Image simulation in high resolution transmission electron microscopy considering atom as an electrostatic interferometer

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Introduction to image simulation

Aberration corrected FEI TITAN^{3TM} 80-300 kV

Simulated HRTEM images

MoS$_2$ BN

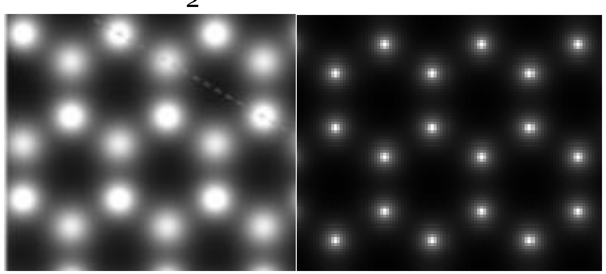
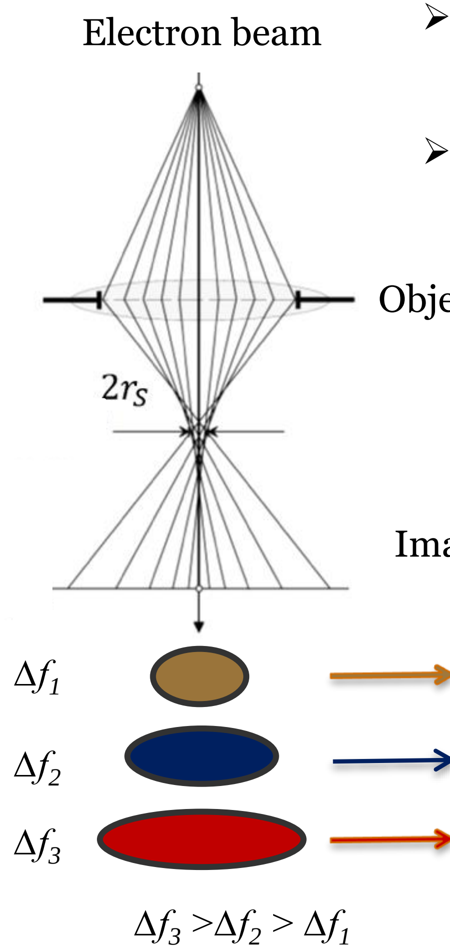
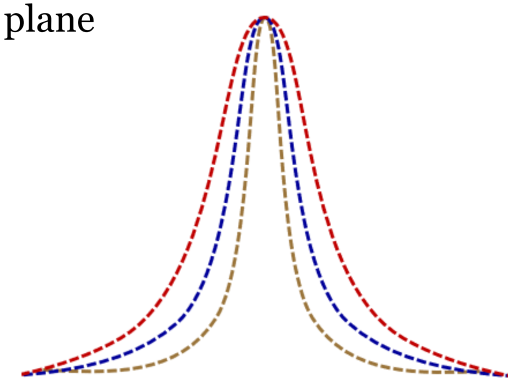


Image formation in TEM





- e- beam passing through the sample contains all the information
- With varying defocus (Δf), changes in FWHM is expected

Existing methods of image simulation

1. Zernike phase object and WPOA

Zernike phase object $F(x) = e^{i\phi(x)}$ or $\sim 1 + i\phi(x)$

WPOA image intensity $I(x,y) = \{1 + 2\phi(x)\}$

$$I(x,y) = 1 + 2\sigma\phi_p(-x,y) * \mathcal{F}\{sin\chi(u,v)P(u,v)\}$$

- Pure phase/weak scattering object
- Intensity has linear dependency on the phase
- Without the WPOA, no information available at the image plane

2. Atomic scattering factor

Moliere scattering factor

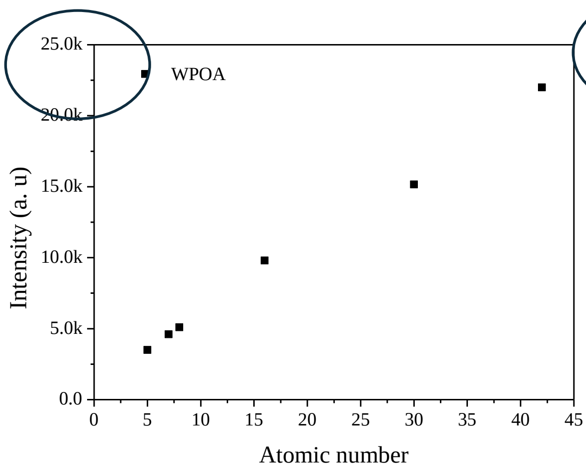
$$f_e(k) = \frac{2\pi i}{\lambda}\int_0^\infty J_0(2\pi kr)\{1 - \exp[i\sigma\int V(x,y,z)dz]\}rdr$$

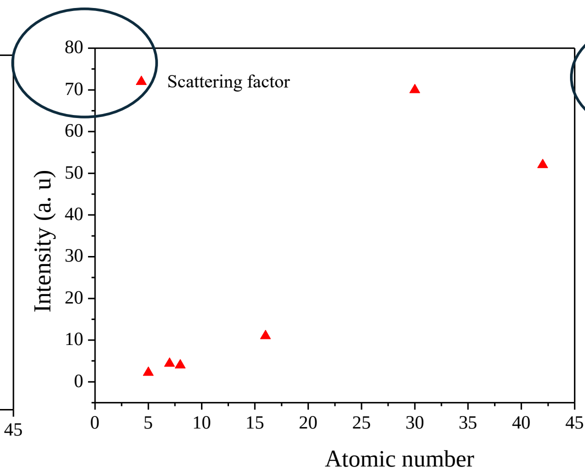
Intensity

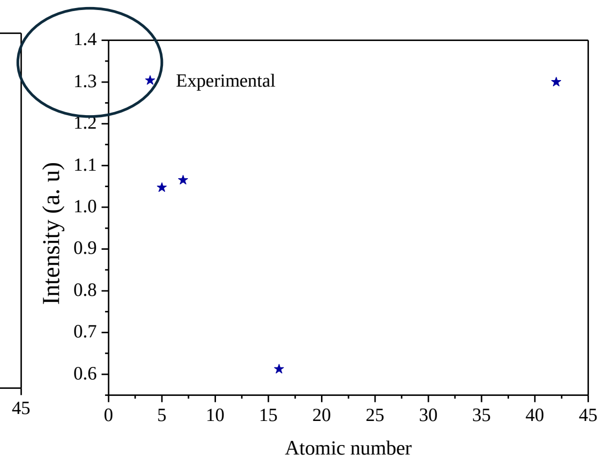
$$g(x) = \left|1 + 2\pi i\int_0^{k_{max}} f_e(k)\exp[-i\chi(k)]J_0(2\pi kr)kdk\right|^2$$

- Moliere scattering factor is considered
- Intensity values are calculated for

Theory v/s experiment

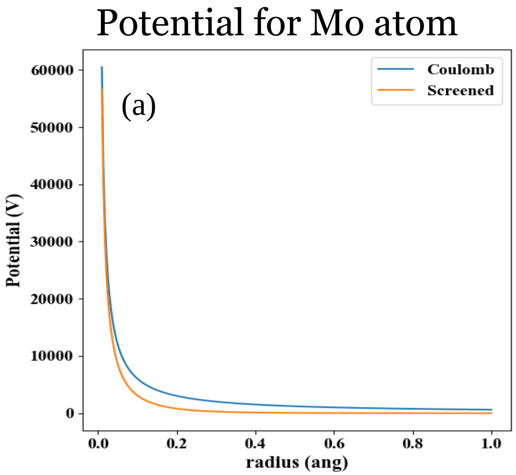


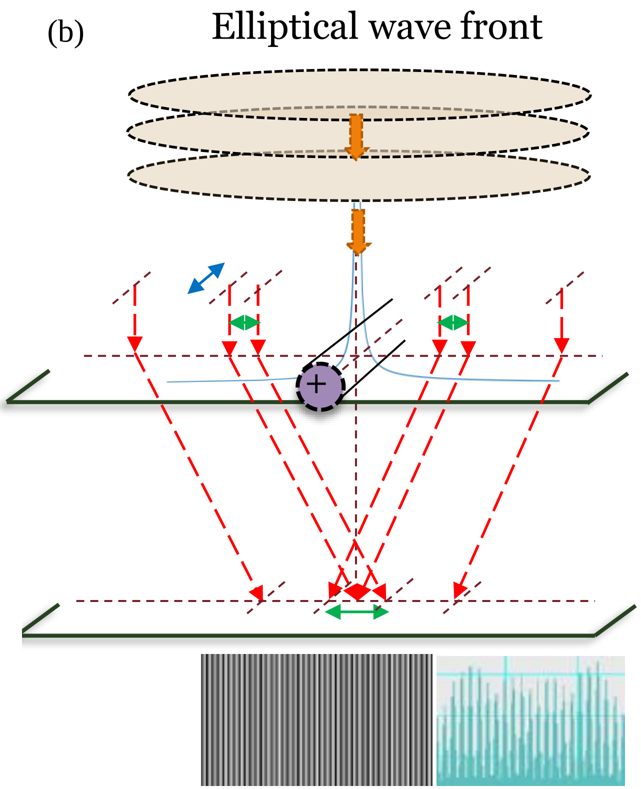


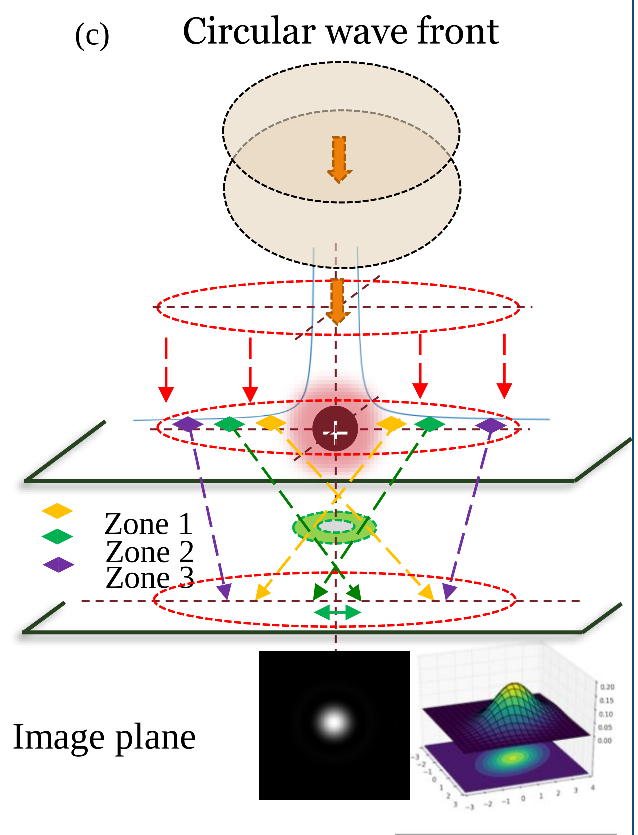


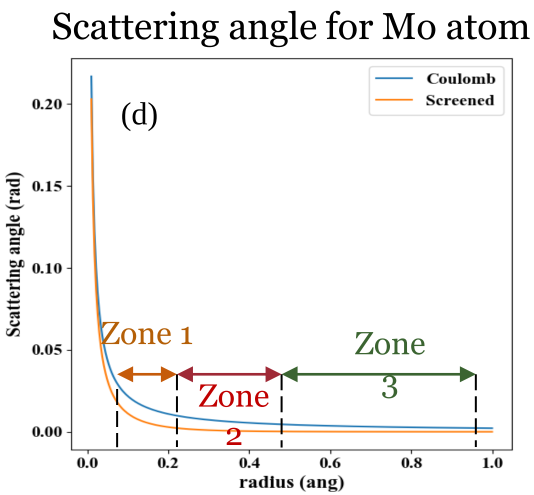
- WPOA intensity varies linearly and it is very high
- Scattering factor based intensity is not linear and it is still high
- Experimental data shows change in intensity is non-linear

Introducing a new method : Atom as an electrostatic interferometer









$$I_{rad\ int}(r) = a_1^2 + a_2^2 + 2a_1a_2\cos(2\pi q_c r) * 2\pi(r_{max} - r)$$

- Off-axis e- holography : Elliptical wave front and interference due to single pair of scattering wave vectors
- New method : Circular wave front and interference due to a range of scattering wave vectors
- Zones are based on the same range of scattering angles & intensity from different zones scaled as 2πr
- Modified intensity equation with the flux balance calculates the image pattern

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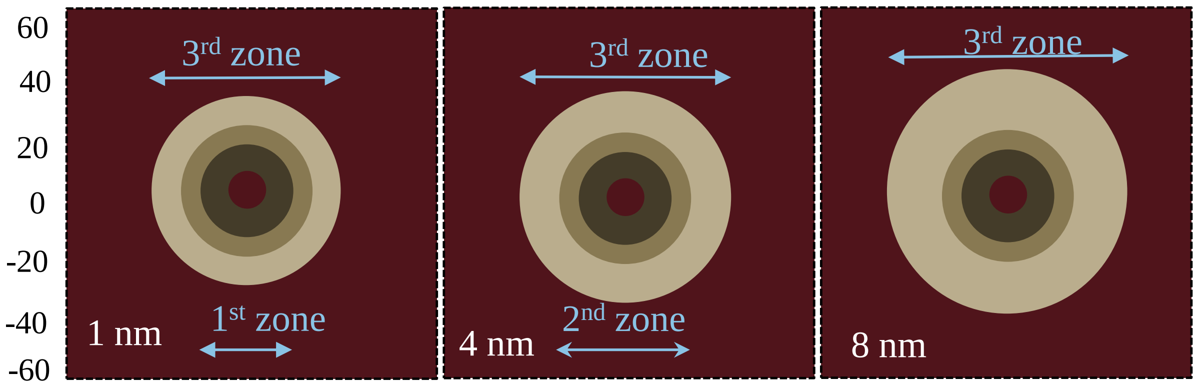
Different zones and corresponding intensity pattern



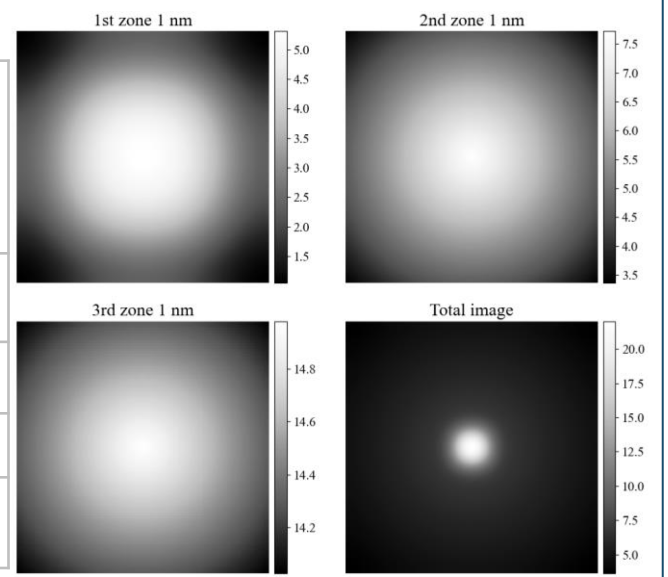
- Zones with varying defocus (Δ*f*) of 1, 4 and 8 nm
- Width of 3rd zone is increasing as Δ*f* increases
- Image of an atom calculated as a sum of all zones

Mo (Z=42)

Radial distance (pm) & zones	Rim width (pm)	Mean scattering angle (rad)	Length on optic axis (nm)	Intensity (with flux balance)
1-1.77	0.77	0.1092	1	6.82
1.77-8.37	6.6	0.0275	1	7.61
8.76-9.54	0.78	0.0092	1	13.73
8.76-15.36	6.60	0.0067	4	9.93
8.76-18.85	10.09	0.0061	8	11.03

B (Z=5)

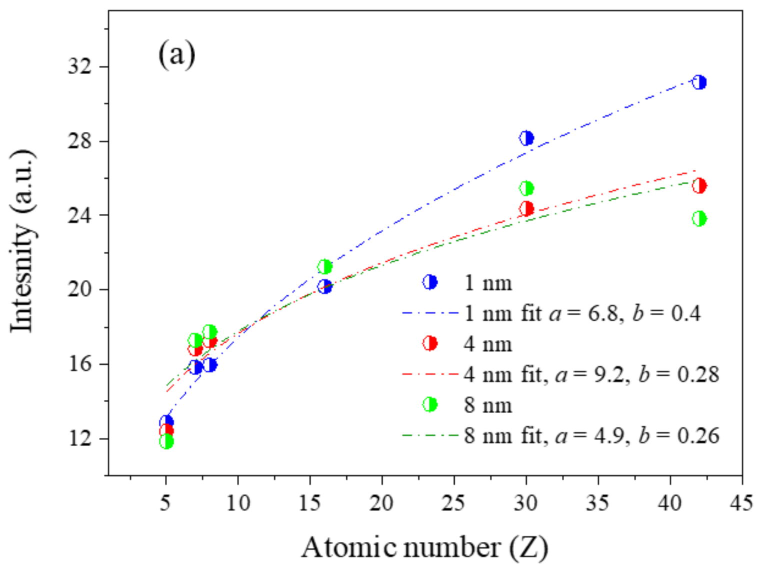
Radial distance (pm) & zones	Rim width (pm)	Mean scattering angle (rad)	Length on optic axis (nm)	Intensity (with flux balance)
1-2.16	1.55	0.014	1	5.09
2.16-4.49	1.64	0.0069	1	7.77
2.16-7.99	6.21	0.0052	4	7.31
2.16-10.31	8.93	0.0049	8	6.76

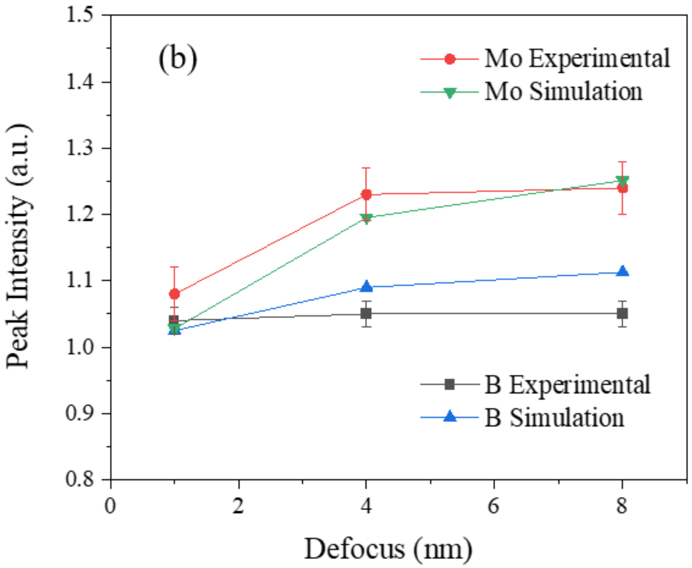


Results and discussion

Comparison of the experimental results with the new method of image simulation

Without aberration | **With aberration**





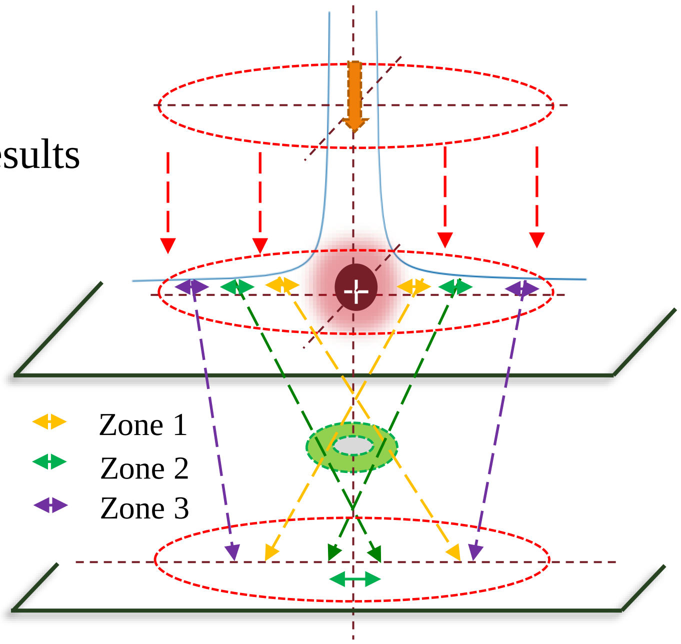
- Peak intensity falls significantly compared to the ideal lens case after considering the aberration
- Simulated result with aberration is in good agreement with the experimental data
- Intensity calculated is proportional to $Z^{03\sim0.4}$

$I = a\,Z^b$ **b ≈ 0.3-0.4**

Summary

- New method of image simulation is introduced in HRTEM considering atom as an electrostatic interferometer and the results match well with the experimental values.
- Intensity is proportional to $Z^{0.4}$.

$$I_{rad\ int}(r) = a_1^2 + a_2^2 + 2a_1a_2\cos(2\pi q_c r) * 2\pi(r_{max} - r)$$



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