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Vibration-Corrected Electron Ptychography

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Far-field electron ptychography is considered to be one of the most powerful phase retrieval techniques currently available for electron microscopists. Recently it was shown that ptychography is capable to surpass the Abbe resolution limit [1] and resolve specimens features as fine as the blurring due to the vibrations of the atoms [2]. A rather simple mathematical model of coherent diffraction pattern formation standing behind conventional algorithms [1,2,3,4] does not account for any motion or entangled states [3,4]. In order to overcome the resolution limit caused by the lattice vibrations we utilize the mixed-object formalism initially proposed in 2013 for x-Rays [4], but never applied to electron microscopy data. In contrast to conventional ptychography [1,2] that treats a single transmission function of a specimen, mixed-object ptychographic reconstruction considers a sequence of entangled transmission function states, each producing a coherent diffraction pattern via a multislice simulation [2,3]. The total diffraction pattern corresponding to the entangled system is formed as an incoherent sum over the states [3,4].

For the tests of mixed-object ptychography we used a 4D-STEM dataset [6] of a monolayer MoS₂ acquired in the Nion Hermes microscope at an accelerating voltage, convergence semi-angle, scan step and electron dose of 60 kV, 33 mrad, 0.2 Å and 5.3e6 $e^{-}/^{2}$, respectively.

To evaluate the resolution of the ptychographic reconstructions we propose a novel approach, akin to the Young fringe resolution test widely applied in TEM imaging [7]. We perform two ptychographic reconstructions with different initial guess for the object, e.g. uniform prior. Then the two independent results are shifted with respect to each other and the Fourier intensity of the difference is computed. The arising interference fringes indicate the range of spatial frequencies identical in the two results, allowing to conclude how deterministic a particular reconstruction is. Further, in contrast to conventional resolution tests, e.g. visibility of the Fourier peaks [1,2], the proposed approach allows to include aperiodic features that are crucial for a moving specimen.

Assuming a single illumination mode [2,4] we conducted pairs of ptychographic reconstructions in two scenarios: one involving a single-state and the other involving 10 entangled states of the transmission function. After 500 iterations of the gradient-descent [3] the achieved resolution was estimated. As a result, two independent pure-state reconstructions appear to produce identical information up to 1.9^{-1} , while the mixed-object reconstructions contain deterministic information up to 2.3^{-1} .

Even with a monolayer specimen that is not supposed to produce a noticeable amount of incoherent scattering, we show that considering multiple entangled states of the transmission function makes the underlying model more realistic and improves the quality of the ptychographic fit. Thus, we liberate ptychography from atomic vibrations, its last known resolution limit [2,3].

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- [3] A. Gladyshev et al., doi:arXiv:2309.12017⊠
- [4] P. Thibault & A. Menzel, doi:10.1038/nature11806🛛[5] P. Godard et al., doi: 10.1364/OE.20.025914🕮
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