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Focal Length Calculation of Transmission Electron Microscope Magnetic Lenses using CST Particle Studio

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Abstract **Original Research Article**

In this paper, we have described a method for calculating the focal length of a magnetic lens based on the simulation of the electron path and the magnetic field distribution in the objective lens of transmission electron microscope using CST Particle Studio, an electromagnetic field and electron orbit analysis program. The results of the proposed focal length calculation method are verified by the results of the correlation experiment of the microscope. The magnetic field distribution varies with the focal length and the magnification varies with the focal length. The accuracy of the design method was verified by comparing the maximum magnification measured through simulation and image observations, focusing on the detailed design of the pole□piece, and analyzing the effect of pole-piece design parameters on the magnetic lens focal length, among many factors affecting this magnetic field distribution.

Keywords: Transmission Electron Microscopy (TEM); Magnetic Lens; CST particle Studio; Focal length; Objective lens.

1. Introduction

The principle of electron microscope is to form a image using an electron beam and an electron lens instead of a light beam and an optical lens in an optical microscope. The design and focusing characteristics of magnetic lenses determine the main parameters of electron microscope. The EO system of transmission electron microscopy can be divided into illumination and imaging systems, including the electron gun, focusing lens, imaging system, sample chamber, objective lens, intermediate and projective lens. In an electro□optical system, lenses are the most important components and the lens that plays a crucial role among lenses is the objective.

Hence, we intend to study the properties of magnetic lenses in depth through the calculation of the focal length of the objective lens.

The magnification of the transmission electron microscope can be controlled arbitrarily by adjusting the lens current, which is immediately due to the change in the focal length of the lens. Thus, the maximum magnification is obtained from the minimum focal length of the lens. Therefore, the focal length of the magnetic lens is the most important design parameter of transmission electron microscope.

In the analysis of previous studies on focal length calculation, the authors [1-5] studied the bell shape distribution of axial magnetic field in magnetic lenses, presented the trajectory equation, focal length and aberration calculation formula, and the authors [6~9] analyzed the effect of pole piece diameter and gap distance on the magnetic field distribution and presented a numerical table for focal length calculation. In addition, there are many studies in the literature on the method of calculating the focal length of magnetic lenses in transmission electron microscope, but these calculations are empirical, given only the pole-piece diameter *D*, the gap *S*, and the number of excitation turns *NI* in the magnetic lens, and the effect of various factors on the focal length is not mentioned, such as the change of the other structural dimensions of the magnetic lens, the change of the magnetic lens material, and the change of the magnetic circuit configuration.

In magnetic lenses, of course, the pole-piece diameter *D* and the gap *S* are important factors, but the magnetic circuit constituting the magnetic lens, the position of the magnetic flux-making coil, and other structural dimensions of the magnetic lens will influence the magnetic field distribution and the focal length of the magnetic lens. Therefore, the conventional focal length calculation method presents many problems in the design of real magnetic lenses. Hence, we have proposed a new method to construct a practical magnetic circuit and calculate the focal length by simulating the magnetic field distribution and trajectory of the magnetic lens.

2. Theoretical study for focal length calculation in magnetic lenses

The study of electron optical systems essentially is to determine the conditions under which the electron wave passing through an electronic lens meets the requirements of perfect imaging. In the design of magnetic lenses, focal length is the most important design parameter, and the intensity of the lens, i.e. magnification, is determined by the focal length. Therefore, how to determine the focal length is a key issue. According to [10], if 10% error is allowed, the focal length in the strong lens is calculated by the following equation:

$$\frac{f}{\sqrt{S^2+D^2}} = 31\frac{U_r}{(NI)^2} + 0.19 \qquad (1)$$

For a weak lens, the focal length is calculated by

$$\frac{f}{S+D} = \frac{25U_r}{(NI)^2} \qquad (2)$$

where f -focal length

S, D - pole piece gap distance, pole piece hole diameter

NI -excitation ampere-turns

$U_r=U_0(1+0.978\times10^{-6}\,U_0)$, relativistic correction accelerating voltage

If $\frac{U_r}{(NI)^2} = 0.001 \sim 0.005$, we consider a strong lens.

When $S/D<2$, minimum projection focal length is calculated by the following formula [10]:

$$f_{p\min} = 0.05(S^2+0.56D^2)^{1/2} \qquad (3)$$

It can be seen that decreasing the pole-piece diameter *D* and the air-gap *S* and increasing the field ampere-turns *NI*, without any other restriction, leads to a higher flux density in the air-gap and a shorter lens focal length.

We have studied the objective lens design and compare the results of the proposed method with the results of the focal length calculation using Eqs. (1) and (2).

Using Eqs. (1), (2), and (3), the focal length is determined if only the pole piece diameter *D* and the gap *S* are determined, and it is impossible to express the influence of various factors on the magnetic field distribution in a mathematical expression.

However, the effect of these factors on the focal length of the lens is never small, and empirical equations alone cannot be used to make a detailed design, but they can not lead to practical solutions, such as how to construct a magnetic circuit at design time, how to perform the electron optical parameter design of the lens in detail, and how the magnetic field.

Hence, we have proposed a new method of calculating focal length that can build the same environment as reality using simulation tools and analyze the effects of them on focal length, the most important characteristic parameter of the lens, by changing all possible parameters.

We have focused our research on how to design the pole-piece, including the pole-piece diameter *D* and the gap *S* of the magnetic lens, among many factors. To consider the variation of the axial maximum flux density value and focal length when other parameters of the piece are varied, we performed magnetic field distribution and trajectory calculations using finite element analysis software.

CST (computer simulation technology) Studio Suite 2024 has CST Microwave Studio, CST EM Studio, CST Particle Studio, and other applications, CST Cable Studio, CST Design Studio, CST PCB Studio, etc., and is widely used worldwide for electromagnetic field analysis and problem solving in the field of application. In CST Particle Studio, the various components of the rigid body can be easily modeled in three dimensions, and various settings for electric, magnetic and electron sources can be established, especially in CST Particle Studio, where the electron trajectory can be calculated under the calculated electromagnetic field distribution. Hence, we can use CST Particle Studio to obtain axial paramagnetic field distribution, electron trajectory and hence focal length by varying the acceleration voltage, lens excitation conditions, coil position, magnetic circuit, and the structure dimensions of the pole-piece.

3. Calculation of magnification

With an ideal lens model, we can establish the concept of perfect imaging.

There are six main planes in the electron lens: two focal planes, two principal planes and two nodal planes. Figure 1 shows the main surfaces of the strong lens, the focal and focal distances.

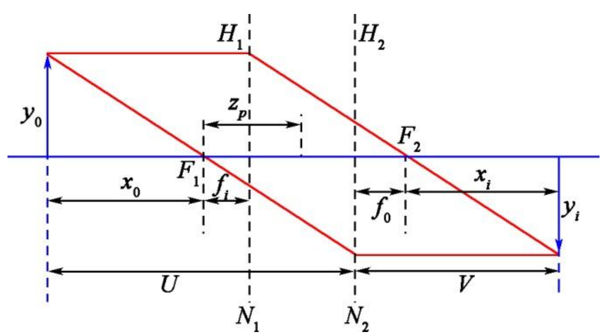


Fig. 1. Main surfaces of the strong lens and focal and focal lengths.

Nodal surfaces-(N_1, N_2), principal surfaces-(H_1, H_2), focal planes-(F_1, F_2), lens focal length- f_i, f_o, object focal length-z_p

Here, the focal plane is a plane normal to the axis passing through the focus, the principal plane with a transverse magnification of 1, and the nodal plane with an angular magnification of 1, which coincides with the principal plane in the case of a magnetic lens.

Calculating the object distance and phase distance from the principal planes H_1 and H_2, the focal calculation formula for thin lenses is;

$$\frac{f_i}{U} + \frac{f_o}{V} = 1 \quad (4)$$

If the refractive index is equal in the object and phase space, then

$$f_i = f_o = f \quad (5)$$

$$\frac{1}{U} + \frac{1}{V} = \frac{1}{f} \quad (6)$$

In Eq. (6), the sign is defined as +(-) when the object is on the left (right) of H_1 and +(-) when the object is on the right (left) of phase H_2.

In a converging lens, both focal lengths are positive and all magnetic lenses have a converging effect on electrons and positrons.

The transverse magnification is

$$M = \frac{y_i}{y_o} = -\frac{V}{U} \quad (7)$$

From Eqs. (6), (7)

$$M - 1 = -\frac{V}{f} \quad (8)$$

From Eqs. (6), (7), (8), the imaging relationship is

① $U < f$ The image is imaginary, just standing and expanding.

② $f < U < 2f$ The image is real image , inverted and magnified.

③ $U > 2f$ The image is real image, inverted and reduced.

From Eq. (8), it can be seen that for fixed and large magnification, the magnification is inversely proportional to the lens focal length.

At high magnification, the value of should be slightly larger, and for high-resolution objective, the value of and should be about 1 mm.

Hence, we calculate the magnification of each lens using Eqs. (7) and (8).

On the other hand, from the focal length calculations introduced above, it can be seen that decreasing the aperture of the lens and increasing the field ampere-turns *NI*, in the absence of other factors, leads to a higher flux density in the air gap and a shorter lens focal length.

Therefore, the total magnification of the electron microscope can be improved by reducing the pole-piece porosity of the lenses and increasing the lens current.

4. Calculation of focal length of magnetic lens through simulation

Using CST Particle Studio, the magnetic field distribution in the real transmission electron microscope is simulated and the electron track data are obtained. Using this trajectory data, the focal length is calculated. Figure 2 shows the method of focal length determination by ray-drawing for objective and projective lenses.

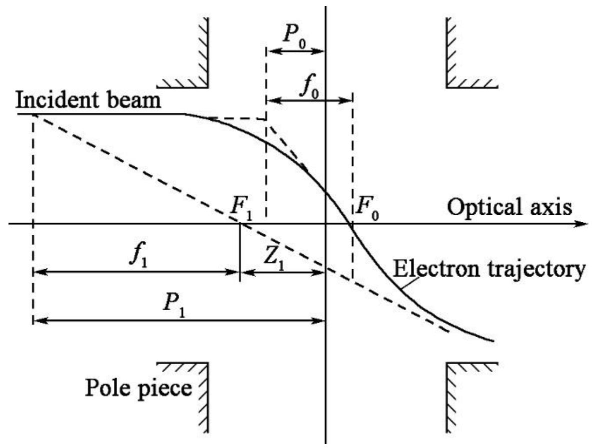


Fig.2. Calculation of focal length for objective and projective lenses

The focal length of the objective lens is calculated by setting the point where the incident electron beam parallel to the optical axis intersects the optical axis as the focal point and the point of intersection of the tangent drawn at the focal point with the tangent drawn at the focal point and the elongation drawn at the parallel electron beam as the principal position. The focal length of the projection lens is calculated by taking the point at which the tangent intersects the axis with the focal point of the projection lens and the point at which the tangent intersects the incident parallel electron beam when the incident electron beam intersects the axis.

In Fig. 2, F_0 is the objective focus, F_1 is the projectile focus, P_0 is the distance from the center to the main objective plane, P_1 is the distance from the center to the projectile principal plane, f_0 is the objective focal length, f_1 is the projectile focal length, Z_0 is the objective focal position, and Z_1 is the projectile focal position.

The computed focal length calculation results from the CST Particle Studio were compared with Eq. (1) by processing the computed parallel electron beam trajectory data in Matlab, a mathematical analysis program, according to the method of focal length determination in the above-mentioned electron optical theory. We have proved the limitations of the previous method by showing that the effect of the focal length of the objective lens of a 100 KV transmission electron microscope, except S and D, is not negligible. The simulation parameters were set to 764 turns, current 6A, and resistor of the objective lens 11.7Ω, acceleration voltage -100 KV.

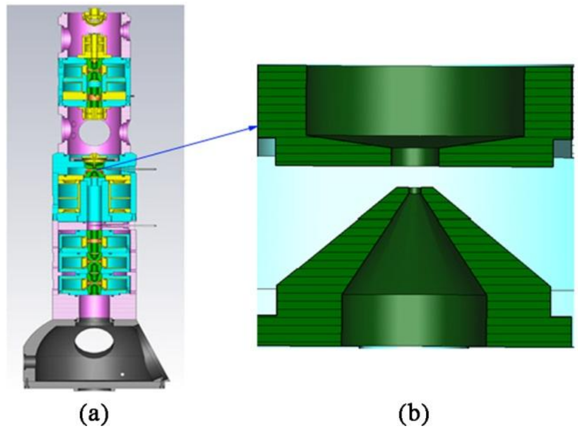


Fig. 3. The structure of transmission electron microscopy, (a); Internal structure,

(b) The structure of objective lens.

The magnetic lens material was used as an iron cobalt alloy (49% Co-49% Fe-2%V alloy) with high permeability and a saturation flux density of about 2.3 T.

Figure 3 shows the transmission electron microscope internal structure for calculations and thethree-dimensional Structure of objective lens.

The mesh for the magnetic field distribution was 2,716,416 for the tetrahedral mode and 8,889,741 for the trajectory calculation, which was relatively high in the number of mesh to ensure accuracy. The trajectory was calculated when generating an electron with energy of 100 KeV. Except for the manufacturing fixtures, the geometric parameters were set as shown in Fig. 4.

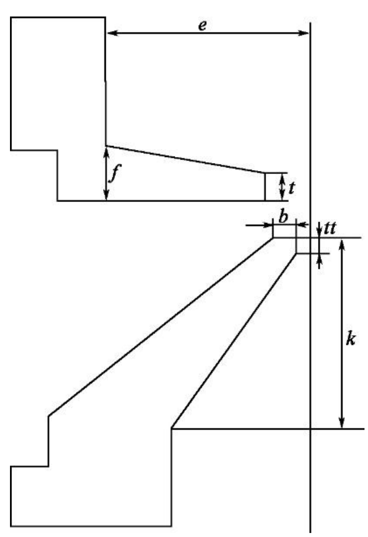


Fig 4. Geometric parameters of objective lens

Here, considering the range of manufacturing changes such as the lower pole-piece diameter 2 mm, outer diameter 26 mm, etc., *b* is determined by parameter variation between 2 to 5, t, *tt* between 1 to 4, *e* between 16 to 23, *f* between 5 to 12 and *k* between 19 and 24, and the optimum design is used to determine the parameter values that maximize the axial magnetic field.

The optimization function of the CST Particle Studio derives the optimal value given the parameter variations and the objective function.

However, the accuracy of the results is improved by reducing the range of variations, but due to the lack of over-fitting time, we have performed optimization simulations at level 4 for six factors.

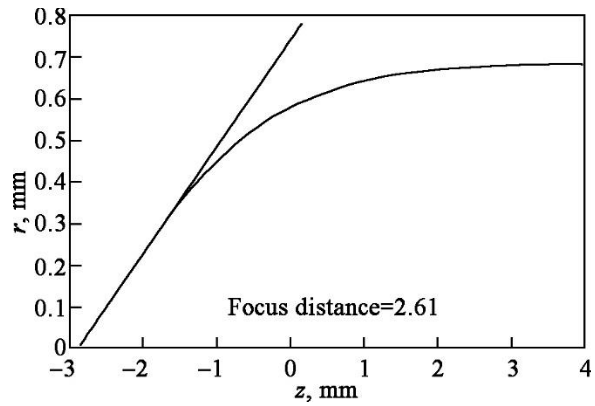
Thus, in this study, we compared the focal length values in the initial and optimum configurations by determining the geometric parameters with the largest axial maximum flux density values, varying other factors except D_1, D_2 and S.

Table 1 shows the optimum values found by changing the structure of the initial lens.

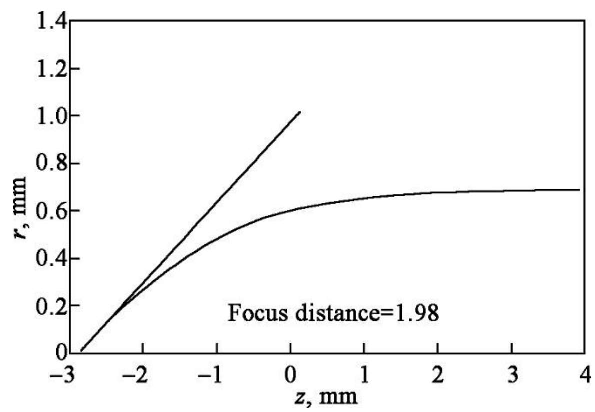
Table 1. Final parameters of objective lens (mm)

b	*t*	*tt*	*e*	*f*	*k*
2	1	1	16	3	24

Fig.5 shows the results of the focal length calculation for the initial and optimum configuration of the objective lens using Matlab, and the comparison is given in Table 2.



a)



b)

Fig.5. Calculation of focal length in the initial structure and optimum structure of the objective lens, (a); Initial structure, (b); Optimum structure

Table 2 Comparison of the characteristic parameters in the initial and optimum structure of the objective lens.

	Maximum axial magnetic field strength (T)	Focal length(*mm*)
Initial structure	1.1	2.61
Optimum structure	1.23	1.98
Calculated difference	0.13	0.63

The optimization of other factors except *S* and *D* for the objective lens resulted in a magnetic field strength as high as 0.13 T and a focal length as short as 0.63 mm.

The results of the CST Particle Studio were compared by calculating the focal length calculation when 10% error in the strong lens was allowed.

The focal length calculation by Eq. (1) for the optimized pole-piece structure parameters S = 3.5 mm, D =(8+2) /2 = 5 mm and the accelerating voltage U = 100KV is f = 2.15 mm, and our calculation is 2.61 mm for the initial structure and 1.98 mm for the optimum structure. It can be seen that the effect of changes in other factors except S and D on the focal length is not negligible.

5. Correctness verification of the calculation method.

To evaluate the accuracy of the simulation by CST particle studio, the maximum flux density in the air gap in the objective initial structure was measured.

The measured air gap maximum flux density with varying objective excitation current of 0.5A is shown in Table 3, and compared with the simulated results.

Table 3 Comparison of magnetic field measurements and simulated values for objective lenses.

Current[A]	Air gap maximum flux density[Gs]		Error analysis	
	Measuring result	Simulation calculated result	Absolute error[Gs]	Relative error[%]
0.45	910	1000	90	9.8
1.05	2100	2200	100	4.7
1.5	3100	3210	110	2.6
2.0	3900	3950	50	1.2
2.5	5820	6000	180	3
3.0	7400	7600	200	2.7
3.5	8600	8760	160	1.8

The simulation results are different from the measurements made by the existing microscope because the magnetic field is calculated under ideal conditions. The value of the maximum flux as the sensor moves in the air gap is recorded as a measurement, which is expected to be caused by the uncertainty of this measurement. The results of the error analysis show that the errors between the simulated and measured values are relatively small and the reliability of the simulation design is high. It is impossible to measure the focal length in a real lens. However, given the distance between the microscope's lenses, the minimum focal length of the lens, the maximum magnification can be calculated. This was verified the accuracy of the focal length calculation method by comparing with the maximum magnification actually obtained through microscopic observation.

The distance between the existing hard-body magnetic lenses is

D_{01}=217 (Distance of objective lens-middle1 lens)

D_{12}=63 (Distance of middle1 lens-middle2 lens)

D_{2p}=66 (Distance of middle2 lens-projective lens)

L_p=290 (Distance of projective lens-fluorescent plate)

The maximum magnification calculations are shown in Table 4.

Table 4. Results of magnification calculations by conventional and new methods of calculation

	Structure dimension		Excitation condition			Conventional method		Simulation method	
	Gap diameter (mm)	Diameter (mm)	Number of turns(T)	Current (A)	NI (AT)	Focal length (mm)	Magnification (times)	Focal length (mm)	Magnification (times)
Objective lens	3.5	5	764	6	4584	2.15	96.59	2.61	80.1
Middle1lens	12	20	1280	2.4	3072	9.32	5.87	9.655	6.2
Middle2lens	1.8	6	1260	1.28	1612	8.24	7.3	9.279	6.5
Projective lens	2.8	2.8	1280	1.28	1638	5.73	50.6	5.51	52.7
Total magnification						209443		170117	

The structural dimensions and excitation conditions of each lens are shown, and the focal length calculation and magnification calculation by conventional and simulated methods are presented. The objective was tested in the initial configuration, and the objective was calculated from the excitation conditions by the strong lens formula and the other lenses by the weak lens formula.

Given the maximum magnification of the microscope calculated based on the conventional method is 209,000 times, the maximum magnification of the microscope calculated based on the proposed focal length calculation method is 170,000 times, and the maximum magnification of the microscope attainable through microscopic correlation is 172,000 times.

This difference can be attributed to other factors, such as the influence of other factors, magnetic circuit architecture, etc., except S and D in the lens.

It was verified that the new proposed focal length calculation method is a superior method that well reflects the practical problems in design of transmission electron microscope.

6. Conclusions

In this paper, we have proposed a new method for calculating the focal length of magnetic lenses in transmission electron microscopy using CST Particle Studio.

Using the simulation tool, the structure dimensions, excitation conditions, and material settings were constructed as realistic conditions, the magnetic field distribution was calculated accordingly, and the focal length was determined from the trajectory data according to the method of calculating the focal length according to the electro-optical theory. The advantage of this method is that, unlike conventional focal length calculation, it can improve the accuracy of the magnetic lens design by considering all the factors affecting the focal length. The accuracy of the measurement method is verified by comparing the simulation results and the measurement results. The new solution in this paper is to build a practical environment to perform simulations and derive the focal length using the data from them. The calculation of magnification by applying the method of focal length calculation to magnetic lenses of a 100KV transmission electron microscope revealed that the magnification measured by correlation observation is close to that measured by the method.

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