Multiphysics Simulation for TEM Objective Lens Evaluation & Design

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Introduction

- Transmission Electron Microscopes (TEMs) are used extensively in both physical and life-sciences to examine micron- to atomic scales.
- Much of the performance of a TEM is dictated by the construction of the pole-piece within the objective lens (OL) shown in figure 1.
- Academics may be hesitant to propose substantial hardware modifications due to fears of voiding the warranty, high cost, and potential downtime.

This work proposes a simple, low-risk, and low-cost method to explore novel designs and evaluate their advantages or disadvantages via;

- COMSOL Multiphysics™ [1], a simulation package readily available in many universities, is well-documented with numerous example models to learn from.

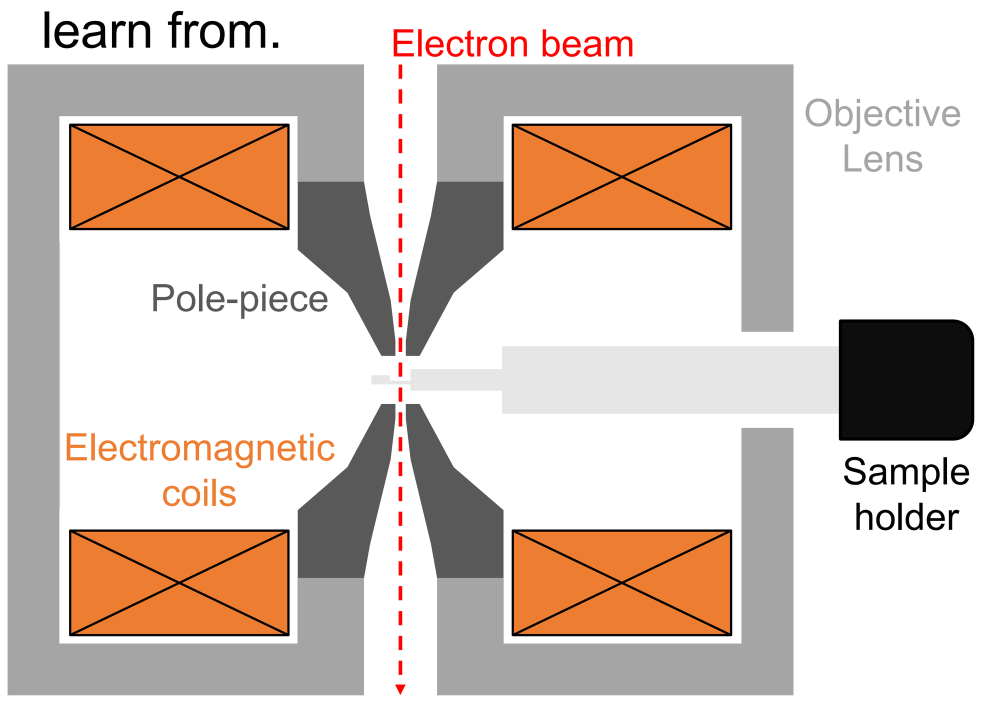


Figure 1: *Sketch of a TEM Objective Lens, with a sample holder inserted. The electron beamline is marked in red.*

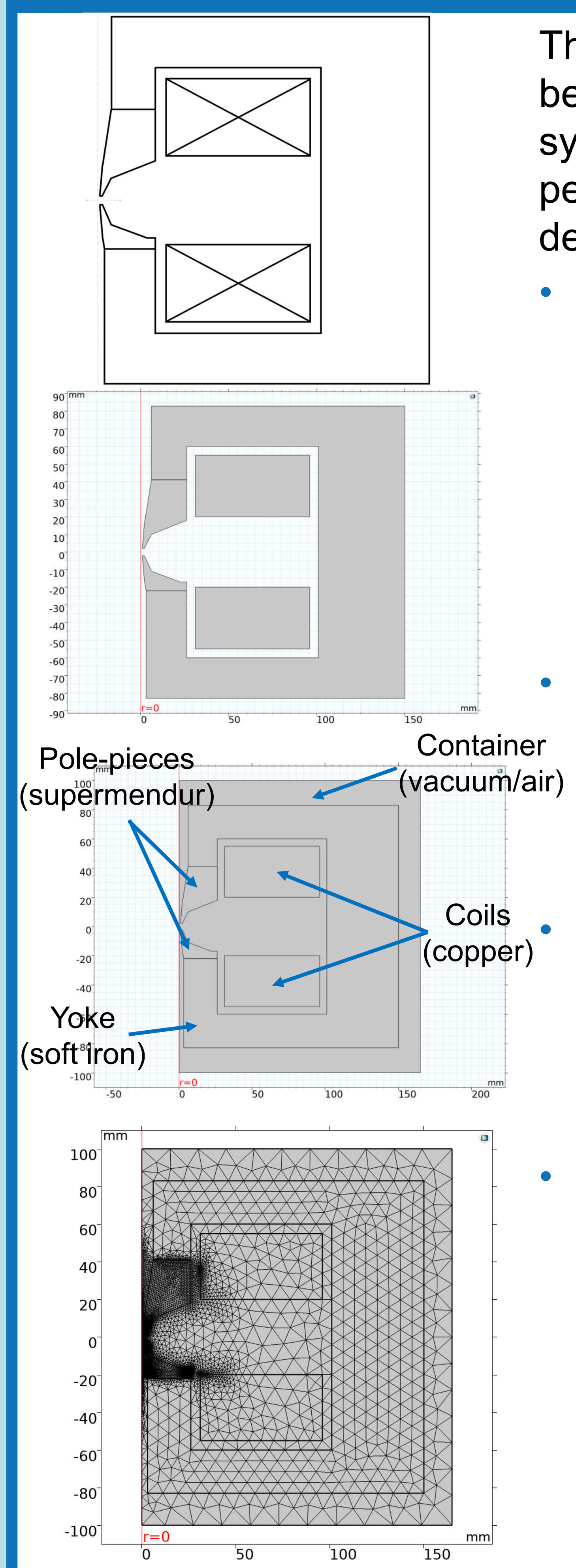
- Using a CAD program such as SolidWorks™ [2], this enables the creation of a "virtual-twin" of current electron optics or the development of new concepts.

We hope that making these tools more open reduces the barrier to entry and will encourage innovation outside of the main TEM manufacturers, leading to a more sustainable and growing field.

Methods

Though 3D models can be simulated, the OL can be approximated as being cylindrically symmetrical and a 2D simulation can be performed, saving computation time. Figure 2 details the steps followed;

- The geometry is first modelled in a CAD software such as SolidWorks™. Here, an immersion lens was modelled, but the same method could equally be used for a snorkel lens, or indeed other optics. Alternatively, COMSOL has native support for creating the geometries, which is useful if access to or knowledge of a CAD software is prohibitive.
- Each domain is then assigned a material from the COMSOL material library, such as *copper*, *soft iron*, or *supermendur*. Alternatively, custom properties can be entered, such as from a supplier of one of the metals.
- An *external current density* is added to each coil, and magnetic fields added elsewhere, either using the *B-H curve* (for the magnetic circuit), or *relative permeability* (for the remainder) as the *constitutive relation*.
- A mesh is generated. The fineness of this mesh should be adjusted to converge to a solution where a finer mesh no longer changes the solution beyond a given tolerance, but for now a fairly coarse one can be used. The mesh can be finer in areas of interest, as have been done here in the pole-piece and sample region.



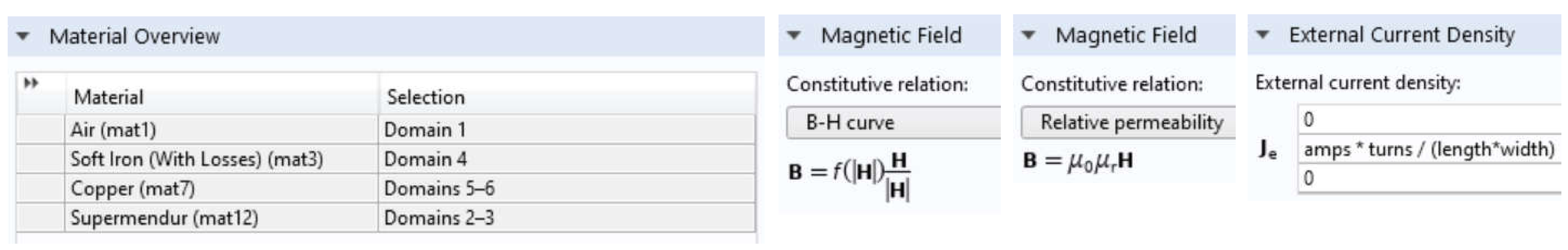


Figure 2: *Simulation methodology. The geometry is first modelled in SolidWorks and then imported to COMSOL. A container is added, and a mesh generated, in this case with a higher meshing in the region of interest (the pole-piece). The relevant materials and physics are then added to each domain.*

Results

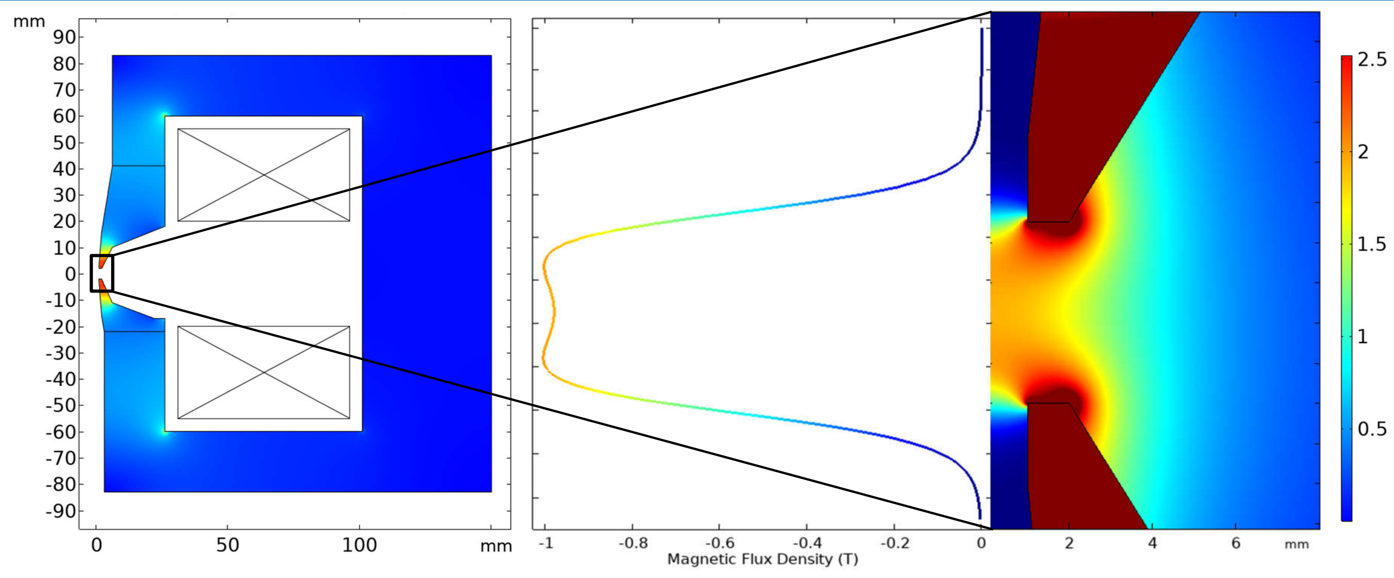


Figure 3: *(Left) The simulated magnetic flux density in the objective lens of a TEM. (Middle) Magnetic flux density along the optical axis. (Right) Zoom to show the concentration of flux density at the pole-piece tips. The vacuum sample region has also been included. Colourmap indicates magnitude of flux.*

- In figure 3, magnetic flux density can be seen to concentrate in the pole-pieces as would be expected. Localisation of flux-density indicates validity of the 'thin-lens' approximation (z-FWHM).
- By plotting the magnetic flux density along the optical axis, we can obtain the flux curves for various different lens excitation values, as seen in figure 4a. This shows that at a gap size of 1.5 mm the pole-piece is saturated just below 1000 AT, where the FWHM begins to widen, and thus aberrations are introduced [3].
- Alternatively figure 4b shows that keeping a constant excitation, but adjusting the gap, has a strong effect on the quality of the magnetic field generated, and the thin-lens approximation is not suitable for larger gaps.

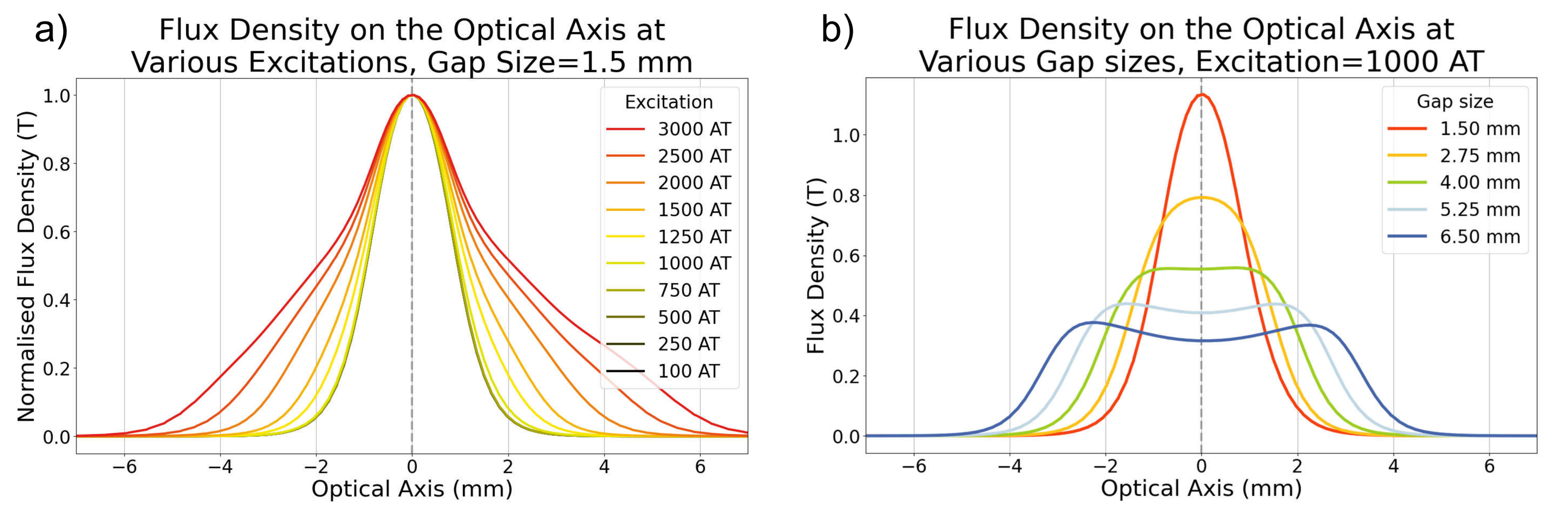


Figure 4: *Simulated flux curves along the optical axis for various levels of lens excitations (a), and gap sizes (b). This lens saturates just below 1000 AT, where the FWHM of the curve begins to increase. The thin lens approximation is not suitable for larger gap sizes, where significant aberrations are introduced.*

- By tuning the wealth of parameters available, such as pole-piece tip geometry, materials, or gap size, the specification of the lens can be designed to fit the requirements needed.
- Charged particle tracing can be added to analyse the electron trajectories, as can be seen in figure 5. These can be used to calculate preliminary aberration coefficient estimates.

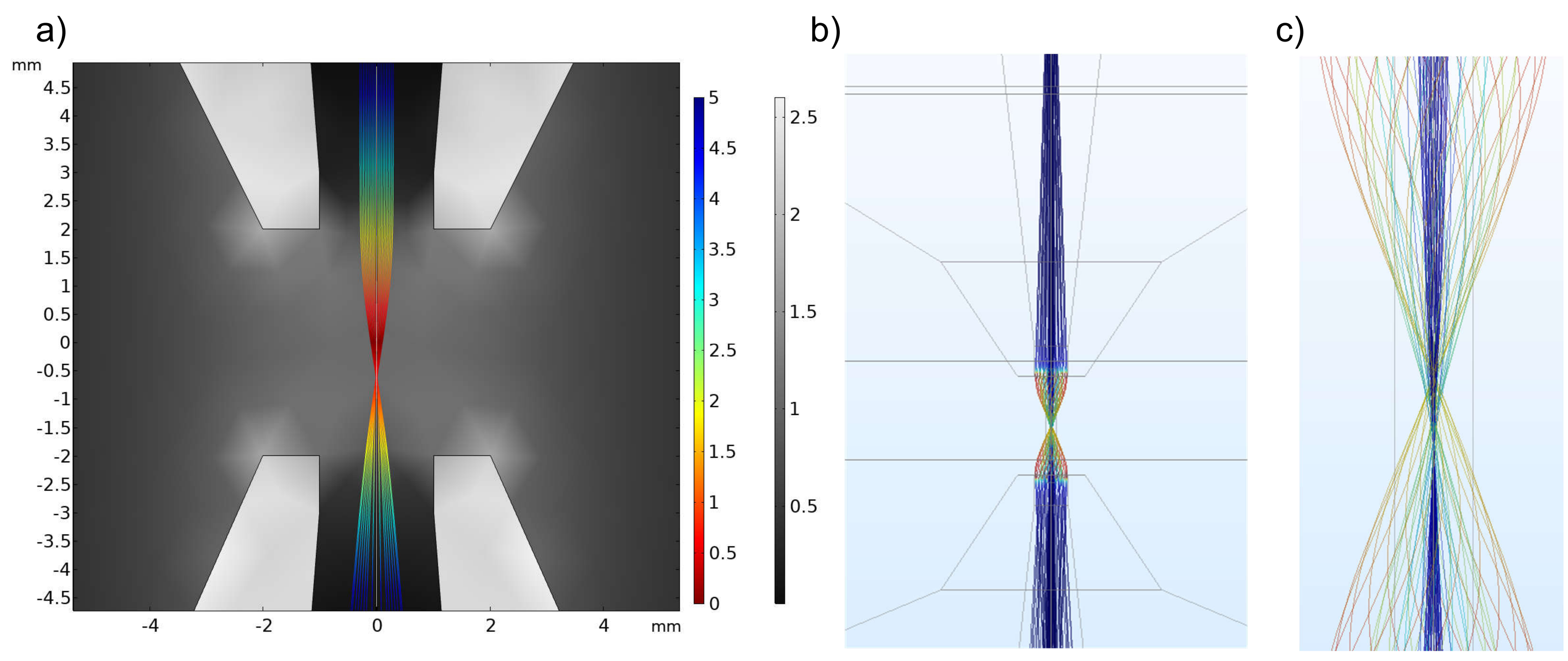


Figure 5: *Charged particle tracing simulations in (a) 2D and (b & c) 3D. In both cases, the crossover point is visible, with the spiralling trajectories visible for the 3D case. Rainbow colourmap in (a) represents vertical distance from the sample midplane for clarity, while black & white colourmap represents the magnetic flux density. Colourmap in (b&c) represents radial distance from central axis.*

Conclusions

- We have shown that COMSOL can be used to simulate both the magnetic fields within TEM objective lenses, and the particle trajectories induced by these magnetic fields. Various parameters can then be tuned to adjust the design of the lens, enabling high quality custom lenses.
- This methodology reduces the barrier to entry for exploring novel lens designs, as well as other components within the TEM, enabling grassroots innovation and allowing for a richer knowledge of TEM imaging conditions.
- Our approaches will guide and accelerate the design and capabilities of next generation TEM lenses in an accessible and sustainable manner.

References & Acknowledgements

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[2] SolidWorks 2021, www.solidworks.com. Dassault Systèmes, Vélizy-Villacoublay, France.

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