# Overfocused-probe ptychography of a 40 nm sample

Spectra Ultra, 300 kV, EMPAD (128 × 128 px). Experiment-design note, 2026-10-02 (version 2: aligned with the literature setting). Based on the 300 kV camera-length calibration in this folder (data 2026-08-21).

## Recommendation

| Setting | Value | Why |
|---|---|---|
| **Accelerating voltage** | 300 kV | as calibrated |
| **Probe semi-convergence α** | 21.5 mrad | as in the literature (21.4 mrad) |
| **EMPAD camera length** | 550 mm | BF disc ≈ 0.63 of the detector width (literature 2/3); window 3.68 nm |
| **Overfocus C1 (CEOS sign)** | +20 nm | as in the literature; under this camera length's +46 nm limit |
| **Scan step** | 0.4–0.5 Å | 94–95 % overlap (literature 0.41 Å, ≈ 95 %) |
| **Expected BF disc radius** | ≈ 40 px | check on the EMPAD before collecting (Figure 5) |

- Probe: 0.86 nm at the entrance surface, 2.58 nm at the exit, which is 0.70 of the 3.68 nm window: inside the loose limit, above the strict one (Section 2).
- Field of view at 0.41 Å: 5.2 nm for a 128 × 128 scan, 10.5 nm for 256 × 256 (about 21 Mx and 10.5 Mx, scaling the 1.8 Mx = 2.38 Å / 256 px setting in the calibration notes). A 256 × 256 scan at 1 ms per frame takes about 65 s; plan the dose accordingly.
- Alternative without overfocus: focus at mid-depth (about 20 nm into the sample). The probe stays ≤ 0.9 nm through the whole thickness and the shorter camera lengths (wider detector range) become usable.

## Comparison with the literature setting

The setting used in the literature for multislice electron ptychography with the EMPAD (as given by the facility): 300 kV, 21.4 mrad, 20 nm defocus, 128 px EMPAD, 0.41 Å scan step, bright-field disc diameter about 2/3 of the detector width. With this microscope's 300 kV calibration:

| | Literature | This plan (550 mm) | 430 mm (version 1) |
|---|---|---|---|
| **α** | 21.4 mrad | 21.5 mrad | 21.5 mrad |
| **BF disc diameter / width** | 2/3 = 0.67 | 0.63 | 0.50 |
| **Angle per pixel** | ≈ 0.50 mrad/px (implied) | 0.535 mrad/px | 0.672 mrad/px |
| **Detector edge** | ≈ 1.5 α | 1.6 α | 2.0 α |
| **Window W** | ≈ 3.93 nm | 3.68 nm | 2.93 nm |
| **Defocus / C1** | 20 nm | +20 nm | +15 nm |
| **Scan step** | 0.41 Å | 0.4–0.5 Å | 1.5–2.0 Å |
| **Overlap (entrance)** | 95 % | 94–95 % | 69–77 % |

- What changed from version 1: version 1 asked for a detector edge of 2α and 70–80 % overlap. The literature works with the edge at about 1.5α and ≈ 95 % overlap; the dense scan recovers the information, and the larger window suits a thick sample. So 550 mm and a fine step are the better choice.
- 550 mm is the longest calibrated camera length and gives 0.63 of the width; the literature's 2/3 would be about 580 mm, between calibrated values. Use 550 mm, or calibrate the next camera length if one is offered.
- Papers differ in the defocus sign convention: check whether the paper's 20 nm means overfocus before copying it, and match it to the CEOS sign with the nudge test (checklist, item 1).
- The literature sample may be thinner than 40 nm; for a thick sample the exit-surface probe is the constraint (Section 1).

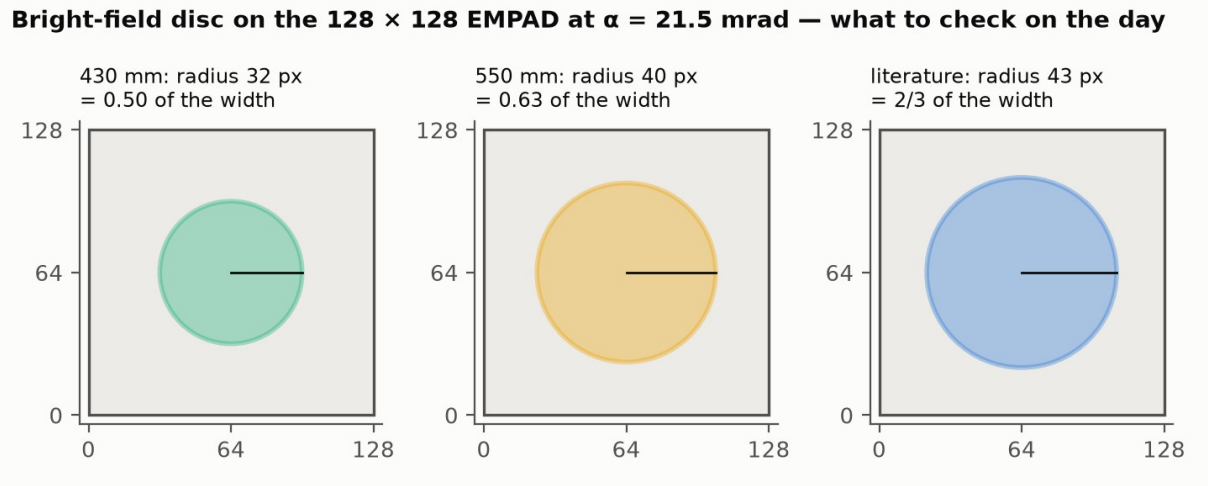



*Figure 5. The bright-field disc on the 128 × 128 EMPAD at α = 21.5 mrad. 550 mm comes closest to the literature's 2/3 of the width.*

## 1. Why the sample thickness limits the overfocus

With overfocus the probe crossover sits above the entrance surface, so the probe keeps widening on its way through the sample. Its geometric diameter at depth z below the entrance surface is $D(z) = 2\alpha(C1 + z)$; at the exit surface of a 40 nm sample it is $2\alpha(C1 + 40\ \text{nm})$. The reconstruction can only hold a probe that fits inside its real-space window $W = \lambda / \Delta\theta$, where $\Delta\theta$ is the EMPAD's angle per pixel. A probe larger than the window wraps around and the reconstruction fails or converges poorly.

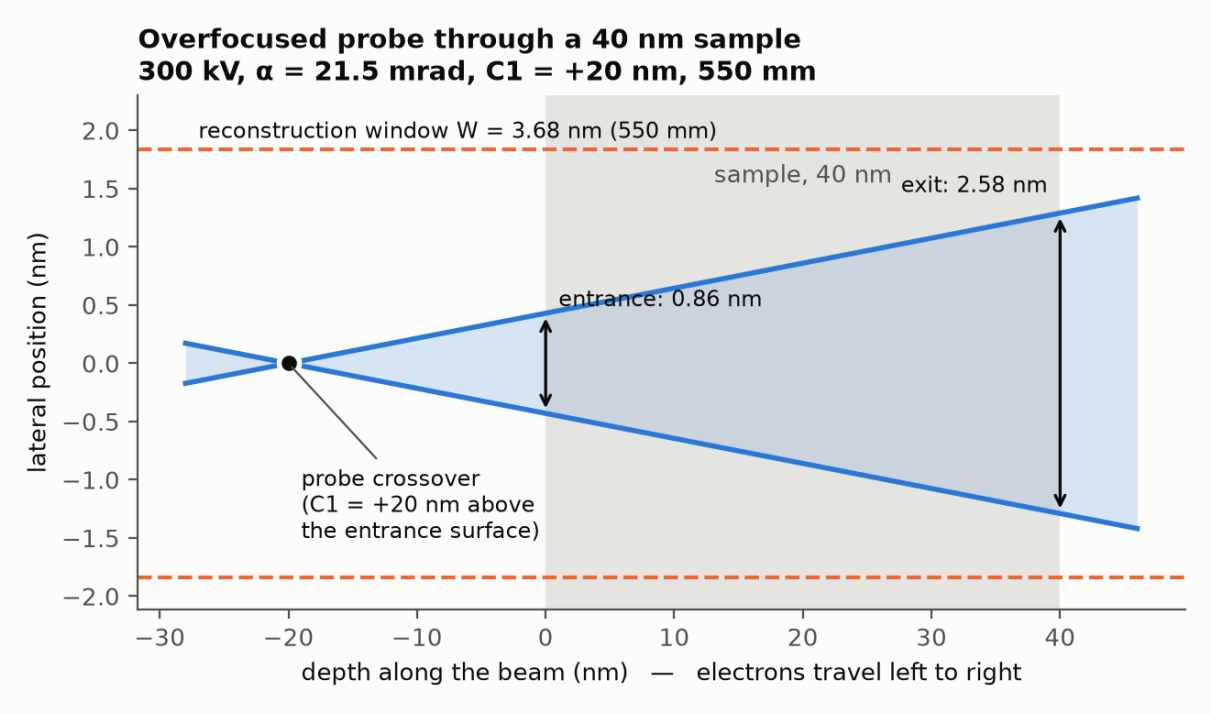



*Figure 1. The recommended geometry to scale: C1 = +20 nm at 550 mm. The probe grows from 0.86 nm at the entrance to 2.58 nm at the exit, inside the 3.68 nm window.*

## 2. How much overfocus fits

Two rules of thumb bound the largest usable C1: a strict one (exit probe ≤ half the window, safe against probe tails) and a loose one (exit probe ≤ the window). Solving $2\alpha(C1 + t) \le f \cdot W$ gives $C1_{max} = f \cdot W / (2\alpha) - t$, with f = ½ or 1.

| Camera length | mrad/px | Window W | Detector edge | BF radius | C1 max strict | C1 max loose |
|---|---|---|---|---|---|---|
| **270 mm** | 1.058 | 1.86 nm | 68 mrad (3.1 α) | 20 px | — | +3 nm |
| **340 mm** | 0.851 | 2.31 nm | 54 mrad (2.5 α) | 25 px | — | +14 nm |
| **430 mm** | 0.672 | 2.93 nm | 43 mrad (2.0 α) | 32 px | — | +28 nm |
| **550 mm** | **0.535** | **3.68 nm** | **34 mrad (1.6 α)** | **40 px** | **+3 nm** | **+46 nm** |

At 21.5 mrad, 550 mm leaves the most room: the loose limit is +46 nm, so the literature's 20 nm fits with margin. At 270–340 mm almost no overfocus fits a 40 nm sample.

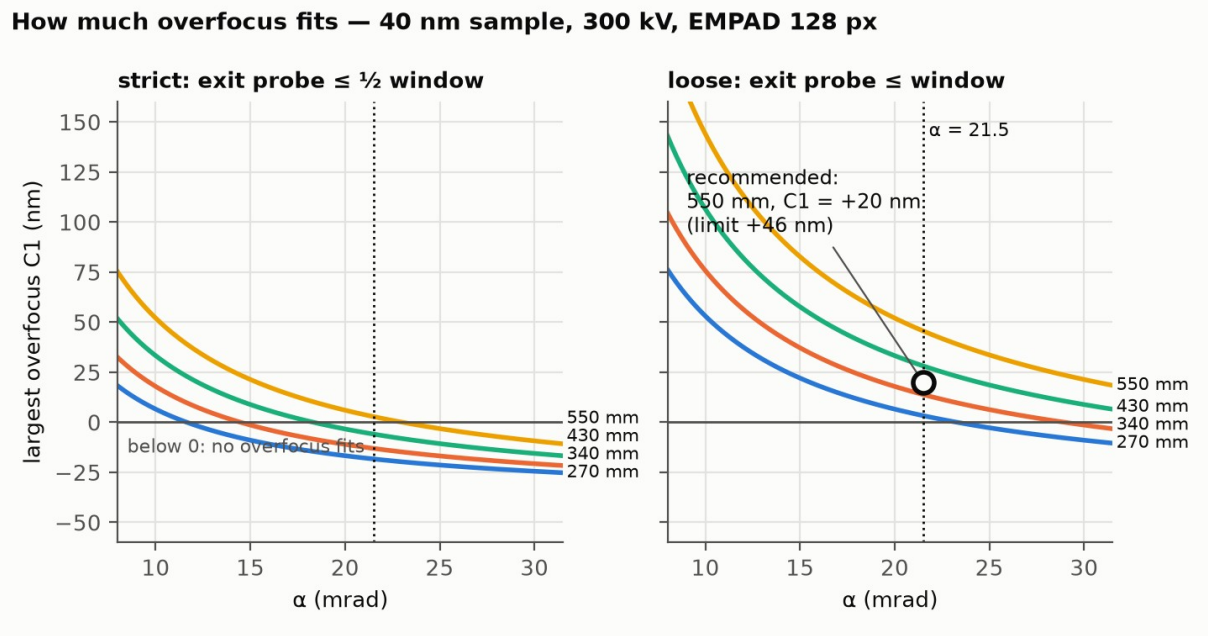



*Figure 2. Largest overfocus vs convergence angle for each camera length; left the strict limit, right the loose limit. Below zero no overfocus fits. The ring marks the recommendation (C1 = +20 nm at 550 mm, against that camera length's +46 nm limit).*

## 3. Scan step and overlap

Neighbouring probe positions must overlap. 70 % is the minimum usually quoted; multislice work on thick samples uses much denser sampling, about 95 % in the literature setting. With overfocus the probe is smallest at the entrance surface, so that is where the overlap 1 − step / D(entrance) is checked. It depends on α, C1 and the step, not on the camera length.

| C1 | Probe entrance → exit | 0.41 Å | 0.5 Å | 1.0 Å | 2.38 Å |
|---|---|---|---|---|---|
| **+10 nm** | 0.43 → 2.15 nm | 90 % | 88 % | 77 % | 45 % |
| **+15 nm** | 0.64 → 2.37 nm | 94 % | 92 % | 84 % | 63 % |
| **+20 nm** | **0.86 → 2.58 nm** | **95 %** | **94 %** | **88 %** | **72 %** |

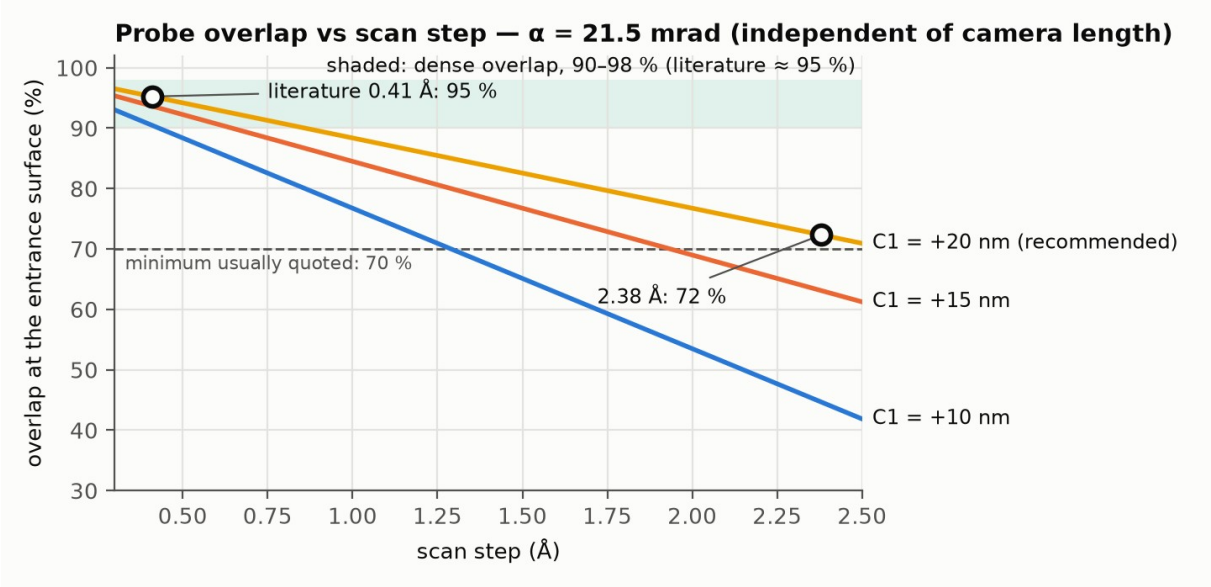



*Figure 3. Overlap vs scan step at α = 21.5 mrad. The recommended C1 = +20 nm with the literature's 0.41 Å step gives 95 %; the 2.38 Å step from the calibration notes gives 72 %.*

## 4. Before collecting — checklist

1. Confirm the C1 sign once on this column: note the TEM UI Defocus, apply a small known C1 (e.g. +20 nm) in DCORprime, read Defocus again. If it rose by about 20 nm, C1 > 0 is overfocus (CEOS convention). If it fell, the sign is reversed here and overfocus needs C1 < 0.
2. Check the bright-field disc on the EMPAD at 550 mm: radius about 40 px, diameter about 0.63 of the width (Figure 5). A different size means α or the camera length differs from the calibration, and the numbers above shift.
3. Set the reconstruction's starting probe to C1 = +20 nm with the matching sign convention (PtyRAD and AutoACEM's twin: overfocus positive; abTEM: defocus = −C1).
4. Set the scan for a 0.4–0.5 Å step (magnification and scan size, see Recommendation) and plan the dose for the dense scan.

## 5. Caveats

- The limits come from rules of thumb (exit probe ≤ ½ or 1 × window, geometric probe size), not from measured reconstruction failures. Diffraction broadening (≈ λ/α ≈ 0.09 nm) is ignored.
- The C1 sign relation between DCORprime and the TEM UI Defocus is not yet verified on this microscope.
- The 300 kV calibration (1.058 mrad/px at 270 mm) disagrees by 1.6× with the 1.689 mrad/px measured from an 80 kV dataset (docs/SITE-FACTS.md §3 in the AutoACEM repository). The calibration file states the angle per pixel is independent of voltage, but these two measurements show the nominal camera length does not give the same real camera length at every voltage: use the calibration for the voltage in use.
- The calibration was measured with a 30 mrad probe; the BF radii at 21.5 mrad are scaled from it.

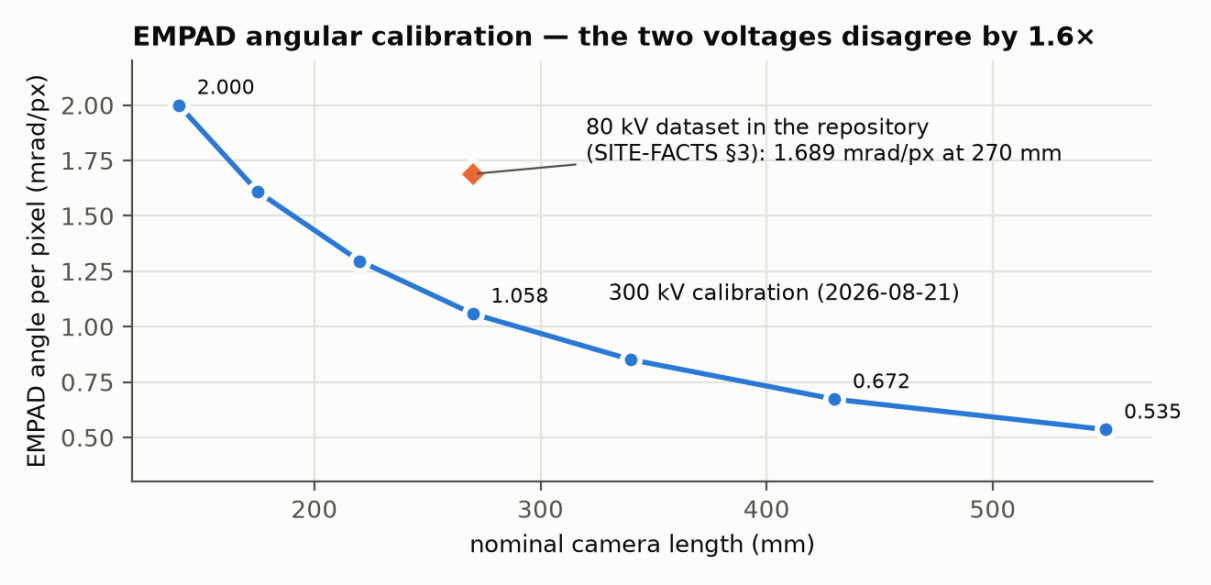



*Figure 4. EMPAD angle per pixel vs camera length at 300 kV (calibration in this folder), with the 80 kV value used so far in the AutoACEM repository.*

## Formulas and inputs

- λ = 1.9687 pm (300 kV); t = 40 nm; α = 21.5 mrad; EMPAD 128 px (64 px from axis to edge).
- Window W = λ / Δθ;  detector edge = 64 × Δθ;  BF disc radius = α / Δθ.
- Probe diameter D(z) = 2α(C1 + z), z measured down from the entrance surface; C1 > 0 = crossover above the sample.
- C1_max = f·W / (2α) − t, f = ½ (strict) or 1 (loose);  overlap = 1 − step / D(0).