

## ЕЛЕКТРОНІКА ТА ІНЖЕНЕРІЯ

<https://doi.org/10.23939/ictee2023.02>

### GRAPHENE – GOLD GRATING-BASED STRUCTURE TO ACHIEVE ENHANCED ELECTROMAGNETIC FIELD DISTRIBUTION

R. Kuzyk, O. Ilin [SCOPUS ID: 57222185168], I. Yaremchuk [ORCID: 0000-0002-7072-5950]

*Lviv Polytechnic National University, 12, S. Bandery str., Lviv, 79013, Ukraine*

Corresponding author: I. Yaremchuk (e-mail: [iryna.y.yaremchuk@lpnu.ua](mailto:iryna.y.yaremchuk@lpnu.ua))

*(Given 10 September 2023)*

In this work, the field distribution in structures such as a gold grating, a graphene layer, and a silicon substrate was studied. The conditions for maximum electromagnetic field distribution (absorption) by this structure to use in photonics and electronics devices were established. The magnitude of the electromagnetic field of a gold diffraction grating with a graphene layer increases with decreasing slit width. At the same time, an increase in the period leads to small changes in the electromagnetic field distribution. The maximum value of the distribution of the electromagnetic field is increased significantly, almost twice reducing the thickness of the graphene layer.

**Key words:** *grapheme; silicon; grating; surface plasmon resonance; field distribution.*

#### 1. Introduction

Modern trends in the development of materials and technologies show the relevance of creating submicron dimensions objects. Nanostructured plasmonic interfaces are of decisive importance for determining the properties and functionality of nanomaterials and devices based on them. It is increasingly recognized that the study and research of such nanostructures allow tuning of materials and interface properties at different scales, including the scientific fields of physics, chemistry, and nanotechnology. The study and development of plasmonic nanostructures not only satisfies the need to create materials with unique linear and nonlinear optical properties, but also helps to find the answer to how the properties of a substance change during the transition from individual atoms and molecules to organized nanostructures, and then to the solid state [1]. The interest of physicists, chemists, and materials scientists in nanoscale materials is associated with the formulation of fundamentally new scientific problems and with the prospects of searching for new physical phenomena and developing new quantum devices and systems with broad functional properties for opto- and nanoelectronics, measurement technology, information technology, and communications [2, 3]. Graphene and gold are promising materials for creating such metasurfaces.

Enhanced light transmission using nanostructured metals has always been of great interest in the field of plasmonics [1, 4]. Through the effects of the near field, it is possible to increase or decrease the transmission of electromagnetic waves. The extreme transmission of light through single subwavelength apertures [5] or arrays of nanoholes [6] has been extensively studied. With similar motives,

electromagnetic transmission through a metal film [7] using surface plasmons has also been proposed. Much of the work on extended transmission is frequency-selective due to size-dependent optical resonant frequencies.

Recently, the field of graphene plasmonics [8] has emerged, which offers new methods for controlling the near field of light-matter interaction, allowing new devices to perform total absorption [9], light modulation [10], plasmonic antennas and nanocavities [11]. In particular, the optical properties of graphene can be tuned using gating or doping, making it a promising material platform for achieving active control of nanoplasmonics.

Metallic gratings with graphene provide enhanced NIR transmission. However, numerous calculations and simulations show that surface plasmonic polaritons excited at the graphene/metal grating interface are responsible for the enhanced field distribution over a wide range of wavelengths. NIR radiation transmitted through plasmonic gratings with narrow slits can be amplified over a wide frequency range by excitation of surface plasmons in continuous graphene. This type of hybrid structure opens new possibilities for investigating and controlling the propagation of surface plasmons in a solid graphene sheet.

Graphene has attracted the attention of many researchers due to its excellent electrical, mechanical, optical, and thermal properties [12]. Graphene is one of the most significant of all two-dimensional (2D) materials due to its important properties such as high thermal conductivity, high transparency, high electrical conductivity, high carrier mobility, low contact resistance, and mechanical flexibility. These properties make graphene an exciting material for future electronics and are used in a variety of electronic and photonic devices such as transistors, electrodes, gas sensors, photodetectors, solar cells, microwave mixers, rectifiers, and some integrated circuits schemes [13]. These graphene-based devices combine the benefits of graphene and semiconductor technology.

The absorption of light by graphene photonic devices is insufficient due to the weak interaction of light-substance in the material with the thickness of the atomic layer. To enhance the light-matter interaction in graphene photonic devices, researchers have proposed integrating graphene with various photonic structures, such as plasmonic structures, optical fibers, and photonic integrated circuits [14].

It is possible to enhance the transmission (absorption) in the NIR from arrays of gold nanoslits by coupling with graphene. Optical gratings are commonly used to excite surface plasmons. Arrays of gold nanoslits provide an ideal scaffold to compensate for the momentum mismatch of surface plasmon excitation in graphene. Graphene is placed under a gold grating with silicon as a substrate, which can be performed experimentally by transferring a graphene film to silicon, followed by simulation of gold arrays of nanoslits. Silicon is used as a transparent substrate in the wavelengths of interest.

In this work, we study the field distribution in structures such as a gold grating, a graphene layer, and a silicon substrate. The optimal geometric parameters were determined to establish the conditions for maximum electromagnetic field distribution (absorption) by this structure to use in photonics and electronic devices.

## **2. Results and Discussions**

The study and determination of the optimal geometric values of structures such as a gold grating, a graphene layer, and a silicon substrate to obtain the maximum electromagnetic field distribution was carried out by the finite element method. To calculate the field distribution, the initial parameters are set, namely, the thickness of the gold grating is 120 nm, the grating width is 800 nm, the slit width is 100 nm, the grating period is 1000 nm, and the thickness of the graphene layer is 4 nm. The resonant wavelength was 1100 nm. Gold dielectric constants were used from work [15]. Refractive index of silicon from [16]. The dielectric constant of graphene is used from [17].

The electromagnetic field distribution over the initial parameters is presented in Fig. 1, a. It was determined that the maximum electromagnetic field is  $1.96 \cdot 10^5$  V/m. The thickness of the gold grating has

been increased to 150 nm, while the other dimensions remain unchanged (Fig. 1, b). The result showed that increasing the grating thickness increases the electromagnetic field, which is now equal to  $2.25 \cdot 10^5$  V/m. Therefore, the grating thickness was increased up to 200 nm. The simulation results are shown in Fig. 1, c. The absorption has increased significantly, and now the maximum value of the electromagnetic field is  $2.73 \cdot 10^5$  V/m. Thus, the grating thickness continued to increase with a step of 50 nm, which means that now it is 250 nm. The simulation results are shown in Fig. 1, d. It should be noted that after increasing the thickness of the grating, the maximum value of the electromagnetic field is  $2.74 \cdot 10^5$  V/m. These are insignificant changes, and therefore, the absorption peak can be obtained when the grating thickness is from 200 nm to 250 nm. In the next step, the grating thickness has been reduced to 225 nm. The simulation results are shown in Fig. 1, e.

The calculated maximum value of the electromagnetic field after reducing the grating thickness to 225 nm increased and is equal to  $2.82 \cdot 10^5$  V/m. Therefore, it can be considered as the optimal grating thickness.

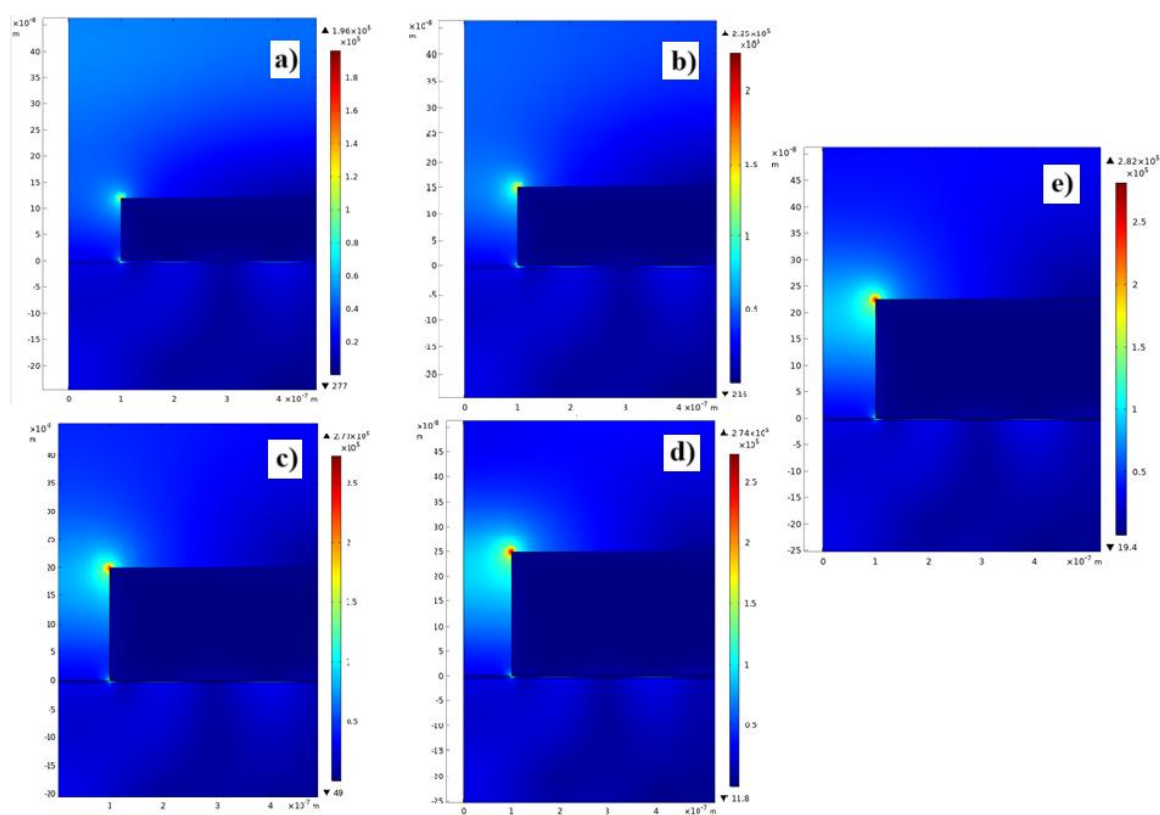


Fig. 1. The electromagnetic field distribution of the grating-based structure, the elements of which have the following dimensions: a – grating thickness is 120 nm, slot width is 200 nm, grating period is 1000 nm, graphene thickness is 4 nm; b – grating thickness is 150 nm, slit width is 200 nm, grating period is 1000 nm, graphene thickness is 4 nm; c – grating thickness is 200 nm, slit width is 200 nm, grating period is 1000 nm, graphene thickness is 4 nm; d – grating thickness is 200 nm, slit width is 200 nm, grating period 1000 nm, graphene thickness is 4 nm; e – grating thickness is 225 nm, slit width is 200 nm, grating period is 1000 nm, graphene thickness is 4 nm

Having determined the optimal grating thickness, a study was carried out at different slit widths to obtain the optimal one. It is already known that the maximum value of the electromagnetic field distribution is  $2.82 \cdot 10^5$  V/m with a slit width of 200 nm. The slit width can be changed by changing the grating width or by changing the grating period. The grating period is increased to 1100 nm. Since the grating width is 800 nm, the slit width will be 150 nm. The simulation results are shown in Fig. 2, a. With the increase in the size of the slit, the maximum intensity of the field decreased to  $2.74 \cdot 10^5$  V/m. Therefore, the width of the slit must be reduced. The grating period is changed to 900 nm, hence the slit size is 50 nm.

The simulation results are shown in Fig. 2, b. The maximum value of the electromagnetic field has increased significantly and now equals  $4.09 \cdot 10^5$  V/m. If we reduce the period to 850 nm, the slit width will be equal to 25 nm. The simulation results are shown in Fig. 2, c. The maximum value of the electromagnetic field has decreased to  $3.84 \cdot 10^5$  V/m, which means that the slit width is too small. We increase the period to 950 nm, while the slit width increases to 75 nm. The simulation results are shown in Fig. 2, d.

The result has improved relative to the previous slit width and now the maximum value of the electromagnetic field is  $4.04 \cdot 10^5$  V/m, but still less than with a slit width of 50 nm since with this slit width the maximum value of the electromagnetic field was  $4.09 \cdot 10^5$  V/m. Therefore, the value of the slit width of 50 nm will be the most optimal.

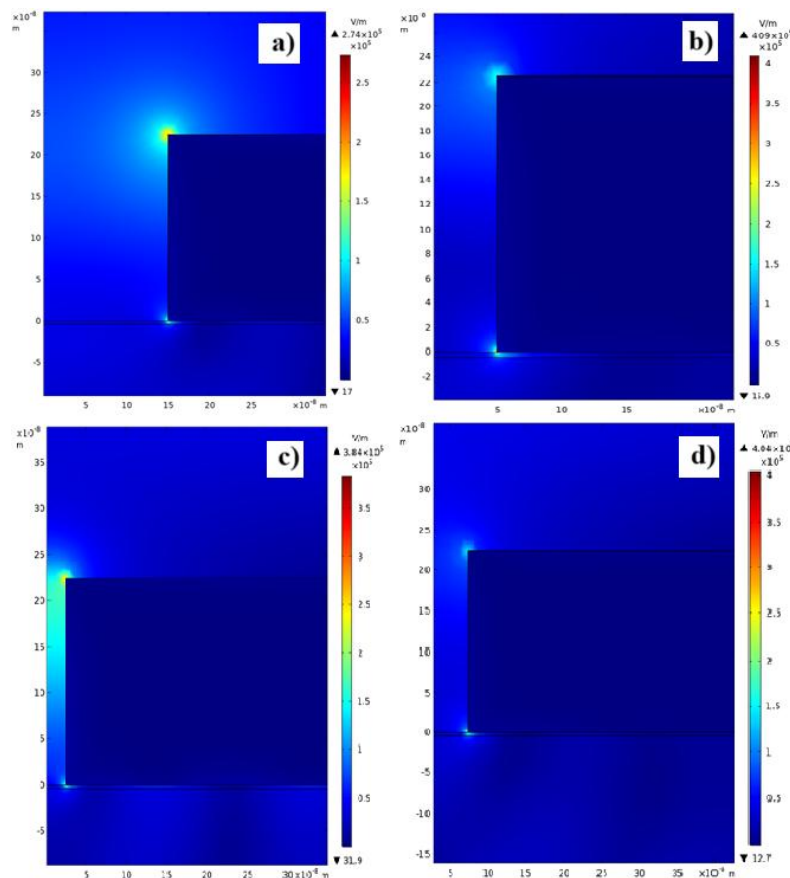


Fig. 2. The electromagnetic field distribution of the grating-based structure and, the elements of which have the following dimensions: a – grating thickness is 225 nm, grating width is 800 nm, slit width is 150 nm, grating period is 1100 nm, graphene thickness is 4 nm; b – grating thickness is 225 nm, grating width is 800 nm, slit width is 50 nm, grating period is 900 nm, graphene thickness is 4 nm; c – grating thickness is 225 nm, grating width is 800 nm, slit width is 25 nm, grating period is 850 nm, graphene thickness is 4 nm; d – grating thickness is 225 nm, grating width is 800 nm, slit width is 75 nm, grating period is 950 nm, graphene thickness is 4 nm

It is necessary to find the optimal value of the grating period having determined the optimal grating thickness and slit width. To keep the slit width constant, it needs to proportionally change the grating width and the grating period. Since it is determined that the peak absorption intensity at a slit width is 50 nm, then the grating width should be 100 nm less, per grating period, since the slit should be the same on both sides. We increase the period up to 1400 nm. The grating width is increased to 1300 nm. The simulation results are shown in Fig. 3, a. The electromagnetic field distribution has slightly decreased from the previous value and is equal to  $4.08 \cdot 10^5$  V/m. Therefore, we can conclude that the grating period is too

large. We decrease the grating period to 1200 nm and the grating width to 1100 nm. The simulation results are shown in Fig. 3, b. The value of the highest value of the distribution of the electromagnetic field has increased to  $4.15 \cdot 10^5$  V/m. Next, we decrease the grating period and grating width in increments of 50 nm. The simulation results are shown in Fig. 3, c. Fig. 3, c shows that the distribution of the electromagnetic field has increased significantly and is now equal to  $4.35 \cdot 10^5$  V/m. We reduce the grating period up to 1100 nm and the grating width to 1000 nm, respectively. The simulation results are shown in Fig. 3, d.

As a result of recent geometric changes, the intensity of the distribution of the electromagnetic field slightly decreased from  $4.35 \cdot 10^5$  V/m to  $4.28 \cdot 10^5$  V/m. Hence, we can conclude that the optimal value of the grating period is 1150 nm, and the grating width is 1050 nm, respectively, since it is necessary to provide a slit width of 50 nm.

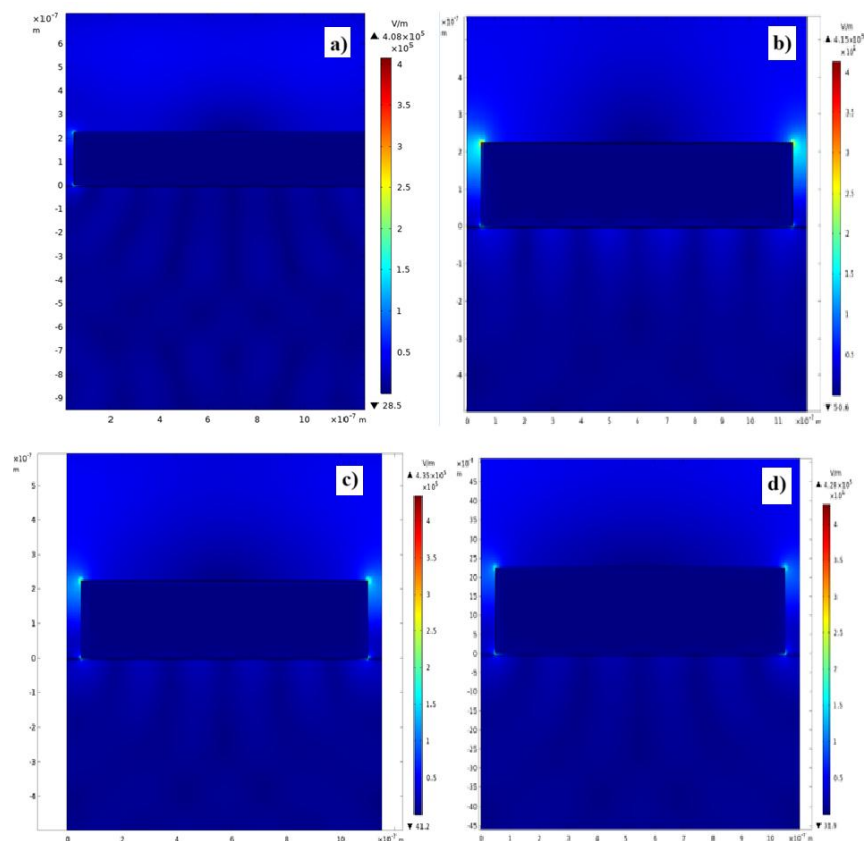


Fig. 3. The electromagnetic field distribution of the grating-based structure, the elements of which have the following dimensions: a – grating thickness is 225 nm, grating width is 1300 nm, slot width is 50 nm, grating period is 1400 nm, graphene width is 4 nm; b – grating thickness is 225 nm, grating width is 1100 nm, slit width is 50 nm, grating period is 1200 nm, graphene thickness is 4 nm; c – grating thickness is 225 nm, grating width is 1050 nm, slit width is 50 nm, grating period is 1150 nm, graphene thickness is 4 nm; d – grating thickness is 225 nm, grating width is 1000 nm, slit width is 50 nm, grating period is 1100 nm, graphene thickness is 4 nm

After all parameter changes, it was determined that with a graphene thickness of 4 nm, a better electromagnetic field distribution value than  $4.35 \cdot 10^5$  V/m can be achieved. Next, it remains to find the optimal graphene thickness and establish the maximum value of the distribution of the electromagnetic field in the researched structure. Let us increase the graphene thickness to 5 nm. The simulation results are shown in Fig. 4, a. As can be seen from Fig. 4, a, the maximum value of the electromagnetic field distribution has been significantly reduced and is now  $3.8 \cdot 10^5$  V/m. Hence the conclusion is that the thickness of graphene should be reduced. This is good because graphene is a layered material and with too many layers, graphene will already be graphite. Let's take the thickness of graphene at 2 nm. The

simulation results are shown in Fig. 4, b. As a result of these changes, the maximum value of the distribution of the electromagnetic field has increased significantly, almost twice as compared to the last calculation, and is now equal to  $6.65 \cdot 10^5$  V/m. We reduced the graphene thickness to 1 nm. The simulation results are shown in Fig. 4, c.

Therefore, this will be the final result for the research structure, since further reductions in the thickness of graphene will lead to a sharp drop in the intensity of the electromagnetic field distribution of  $9.0 \cdot 10^5$  V/m.

### 3. Conclusion

In this work, the study of the electromagnetic field distribution in structures of type the gold grating, the graphene layer, and the silicon substrate at different geometric parameters was carried out. The most intense electric field is observed when the electric field is concentrated both in the upper and lower corners of the grating. The strongest electromagnetic field distribution can be obtained when the grating thickness is in the range from 200 nm to 250 nm, the value of the slit width of 50 nm, the grating period is 1150 nm, and the grating width is 1050 nm at the given parameters. The maximum value of the distribution of the electromagnetic field has increased significantly, almost twice as compared to the last calculation reducing the thickness of the graphene layer. The optimal graphene thickness of 1 nm was determined.

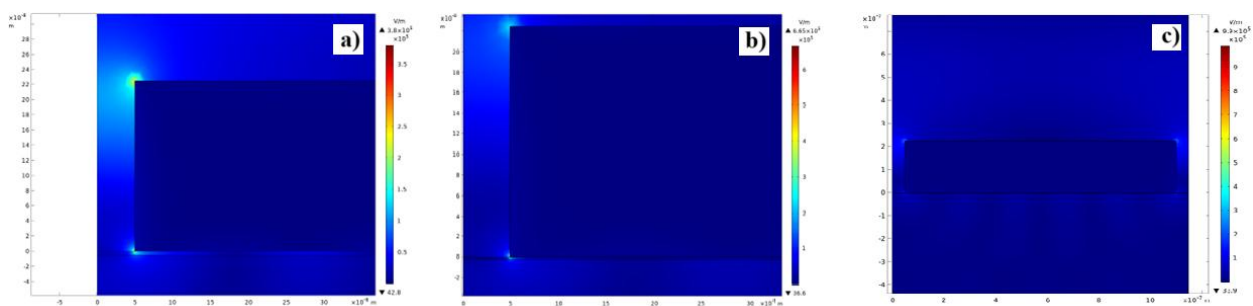


Fig. 4. The electromagnetic field distribution of the grating-based structure, the elements of which have the following dimensions: a – grating thickness is 225 nm, grating width is 1050 nm, slot width is 50 nm, grating period is 1150 nm, graphene thickness is 5 nm; b – grating thickness is 225 nm, grating width is 1050 nm, slit width is 50 nm, grating period is 1150 nm, graphene thickness is 2 nm; c – grating thickness is 225 nm, grating width is 1050 nm, slit width is 50 nm, grating period is 1150 nm, graphene thickness is 1 nm

The magnitude of the electromagnetic field (absorption) of the gold diffraction grating with a graphene layer increases with decreasing slit width. At the same time, an increase in the period leads to small changes in the electromagnetic field distribution. Therefore, the maximum of the electromagnetic field distribution can be tuned by the values of the structures' geometric parameters.

### Acknowledgment

This research was funded by the Ministry of Education and Science of Ukraine and should be acknowledged (Infra 0123U101690).

### References

- [1] Strobbia, P., Languirand, E., & Cullum, B. M. (2015), "Recent advances in plasmonic nanostructures for sensing: a review. *Optical Engineering*", Vol. 54, No. 10, pp. 100902–100902.
- [2] Roduner, E. (2006), "Size matters: why nanomaterials are different", *Chemical Society Reviews*, vol. 35, no. 7, pp. 583–592.
- [3] Kolahalam, L. A., Viswanath, I. K., Diwakar, B. S., Govindh, B., Reddy, V., & Murthy, Y. L. N. (2019), "Review on nanomaterials: Synthesis and applications", *Materials Today: Proceedings*, Vol. 18, pp. 2182–2190.

- [4] Li, X., Zhu, J., & Wei, B. (2016), "Hybrid nanostructures of metal/two-dimensional nanomaterials for plasmon-enhanced applications", *Chemical Society Reviews*, Vol. 45, No. 11, pp. 3145–3187.
- [5] Schuller, J. A., Barnard, E. S., Cai, W., Jun, Y. C., White, J. S., & Brongersma, M. L. (2010), "Plasmonics for extreme light concentration and manipulation". *Nature Materials*, Vol. 9, No. 3, pp. 193–204.
- [6] Liang, C., Yi, Z., Chen, X., Tang, Y., Yi, Y., Zhou, Z., ... & Zhang, G. (2020), "Dual-band infrared perfect absorber based on an Ag-dielectric-Ag multilayer film with nano ring grooves arrays", *Plasmonics*, Vol. 15, pp. 93–100.
- [7] Karmakar, S., Kumar, D., Varshney, R. K., & Roy Chowdhury, D. (2022), "Magneto spectroscopy of terahertz surface plasmons in subwavelength perforated superlattice thin-films". *Journal of Applied Physics*, Vol. 131, No. 22, pp. 223102.
- [8] Kim, B. S., Sternbach, A. J., Choi, M. S., Sun, Z., Ruta, F. L., Shao, Y., ... & Basov, D. N. (2023), "Ambipolar charge-transfer graphene plasmonic cavities". *Nature Materials*, pp. 1–6.
- [9] Echtermeyer, T. J., Britnell, L., Jasnos, P. K., Lombardo, A., Gorbachev, R. V., Grigorenko, A. N., ... & Novoselov, K. S. (2011), "Strong plasmonic enhancement of photovoltage in graphene", *Nature communications*, Vol. 2, No. 1, pp. 458.
- [10] Cui, L., Wang, J., & Sun, M. (2021), "Graphene plasmon for optoelectronics". *Reviews in Physics*, Vol. 6, p. 100054.
- [11] Popov, V. V., Polischuk, O. V., Davoyan, A. R., Ryzhii, V., Otsuji, T., & Shur, M. S. (2020), "Plasmonic terahertz lasing in an array of graphene nanocavities". In *Graphene-Based Terahertz Electronics and Plasmonics* Jenny Stanford Publishing, pp. 587–601.
- [12] Yu, W., Sisi, L., Haiyan, Y., & Jie, L. (2020), "Progress in the functional modification of graphene/graphene oxide: A review", *RSC Advances*, Vol. 10, No. 26, pp. 15328–15345.
- [13] Wang, S., Zhang, D. W., & Zhou, P. (2019), "Two-dimensional materials for synaptic electronics and neuromorphic systems", *Science Bulletin*, Vol. 64, No. 15, pp. 1056–1066.
- [14] Chen, K., Zhou, X., Cheng, X., Qiao, R., Cheng, Y., Liu, C., ... & Liu, Z. (2019), "Graphene photonic crystal fibre with strong and tunable light-matter interaction", *Nature Photonics*, Vol. 13, No. 11, pp. 754–759.
- [15] Fitio, V., Yaremchuk, I., Vernyhor, O., & Bobitski, Y. (2018), "Resonance of surface-localized plasmons in a system of periodically arranged gold and silver nanowires on a dielectric substrate". *Applied Nanoscience*, Vol. 8, pp. 1015–1024.
- [16] Schinke, C., Christian Peest, P., Schmidt, J., Brendel, R., Bothe, K., Vogt, M. R., ... & MacDonald, D. (2015) "Uncertainty analysis for the coefficient of band-to-band absorption of crystalline silicon", *AIP Advances*, Vol. 5, No. 6, pp. 067168.
- [17] Song, B., Gu, H., Zhu, S., Jiang, H., Chen, X., Zhang, C., & Liu, S. (2018). Broadband optical properties of graphene and HOPG investigated by spectroscopic Mueller matrix ellipsometry. *Applied Surface Science*, 439, pp. 1079–1087.

## СТРУКТУРА ГРАФЕН – ЗОЛОТА ГРАТКА ДЛЯ ОТРИМАННЯ ПІДСИЛЕНОГО РОЗПОДІЛУ ЕЛЕКТРОМАГНІТНОГО ПОЛЯ

Р. Кузык, О. Ільїн, І. Яремчук

Національний університет "Львівська політехніка" вул. С. Бандери, 12, Львів, 79013, Україна

У роботі досліджено розподіл поля в структурах типу золота ґратка, графеновий шар та кремнієва підкладка. Встановлено умови максимального розподілу електромагнітного поля (поглинання) цими структурами з метою використання їх у пристроях фотоніки та електроніки. Величина напруженості електромагнітного поля дифракційної ґратки із золота з шаром графену зростає зі зменшенням ширини щілини. Водночас збільшення періоду призводить до невеликих змін розподілу електромагнітного поля. Показано, що максимальне значення розподілу електромагнітного поля істотно зростає, майже вдвічі, зі зменшенням товщини графенового шару.

**Ключові слова:** графен; кремній; ґратка; поверхневий плазмонний резонанс; розподіл електромагнітного поля.