

Automated morphological analysis of cellulose nanocrystals

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University of Cambridge

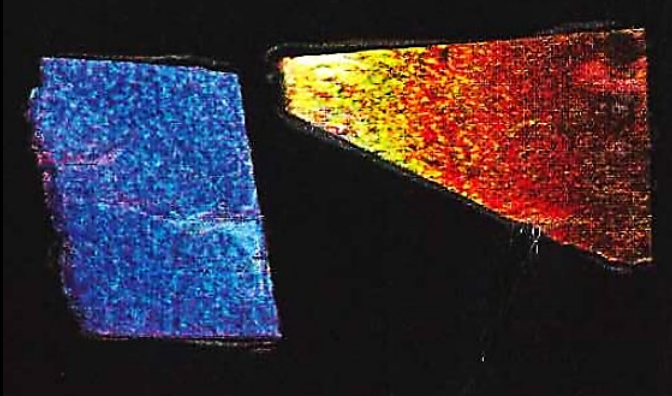


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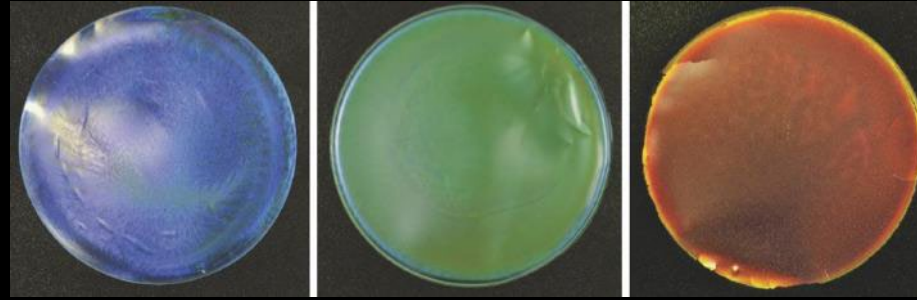


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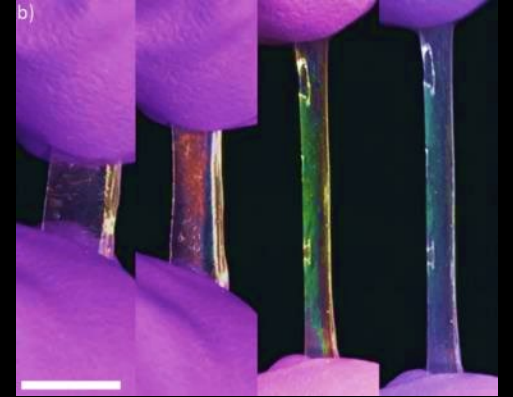
Structural colour using cellulose nanocrystals (CNCs)



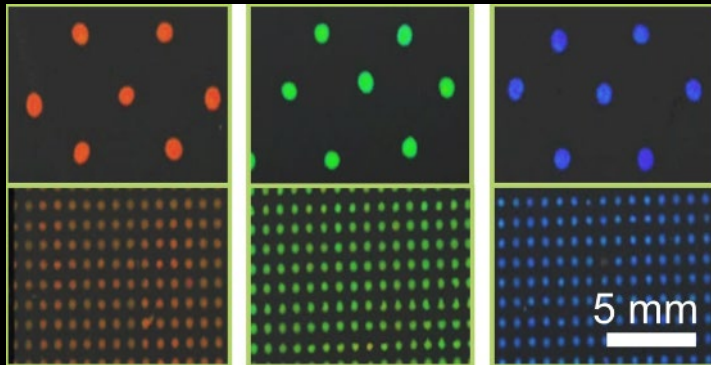
Revol, J.-F et al *J. Pulp Paper Sci.* **24**, 146–149 (1998).



Yao et al., *Adv. Mat.* **29**, 1701323 (2017).



Boott et al., *Angew. Chem. Int. Ed.* **59**, 226–231 (2020).



Zhao et al., *Adv. Func. Mat.* **29**, 1804531 (2019).



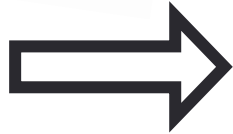
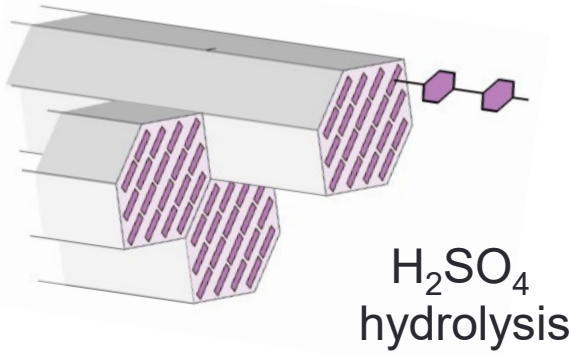
Droguet et al. *Nat. Mater.* **21**, 352–358 (2022).



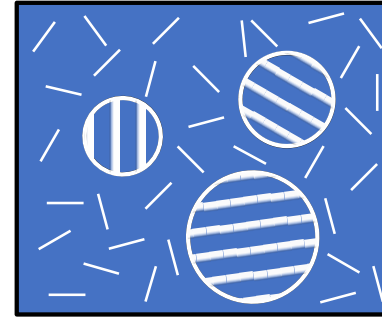
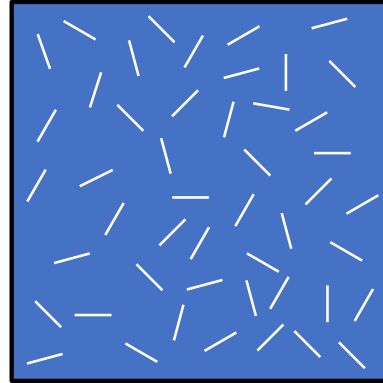
Parker et al., *Nat Commun* **13**, 3378 (2022).

CNC self-assembly for photonic films

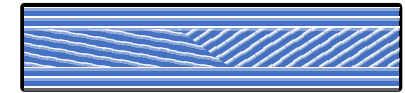
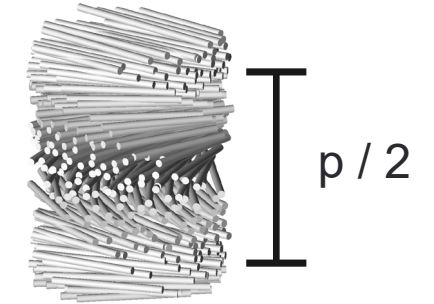
Native cellulose microfibrils



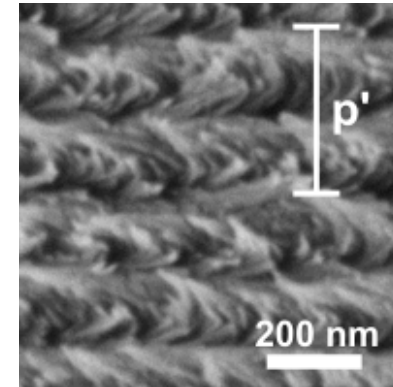
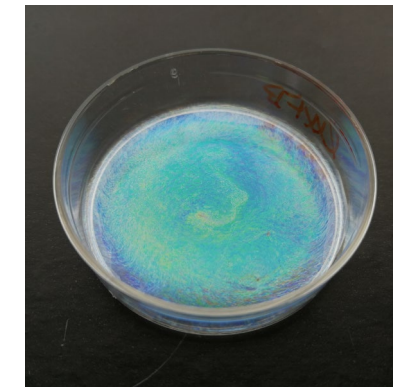
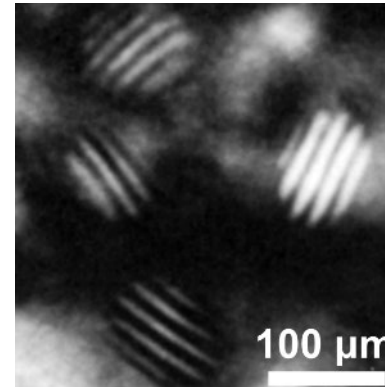
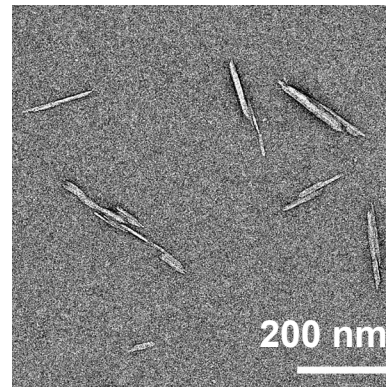
Chiral nematic (cholesteric) liquid crystal



CNC photonic films

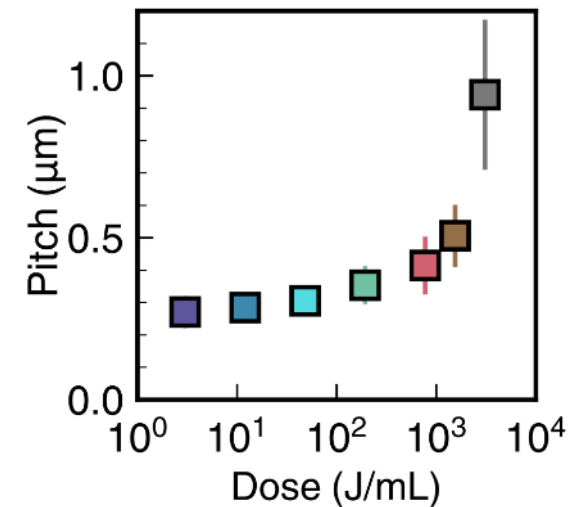
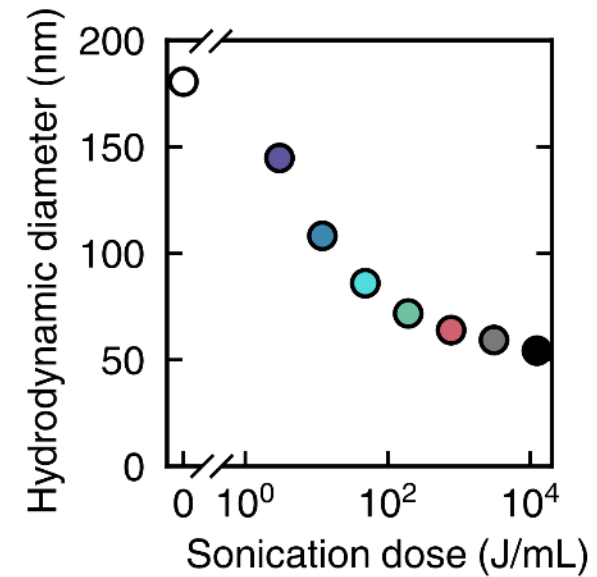
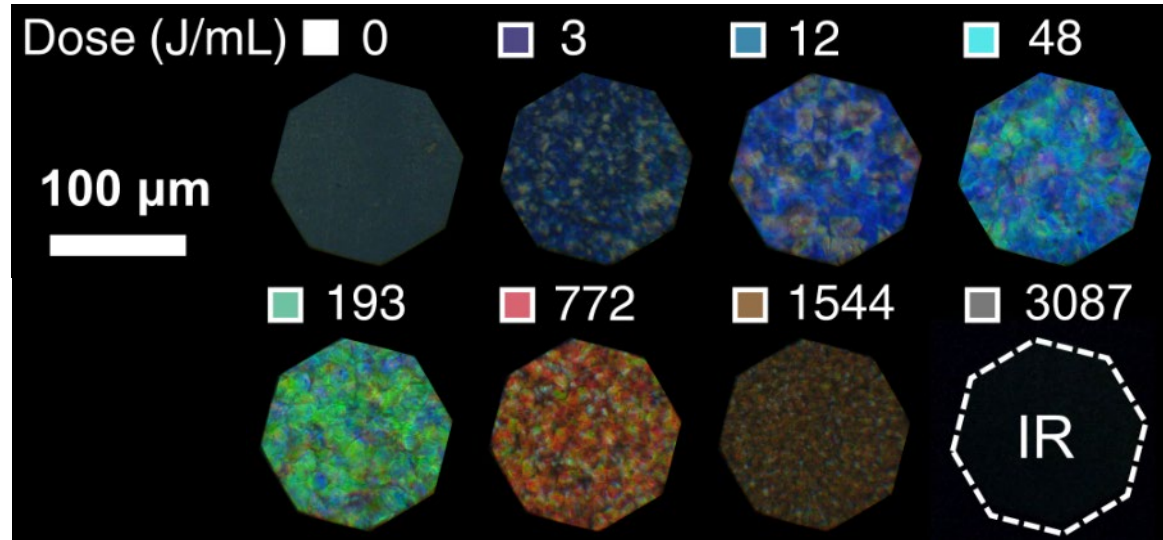
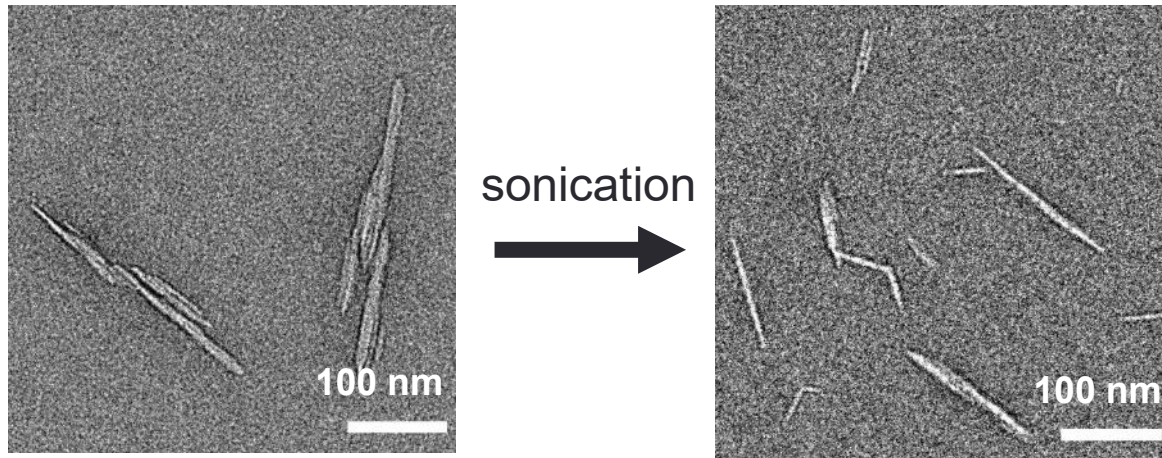


CNC concentration



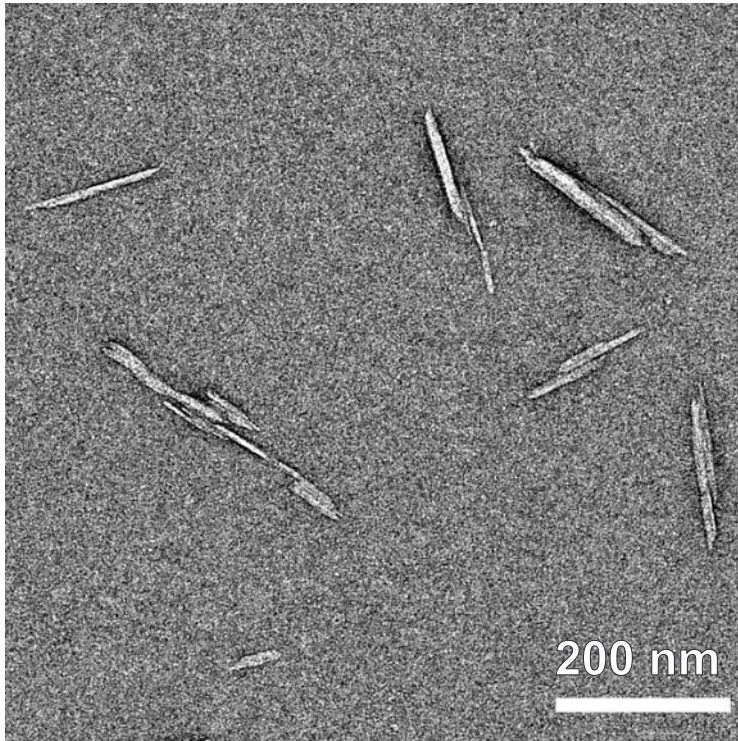
How does the final film colour relate to the initial formulation?

Ultrasonication increases the pitch and red-shifts film colour

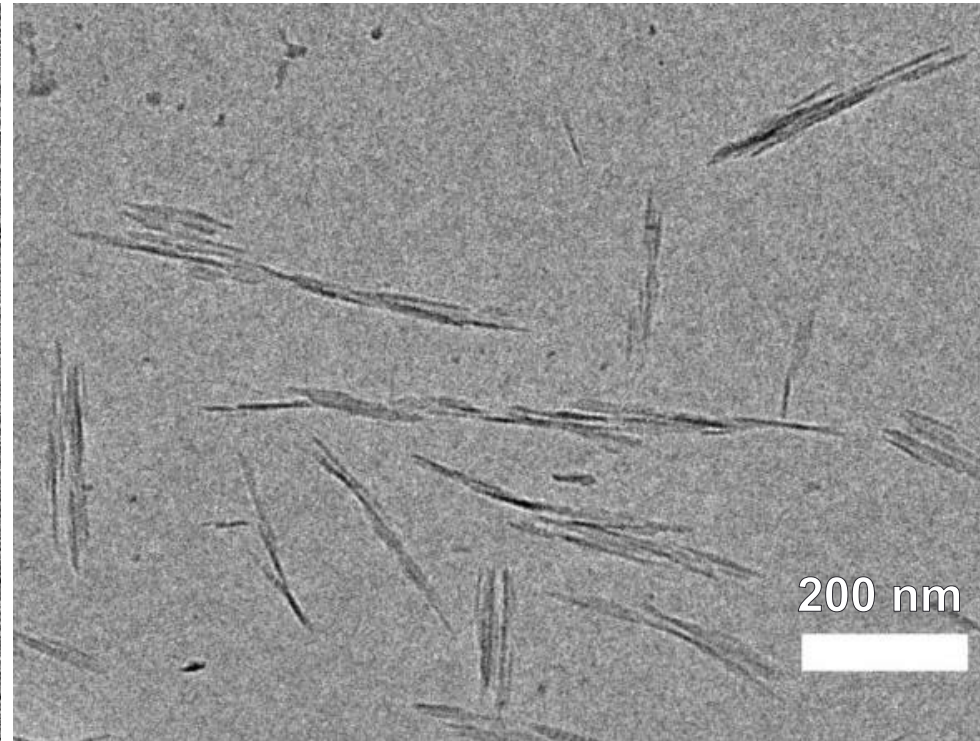


Many cotton CNCs have a native “bundle-y”, agglomerated structure

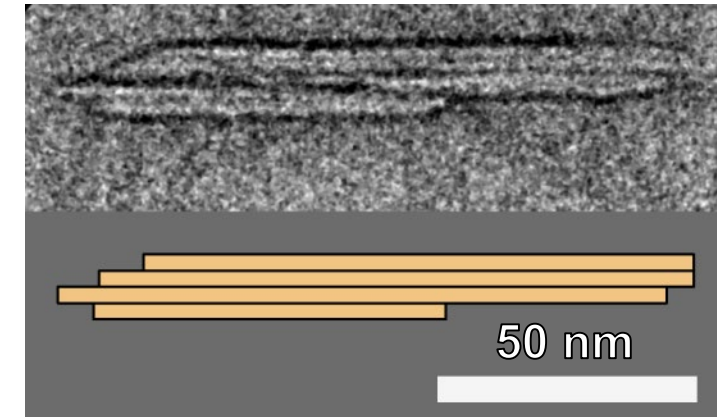
TEM



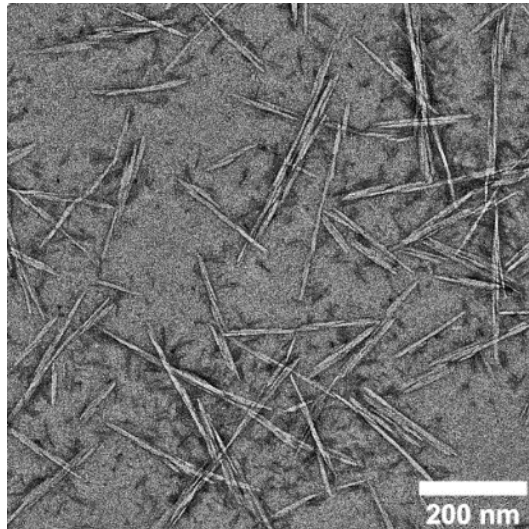
Cryo TEM



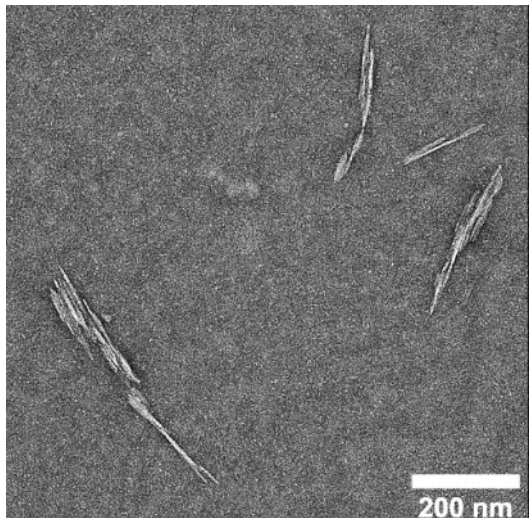
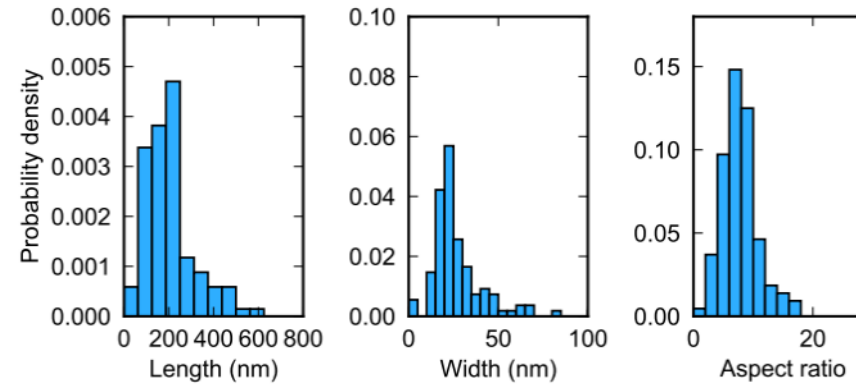
Composite multi-crystallite particles



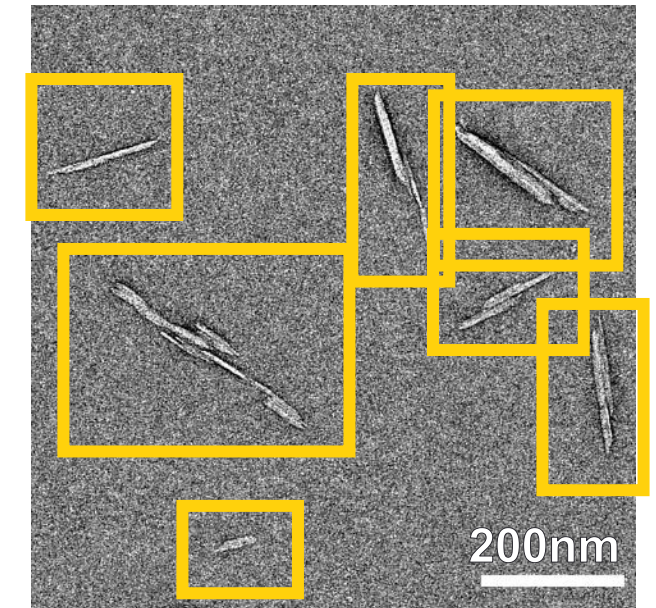
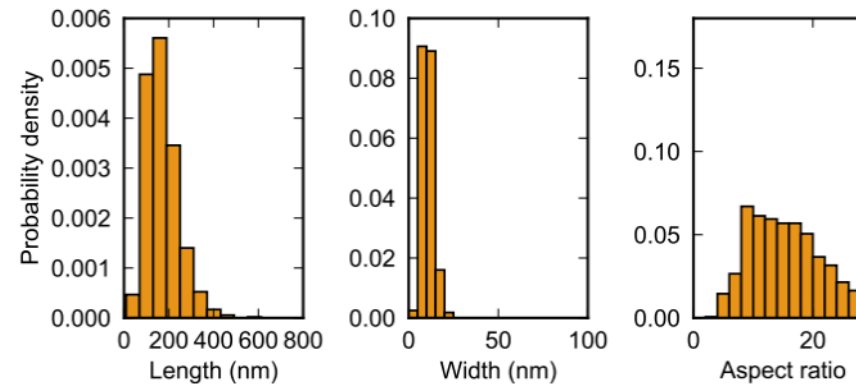
The subjectivity of manual CNC size measurements from TEM images



Researcher 1



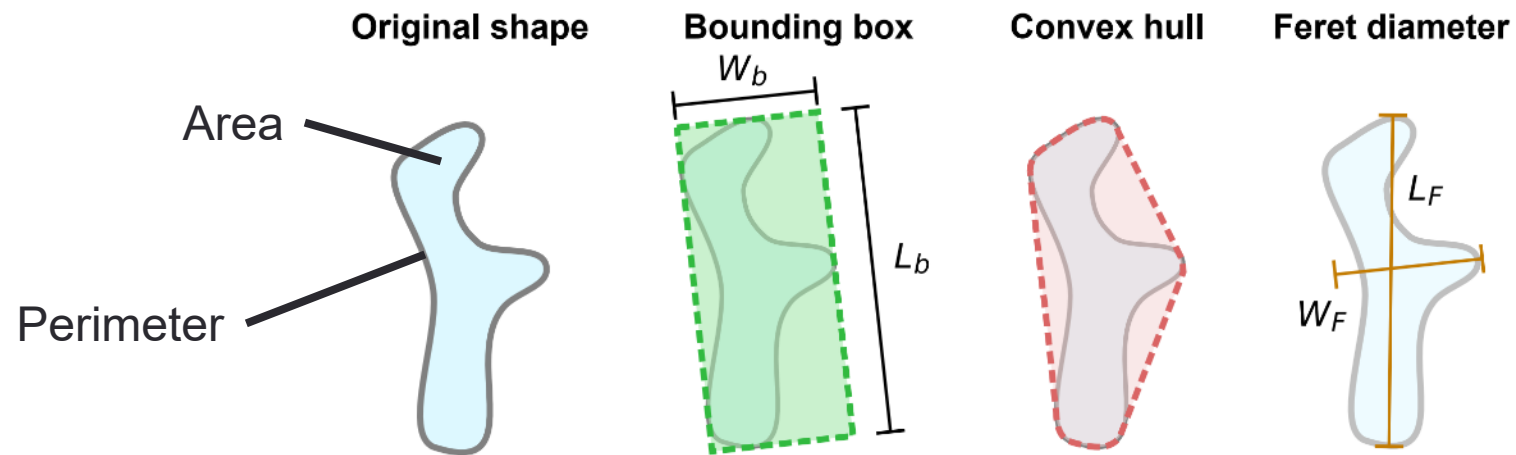
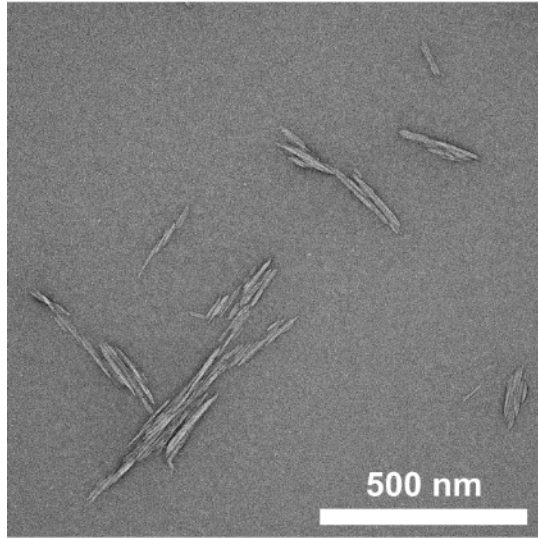
Researcher 2



Assume any distinct object = "CNC particle"

Extracting CNC morphology from TEM images

Original TEM image



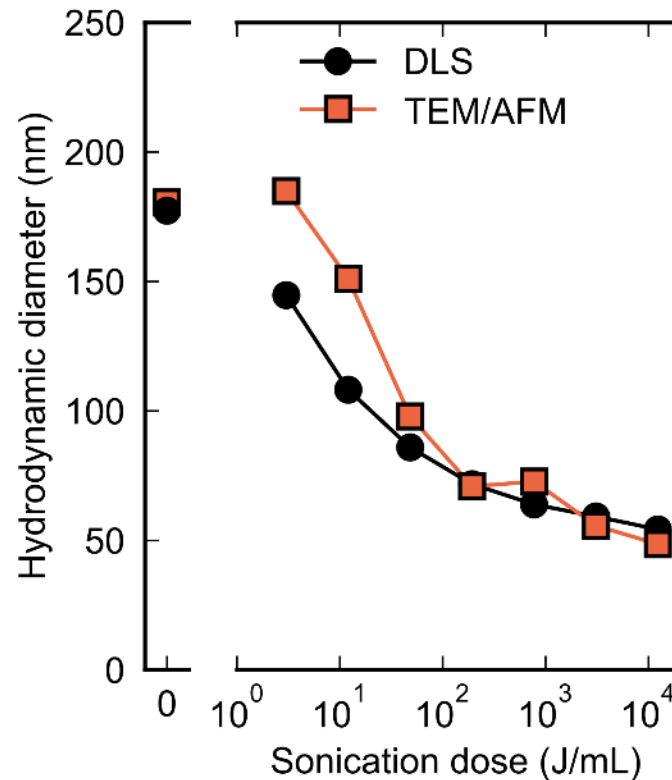
Relating individual and ensemble measurements

TEM/AFM: lots of info on 100s of CNCs

DLS/turbidity: limited info on 100000.....s of CNCs

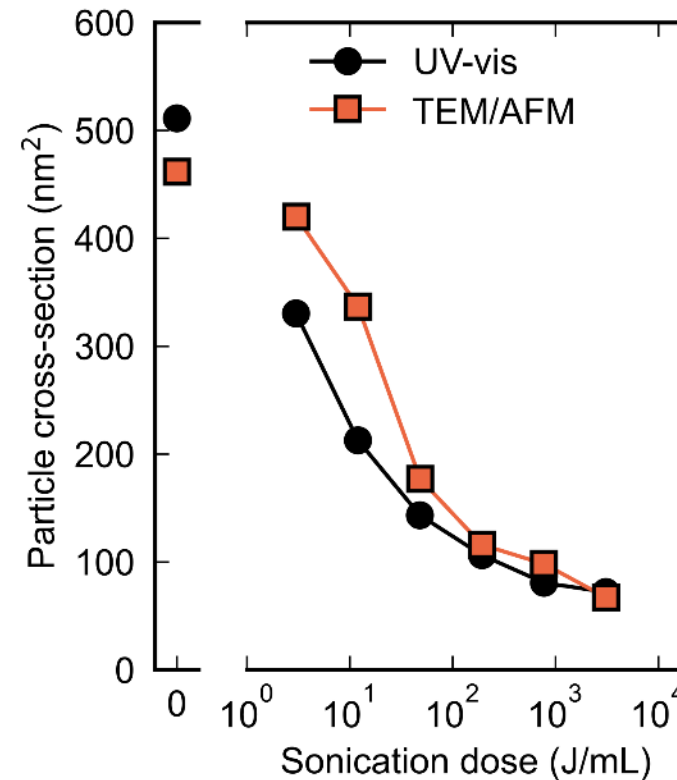
Dynamic light scattering (DLS)

Mean hydrodynamic diameter

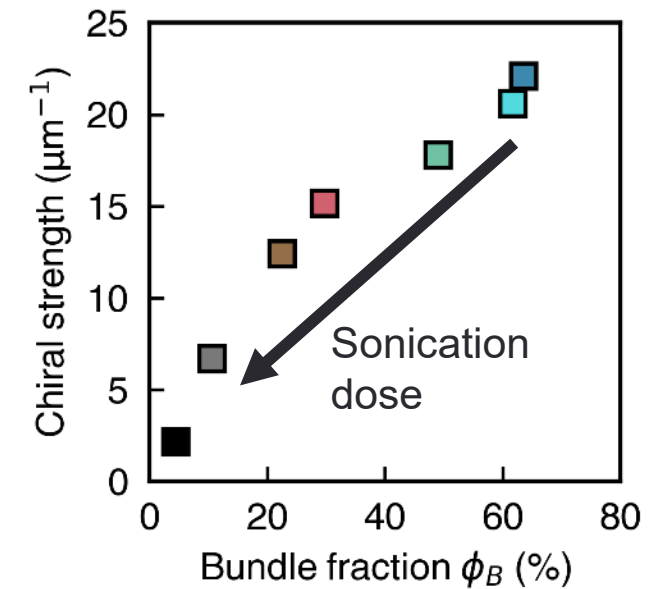
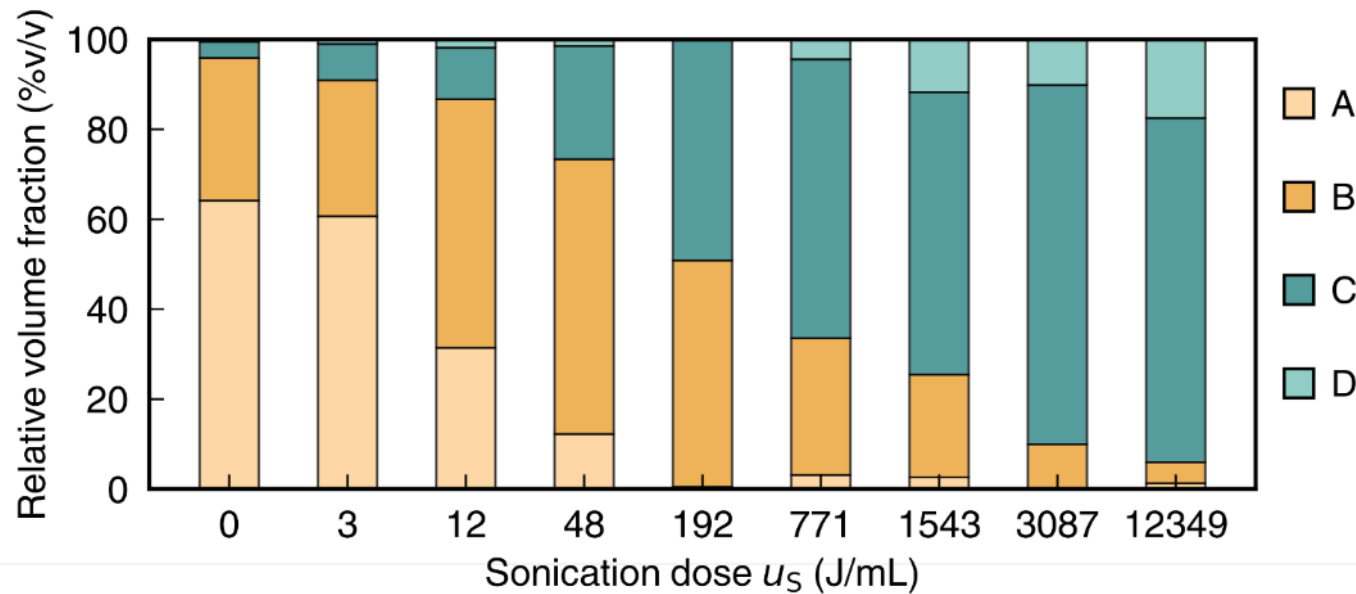
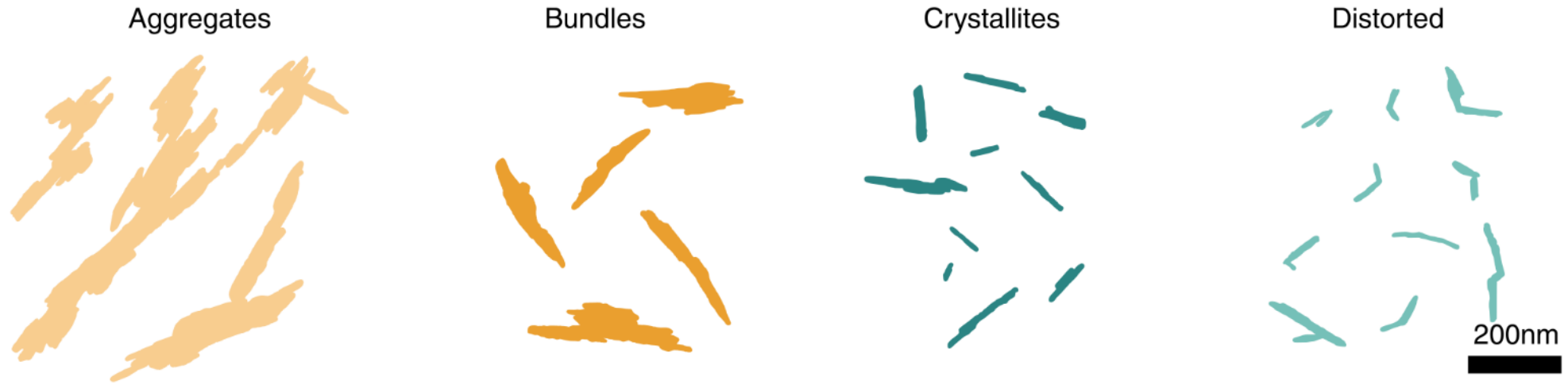


Turbidimetry (UV-vis transmission)

Estimate mean CNC cross-section

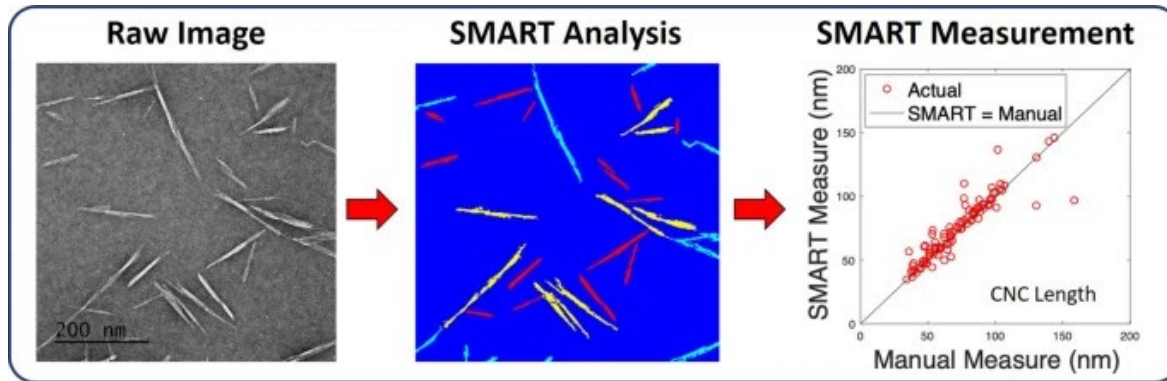
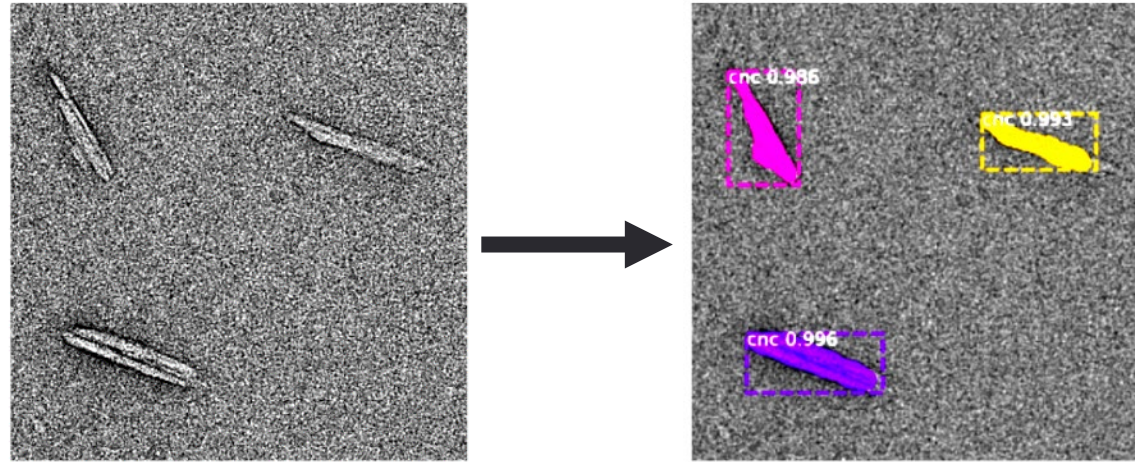


Chiral self-assembly is driven by “bundled” CNCs

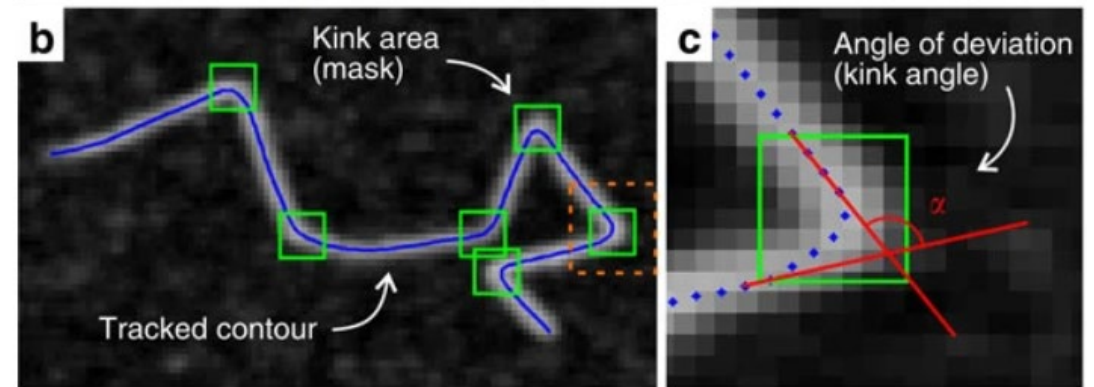


Automating EM characterisation of cellulose nanomaterials

Aim: **automatically** acquire CNC shapes



Yucel, S.; et al *Cellulose* **2021**, 28 (4), 2183–2201



Usov, I. et al *Nat Commun* **2015**, 6 (1), 7564.

Finding CNCs in TEM images, as a computer vision task

Classification

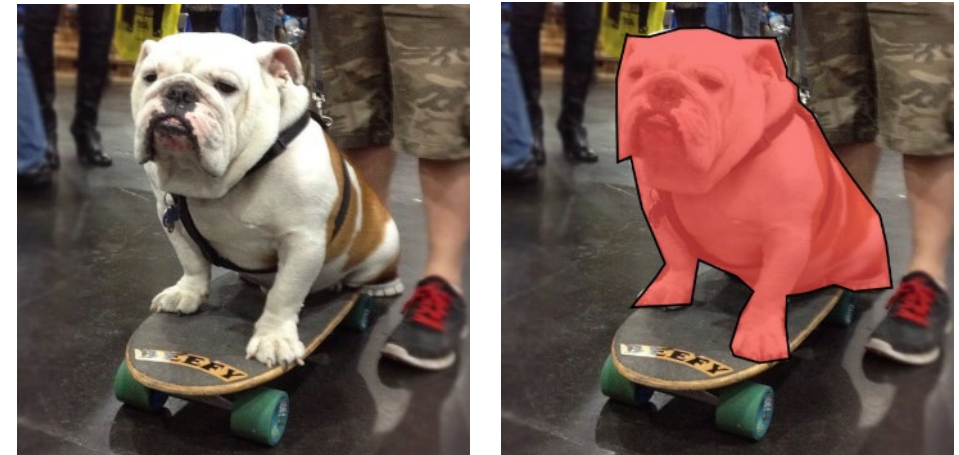


Example: COCO dataset

Multi-label instance segmentation

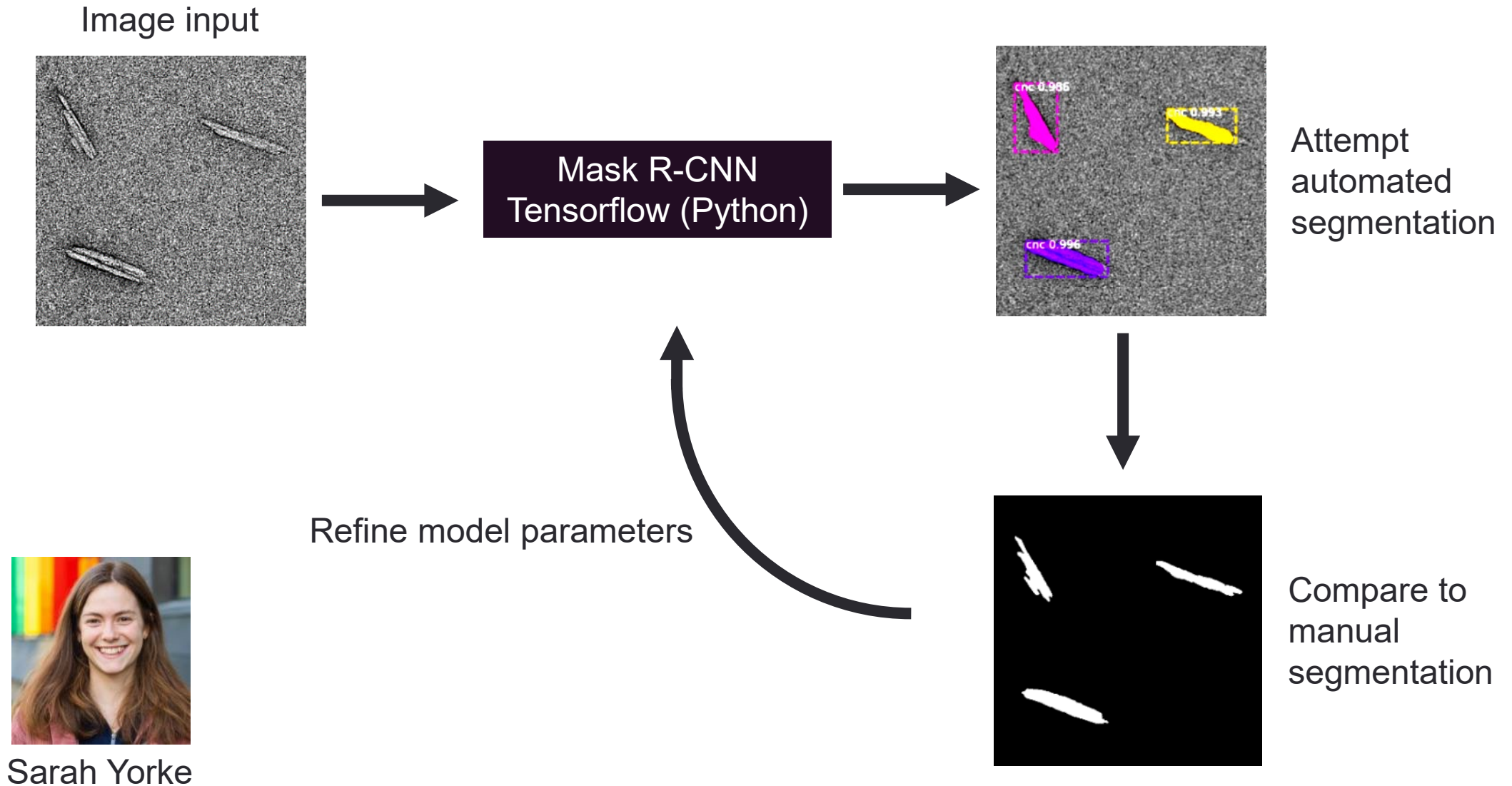


Binary instance segmentation



Aim with CNCs: automated binary instance segmentation

Automated image segmentation using Mask R-CNN

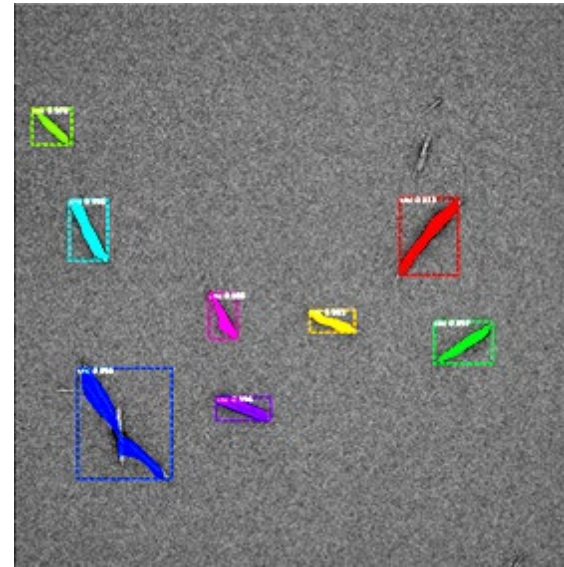
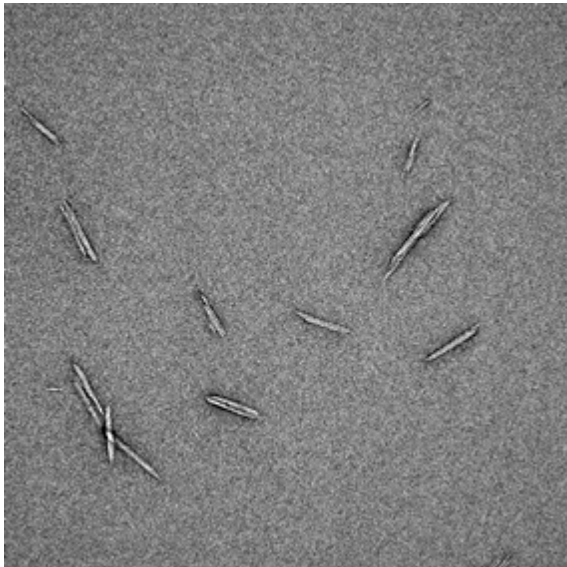


A first look at the automated segmentation results

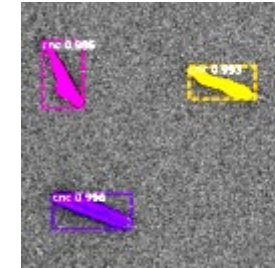
GPU: NVIDIA GeForce GTX 1080

180 training images

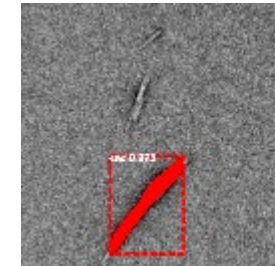
30 epochs (training rounds)



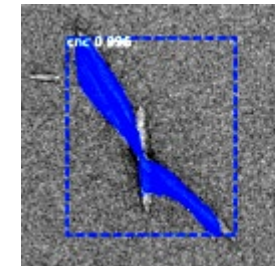
Many “good outlines”



Missing small particles

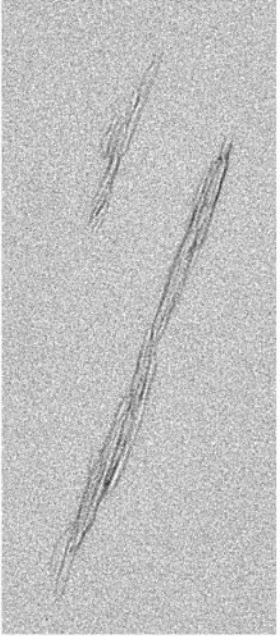


Irregular shapes



Quantifying model performance

Original

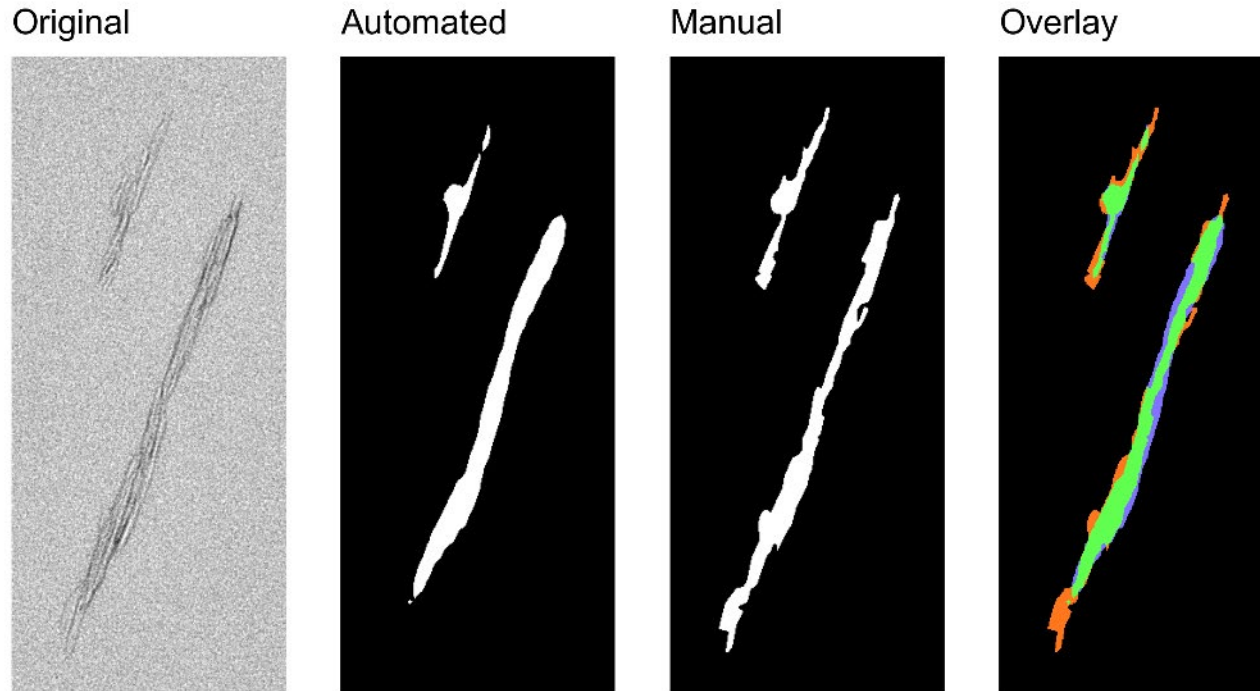


	Positive	Negative
True	True positive	True negative
False	False positive	False negative

Q1. Does the model think this pixel is CNC?
Positive (CNC) or negative (not CNC).

Q2. Did the model answer correctly?
True or False

Quantifying model performance



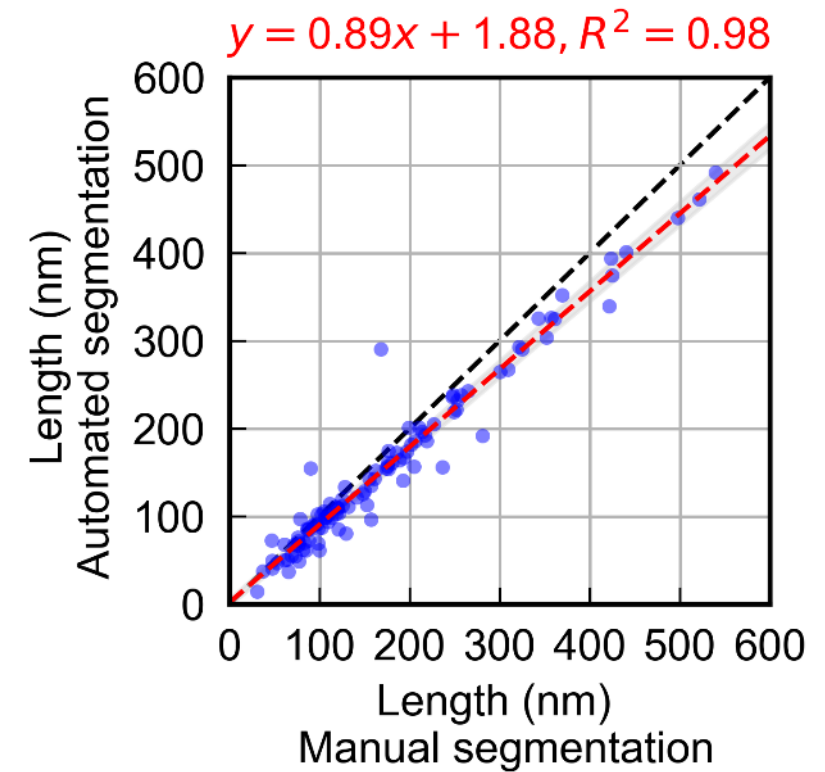
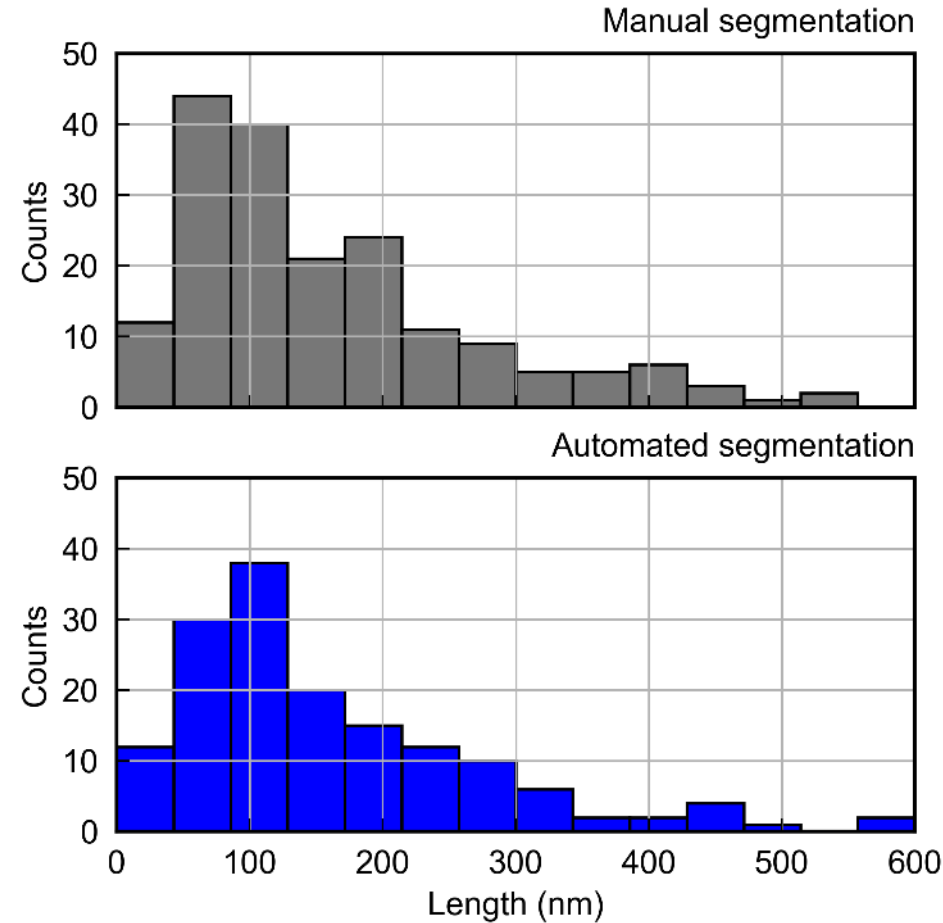
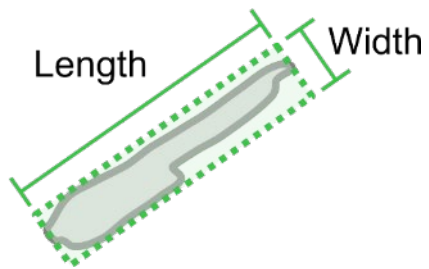
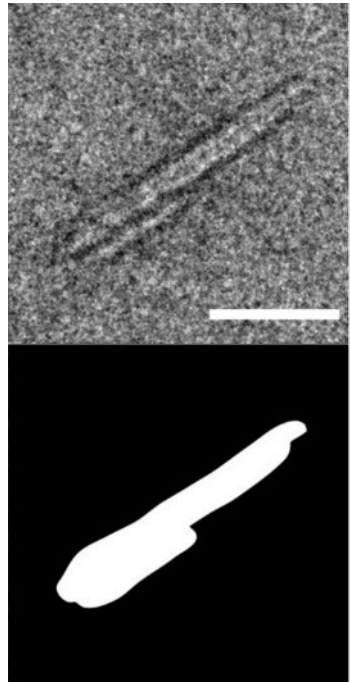
	Positive	Negative
True	True positive	True negative
False	False positive	False negative

Precision = $\frac{\text{TP}}{\text{TP} + \text{FP}}$ 91%

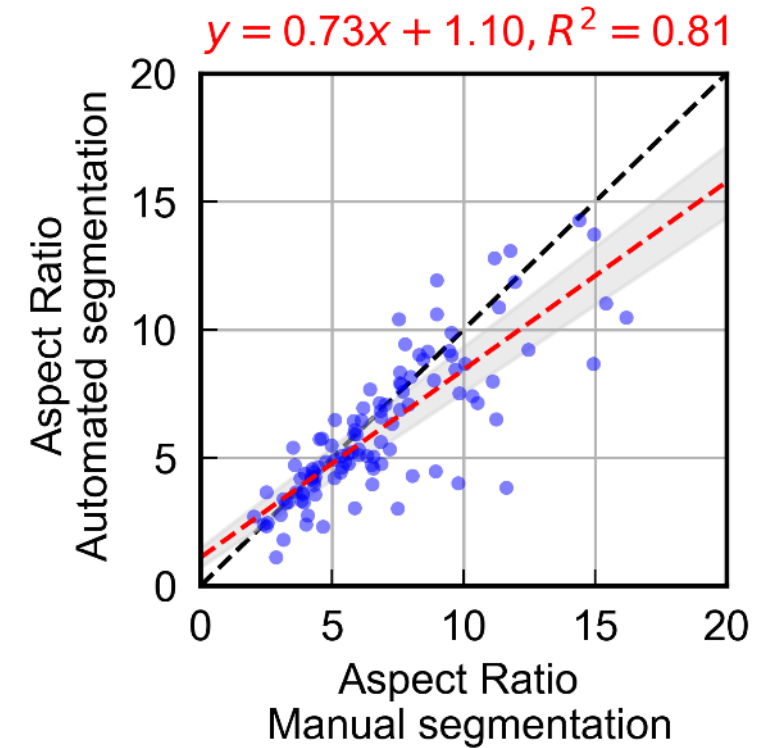
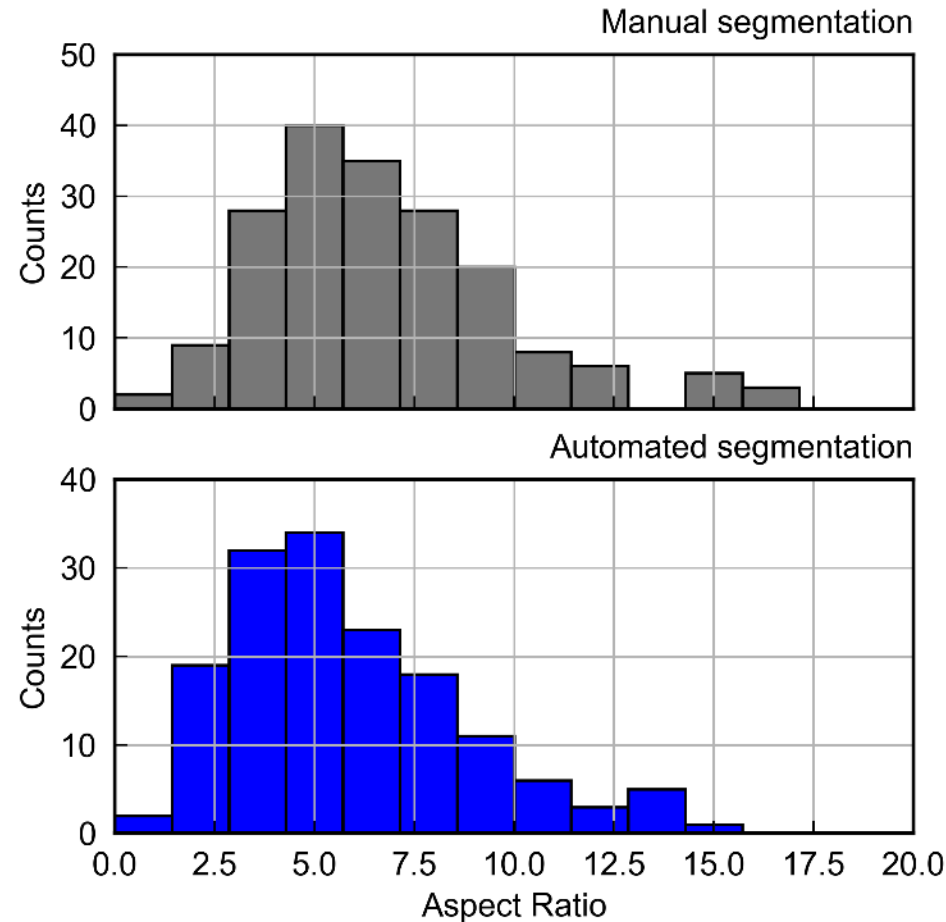
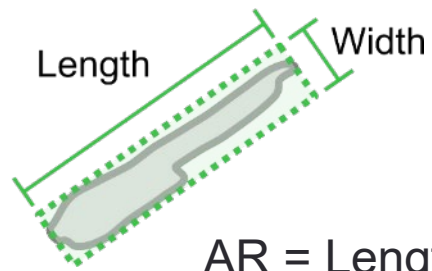
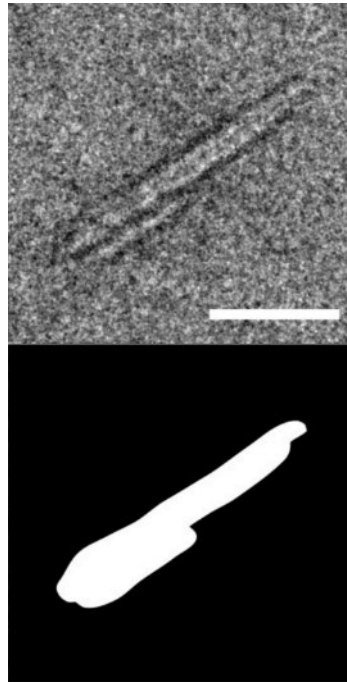
Recall = $\frac{\text{TP}}{\text{TP} + \text{FN}}$ 78%

$$F_1 = \frac{2}{\text{recall}^{-1} + \text{precision}^{-1}} \quad 84\%$$

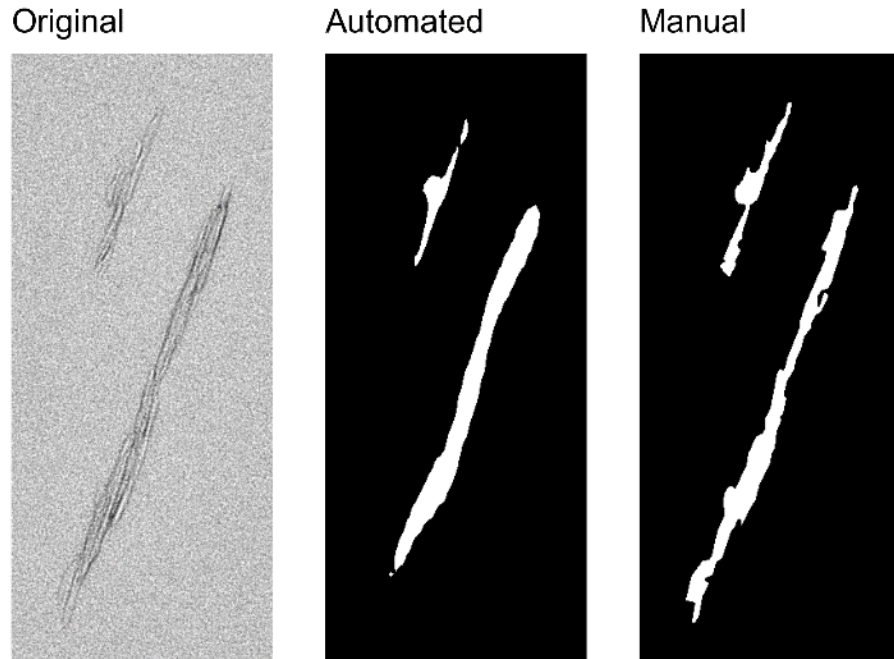
Automated segmentation gives comparable CNC length values



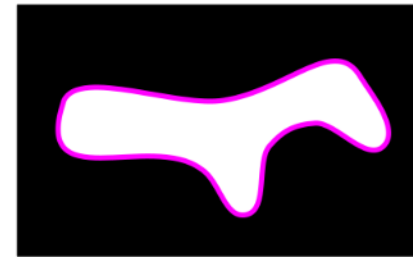
Lower aspect ratio values from automated segmentation



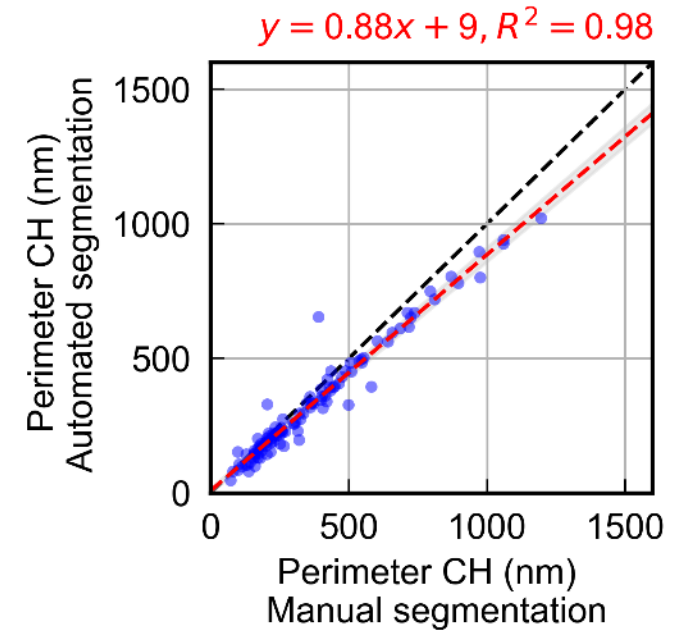
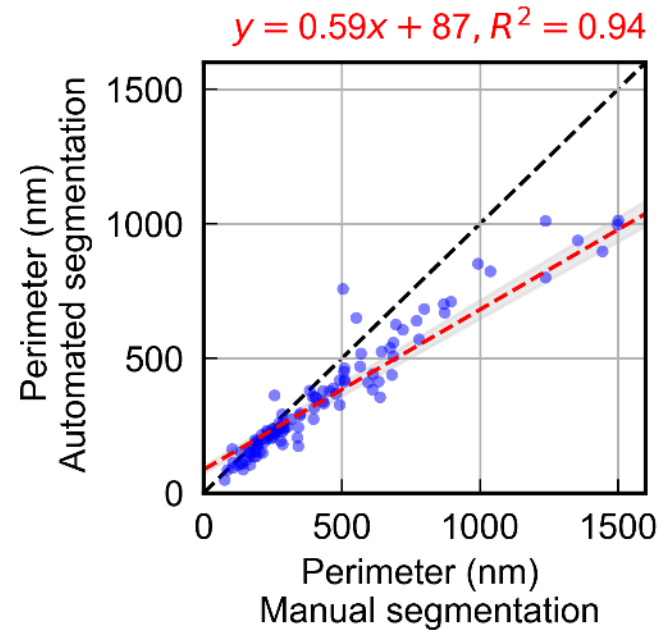
Auto-segmented shapes have simplified morphology



Original shape



— Perimeter

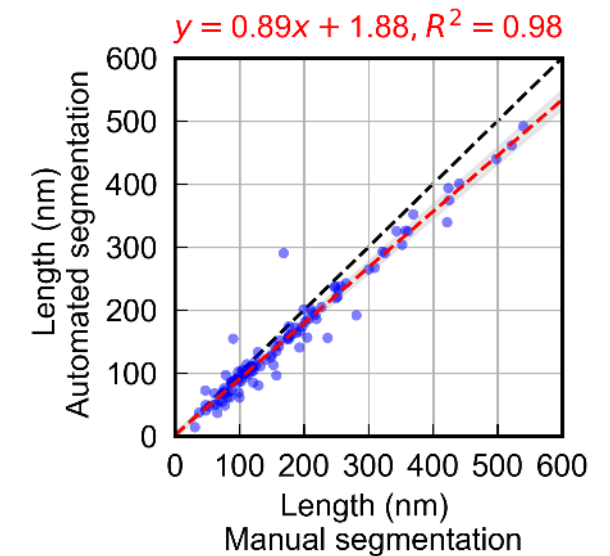
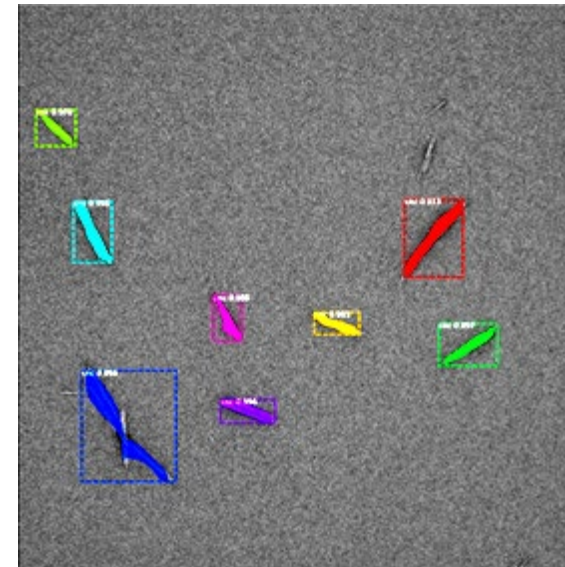
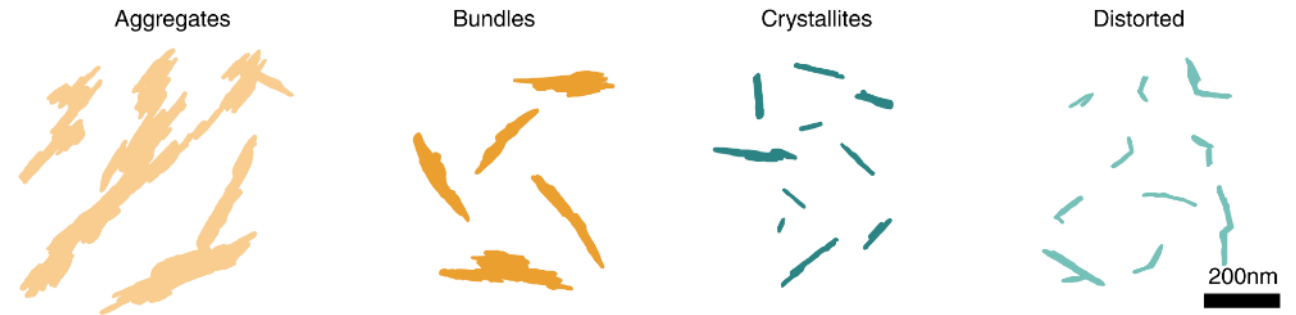


Summary

Morphology of individual CNCs important for understanding their chiral self-assembly

Automated instance segmentation of CNCs is possible using mask R-CNN

Morphological properties comparable to manually-labelled images



Acknowledgements



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**Engineering and
Physical Sciences
Research Council**