Supplemental information for “Ptychography removes spectral distortions intrinsic to conventional zone-plate based x-ray spectromicroscopy”

Matthew A. Marcus,1[[1]](#footnote-1) David A. Shapiro,1 and Young-Sang Yu1

*Advanced Light Source, Lawrence Berkeley Laboratory, 1 Cyclotron Road, Berkeley CA USA 94720.*

*Apodization*

 To investigate the effects of apodization, we modeled the zone plate considered for the polymer system (Figs. 1,2) with the field transmission function multiplied by a function of radius on the zone plate which vanishes at the inner edge, outer edge or both. These functions are given by

 

where  is the radial coordinate on the zone plate and the cutoff radii  are given by:

 

where *a,b* are outer and inner radii of the zone plate. These cutoffs are chosen so that  at the edge not being apodized. Of course  when no apodization is done. The constant factor in is chosen so that the maximum value of  is 1, Images of the apodized zone plates and their resulting knife-edge profiles are shown in Figure S1. Apodizing the inner edge alone seems to produce no diminution of the tails, while apodizing the outer edge or both reduce the tails by 30-40%. For comparison, we consider a Gaussian probe whose error-function knife-edge curve has a 10-90% width the same (64nm) as that of the un-apodized zone plate.

 For each case (none, inner, outer, both, Gausian), we calculated a simulated knife-edge profile and performed the same kind of fits as described in the section “Calculation of simulated STXM spectra”, using the polymer references, with  and  as in Figure 3. We then plotted the fitted and knife-edge weighted fitted fractions of Reference 2 (minority component) for each apodization (Figure S2) as well as the spectrum and its fit at a position of *x*=-200nm (Reference 2[P3HT]-rich side, Figure S3). The knife-edge weighted fitted fractions are what one would naively expect as the result of convolving a step-function composition with the probe. All probes result in erroneous results near the midline, because even when the probe is centered on the Reference 1 [PC61BM] side, some light gets through on the thinner Reference 2 side and distorts the results. This is the hole effect. However, with a true Gaussian probe, the effect is confined to within 100nm of the interface, while the zone plates, however apodized, produce the erroneous impression of significant amounts of the second component where there is none, even 300nm from the interface. Even if both edges are apodized, the improvement over the un-apodized case is relatively modest. It is, of course, possible that a different form of  would yield better results.

 Similarly, when we look at the “measured” spectrum vs. a linear fit, we see that the inner-apodized zone plate performs like the un-apodized zone plate, the outer-apodized and both-edges-apodized zone plates perform almost alike, and the Gaussian probe is better than all.

none inner outer both Gauss

x (m)

Figure S1. Knife-edge profiles of the simulated non-apodized zone plate, zone plates apodized at inner, outer and both edges, and an ideal Gaussian zone plate. The illumination profiles for the zone plates are shown. Only the left half of the knife-edge profile is shown because the right half is the same, only flipped in X and Y.



Figure S2. Fraction of P3HT (component 2) measured in the PC61BM/P3HT model system in which the effective thicknesses of the two phases differ (OD1 = 1 and OD2 = 0.01), simulated for the different probe conditions. Dashed lines are the knife-edge profiles, weighted by the OD2 and solid lines the fits. The peak around *x*=0 is due to the hole effect, while the long tail to the right is due to the tail of the knife-edge response, as seen from the fact that the Gaussian probe doesn’t show this effect.



Figure S2. Spectra extracted from the polymer simulation at a position *x*=-0.2m, for the various probes. Solid lines are the spectra while dotted lines show the linear fits of the spectra to the reference spectra. Note that the deviation from fit is much less for the outer- and both-edge-apodized zone plate than for the un-apodized, and less still for the Gaussian probe.

1. Electronic mail: mamarcus@lbl.gov Phone 510 495 2106 [↑](#footnote-ref-1)