Cumhuriyet Sci. J., 44(2) (2023) 377-383
DOI: https://doi.org/10.17776/csj.1185157

Cumhuriyet Science Journal

| csj.cumhuriyet.edu.tr | Founded: 2002 ISSN: 2587-2680 e-ISSN: 2587-246X Publisher: Sivas Cumhuriyet University

Numerical Investigation of Diffraction Patterns of Small Size Apertures Using Light Sources From Xuv to The Visible Region: Simulation for The Small Size Structures

Muhammed Sayrac [1,a,*], **Emine Kaynar** [1,b], **Fatih Ungan** [2,c]

[1] Department of Nanotechnology Engineering, Faculty of Engineering, Sivas Cumhuriyet University, Sivas, Türkiye.
[2] Department of Physics, Faculty of Sciences, Sivas Cumhuriyet University, Sivas, Türkiye.
*Corresponding author

Research Article

History
Received: 06/10/2022
Accepted: 06/06/2023

ABSTRACT

In the present work, a computer simulation program generates Fresnel diffraction patterns from small-size apertures using illumination wavelengths from extreme ultraviolet (XUV) to the visible region suggesting that it can be used to model a wide range of experimental setups. By being able to simulate diffraction patterns for such a broad range of wavelengths, the program can be used to investigate the effects of varying wavelengths and aperture size on the resulting pattern. By using a computer simulation program that can generate Fresnel diffraction patterns across a wide range of wavelengths, one can explore how different wavelengths of light interact with various aperture sizes. This allows one to investigate the effects of changing these parameters on the resulting diffraction pattern. The computer simulation program generating Fresnel diffraction patterns from square apertures by using the illumination wavelength sources from XUV to the visible region has been studied. Changing the aperture-screen distance, the illumination wavelength, and the aperture size provides a clear transition of diffraction patterns from the Fresnel to the Fraunhofer region. The diffraction patterns obtained by the Fresnel integral method have been compared with that simulated by the Fraunhofer calculation. There is a good agreement between the results. The structural similarity index (SSI) exhibits that comparing the diffraction images produced with both approaches agree.

Keywords: Diffraction. Optics. Numerical simulation. Micron/nanostructures. XUV radiation.

[a] *muhammedsayrac@cumhuriyet.edu.tr* *https://orcid.org/0000-0003-4373-6897*
[b] *emineekaynar@hotmail.com* *https://orcid.org/0000-0002-0050-348X*
[c] *fungan@cumhuriyet.edu.tr* *https://orcid.org/0000-0003-3533-4150*

Introduction

Optics is one of the important fields of physics that studies the properties of light. It plays an important role in technical applications such as communication and information sciences. In optics, the diffraction of light plays a paramount role in solving optical problems that do not usually reach an agreement with an exact solution. Therefore, numerical methods make it easy to investigate simpler cases. When the optical wave encounters an aperture, diffraction of light occurs [1]. Diffraction is classified known as Fraunhofer (far-field) and Fresnel (near-field) diffraction. The Fraunhofer diffraction pattern occurs when the aperture-observation screen distance is large. However, the Fresnel diffraction pattern appears when the aperture-screen distance is short [2, 3]. Diffraction and propagation of the optical field from an aperture were calculated by using Helmholtz-Kirchhoff [4] and Rayleigh-Sommerfeld integrals [5]. The Fresnel and Fraunhofer diffraction patterns were obtained by using the Fourier transform method [6] and the two-dimensional Fast Fourier transform method [7, 8].

The calculation of the diffraction integral is possible with minimum effort due to the personal computer and packaged mathematical software. In this paper, the diffraction patterns have been obtained by using Matlab software (R2017b 9.3.0.713579 (x64)) in the XUV and visible region. [9]. The Fresnel and Fraunhofer diffraction patterns have been simulated for a nano or micron size aperture by using the radiation source from 4nm to 600nm (corresponding to photon energy from ~310eV to 2eV) [1, 10-12]. This paper aims to study diffraction phenomena further for small-size structures by using short-wavelength radiation. The "soft x-ray region" of 4nm corresponds to the water window region in which water is transparent to extreme ultraviolet (XUV) radiations. Therefore, the wavelength region has a crucial role in viewing water-dominant biological samples, and the diffraction of light has a vital role in life science. On the other hand, this phenomenon is complex for studies in the short wavelength region, and it is not easy for laboratory experiments. For this reason, the simulation approaches facilitate viable alternatives and bring an idea for pre experiments studies. Over the last 20 years, the optics field including coherent XUV beamlines has brought opportunities that study in several disciplines from biological imaging [13-15] to material science [16, 17], and astrophysics [18] to high energy plasmas [19-21]. Also, it is useful to science and engineering students who deal with Fresnel diffraction, especially in short-wavelength regions. Therefore, the implementation of a diffraction model for a small-size aperture by using a short-wavelength source is important.

The diffraction patterns discussed the Fraunhofer diffractions of the single slit at the visible or infrared region, however, the diffraction patterns at the XUV region were not mentioned. The paper introduces a simulation for Fraunhofer and Fresnel diffraction at a wavelength range from XUV to the visible region. The simulation program is compiled by several input parameters, namely the aperture-screen distance, the illumination wavelength, and the aperture size. The simulation program demonstrates how a diffraction pattern changes with varying input parameters from the Fraunhofer to the Fresnel region at the short wavelength region. Optical diffraction has been studied by several researchers in the visible wavelength region [12, 22-28]. In this paper, the diffraction patterns from small-size apertures (nano/micron-size objects) at the short-wavelength regions have been studied. This is the novelty of this paper for studying diffraction patterns from small-size structures illuminated by monochromatic light. In addition, diffraction patterns obtained by the Fresnel and the Fraunhofer methods have been compared by using the structural similarity index (SSI). The SSI is used for metric measure the similarity between two patterns. The concept of SSI is introduced in Section 4. Both approaches produce similar patterns for the same input parameters. The rest of the paper is organized as follows. Section 2 gives basic diffraction theory. Section 3 describes the simulation results. Section 4 compares simulation results obtained by the Fraunhofer and Fresnel diffraction methods. Finally, the conclusion is drawn in Section 5.

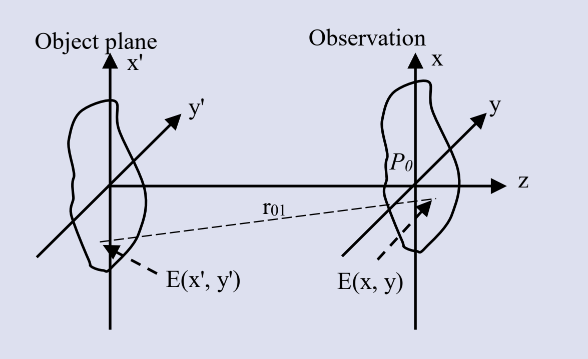

Figure 1. Schematic diagram of diffraction [1, 11]

Basic Diffraction Theory

Light propagation and diffraction have been described by using the Huygens-Fresnel principle by several researchers [4, 6-8, 10, 12]. The fundamental calculation of Fresnel diffraction from a rectangular aperture is that a light wave passes through an aperture and the total electric field at any point in the xy-plane can be obtained by the Huygens-Fresnel Principle for rectangular coordinates, Fig. 1 [1, 11]. The diffracted light is observed on the screen located at a distance. By using the Huygens-Fresnel principle, the total field in the xy-plane is integral to the fields of all the wavelets produced in each part of the aperture in the x'y'-plane [1, 10, 12] and can be described as follows

$$E = \frac{-iE_u}{2}\left[C(u)+iS(u)\right]_{\alpha_1}^{\alpha_2}\left[C(v)+iS(v)\right]_{\beta_1}^{\beta_2} \qquad (1)$$

where E_u is the unobstructed electric field at P_0. *C* and *S* are the Fresnel integrals and two-dimensional variables are defined $u = y\left[\frac{2(r_{01}+P_0)}{\lambda r_{01}P_0}\right]^{0.5}$ and $v = z\left[\frac{2(r_{01}+P_0)}{\lambda r_{01}P_0}\right]^{0.5}$.

λ is the wavelength, and r_{01} is a vector from an aperture point to a parallel screen. *E(x', y')* and *E(x, y)* are electric fields on the aperture and the screen, respectively. There are two approximations: (i) the dimensions of the diffraction geometry are larger than the illumination wavelength (λ). (ii) The observation screen distance is many wavelengths from the aperture ($r_{01} >> \lambda$)

Taking the square of the electric field, Eq. 1 gives the illumination intensity *I* and can be written as,

$$I = \frac{I_u}{4}\left\{\left[C(\alpha_2)-C(\alpha_1)\right]^2+\left[S(\alpha_2)-S(\alpha_1)\right]^2\right\}\times \\ \times\left\{\left[C(\beta_2)-C(\beta_1)\right]^2+\left[S(\beta_2)-S(\beta_1)\right]^2\right\} \qquad (1)$$

I_u is unobstructed intensity corresponding to the square of E_u, and $\alpha = \sqrt{\frac{2}{\lambda z}}(x'-x)$ and $\beta = \sqrt{\frac{2}{\lambda z}}(y'-y)$ are coefficients. α and β indicates the position of the edges of the structure in the *x* and *y* direction, respectively.

The derivation of the Fresnel integral method is given in a detailed manner [10, 12]. When the distance between the aperture to the observation screen is increased, the Fresnel diffraction region gradually approaches the Fraunhofer diffraction region. In the simulation part, the Fresnel diffraction integral has been used, Eq. 2 [10]. Input parameters namely the aperture to screen distance, the illumination wavelength, and the aperture size have been changed, and the diffraction patterns vary with changing input parameters.

Simulation results

The input parameters of the simulation program are as follows: the width of the aperture in millimeters, the wavelength in nanometers, and the aperture to screen distance in millimeters. For Fig. 2-4 (a-d), the upper figures correspond to 2D diffraction patterns, and the lower ones are for 1D normalized intensity distribution of diffraction patterns. To compare the diffraction patterns, we gradually increase the aperture to screen distance, Fig. 2. Figure 2 shows the diffraction patterns for the increasing aperture to screen distance. The illumination wavelength and the aperture size are kept constant at 32nm and 0.1mm×0.1mm, respectively. The transition of diffraction patterns from the Fresnel regime to the Fraunhofer regime is expected, Fig.2 (a)-(d). When the aperture-screen distance is increased, the Fresnel diffraction pattern gradually changes into the Fraunhofer diffraction pattern. Aperture size is about 3100 wavelengths wide, and the screen has been placed from the aperture about 0.3million to 43million wavelengths away, Fig. 2 (a) 0.3million, (b) 2.2million, (c) 22milllion, and (d) 43million. For the case of a large aperture to screen distance, the diffraction patterns resemble a Fraunhofer diffraction pattern (Fig. 2(d)). On the other hand, for the smallest aperture to screen distance, a Fresnel diffraction pattern is obtained, (Fig 2(a)).

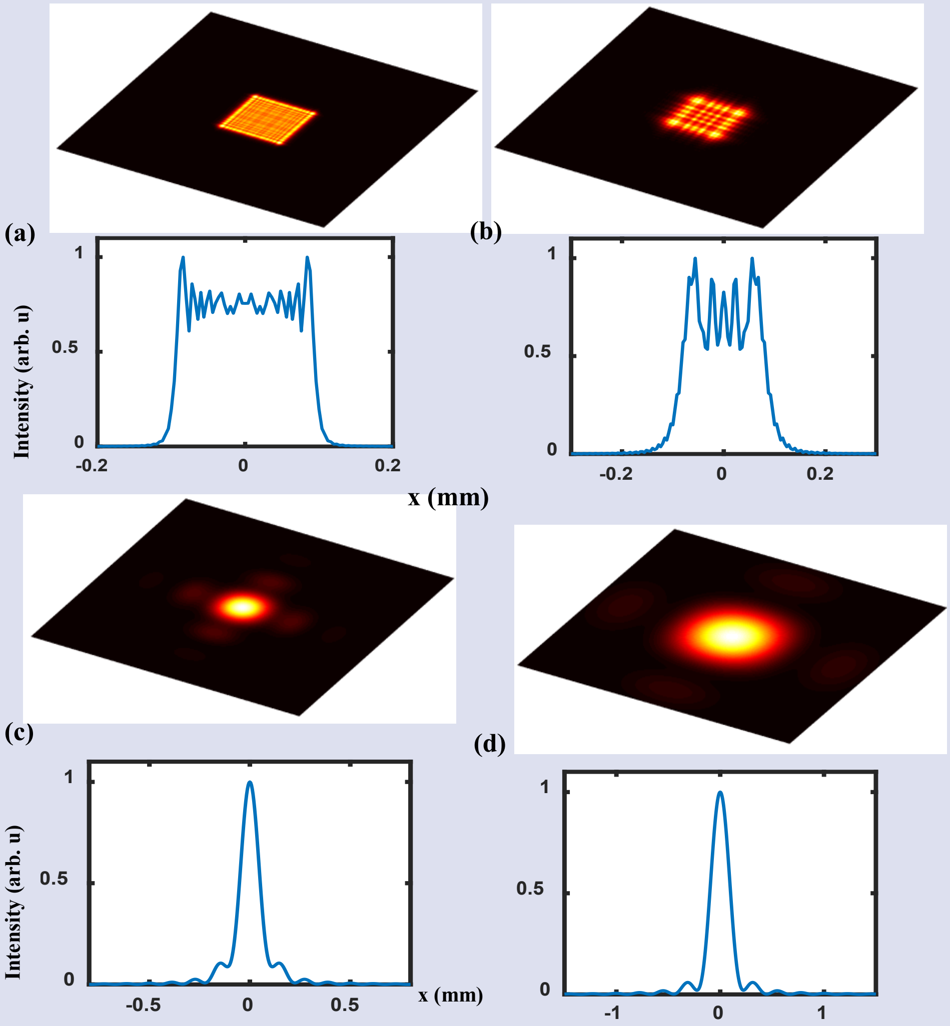

Figure 2. Diffraction patterns for increasing the aperture-screen distance. (a)10mm, (b)70mm, (c)700mm, (d)1400mm. The aperture size is 0.1mm×0.1mm, and the illumination wavelength is 32nm

Moreover, the effect of the change of wavelength on the diffraction patterns is observed, in Fig. 3. Figure 3 presents diffraction patterns (upper figures Fig. 3 (a-d)) for a fixed aperture size of 0.1mm×0.1mm and for the apertures to screen distance of 700mm. The illumination wavelength gradually increases from 4nm to 600nm wavelength. Thus, the aperture width varies from 25×10^3 to 160 wavelength size, and the distance between the aperture-observation screen changes from 175 to 1 million wavelengths away, Fig. 3 (a)-(d). When the aperture size and the aperture-to-screen distance are constant, the Fresnel diffraction patterns are generated at the short wavelength region. An increase in the illumination wavelength generates the Fraunhofer diffraction patterns, Fig. 3. A clear transition from the Fresnel regime to the Fraunhofer regime is observed with the increment of wavelength from 4nm to 600nm, Fig 3

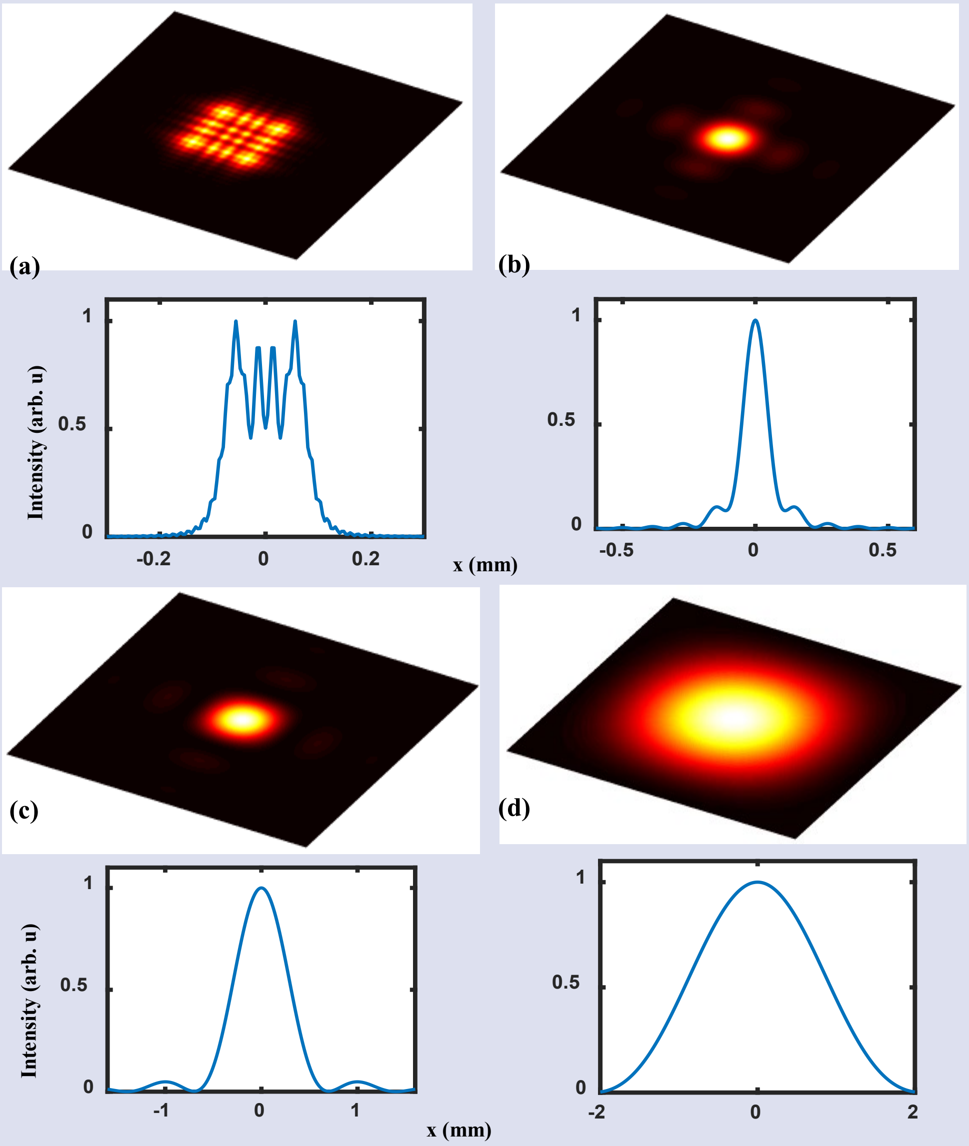

Figure 3. Diffraction patterns for increasing wavelength. (a) 4nm, (b) 32nm, (c) 200nm, (d) 600nm. The aperture size is 0.1mm×0.1mm, and the aperture-screen distance is 700mm

For a final investigation, we have studied the effects of change in the aperture sizes. The effect of a change in the aperture size is investigated. Figure 4 presents diffraction patterns of increasing aperture sizes from nano to micro size while keeping the illumination wavelength and the aperture-screen distance constant. The illumination wavelength is 4nm, and the aperture to screen distance is 700mm. The aperture size changes from 500nm to 100µm. The aperture-screen distance corresponds to about 175 million wavelengths, and the aperture size varies from 125 to 25000 wavelength size, Fig. 4 (a)-(d). For the smallest aperture size, the diffraction pattern resembles the Fraunhofer diffraction patterns (Fig. 4(a)), while the Fresnel diffraction pattern is obtained for the largest aperture size (Fig. 4(d)). Figures 2-4 agree with the rule that the aperture size, the illumination wavelength, and the aperture-screen distance have effects on the diffraction patterns [1, 11]. A practical comparison, if a satisfies the relation of $r_{01} < a^2/\lambda$, the Fresnel diffraction occurs. The relation $r_{01} > a^2/\lambda$ gives the Fraunhofer diffraction [10]. Here r_{01}, a, and λ are the aperture-screen distance, the aperture size, and the illumination wavelength, respectively. The relation for the occurrence of Fresnel and Fraunhofer diffractions can be immediately checked by using the above numerical formula. The real-time observation is obtained that the diffraction patterns change from Fresnel to Fraunhofer regime for the increasing input parameters of aperture-screen distance and the illumination wavelength, Fig. 2-3. Variations from Fraunhofer to Fresnel diffraction regime are obtained for increasing the aperture size, Fig. 4.

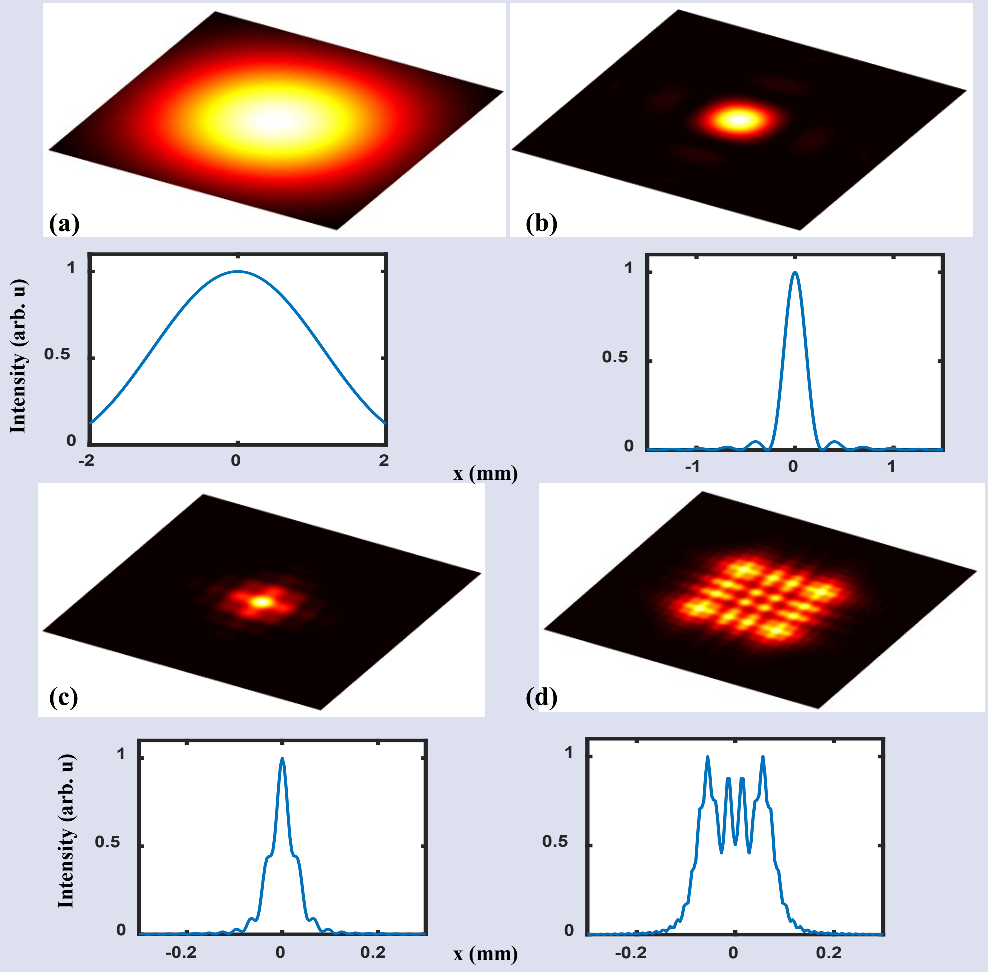

Figure 4Diffraction patterns for increasing aperture size. (a) 500nm×500nm, (b) 5000nm×5000nm, (c) 50000nm×50000nm, (d) 100000nm×100000nm. The illumination wavelength is 4nm, and the aperture-screen distance is 700mm

Figures 2-4 agree with the rule that the aperture size, the illumination wavelength, and the aperture-screen distance have effects on the diffraction patterns [1, 11]. A practical comparison, if a satisfies the relation of $r_{01} < a^2/\lambda$, the Fresnel diffraction occurs. The relation $r_{01} > a^2/\lambda$ gives the Fraunhofer diffraction [10]. Here r_{01}, a, and λ are the aperture-screen distance, the aperture size, and the illumination wavelength, respectively. The relation for the occurrence of Fresnel and Fraunhofer diffractions can be immediately checked by using the above numerical formula. The real-time observation is obtained that the diffraction patterns change from Fresnel to Fraunhofer regime for the increasing input parameters of aperture-screen distance and the illumination wavelength, Fig. 2-3. Variations from Fraunhofer to Fresnel diffraction regime are obtained for increasing the aperture size, Fig. 4.

Diffraction pattern using the Fraunhofer diffraction method

The diffraction patterns in the previous section are obtained using the Fresnel integral method [10]. In this section, the diffraction pattern obtained by using the Fraunhofer diffraction calculation is compared with that obtained by using the Fresnel integral for nano/micron size structures of the monochromatic light. The Fraunhofer diffraction studied by many researchers [2, 11, 26] is given by

$$I = I_0(\sin(\alpha)/\alpha)^2(\sin(\beta)/\beta)^2 . \qquad (2)$$

where I_0 is the intensity. $\alpha(=2\pi aX/R\lambda)$ and $\beta(=2\pi bY/R\lambda)$ are coefficients. *a* and *b* correspond to the aperture size, and *R* is the aperture-observation screen distance. The simulation using Eq. 3 compares the Fresnel diffraction with the Fraunhofer diffraction method. Figure 5(a) resembles the Fraunhofer diffraction image obtained by Eq. 3. Figure 5(b) is calculated by the

Fresnel integral method (Eq. 2) for the same parameters used for Fig. 5(a). Figure 5 (a)-(b) are well-known diffraction patterns of Fraunhofer diffraction [2, 11].

Figure 5 (b) obtained by the Fresnel integral method (Eq. 2) resembles that of the diffraction pattern presented in Fig. 5 (a) (Eq. 3) obtained by the Fraunhofer calculation method. This shows that the diffraction patterns produced using illumination wavelength in the XUV region are correct. In Fig. 5, the input parameters are the following: the illumination wavelength is 500nm, the aperture size is 1mm×1mm, and the aperture to observation screen distance is 1000mm.

Figure 5 proves that the diffraction images obtained by using the Fraunhofer calculation are perfectly matched with that obtained by using the Fresnel integral method. Measurements for diffraction pattern quality obtained by the Fraunhofer and Fresnel diffraction methods are presented in Fig. 5.

Structural Similarity Index (SSI)

SSI measures the similarities between two images (a reference image and a sample image) based on three features: luminance, contrast, and structure. The signals coming from the reference and the sample images are represented mathematically. The first feature of luminance is the measurement by averaging over all pixel values. Then, contrast is measured by taking the square root of the variance of all the pixels from the images. Finally, the structure is a comparison function by dividing the input signal by its square root of variance. After the three features are determined, the comparison function combines them and produces the similarity index value [31].

In the scope of this study, the calculation of SSI between the two patterns in Fig. 5 (a)-(b) is performed. Figure 5 (a) is used as a reference image, and Figure 5 (b) acts as a sample image. Figure 5 (c) shows that each calculation generates diffraction patterns in the Fraunhofer region and displays SSI. SSI index value is 0.57. Thus, the diffraction images in the XUV region obtained by using Fresnel integral method must be correct.

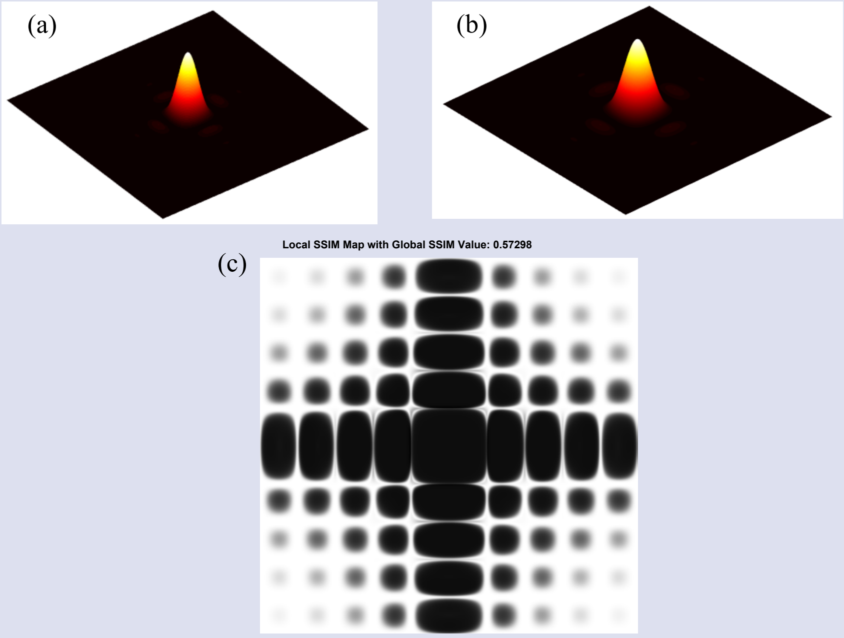

Figure 5. (a) 3D intensity distribution of the Fraunhofer diffraction image generated by using Eq. 3. (b) Simulation result of the Fresnel integral (Eq. 2) using the same simulation input parameters of Fig. 5 (a). (c) Structural similarity index (SSI) for Fig. 5 (a)-(b)

Conclusions

This paper describes that the diffraction images are generated in the Fresnel and the Fraunhofer region by using illumination wavelength from XUV to the visible region. The basic diffraction theory is described. The simulated 2D diffraction images and 1D diffraction intensity distribution for small-size apertures (nano-micron size) and different wavelength sources (from 4nm to 600nm) are presented in the results. The Matlab software simulates the diffraction patterns. The transition from the Fresnel to Fraunhofer region is observed with varying input parameters, namely the aperture-screen distance, the aperture size, and the illumination wavelength.

The diffraction images are obtained from the nano or micron-size structures at a different aperture-screen distance by using the illumination wavelength from 4nm to 600nm. The Fresnel and Fraunhofer diffraction methods produce diffraction images, and both methods generate similar diffraction patterns, Fig. 5. The structural similarity index (SSI) for comparing diffraction images obtained by the Fraunhofer and the Fresnel calculation has been performed. The diffraction patterns obtained with both approaches resemble. Thus, the Fresnel diffraction images produced by using short-wavelength sources presented in Section 3 are correct.

Acknowledgment

This work is supported by the Scientific Research Project Fund of Sivas Cumhuriyet University under project number [M-2021-819].

Conflict of interests

The authors state that did not have a conflict of interest.

References

[1] Goodman, J. W.: Introduction To Fourier Optics. McGraw-Hill Science, McGraw-Hill Science (1996).

[2] Born, M., Wolf, E.: Principles of Optics: Electromagnetic Theory of Propagation Interference and Diffraction of Light. Cambridge University (1999).

[3] Ball, C. J.: An Introduction to the Theory of diffraction. Pergamon Press, New York (1971).

[4] Rudolf, P. G., Tollett, J. J., McGowan, R. R.: Computer modeling wave propagation with a variation of the Helmholtz-Kirchhoff relation. *Appl. Opt*. 29, 998-1003 (1990).

[5] Räsänen, J., Abedin, K. M., Kawazoe, M., Tenjimbayashi, K., Eiju, T., Matsuda, K., Peiponen, K. E.: Computer simulation of the scatter plate interferometer by scalar diffraction theory. *Appl. Opt.* 36, (1997) 5335-5339.

[6] Dodds, S. A.: An optical diffraction experiment for the advanced laboratory. *Am. J. Phys*. 58, (1990) 663.

[7] Dauger, D. E.: Simulation and study of Fresnel diffraction for arbitrary two-dimensional apertures. *Comput. Phys*. 10, (1996) 591-604.

[8] Trester, S.: Computer-simulated Fresnel diffraction using the Fourier transform. *Comput. Sci. Eng.* 1, (1999) 77-83.

[9] MATLAB version 9.3.0.713579. The Mathworks, Natick, Massachusetts (2017).

[10] Abedin, K. M., Islam, M. R., Haider, A. F. M. Y.: Computer simulation of Fresnel diffraction from rectangular apertures and obstacles using the Fresnel integrals approach. *Opt. Laser Technol*. 39, (2007) 237-246.

[11] Hecht, E.: Optics. Pearson (2016).

[12] JDíaz, J. A.: Comment on “Computer simulation of Fresnel diffraction from rectangular apertures and obstacles using the Fresnel integrals approach”. *Opt. Laser Technol.* 121, (2020) 105819.

[13] Seibert, M. M., Ekeberg, T., Maia, F. et al.: Single mimivirus particles intercepted and imaged with an X-ray laser. *Nature* 470, (2011) 78-81.

[14] Chapman, H., Fromme, P., Barty, A. et al.: Femtosecond X-ray protein nanocrystallography. *Nature* 470, (2011) 73-77.

[15] Helk, T., Zürch, M., Spielmann, C.: Perspective: Towards single shot time-resolved microscopy using short wavelength table-top light sources. *Struct. Dynam*. 6, (2019) 010902.

[16] Chapman, H., Barty, A., Bogan, M., et al.: Femtosecond diffractive imaging with a soft-X-ray free-electron laser. *Nature Phys*. 2, (2006) 839-843.

[17] Milathianaki, D., Boutet, S., Williams, G. J., et. al.: Femtosecond Visualization of Lattice Dynamics in Shock-Compressed *Matter. Science* 342, (2013) 220-223.

[18] Savin, D. W., Brickhouse, N. S., Cowan, J. J., et. al.: The impact of recent advances in laboratory astrophysics on our understanding of the cosmos. *Rep. Prog. Phys*. 75, (2012) 036901.

[19] Beye, M., Schreck, S., Sorgenfrei, F., Trabant, C., Pontius, N., Langeheine, C. S., Wurth, W., Föhlisch, A.: Stimulated X-ray emission for materials science. *Nature* 501, (2013) 191-194.

[20] Rudek, B., Son, SK., Foucar, L. et al.: Ultra-efficient ionization of heavy atoms by intense X-ray free-electron laser pulses. *Nat. Photonics* 6, (2012) 858-865.

[21] Lopez, M. R., Faenov, A., Pikuz, T. et. al.: Coherent X-ray beam metrology using 2D high-resolution Fresnel-diffraction analysis. *J. Synchrotron Rad*. 24, (2017) 196-204.

[22] Makris, K. G., Psaltis, D.: Huygens–Fresnel diffraction and evanescent waves. *Opt. Commun*. 284, (2011) 1686-1689.

[23] Cui, Y., Zhang, W., Wang, J., Zhang, M., Teng, S.: Fresnel diffraction of aperture with rough edge. *J. Optics* 17, (2015) 065607.

[24] Tan, J., Lu, Z., Liu, J., Jin, P., Wang, Y.: Analysis of Fraunhofer diffractive characteristics of a tilted metallic mesh for its effect on optical measurement. *Meas. Sci. Technol.* 18, (2007) 1703-1709.

[25] Abedin, K. M., Rahman, S. M. M.: Computer simulation of Fresnel diffraction from double rectangular apertures in one and two dimensions using the iterative Fresnel integrals method. *Opt. Laser Technol*. 44, (2012) 394-402.

[26] Zhang, Z., Bai, H., Yang, G., Jiang, F., Ren, Y., Li, J., Yang, K., Yang, H.: Computer simulation of Fraunhofer diffraction based on MATLAB. *Optik* 124, (2013) 4449-4451.

[27] Stevanovic, N., Markovic, V. M., Nikezic, D.: New method for determination of diffraction light pattern of the arbitrary surface. *Opt. Laser Technol*. 90, (2017) 90-95.

[28] Markovic, V. M., Stevanovic, N., Nikezic, D.: Propagation of light from dipole source and generalization of Fresnel-Kirchhoff integral. *Optik* 180, (2019) 447-454.