

A deep learned nanowire segmentation model using synthetic data augmentation

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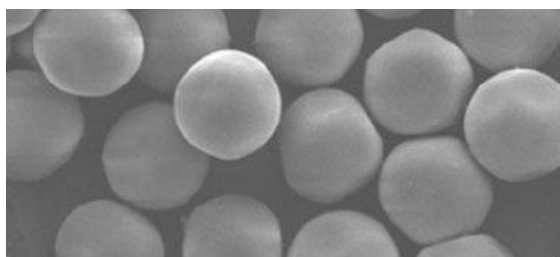
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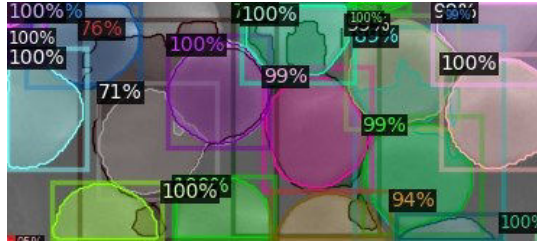
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Supplementary Note 1: Additional information on the extension of the deep learning model to account further instance classes

In the present work, the model presented leverages a pre-trained machine learning model that is trained on the large-scale COCO-Dataset with classes and labels of common daily objects. Based on the pretrained weights (for which the algorithm already has learned some general sense of features of objects with various shapes), we fine-tune and optimize the network by introducing the information of optical density-based synthetic nanowire data. This way effectively adds additional constraints in the network training and reinforces the model to learn the newly introduced training data of nanowires. Adding a new class of objects is relatively cheap in terms of computing time, especially with our given synthetic data generation workflow. The nanowires in real images, as in STXM and SEM images, are not exactly regular and straight nanowires, compared to the synthetic dataset. However, the trained algorithm is capable of segmenting non-regular instances, demonstrating the functionality of the present approach. Below we further show a test case for non-nanowire objects with our interactive web application: We see that the trained algorithm can detect spherical objects, by segmentation foreground objects and differentiating the particle boundaries. The results are, of course, not sufficiently good in the overlapped regions, since the model was not trained on spherical particles and their overlaps. One could, therefore, include a training dataset of spherical particles for the model to learn a second class, namely, e.g., nanospheres to enhance the prediction of spherical objects.



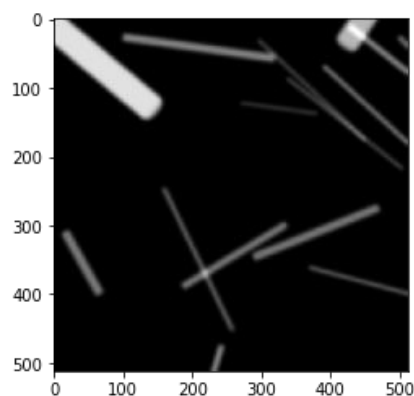
Supplementary Figure 1. Example SEM image of spherical particles with touching boundaries. We note here that the overlapped areas are not visible as in our optical density-based image dataset.



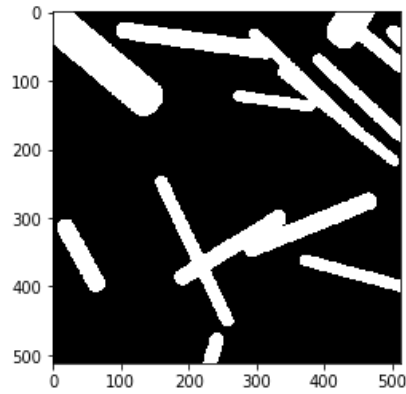
Supplementary Figure 2. Instance segmented image using the current model based on the synthetic dataset of nanowires. The results are not sufficiently good in the overlapped regions; However, the shapes of spheres are well captured. Including further training dataset of spherical objects in the synthetic training dataset can be instrumental to achieve a better performance, especially at the touching boundaries.

Supplementary Note 2: Exemplary segmentation results using Watershed algorithm

The watershed algorithm usually performs well at instance segmentation of similar **touching** objects, where the overlaps are not strictly visible unlike in our optical density-based images. Furthermore, one must firstly segment the foreground information, accompanying several steps of noise removals. Connected component labeling and distance transformation mapping have to be applied to provide initial marker areas (basins) for the watershed algorithm. Such steps can heavily involve manual tuning for complex microscopy images, counteracting efficient image analysis steps. Heavy manual preprocessing steps are spared in our approach by providing images containing different nanowires, that are labeled within noisy images, which can contain different sets of noise sources that are introduced in a synthetic manner. To provide some demonstrative cases using the watershed algorithm, we show below how a marker (connected-components-labeling) based watershed algorithm works on one of our relatively simple synthetic images following the OpenCV implementation in supplementary reference 1. The first step demonstrates the thresholding and segmentation of the foreground object.

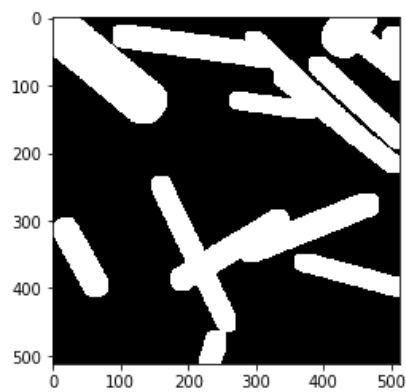


Supplementary Figure 3. Example of a simple synthetic image from our synthetic dataset with only few overlaps without any noises for testing purpose of the Watershed algorithm.

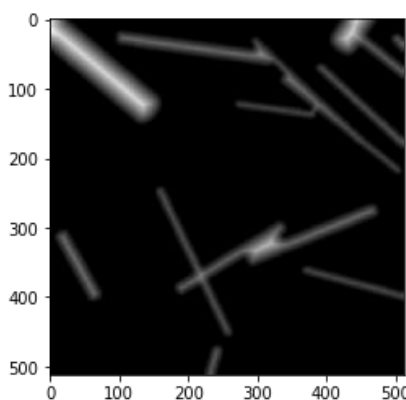


Supplementary Figure 4. Binary thresholding of the foreground nanowires from Supplementary Figure 3.

Further steps include dilate operation of thresholded image for further boundary marking, and distance transformation of foreground image.

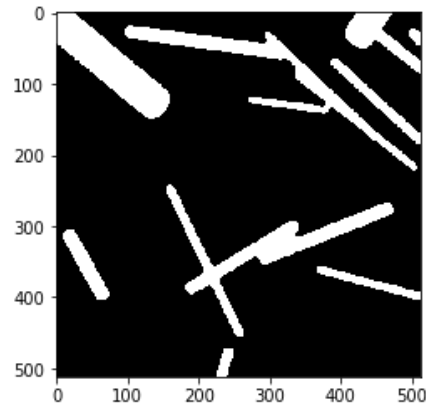


Supplementary Figure 5. Dilation of the thresholded image from Supplementary Figure 4. Dilation operation adds further pixels on the object boundary, which enlarges the object.

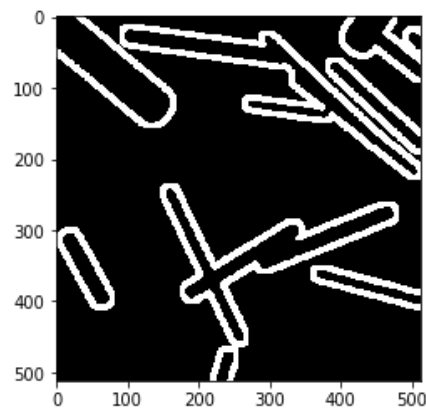


Supplementary Figure 6. Distance transformation of the previous image. Distance transformation generally maps the distance of the foreground object to its surrounding background.

Then we threshold the distance transformed image to extract the sure foreground image and subtract it with the dilated image to get the particle boundaries.

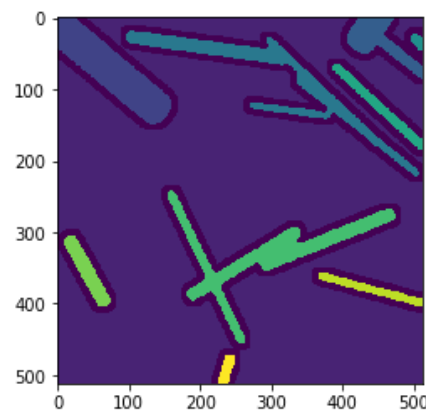


Supplementary Figure 7. Threshold of the distance transformed image to extract the sure foreground image as basis.

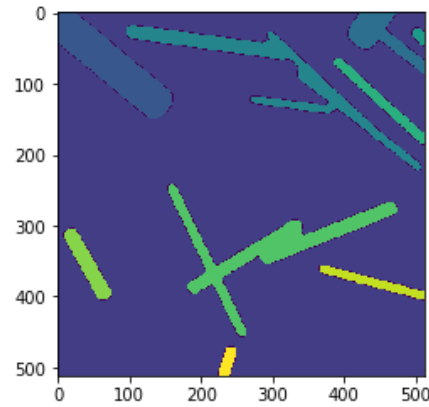


Supplementary Figure 8. Particle boundary extraction by subtract the sure foreground image in Supplementary Figure 7 from dilated image in Supplementary Figure 5.

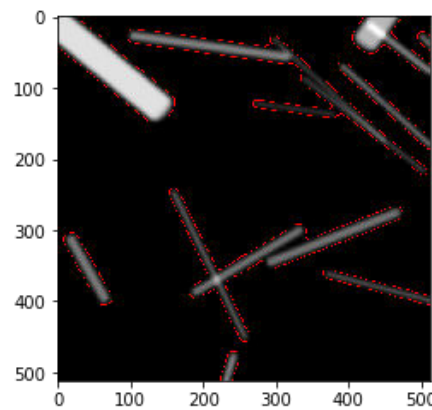
We further performed the connected component labeling algorithm to the sure foreground image and the obtained information served as a marker for the watershed algorithm. The obtained results are shown below:



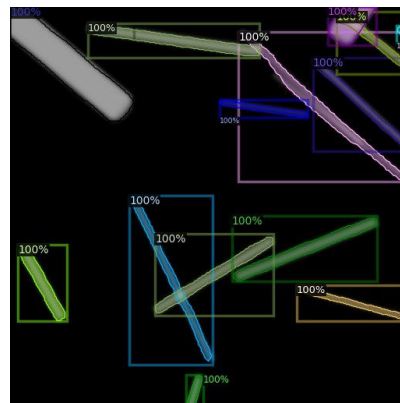
Supplementary Figure 9. Connected-Component-Labeling is performed for Supplementary Figure 8. The algorithm basically finds and marks the individually closed particle boundaries and assigns them consecutive numbers to determine different instances.



Supplementary Figure 10. Final mask image after application of Watershed algorithm with individual instances masked with different color scheme.



Supplementary Figure 11. Final boundaries of individually marked instances.



Supplementary Figure 12. Our model prediction with bounding boxes and masks in color. All overlapped nanowires are successfully detected and segmented as individual instances.

Looking at the results using the aforementioned procedure with a Watershed algorithm, it is clear that using a watershed algorithm -that relies on distance map as markers- is not sufficient at detecting overlapping nanowires, while it performs well for isolated ones. The issue lies in the pixels in the boundary regions, which are not clearly defined for the Watershed through the distance map. This could lead to false segmentation in complex microscopy images, where the boundaries can be blurred by limited spatial resolution, particle defects, and overlapping regions. Our synthetic data model can detect overlapped objects (for which it is trained to do so), whereas traditional algorithms

such as thresholding + connected component analysis are unable to accomplish this objective. The Watershed algorithm can indeed separate touching structures; however, it tends to overestimate/underestimate the boundary in real microscopy images and is prone to noise contamination, with additional preprocessing steps that need to be carried out in advance. However, it must be mentioned that further markers can be used for the watershed algorithm, including manual annotation, which might improve the segmentation results presented above.

Supplementary Note 3: Training results with a small set of real images included

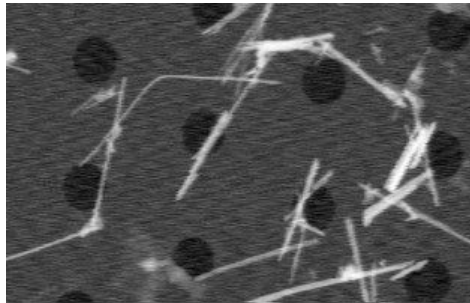
A model has been trained utilizing experimentally generated images. One of the main limitations arises from the limited number of images that can be generated with sufficient variability to train a model. Since the experimental data are limited and hard to label, we included 36 images derived from one real ptychography image, which was cropped in 9 smaller images and augmented with 3 times of 90% rotation each step. This dataset was included additionally into the training dataset size of 500 images for our model training. Adding a small amount of experimental data to the synthetic data in the training stage resulted in a negligible change in terms of AP performance within the large number of training dataset sizes. The difference in AP was within the margin of error (The AP dropped around 0.25), therefore we did not include any of the real images into the training dataset, instead, we used a pure synthetic data set to train our model.

Supplementary Note 4: Training results with smaller learning rates

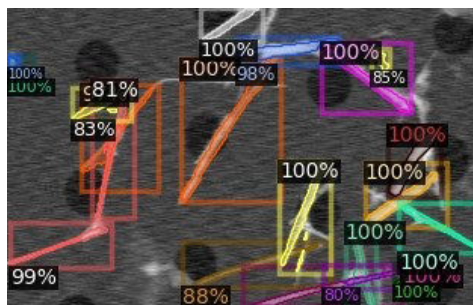
In the present work, the model presented leverages a pre-trained machine learning model that is trained on the large-scale COCO-Dataset with classes and labels of common daily objects. Based on the pre-trained weights, we optimize the network by introducing the information of optical density-based synthetic nanowire data. Such a way effectively adds additional constraints in the network training and reinforces the model to learn the newly introduced training data of nanowires. Therefore, in contrast to training a new network from scratch, where an extremely large dataset would be needed, we chose a comparably larger learning rate of 0.01, 0.02, 0.03 for a certain number of epochs to see how the model reacts to our dataset. We found that with a learning rate of 0.02 and the corresponding epoch numbers and training dataset size, the model performs optimally in our case. To test the model how it reacts to smaller learning rates, we further additionally trained two models with learning rates of 0.005 and 0.001 while keeping other hyperparameters fixed. The resulting AP BOX/SEGM decreased roughly 3 for each synthetic, X-ray ptychography and STXM image and can be found in the supplementary table 1 of hyperparameter study results. The default hyperparameter setting of model #7, has been used to vary the learning rate of 0.005 and 0.001.

Supplementary Note 5: Further statistical results for exemplary image samples

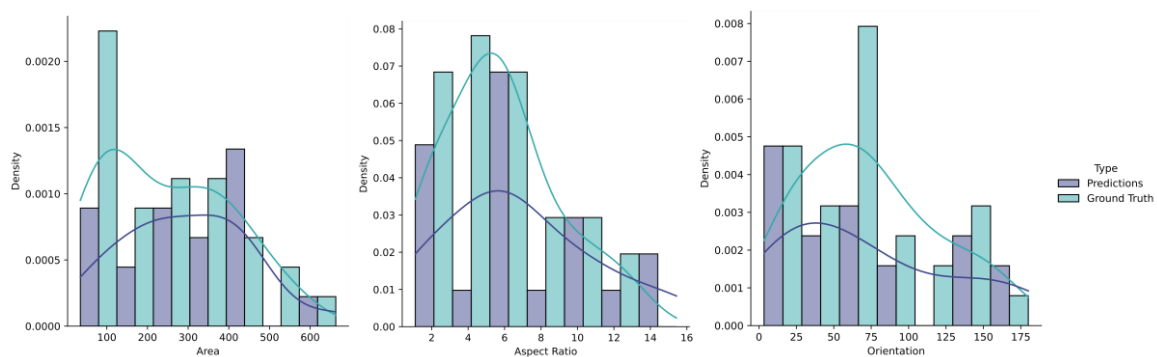
In the following, more STXM and SEM segmentation samples are presented along with the corresponding statistics. This is facilitated using our developed web-based interactive segmentation tool.



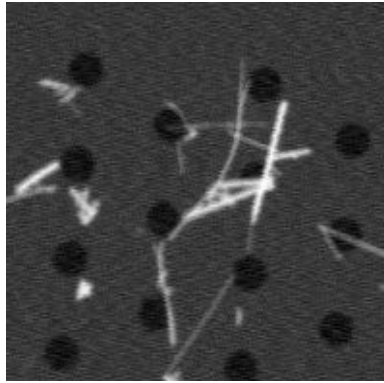
Supplementary Figure 13. A sample STXM image on substrate.



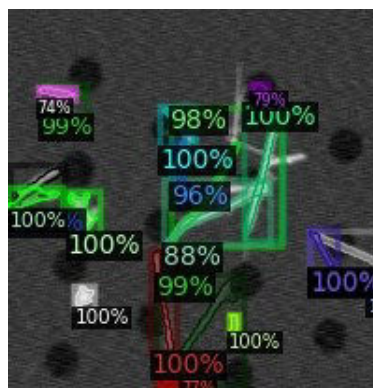
Supplementary Figure 14. Model prediction results on the sample image; The model results here are even insensitive to the substrate with black holes in the background and can predict the nanowires, including overlaps across the substrate holes. The long, curved nanowire, as well as some densely connected nanowires have not been well segmented, leading therefore to statistical deviations as shown in the following statistics.



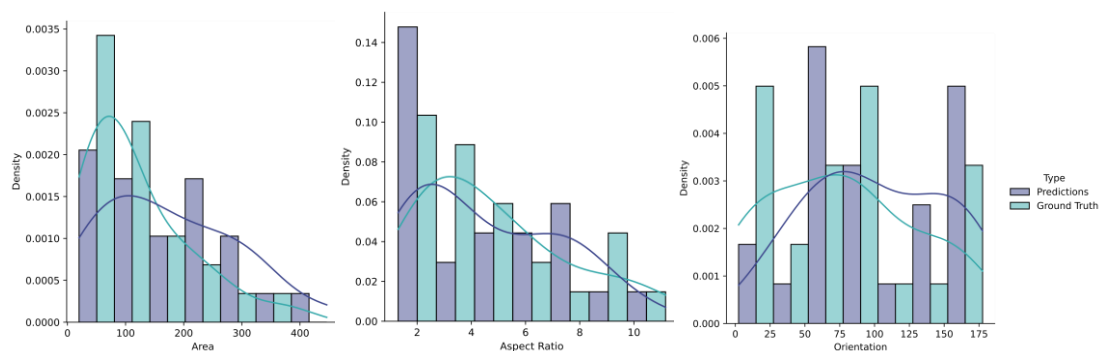
Supplementary Figure 15. Statistics from the exemplary image with histogram and KDE curves as functions of particle area size, aspect ratio, and relative orientation to horizontal axis.



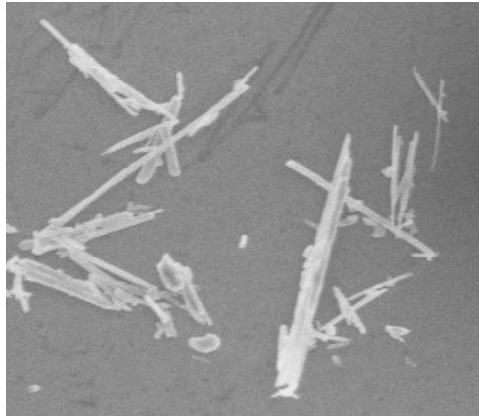
Supplementary Figure 16. Another sample STXM image on substrate.



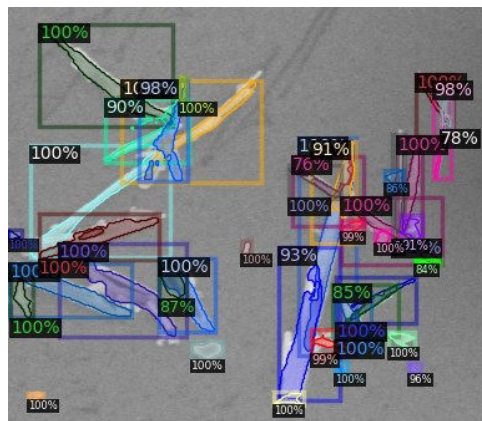
Supplementary Figure 17. Model prediction results on the sample image; The model results here are again insensitive to the substrate with black holes in the background and can predict the nanowires, including overlaps across the substrate holes. The model predicts this image to a great extent. The results are in qualitative and quantitative agreement. Little inconsistency still exists for small, densely nanowires in the left regions, where multiple particles are predicted as one. However due to the low resolution of the image, visual evaluation is difficult and will not be further elaborated.



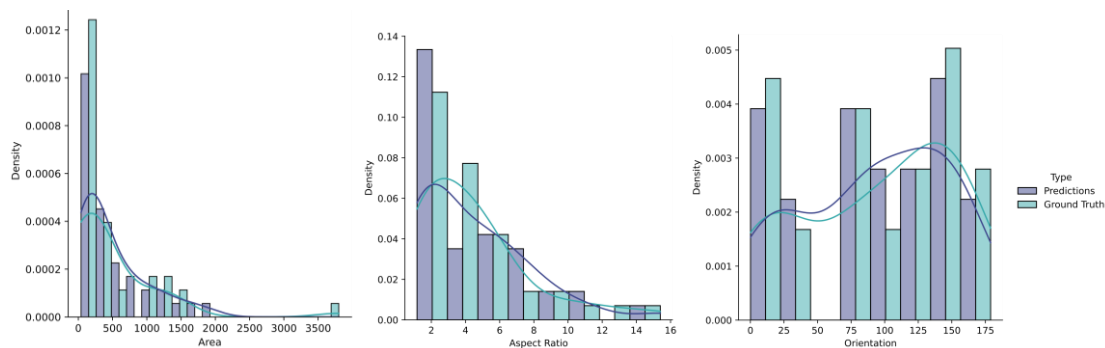
Supplementary Figure 18. Statistics from the exemplary image with histogram and KDE curves as functions of particle area size, aspect ratio, and relative orientation to horizontal axis. Higher density in the ground truth is observed in the respective number ranges due to manual separations of smaller nanowires, where the model predicts multiple nanowires as one single instance, presumably due to the comparably lower resolution of the image.



Supplementary Figure 19. A sample SEM image.



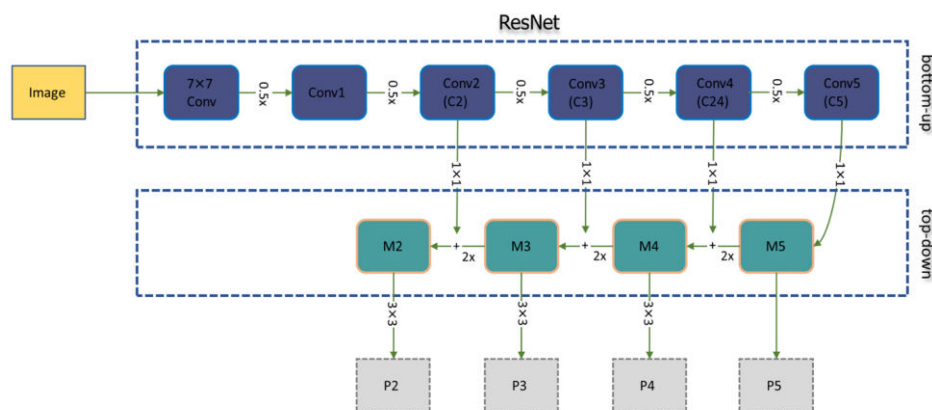
Supplementary Figure 20. Model prediction for the sample image; upon visual assessment, multiple nanowires are attached and melted together. This complicates the model prediction. The isolated, as well as cross orientated nanowires are well captured, whereas the attached nanowires are segmented as single instances and to less satisfaction.



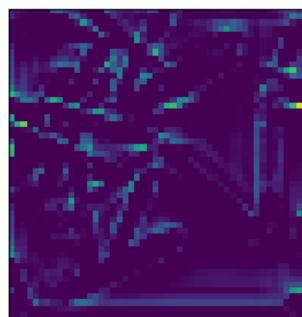
Supplementary Figure 21. Statistics from the SEM image. The statistical results show good qualitative, and quantitative agreement for the SEM image, but smoothed out in presence of many nanowires. Underestimation of the model leads to fewer number of nanowires thus leading to minor deviation in the statistics.

Supplementary Note 6: Details on the FPN Backbone

One of the main problems in object detection is detecting objects at different scales mainly for small objects. Image pyramids [2] were introduced by using the image at different scales to detect objects. This method comes with a significant cost in time and memory for end-to-end training. An alternative for this method is to use a pyramid of feature maps rather than the image, which enables object detection in a wide range of scales. These feature pyramids are considered scale-invariant since the object's scale is offset by shifting the level of the pyramid [3]. FPN is then constructed of two pathways, a bottom-up and a top-down pathway [3]. The bottom-up pathway is the well-known ConvNets, known for feature extractions, which encode the image to low-resolution feature maps with increasing semantic features and detecting high-level structures when going up (see supplementary figure 22). This part constructs the backbone of FPN which is usually different variants of Residual networks (ResNet) [4]. The top-down path constructs layers with higher spatial resolutions while combining the enriched semantic features of the bottom-up layers to lead final feature maps for further instance segmentation.



Supplementary Figure 22. General architecture of feature pyramid network with ResNet as backbone, redrawn based on [5]; The bottom-up path constructs layer with decreasing spatial scale (illustrated with 0.5x) with increasing semantic feature from C1-C5 layer, the top-down path M5-M2 constructs layers with increasing spatial resolution (illustrated with 2x) and combines the low-resolution, but high semantic features from bottom-up path (1x1) to create final feature maps (3x3), more details can be found in [3]



Supplementary Figure 23. A feature map from P3 level shown after the operation.

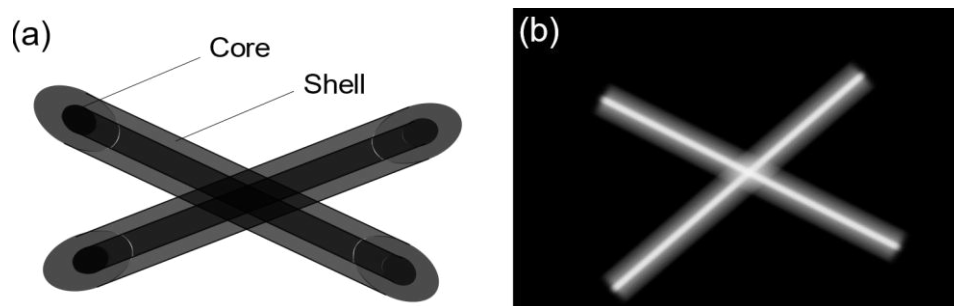
Supplementary Note 7: Additional information on model training/prediction speed

The time for generation is, after building the workflow, to a neglectable extent. The ML algorithm is purely trained on this dataset with a pre-trained network structure and backbone and took 5 to 10 hours (depending on the epoch numbers and dataset size) on four A100 Tesla cards.

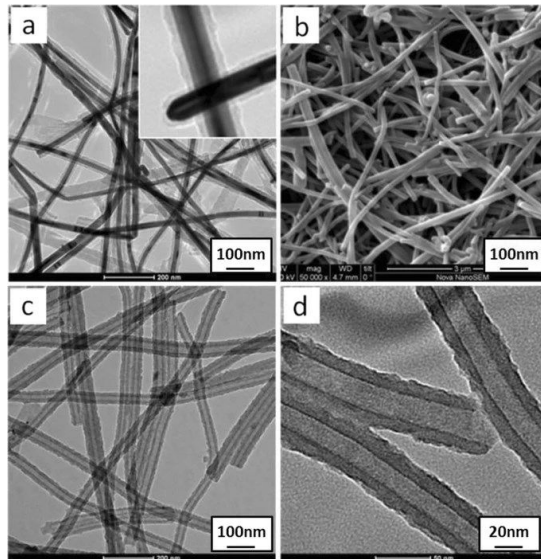
Regarding the speed performance, for comparison, ground truths are generated by human labeling, taking approx. tens of seconds for one nanowire, depending on the resolution of the image and coarseness of polygons (i.e, for a circular object, numbers of straight lines that are used to approximate the object) drawn on the instance object. The steps within human labeling using MakeSense.AI include uploading the desired image and drawing polygons around the instance. If multiple instances are available, multiple polygons are independently drawn. Ideally, the number of polygons drawn is equal to the particles visible in the image. After masking the instances, polygons are exported for further post-processing as determination of area size, orientation, or aspect ratios. The above steps would result in tens of seconds up to minutes for one image. Regarding this point, ML-method outperforms human segmentation, especially when it comes to large-scale, multi-particle, and low contrast images. The current inference speed, run on a CPU (AMD ryzen 3700x) is 3.4 seconds and on a GPU (RTX 2070 super) is 1.2 seconds plus post-processing steps of 1-2 seconds.

Supplementary Note 8: Additional information on extension of the current model to segmentation of coaxial or hierarchical structures

In principle, the framework is not bound to any specific structures if the structures can be created or synthesized. Based on the example of a STXM image, which maps the nanowires into optical intensity values, the synthetic image can be generated by creating coaxial, or hierarchical structures, for example, a core-shell nanowire of different materials, see illustration in the Supplementary Figure 23. Performing the optical density compression step as mentioned in the manuscript, we believe that our approach can be applied to real STXM, SEM images of coaxial structures as in Supplementary figure 25 [6] as well.



Supplementary Figure 24. (a) Illustration on generating synthetic data for coaxial core-shell nanowires (b) Illustration of optical intensity-based mapping step



Supplementary Figure 25. Example microscopy images of typical coaxial nanocomposites from [6]

Supplementary table 1:

AP BBOX

#	Epoch	LR	ROI head	Dataset	NMS	IOU	Synthetic Dataset							Ptychography							SXTM							SEM						
							AP	AP50	AP75	APs	APm	API	AP	AP50	AP75	APs	APm	API	AP	AP50	AP75	APs	APm	API	AP	AP50	AP75	APs	APm	API				
							1	250	0.02	256	250	0.7	0.6	89.442	96.027	93.853	82.205	92.259	77.576	36.566	60.935	37.33	21.04	47.024	82.525	27.267	54.404	23.423	25.228	37.774	nan	27.61	51.8	22.884
22*	500	0.005	256	750	0.7	0.6	90.951	93.719	93.627	85.161	93.16	79.148	36.092	61.201	39.678	22.716	42.525	72.667	26.386	51.151	24.184	18.439	47.485	nan	20.639	50.073	15.423	13.56	40.777	13.175				

AP SEGM MASK

#	Epoch	LR	ROI head	Dataset	NMS	IOU	Synthetic Dataset							Ptychography							SXTM							SEM						
							AP	AP50	AP75	APs	APm	API	AP	AP50	AP75	APs	APm	API	AP	AP50	AP75	APs	APm	API	AP	AP50	AP75	APs	APm	API				
							1	250	0.02	256	250	0.7	0.6	87.392	96.013	93.628	86.179	88.027	89.052	38.091	57.648	37.33	18.274	47.283	85.05	21.791	51.877	17.587	20.862	28.877	nan	12.927	23.126	5.206
22*	500	0.005	256	750	0.7	0.6	87.532	93.718	93.523	88.209	87.687	85.867	36.179	60.384	39.678	24.404	48.188	67.701	18.484	46.484	17.308	12.417	34.034	nan	8.786	29.386	0.054	5.45	18.13	7.521				

Supplementary reference:

1. OpenCV documentation, https://docs.opencv.org/4.x/d3/db4/tutorial_py_watershed.html.
2. Adelson, E. H., Anderson, C. H., Bergen, J. R., Burt, P. J. & Ogden, J. M. Pyramid methods in image processing. *RCA engineer* 29, 33–41 (1984).
3. Lin, T.-Y. et al. Feature pyramid networks for object detection. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, 2117–2125 (2017).
4. He, K., Zhang, X., Ren, S. & Sun, J. Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, 770–778 (2016).
5. Jonathan Hui. Understanding Feature Pyramid Networks for object detection (FPN) <https://jonathan-hui.medium.com/understanding-feature-pyramid-networks-for-object-detection-fpn-45b227b9106c>
6. Zhu, Hongmei, and Xuchuan Jiang. Development of a General Fabrication Strategy for Carbonaceous Noble Metal Nanocomposites with Photothermal Property. *Nanoscale research letters* 15.1, 1-11 (2020).

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