

## Computation cost in imaging simulation

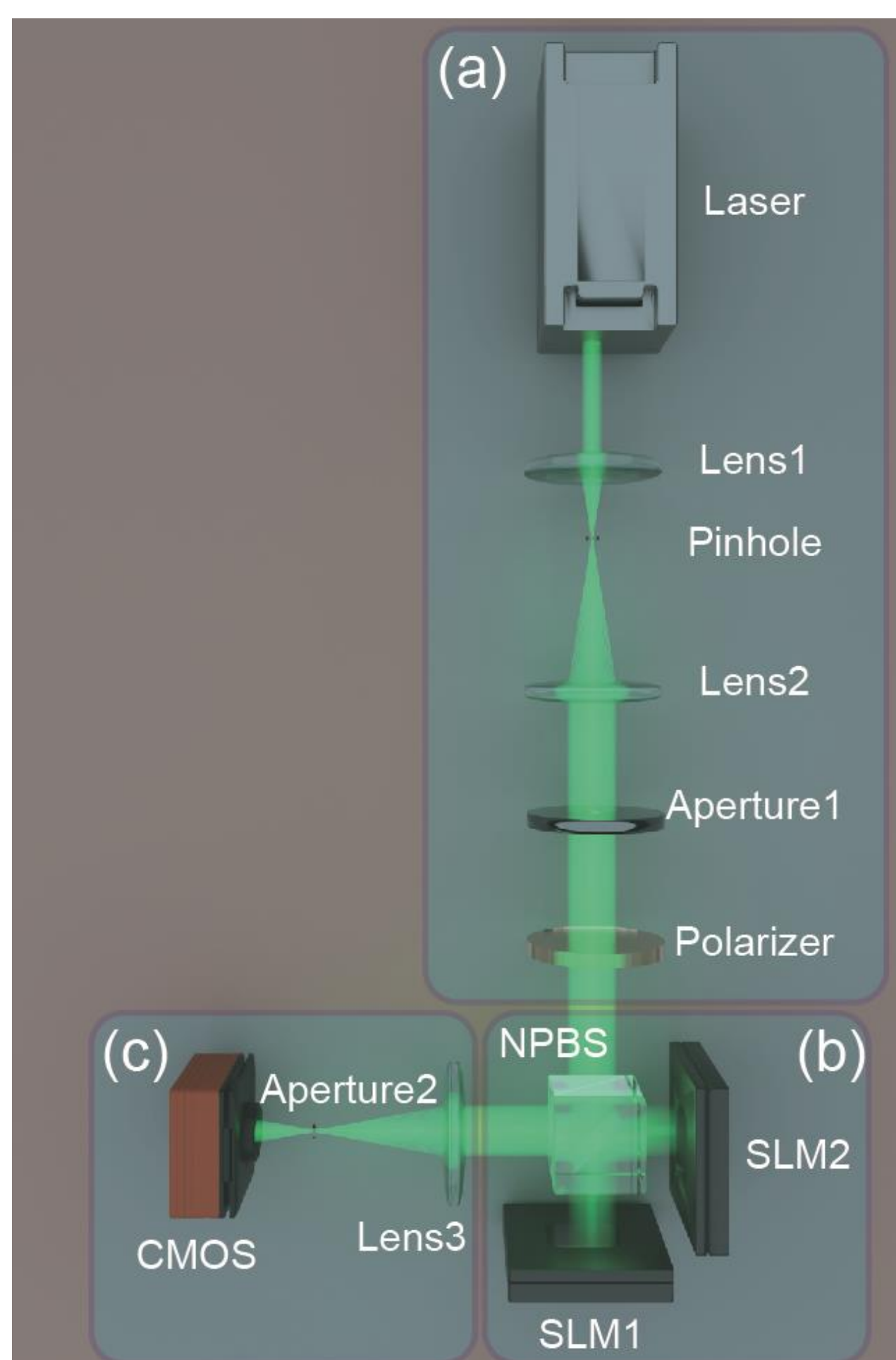
The transmission electron microscope (TEM) is an important tool for condensed material and nanostructure characterization due to its ability to directly imaging atoms in real space. However, image formation in transmission electron microscope (TEM) is inherently complex and governed by multiple coupled physical processes. Thus, electron imaging simulation remains one of the most widely used approaches for interpreting S/TEM images in terms of structure, composition, and bonding.

Currently, electron imaging simulations are conventionally performed through numerical computation on electronic computers. These calculations are typically time-consuming, as they require repeated large-scale matrix operations, such as matrix multiplication and convolution, to model probe formation, dynamical propagation through the crystal, and the formation of the final image.

Therefore, here we report a prototype platform for simulating electron imaging within the multislice formalism using optical computation to accelerate image simulation and structure analysis process in TEM.

## Simulation examples

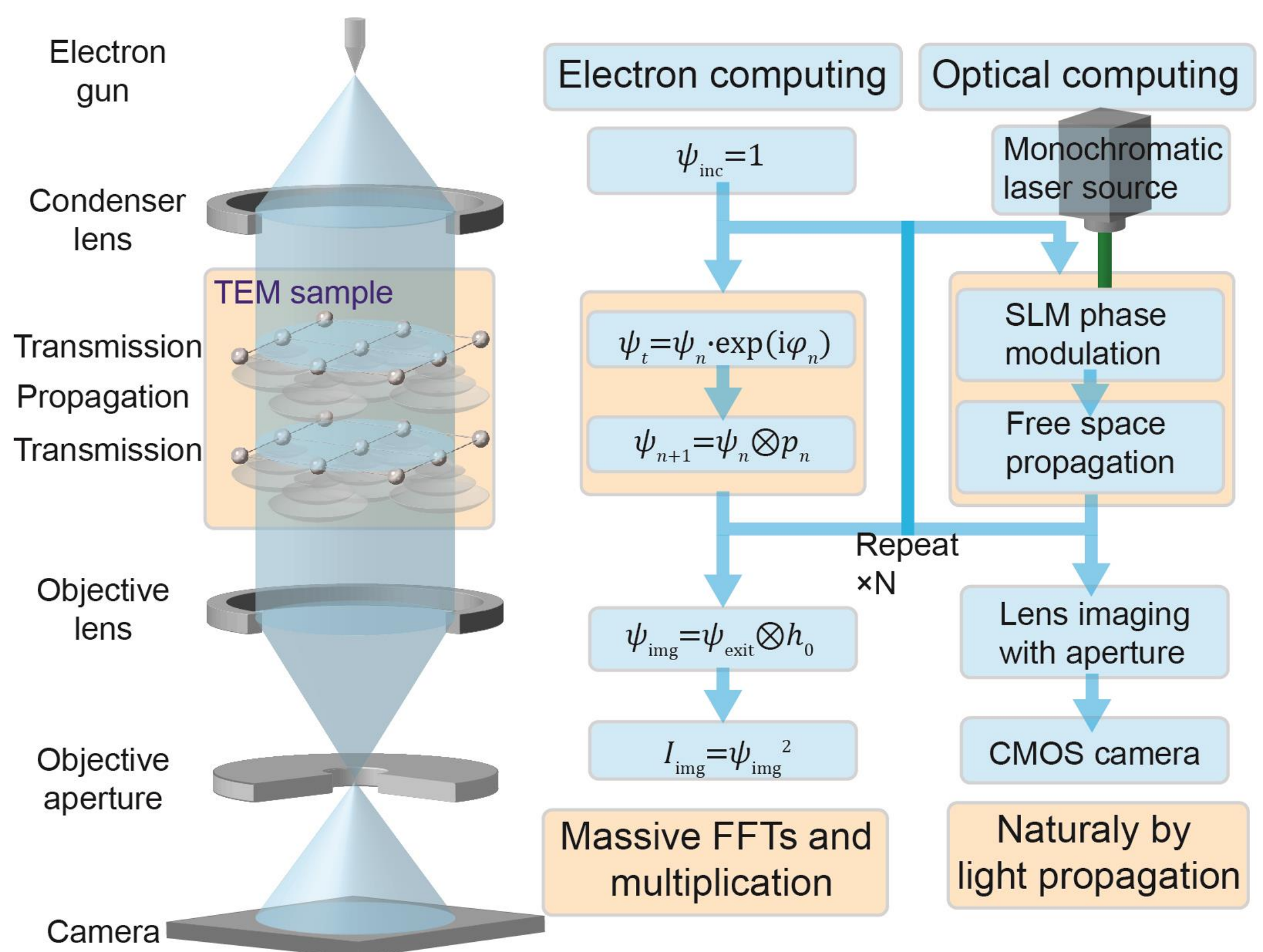
Employing the similarity, in experiment we build the optical computer as shown in figure below. From (a) to (c) are respectively: (a) illumination system which generates aligned monochromatic coherent laser as input beam to the system; (b) SLMs placed by an adjustable optical path length  $\Delta z$  connected by a Non-Polarizing Beam Splitter (NPBS), acting as a two-layer transmission-propagation module and (c) the imaging and recording system which simulates the lens imaging process and records the output image. This setup allows the simulation of TEM images of two-layer samples, and simulation examples are shown in following section.



## Reference

- [1] X. Li, Z. Shao, M. Zhu, and J. Yang, Fundamentals of Optical Computing Technology (Springer, 2018).
- [2] J. W. Goodman, Introduction to Fourier optics (Roberts and Company publishers, 2005).
- [3] E. J. Kirkland, Advanced computing in electron microscopy (Springer, 1998), Vol. 12.

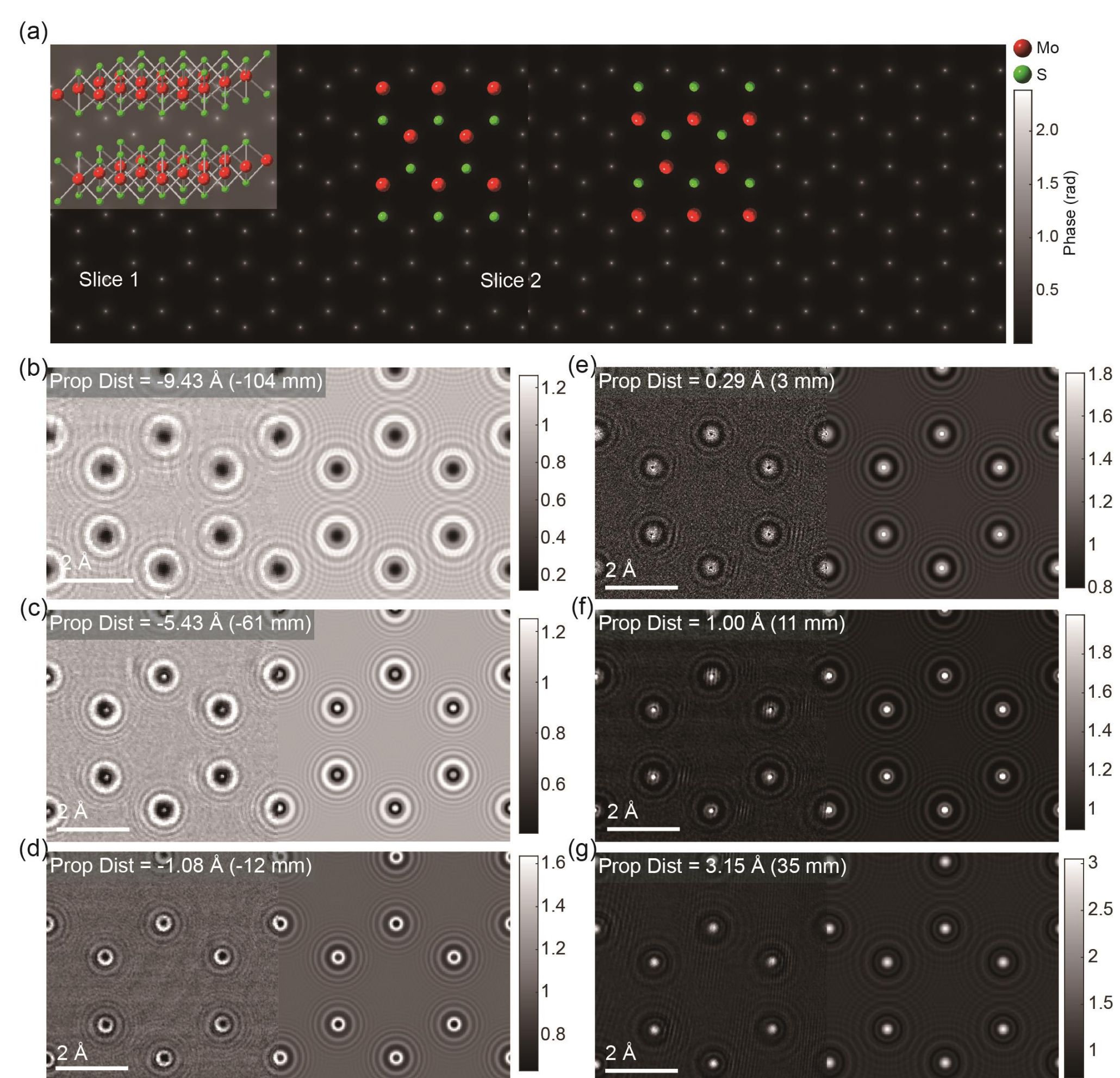
## Optical computer for TEM imaging



In TEM, a very thin sample is illuminated by high energy electrons, where scattering and phase shifts of the electron wavefunction encodes the sample structure. The multislice algorithm models this by slicing the specimen, applying atom phase shifts at each layer and Fresnel propagation between layers. The figure above shows the working principle of optical computing for TEM image simulation.

The fundamental similarity between the wave behavior of photons and electrons enables the simulation of electron scattering through phase modulation of photons implemented with spatial light modulators (SLMs) combined with free-space optical propagation.

## Optical computing principle for TEM imaging



The figure above shows simulated double layer MoS2 TEM images. (a) Projection potential induced phase shift of the two slices and corresponding atomic site. Inset: structure model for two-layer MoS2. (b-g) Wave intensity at different propagation distances in Angstrom and mm given by optical computing method (left) and numerical simulation (right). High level similarity is exhibited in all the images, including brightness at atom centers, contrast features and radius of rings around the atoms. These results demonstrate that optical computing can successfully simulate electron propagation processes, and is therefore capable of image and diffraction pattern simulation for TEM.