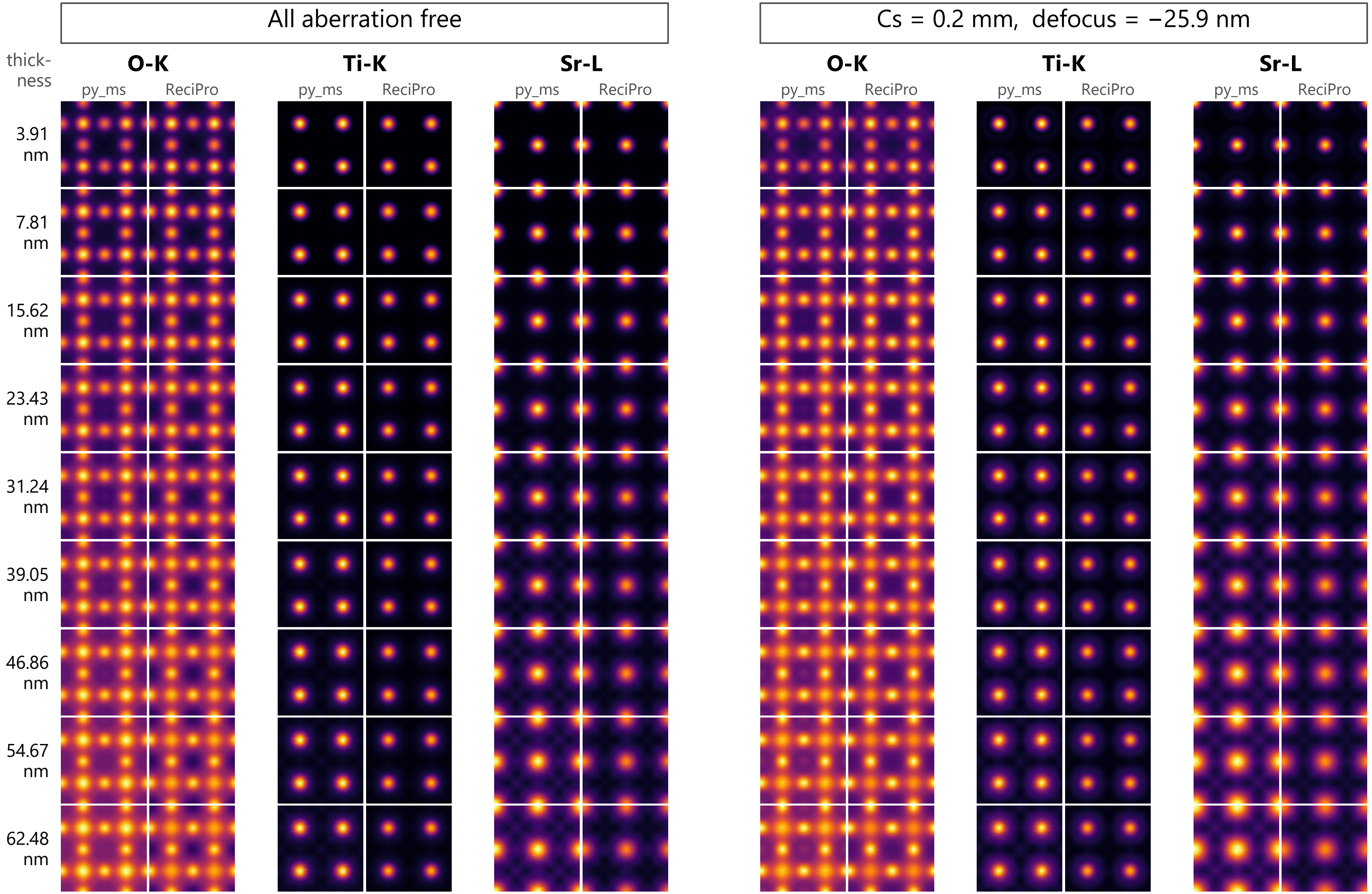
Comparison of STEM-EDX simulations by py_multislice (5e5e4d8) and ReciPro (v4.945)

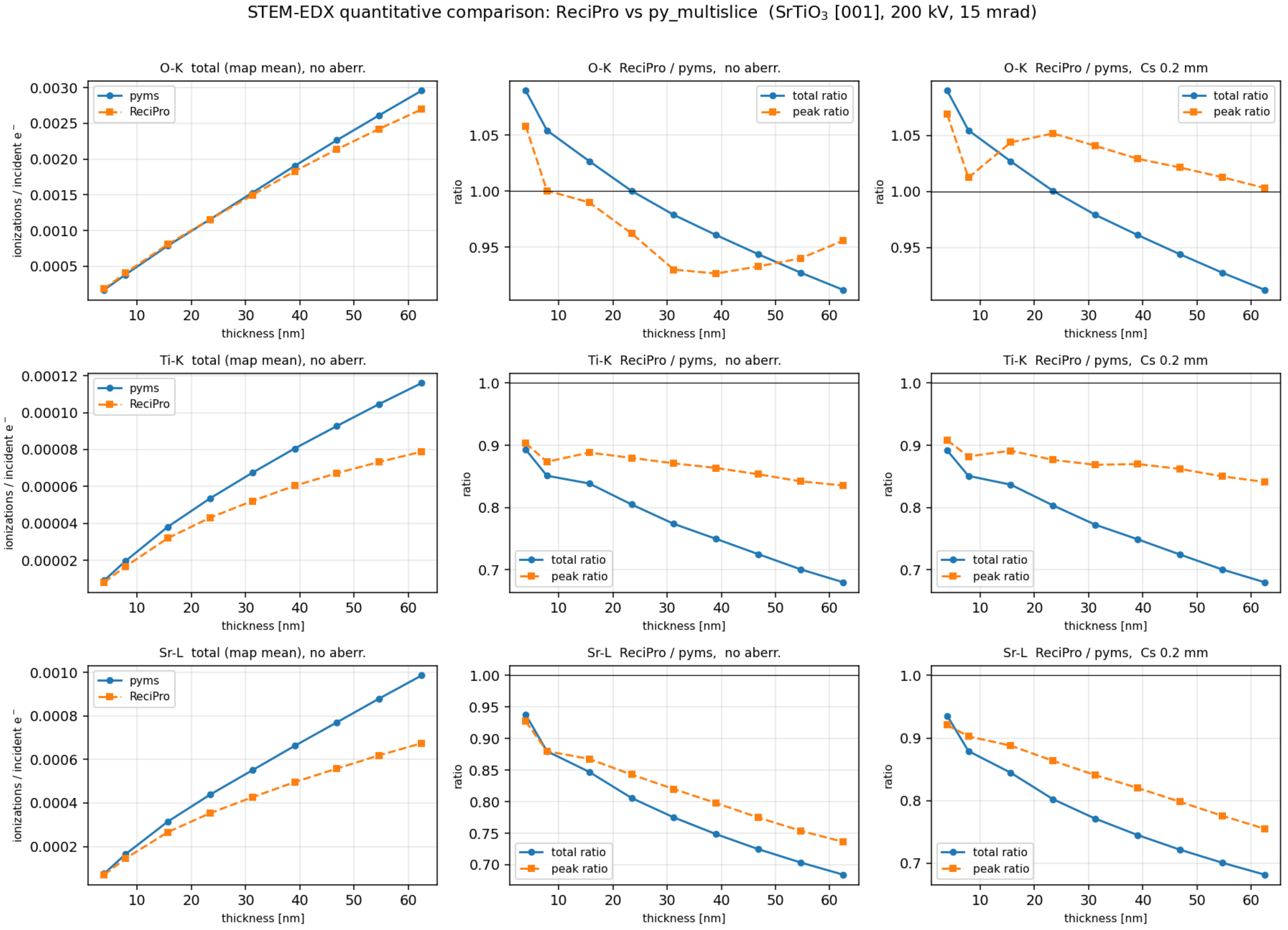
Sample: $SrTiO_3$ [001] ($B = 8\pi^2\langle u^2\rangle$: Sr 0.621, Ti 0.440, O 0.732 Å^2)
Acc. vol.: 200 kV, beam convergence: 15 mrad
Signal: inner-shell ionizations per incident electron; Sr-L = L1+L2+L3

py_multislice conditions: multislice, frozen phonon (25 configurations), 6×6×1 supercell, 384^2 grid, slice a/2, Allen-group parameterised ionization potentials (Sr = 2p + 2s). Computation: 112 min / 105 min per block (NVIDIA RTX 4060).
ReciPro conditions: Bloch wave method, 400 waves, 64^2 probe directions, Δz = 0.195 nm, DHFS–KS23 F(s) + Bote–Salvat σ (dataset v3.0.0). Computation: 6.3 min / 6.3 min per block (Ryzen 9 9950X, 32 threads).



Each panel: one unit cell scanned 32×32 (shown 2×2 tiled). Colour scale is shared within each py_multislice/ReciPro pair, so absolute differences are visible. Times are wall-clock for the same output on one workstation. The physical models differ (absorptive vs frozen-phonon thermal scattering): a practical, not algorithmic, comparison.

Quantitative comparison



	σ ratio pyms / ReciPro (t → 0)	shape agreement |F(q)| ratio, 3.9 nm (q ≤ 3 a*)
O-K	0.92	0.96 – 1.11
Ti-K	1.12	0.995 – 1.007
Sr-L	1.07	0.978 – 0.990

- Normalized map shapes agree to 1–2 % (Ti-K, Sr-L) in the thin limit; the same holds with Cs = 0.2 mm.

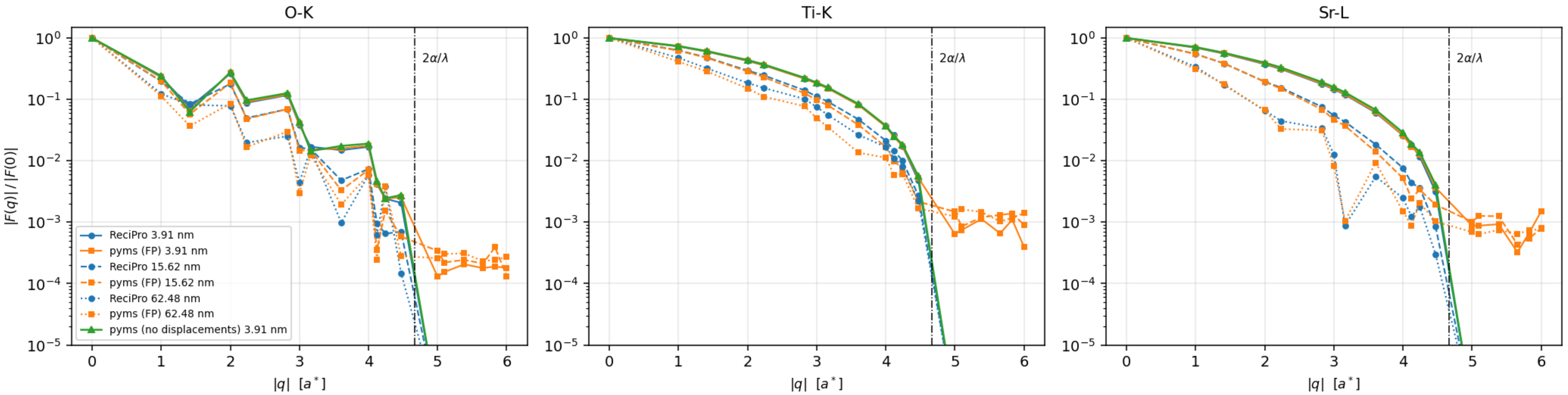
- Totals differ by the cross-section source: Bote–Salvat (ReciPro) vs the Allen-group tables (pyms), ±10–17 % depending on the shell.

- The ReciPro/pyms total falls with thickness (Ti-K 0.90 → 0.68 at 62 nm): ReciPro's absorptive model removes thermally scattered electrons, while frozen phonon keeps them ionizing. This quantifies the practical error of the absorptive approximation for EDX.

- Baseline: ionization dataset v3.0.0 (Dirac bound states, j-resolved L, scalar-relativistic continuum, $s \le 8$ Å^{-1}). Regenerating the v1.0.0 baseline with v3 moves every number on this slide by ≤1 % (thin limit ≤0.3 %) — the remaining differences are set by the σ source and the TDS treatment, not by the form-factor refinement.

Spatial-frequency content — band limit and frozen-phonon aliasing

Spatial-frequency content of the EDX maps (aberration free). ReciPro is exactly zero beyond $2\alpha/\lambda$ as it must be; py_multislice's out-of-band content is frozen-phonon aliasing.



• Both codes are strictly band-limited: the EDX map has no spatial frequency beyond 2α/λ = 4.67 a* at 15 mrad, as required for incoherent STEM imaging — ReciPro and py_multislice (thermal displacements off) both drop to zero there.

• The residual out-of-band floor (~10^{-3}) of the frozen-phonon curves is aliasing of the 6×6 supercell phonon configurations; it disappears when thermal displacements are disabled and is invisible at map level.

• Within the band the normalized Fourier amplitudes of the two codes track each other over three orders of magnitude.