

Optimized probe design for atom identification

Besides providing high resolution images, from which structural information can be learnt, atom species identification is another important function that frequently integrated to a modern microscope. Existing ways of identifying atom species with the help of electrons include energy dispersive spectroscopy (EDS), electron energy loss spectroscopy (EELS). Both methods depend on inelastic scattering that happens when the fast incident electrons transfer energy to the orbital electrons from the material, and thanks to the quantized energy level of the orbitals, the amount of energy differences between them can thus be used to identify the atom species. Elastic scattered electrons also carry information about the atoms that they passed by. The probability for scattering to take place at a certain angle is positively related to the local electric field established by an atom, thus we can compare the amount of electron at different angle as a reference to which atoms are of higher atomic number than the others, e.g. Z-contrast imaging.

However, as the electric fields built by the atoms lack of a quantized property, links between experimental results and models needs to be made so the specie of the observed atom can be determined afterwards. Since electron detection follows Poisson process, with the knowledge of the atom models and the experiment conditions, such as detector geometry and dose, it is indeed possible to carry out the comparison between microscopic images and simulations, and also the probability of error in atom identification can be estimated statistically, which is how likely one would make a mistake in telling atoms apart from each other [1].

In this research, we explore the optimal design in atom identification exploiting only elastic scattering. MULTEM [2], a multislice simulation package, is used to calculate the out-going wave after the interaction with atoms. We begin with the assumption of total control of electron wave amplitude and phase distribution. A searching process that continuously tunes the phase and amplitude distribution of the incident beam is used and the generated beam is fed to MULTEM for out-going wave calculation. We show that in case of no energy loss and electron loss, the difference between waves can be seen as the angle between vectors created by vectorizing the waves (Fig. 1). The result from the searching shows that there exists an upper limit in the power of distinguishing two atoms at a given dose. Then, with more realistic experiment condition, including limited convergence angle and ability to adjust only phase but not amplitude [3], we try to find designs that can bring the probability of error as low as possible. Furthermore, we show that with special designs, atom identification can be done by observing specific features in the out-going electron wave without the help of post-experimental simulation.

References

- [1] A. De Backer, A. De wael, J. Gonnissen, and S. Van Aert, "Optimal experimental design for nano-particle atom-counting from high-resolution STEM images," *Ultramicroscopy*, vol. 151, pp. 46–55, Apr. 2015, doi: 10.1016/j.ultramic.2014.10.015.
- [2] I. Lobato and D. Van Dyck, "MULTEM: A new multislice program to perform accurate and fast electron diffraction and imaging simulations using Graphics Processing Units with CUDA," *Ultramicroscopy*, vol. 156, pp. 9–17, Sep. 2015, doi: 10.1016/j.ultramic.2015.04.016.
- [3] J. Verbeeck, A. Béché, K. Müller-Caspary, G. Guzzinati, M. A. Luong, and M. Den Hertog, "Demonstration of a 2×2 programmable phase plate for electrons," *Ultramicroscopy*, vol. 190, pp. 58–65, Jul. 2018, doi: 10.1016/j.ultramic.2018.03.017.