50 backbone to extract feature maps from SEM scans. The RPN generates ROIs, which are aligned to a consistent size. The Mask R-CNN and uncertainty heads process these proposals for predictions. Ground-truth bounding boxes and masks are converted to numerical values, and both Mask R-CNN and uncertainty losses are computed and combined to yield the overall loss.

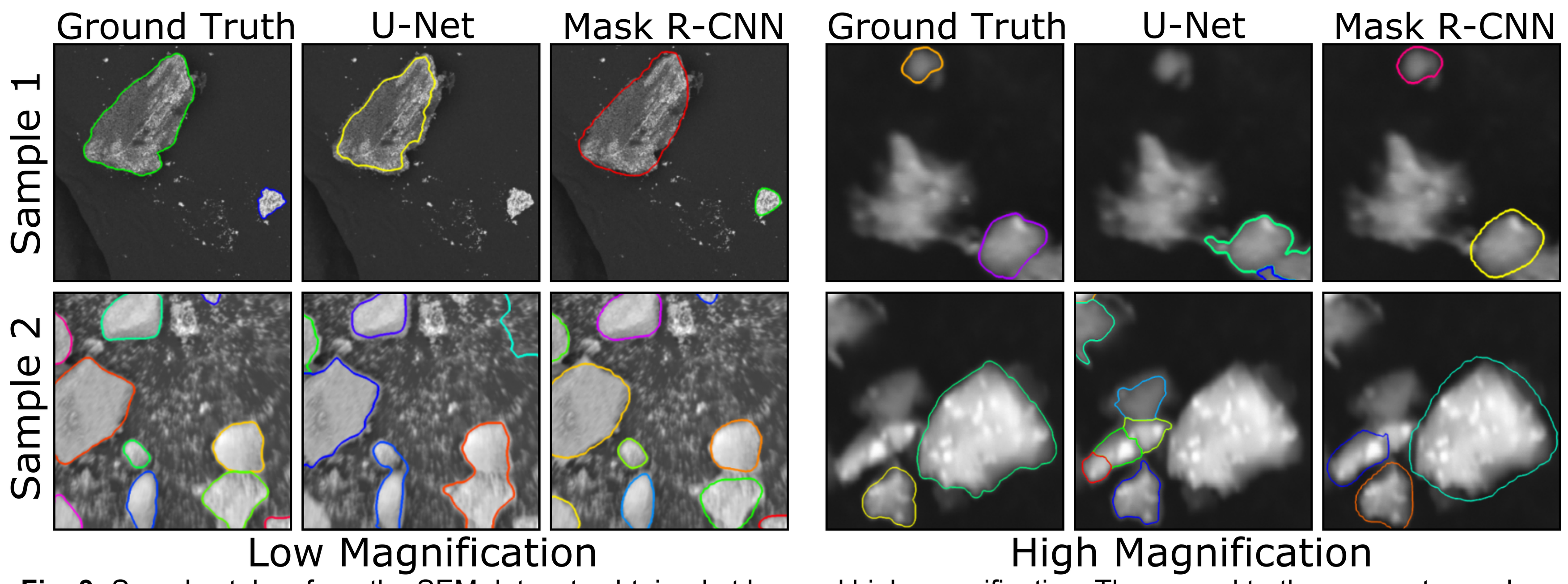

Fig. 3: Samples taken from the SEM datasets obtained at low and high magnification. The ground truth represents overlays that were manually created by domain experts. Overlays predicted by U-Net and Mask R-CNN models are also shown.

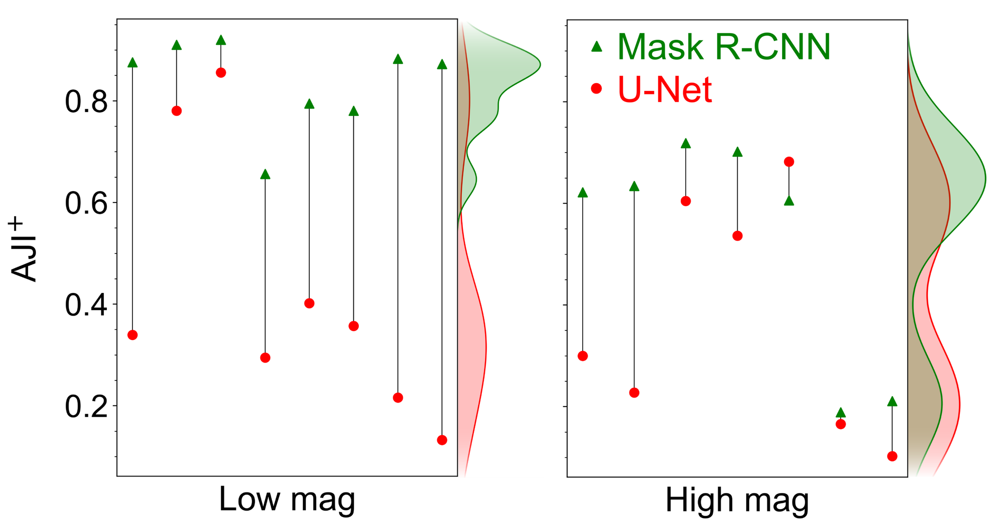

Fig. 4: The AJI+ metric applied to SEM images obtained at low (left panel) and high magnification (right panel). Results from the same image are linked with a black line. A density representation is shown on the right axis of each panel.

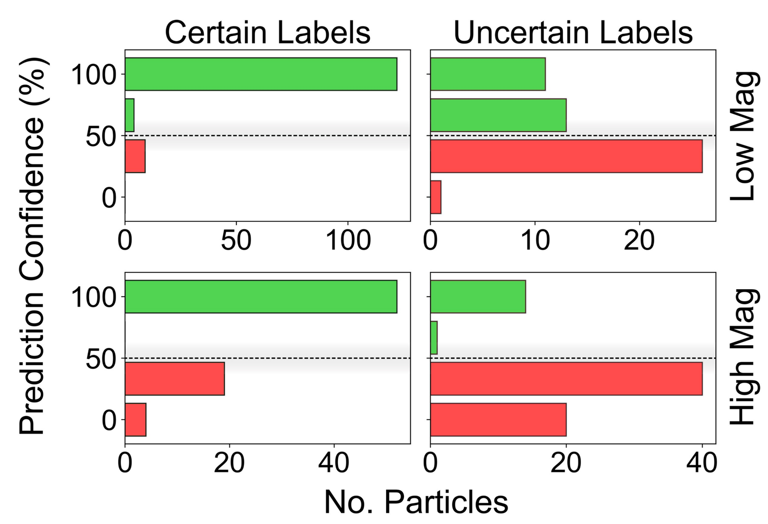

Fig. 5: Mask R-CNN confidence on low and high magnification images for "Certain" and "Uncertain" particles. Left panels: particles that were labeled as "Certain", right panels: particles labeled "Uncertain".

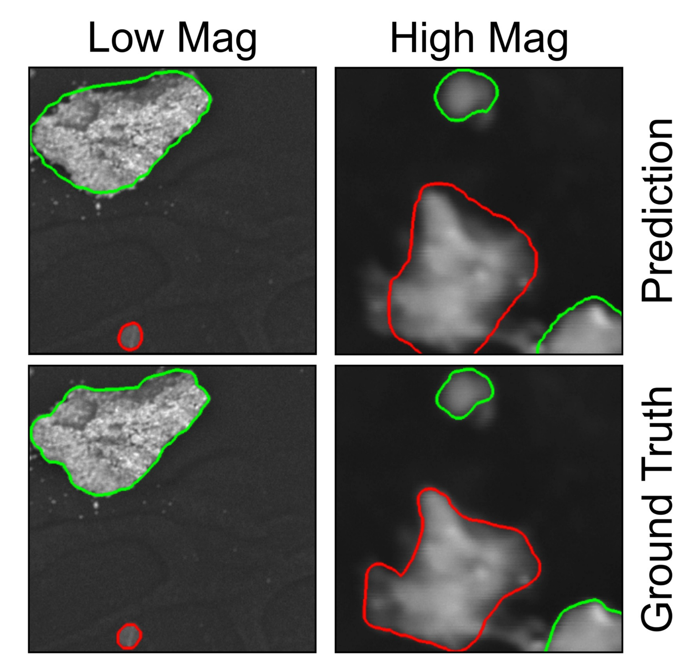

Fig. 6: Samples segmented by the Mask R-CNN. For comparison, the labels provided by domain experts are shown in the bottom panels. Red curves indicate uncertain and green curves certain particles.

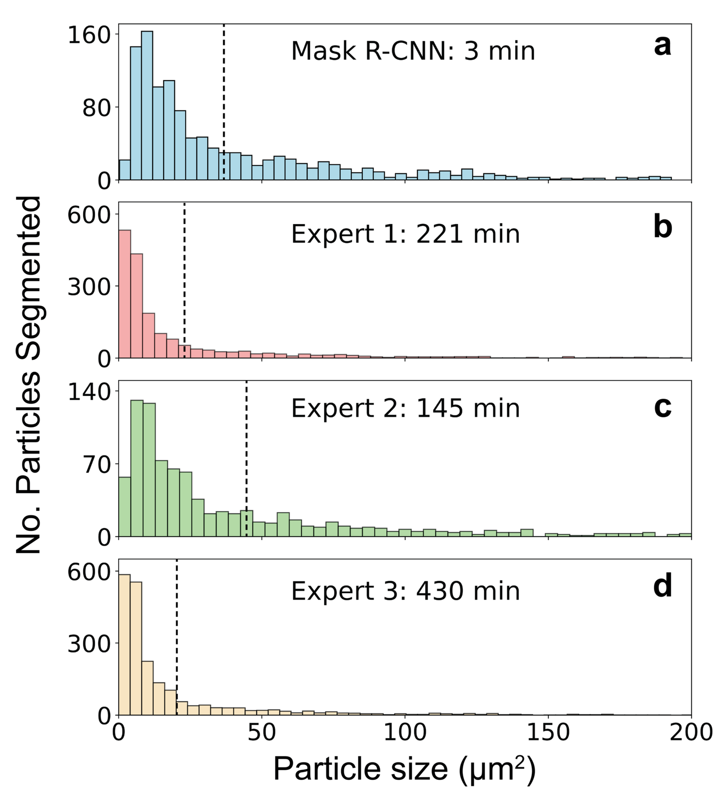

Fig .7: Size distribution of particles that were segmented by (a) the Mask R-CNN model and (b-d) three separate domain experts.

References

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[3]: Rettenberger, Luca, et al. "Mask R-CNN Outperforms U-Net in Instance Segmentation for Overlapping Cells." Current Directions in Biomedical Engineering. Vol. 9. No. 1. De Gruyter, 2023.