InGaAs based gratings for UV–VIS spectrometer in prospective mRNA vaccine research

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Received: 6 June 2022 / Accepted: 13 July 2022 / Published online: 26 July 2022 © The Author(s), under exclusive licence to Springer Science+Business Media, LLC, part of Springer Nature 2022

Abstract
During the outbreak of the COVID-19 illness, mRNA (messenger RNA) injections proved to be effective vaccination. Among the presently available analytical techniques, UV/VIS spectrophotometry is a trustworthy and practical instrument that may provide information on the chemical components of the vaccine at the molecular level. In this paper, we will present a one-dimensional grating of InGaAs as a prospect grating structure for UV–VIS spectrometer that can be used for mRNA vaccine development. The main parameters and the wavelength region used in mRNA vaccine development lies in the range of 200 nm to 700 nm (UV–VIS Range). The incorporation of new materials that are excellent for cutting-edge semiconductor industry procedures for MEMS manufacture, as well as new optimal parameters, will improve the grating and spectrometer’s performance which will enhance the mRNA vaccine development and manufacturing workflows enabled by UV–VIS spectroscopy. Hence we evaluated the feasibility of the materials, Si (Silicon), GaN (Gallium Nitride), InGaAs (Indium Gallium Arsenide) and InP (Indium Phosphide) as a grating material. Reflection spectrum of the proposed structure shows 48% increase compared to the grating made up of Silicon. In order to model wave propagation in one grating unit cell, electromagnetic waves frequency domain interface is used. The periodic constraints of floquet periodicity are used for simulation at both faces of the unit cell. The reflectance of grating with each material as functions of the angle of incidence was plotted. Also we evaluated the effect of grating thickness, groove density, spectral resolution and efficiency over different materials namely Si, GaN, InGaAs and InP. After optimizing geometric parameters, the designed InGaAs based grating achieved a efficiency of 87.45% and can be a reliable prospect for mRNA based vaccine development.

Keywords mRNA vaccine · COVID-19 · Diffraction gratings · Spectroscopy · MEMS · Optical materials

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1 Introduction

Vaccines protect against several diseases as well as save many lives every year. To set off an immune action, lots of vaccines place a damaged or inactivated bacterium right into our bodies. Instead, Messenger RNA (mRNA) injections utilize mRNA produced in a research laboratory to teach our cells how to make a healthy protein or even just a piece of a healthy protein that activates an immune action inside our bodies.

Messenger RNA (mRNA) injections incorporate preferable immunological properties with an outstanding safety and security profile and also the unmet adaptability of hereditary vaccinations. Based upon sitting healthy protein expression, mRNA injections are capable of generating a balanced immune action making up both cellular and humoral immunity while not subject to MHC heliotype constraint. Furthermore, mRNA is an inherently risk-free vector as it is a minimal as well as only short-term carrier of info that does not communicate with the genome. mRNA injections also provide optimum versatility with respect to development due to the fact that any healthy protein can be shared from mRNA without the requirement to change the manufacturing procedure.

Throughout the break out of the COVID-19, mRNA (messenger RNA) injections developed as efficacious vaccines. Study and growth of these vaccinations depends chiefly on their quality and comparable activity to a standard vaccine strategy, which can be examined with innovative analytical techniques. UV/VIS spectroscopy (Ravindran et al. 2020) is one such commonly utilized method that can establish the existence as well as quality of nucleic acids, one of the essential components of mRNA injections. To make certain injection security, it is essential to analyze top quality at every phase of advancement. These assessments enhance vaccine efficacy as well as reduce the chance of failure during development and clinical tests. According to Pfizer, a leading manufacturer of mRNA vaccine, quality assurance as well as testing takes over half of injection manufacturing time (Mascola and Fauci 2020). The lawful responsibility to maintain the effectiveness of items at every phase of manufacturing usually is up to the maker. Hence, analysis of vaccine raw materials and finished product becomes crucial (Crommelin et al. 2021). The global characterization techniques for the infection and its vaccinations is a challenge due to the virus framework, its intrinsic heterogeneity, and the range of biological activities it advertises (Liu et al. 2020). Among currently offered analytical strategies, UV/VIS spectrophotometry is a dependable and convenient tool that can provide information regarding the chemical parts of the vaccination at a molecular degree (Liu et al. 2020; Zhang et al. 2021). This is very important, due to the fact that mRNA vaccinations need highly purified DNA/RNA to keep effectiveness. The purity of nucleic acids can be easily checked by the aid of UV/VIS spectroscopy. Before entering the market, vaccinations have to pass rigorous regulative procedures and must be examined for quality. For liposome-based drug products including mRNA vaccinations, it is necessary to do analytical examinations supported by spectroscopic logical approaches (Koh et al. 2018; Farkash et al. 2021) in order to examine parameters that affect pureness, shelf-life, efficiency, and more. UV/VIS spectrophotometric analysis is considered a conventional method for the determination of nucleic acid. Additionally, it can be made use in the analysis of bacteria, enzymes, proteins, nucleotides, plasmids in addition to the purity of raw materials such as ethanol and sucrose. COVID-19 vaccine manufacturers and quality assurance departments are sharing information about the logical methods that are helping them to standardize injection quality (Schmidt et al. 2021; Ellis et al. 2021).
UV/VIS spectrophotometers can identify all chemical parts of a vaccination raw product if the sample takes in or sends noticeably within the UV or VIS area, (range 200–800 nm) (Sun et al. 2022). The main parameters and the wavelength region used in mRNA vaccine development and manufacturing is listed in Table 1. UV/VIS spectrophotometric analysis is regarded as a standard method for determining nucleic acid content. It can also be used to analyse bacteria, enzymes, proteins, nucleotides, and plasmids, as well as purity/impurity profiles of raw materials like ethanol and sucrose. Because of its flexibility and ease of analysis, it has become the analysis of choice for characterization of both final vaccines and various vaccine components throughout the development chain.

A light supply, grating valve, and detector are the three primary parts of a UV/VIS spectrometer. All of the blocks are vital within the design; however the grating is the most significant part. Diffraction gratings, which break light into several beams traveling in various directions, are widely used in optical components (Wolffenbuttel 2004). Gratings are small optical elements that divide white light into its component wavelengths (Liu and Li 2021). The primary factors for assessing grating performance are grating efficiency, groove density and spectral resolution. The materials that were utilized in the manufacturing process as well as the grating parameters, plays a major role in the performance of the grating. The most common materials are Silicon (Si), Silicon dioxide (SiO₂) (Aspnes and Studna 1983), Poly methyl methacrylate (PMMA), Chromium and Silicon Nitride (Si₃N₄). The incorporation of new materials such as GaN (Gallium Nitride), InGaAs (Indium Gallium Arsenide) and InP (Indium Phosphide) that are excellent for cutting-edge semiconductor industry procedures for MEMS manufacture, as well as new optimal parameters, will improve the grating and spectrometer’s performance. This will enhance the mRNA vaccine development and manufacturing workflows enabled by UV–VIS spectroscopy.

The choice of a grating for a spectrometer is heavily influenced by the spectrometer’s intended application. The identification of grating parameters and boundary conditions is required for the design and fabrication of a diffraction grating for a spectrometer. The complete procedure may be summarised as follows. (a) Determining the wavelength range to be examined (minimum and maximum wavelengths in nm) (b) Choice of the incident angle of the beam upon the diffraction grating (c) Choice of Grating thickness (d) Choice of groove density (e) Calculation of spectral resolution vs grating period (f) Calculation of the grating efficiency. In mRNA vaccine development, the wavelength range is 200 nm to 700 nm. Considering this wavelength range, we tried to optimize the grating design by completing the remaining steps.

| Parameters                          | Wavelength          | References                  |
|-------------------------------------|---------------------|-----------------------------|
| Physiochemical properties          | 200–700 nm          | Gao et al. (2021)            |
| Nucleic acids                       | 260 nm              | Pinhas and Hava (2003)       |
| Proteins                            | 200–300 nm          | Gao et al. (2021)            |
| Chemical components                 | 820 nm              | Pinhas and Hava (2003)       |
| Sucrose                             | 340 nm              | Gao et al. (2021)            |
| Lipids                              | 675 nm              | Pinhas and Hava (2003)       |
| Ethanol                             | 235–340 nm          | Gao et al. (2021)            |
| Bacterial endotoxins                | 340 nm              | Pinhas and Hava (2003)       |
2 Grating in UV/VIS spectrometer

Gratings are manufactured on substrates and have a small optical dimension. As polychromatic light strikes the grating, it is partially scattered, and the dispersed light is driven to the sample material, as illustrated in the Fig. 1. The objective of each grating production system is to realize sensible parameter values (Sugimoto et al. 2020). As a result, high-performance gratings are a prerequisite for high-performance MEMS based spectrometers, and they can be produced with the help of MEMS manufacturing technologies (Pinhas and Hava 2003; Mosca and Targia 2001).

The grating equation can be represented by, Eq. (1)
\[ n\lambda = \Delta (\sin \theta + \sin \theta') \]  
where space among the groove is represented by \( \Delta \), the incidence and diffraction angles determined from the grating standard is denoted using \( \theta \) and \( \theta' \) respectively, \( n \) would be the order of diffraction where as \( \lambda \) is the wavelength of incident light that has been diffracted (Yu et al. 2021). The Eq. (2) is applicable for the diffraction grating’s rectangular profile and requires the solution of the Bessel functions:
\[ \eta_m = j_m^2 \left\{ \frac{\pi d}{\lambda} \cos \alpha + \cos \alpha_m \right\} \]  
where \( \eta_m \) is the mth order diffraction efficiency, \( j_m \) is the Bessel first order function of mth order, \( d \) denotes the grating depth, the \( \lambda \) denotes the incident light wavelength, \( \alpha_m \) is the mth order angle of diffraction and \( \alpha \) is the angle of incidence. Equation (1) is calculated for an optimally reflecting material and should be modified by multiplying by the material’s reflectivity.

The redistribution of energy diffracted into distinct diffraction orders at a specific wavelength is affected by a number of factors, including incident light polarization, angle of incidence, refractive index of the material used to make the grating, and grating period.

Fig. 1 Grating in a spectrometer
InGaAs based gratings for UV–VIS spectrometer in prospective applications. Since infrared light has greater wavelengths than Visible light, it responds differently when propagated through an optical medium. Certain materials like Si, GaN, InGaAs and InP can also be included in both infrared and Visible applications. Hence, the efficiency of an optical grating can be improved by choosing materials that are ideally matched to the applications.

3 Design and theoretical background

A 1-dimensional grating structure’s reflectance can be calculated with the help of the wave equation obtained from the scheme of Maxwell’s equations, expressed by the Helmholtz equation. The Helmholtz equation is written as follows for a one-dimensional grating configuration,

\[
\frac{\partial^2 E_z(x)}{\partial x^2} + \varepsilon_r(x) \frac{\omega^2}{c^2} E_z(x) = 0
\]  

(3)

in which \(E_z(x)\) represents the electric field along its z axis, which varies with propagation direction \(x\), \(\varepsilon_r(x)\) is relative permittivity along the x-axis of a grating substrate, the angular frequency of the radiation is \(\omega\) and \(c\) represents the light’s speed in a vacuum (Galle et al. 2003; Cialla-May and Schmitt 2019).

Equation (3) can be utilized for calculating a one-dimensional grating structure’s field distribution and reflectance. In order to calculating reflectance, the parameters in Eq. (3) such as layer thicknesses and refractive indices of a 1-dimensional grating structure must be chosen correctly.

The optimal solution to Eq. (3) would be

\[
E_j(x) = A_j e^{injkx} + B_j e^{-injkx}
\]  

(4)

in which the amplitudes of waves moving forward and backward are \(A\) and \(B\) respectively. Since the tangential portion of the electric field is taken into account in the case of a 1D grating configuration, boundary settings are defined as the consistency of wave functions and its derivatives. Creating one such equation scheme for every structure interface will result as follows.

\[
E_j(x) = E_{j+1}(x)
\]  

(5)

By using Crammer’s method and a finite size periodic form, we can solve the obtained linear system equations. The following expression can be used to determine the wavelength of maximal reflectance.

\[
\lambda = 2(n_1t_1 + n_2t_2)
\]  

(6)

whereas \(n_2\) and \(n_1\) are the refractive indices of the second and first layers, respectively. \(t_1\) and \(t_2\) are the thicknesses of the first and second layers of air respectively. Solution of Eq. (6) is calculated at various wavelengths with respect to reflectance. The efficiency of transmitted light is denoted by Eq. (7).

\[
\eta_T = (1 - R)^2 e^{-\beta(t_1 + t_2)}
\]  

(7)
whereas $\beta$ is the material’s coefficient of absorption and $R$ is the reflectance. The thicknesses of the odd and even layers are denoted by $t_1$ and $t_2$ respectively, and the grating structure’s diffraction efficiency is denoted by

$$
\eta_d(\Delta \phi_m) = \frac{\sin^2[\pi t((\delta n/\lambda F_{\phi_m})^2 + (\nabla \phi_m^2))^{1/2}]}{1 + [(F_{\phi_m}^2/\lambda N \phi_m/\delta n^2)]}
$$

(8)

where $t$ denotes the grating thickness, $\delta n$ denotes the modulation of the refractive index, given by $(n_1 + n_2)/2$, $\nabla \phi_m$ is shifting away from the Bragg’s angle, $\lambda$ is the signal wavelength, $F_{\phi_m}$ denotes the inclination element, which is equal to $\sin \phi_m$, where $\phi_m$ is the incident Bragg’s angle and $f$ denotes spatial efficiency (Bonod and Neauport 2016). Ultimately, the total transmitted performance of the waveguide $\eta$ is calculated as

$$
\eta = \eta_T \eta_d
$$

(9)

where $\eta_T$ denotes transmitted efficiency of the grating and $\eta_d$ represents diffraction efficiency.

Optical properties describe a material’s reaction to incident electromagnetic radiation (Kyotoku et al. 2010; Chowdhuri et al. 2007). Optical properties such as transmissivity, reflectivity, and absorptivity are due to incident radiation and these are directly related to the material properties (Kita et al. 2017). One common material used for the fabrication of optoelectronic device is Silicon (Rao et al. 2010). After silicon, III–V semiconductor materials such as Indium Gallium Arsenide (InGaAs) (Iqbal et al. 2020), Gallium Nitride (GaN) (Ziane et al. 2015) and Indium Phosphide (InP) (Zheng et al. 2022) have been the fastest-growing, most widely-used and highest-output semiconductor materials for optoelectronic use (Zhou 2021; Amiri and Lazreg 2021). Compound semiconductor materials outperform conventional semiconductor materials in terms of (1) High electron mobility (2) Wide bandwidth (3) High frequency (4) High power (5) High linearity (6) Diversity of material selection (7) Anti radiation. Compound semiconductors are thus used mainly in the production of opto electronic devices, and have great development potential (Gao et al. 2021). The complete refractive index of Silicon (Si), Gallium Nitride (GaN), Indium Gallium Arsenide (InGaAs) and Indium Phosphide (InP) with respect to wavelength is shown in Table 2.

### 4 Results and discussions

The numerical simulation was carried out with the help of COMSOL Multiphysics, and the finite element approach was used to simulate the reflection properties of Si, GaN, InGaAs and InP based fixed gratings (Iqbal et al. 2020; Ziane et al. 2015; Zheng et al.

| Material used for the grating structure | Complex refractive index | References |
|----------------------------------------|--------------------------|------------|
| Si                                     | 3.9766 + 0.030209i       | Rao et al. (2010) |
| GaN                                    | 2.3991                   | Iqbal et al. (2020) |
| InGaAs                                 | 3.9123 + 0.61589i        | Ziane et al. (2015) |
| InP                                    | 3.53635 + 0.3075118i     | Zheng et al. (2022) |
2022; Arosa and Fuente 2020; Xiong et al. 2021). The Finite Element Method (FEM) is a computational technique for approximating the solution of a series of constrained partial differential equations to the boundary conditions of the problem domain. The idea of the technique is to subdivide the problem domain into many simpler parts, named finite elements, in which the parameters describing the domain properties can be considered constant (Kazanskiy et al. 2021). By solving the differential equations on these finite elements and connecting them to the solution of the differential equations on their neighbor elements, an approximation of the whole problem domain is made. The finite element method can be formulated using the weighted residual method (Kwa and Wolenbuttel 1992). Introducing the basic principle of this method, we consider a general partial differential equation on the solution domain.

\[ \nu \phi = f \]  \hspace{1cm} (10)

Here \( f \) represents a given function, \( \phi \) is the function we will solve for and \( \nu \) is the differential operator.

In order to analyze the best material and grating parameters for mRNA vaccine production, we simulated grating structure with different materials namely Si, GaN, InGaAs and InP by employing the appropriate factors, notably the Index of refraction, groove density and thickness (Song et al. 2006).

4.1 Modeling for simulation

Figure 2 depicts a 1D rectangular model and its schematic diagram used for the simulation. Here the grating model have a period, \( \Lambda = 290 \) nm to 340 nm; Material film thickness, \( t = 200 \) nm to 800 nm; tailored slit width, \( a = 450 \) nm, each illustrating a separate grating structure. Table 2 shows the properties of the materials used as an input for the model and other input parameters used in the model are shown in Table 3.

The horizontal and vertical directions are used for periodic boundary conditions (PBC) (Chamoli et al. 2020). Continuity boundary limits for directionality and the flow of radiation are employed in the simulation model. At the time of export, Scattering Boundary Conditions (SBC) was used.

![Geometry of 1D rectangular grating unit cell and its schematic diagram](image)

**Fig. 2** Geometry of 1D rectangular grating unit cell and its schematic diagram
4.2 Reflectance with angle of incidence

In order to analyze the best angle of incidence for grating structure with different materials, we simulated grating structures with different materials namely Si, GaN, InGaAs and InP by employing the appropriate factor, notably the Index of refraction (Wolffenbuttel 2004). For determining the least reflectance corresponding to various wavelengths, we performed a simulation utilizing Eq. (6). Table 3 shows refractive index and the grating design thickness. Using the data in Table 3, we completed simulations for various grating structures to calculate the reflectance in relation to wavelength. Simulated results for various gratings with different angle of incidence are shown in Fig. 3.

The incident light was from 1° to 89° to the top of the gratings and output rays are traced from the surface normal to the grating. Figure 3 demonstrates the computed reflectance light intensity of Si, GaN, InGaAs and InP. All the four materials reveal reflectance where InGaAs as well as InP exhibit almost comparable curve while Si and also GaN reveal low reflectance. From the curve, it is noticeable that InGaAs shows the highest reflectance at all the angle of incidence and we choose 47° as the best selection since beyond that the reflectance has a tendency to increase in an exponential way.

Table 3 Parameters used for simulation

| Parameter                          | Value                        | References         |
|------------------------------------|------------------------------|--------------------|
| Vacuum wavelength of light         | 445 [μm]                    | Song et al. (2006) |
| Grating constant                   | 290 [μm]–340 [μm]           | Dennett et al. (2016) |
| Angle of incidence                 | 47°                          | Wang et al. (2021) |
| Refractive index of Si             | 3.9766 + 0.030209i           | Rao et al. (2010)  |
| Refractive index of GaN            | 2.3991                       | Ziane et al. (2015) |
| Refractive index of InGaAs         | 3.9123 + 0.61589i            | Iqbal et al. (2020) |
| Refractive index of InP            | 3.53635 + 0.3075118i         | Zheng et al. (2022) |

Fig. 3 Reflectance with different angle of incidence
4.3 Reflectance with grating thickness

After choosing the angle of incidence as 47°, we simulated spectral reflectance of all grating units by sweeping its geometric parameter especially grating thickness. We investigated grating thickness in the range of 200 nm to 800 nm with 100 nm steps while maintaining the grating period (340 nm) and angle of incidence (47°) as a constant. From the Fig. 4, it is evident that the reflectance value is not related to grating thickness in the interval of 200 nm to 800 nm. The result also shows that the material properties play an important role in regulating the reflectance of diffraction gratings. Out of the four gratings, InGaAs gratings show high reflectance where as GaN shows the least. Therefore we can conclude that InGaAs is a better choice for fabricating a grating for UV–VIS spectrometer with respect to grating thickness. In order to finalize the material we need to analyze Electric field’s spatial distribution, Groove density and Efficiency.

4.4 Electric field’s spatial distribution of different materials

The calculated electric field spatial distributions for different materials are depicted at Fig. 5. The frequency-dependent complex refractive index \( N = n - ik \) gives the velocity of propagation of an electromagnetic wave through a solid. The velocity is tied to the real part, \( n \), and the extinction coefficient, \( k \), is linked to the decay of the oscillation amplitude of the incident electric field. The interaction between the solid and the electric field of the electromagnetic wave therefore governs the optical characteristics of the solid. A reciprocal relationship exists between diffraction efficiency and the electric field. Out of the four gratings, in GaN gratings, the electric field is maximum inside the grating structure and hence the reflectance is minimum. At the same time InGaAs shows minimum electric filed and hence it is having maximum reflectance. The electric filed distribution also is in hand with the results obtained during the simulation of four gratings with the other two parameters, angle of incidence and thickness of the grating.
4.5 Reflectance with groove density

The simulation results obtained in the preceding section indicate that the proposed structure can be implemented for UV–VIS spectrometer for mRNA vaccine development. To further improve the structure, we investigate the variation in groove density by keeping the angle of incidence at 47° and considering the thickness of 400 nm. Gratings are usually marked by their groove density, the variety of grooves per unit length, typically revealed in grooves per millimeter (g/mm). We swept groove density in the range of 2900 to 3300 with the step of 100 by keeping all other parameters as constant. The result shows that during the entire range, InGaAs shows the better result and out of that groove density of 3300 gives the maximum reflectance and this result also exhibited the potential of InGaAs (Fig. 6).

4.6 Spectral resolution of the grating

In order to fix the grating period to its optimum value, we analysed the spectral resolution of the grating with respect to different grating period throughout the entire wavelength of incident light for a UV–VIS spectrometer. The result is shown in Fig. 7 and it is very clear that grating period of 340 nm shows maximum spectral resolution. That helped us to come to a conclusion that grating period of 340 nm is the best choice for InGaAs based gratings for mRNA research applications.
4.7 Efficiency of grating

A grating’s efficiency is the proportion of incident monochromatic light that is diffracted into the intended order. It is connected to the incidence angle of light, the groove geometry, and the reflectance of the materials used to fabricate the grating. Here we calculated the efficiency of four gratings and plotted the result in Fig. 6. The results demonstrate that InGaAs is showing the highest efficiency of 87.45% by keeping the optimum values obtained from previous simulations, namely angle of incidence of 47°, grating thickness of 400 nm, and grating period of 340 nm (Fig. 8).
In preceding sections, we simulated a 1D grating structure and came to a conclusion that InGaAs is the best choice for fabricating grating for UV–VIS spectrometer with a range of 200 nm to 700 nm. In addition, its geometric parameters were numerically optimised as Angle of Incidence = 47°, Thickness = 400 nm and Period = 340 nm. Based on these simulation findings, we expect that the performance metrics of the InGaAs based grating that will be manufactured in accordance with the designed structure will be extremely satisfactory, in the development of UV–VIS spectrometer for the analysis of various parameters related to mRNA vaccine development.

5 Conclusion

In conclusion, we developed an easy-to-manufacture grating for UV–VIS spectrometer suitable for mRNA vaccine development. The proposed structure is based on a one dimensional grating pattern of InGaAs. In order to model wave propagation in one grating unit cell, electromagnetic waves, frequency domain interface is used. The periodic boundary condition with floquet periodicity is utilised for simulation on either side of the unit cell. The effects of Angle of incidence, Grating thickness, Groove density, Grating period and Efficiency on the characteristics of reflectance have been carefully studied in order to optimise the structure. The strong reflectance of InGaAs and its high efficiency of 87.45% in the interval of 200 nm to 700 nm made the proposed structure highly reliable for mRNA vaccine manufacturing applications. In addition, the proposed structure is simple to fabricate. The aforementioned benefits, particularly high performance in full spectral range needed for mRNA quality analysis, reveal that the recommended structure can be a reliable prospect for mRNA based vaccine development. We plan to manufacture tailored grating in the future for the understanding of affordable yet high-value UV–VIS spectrometer for mRNA research study.

Acknowledgements The author gratefully acknowledges the research facilities at Karunya Institute of Technology and Sciences, Coimbatore and National Institute of Technology, Tiruchirappalli to carry out this research.
Author contributions  All the authors contributed for completing this article. AR and Dr. DN did the simulation and wrote the main text. BKJ prepared the figures. KPP, PP and JA reviewed the manuscript.

Funding  This research received no specific grant from any funding agency.

Data availability  All of the material is owned by the authors and/or no permissions are required.

Declarations

Conflict of interest  The authors have no competing interests as defined by Springer, or other interests that might be perceived to influence the results and/or discussion reported in this paper.

Ethical approval and consent to participate  No human participants and animals were involved in this research.

Consent for publication

I understand journal Optical and Quantum Electronics is a transformative journal. When research is accepted for publication, there is a choice to publish using either immediate gold open access or the traditional publishing route.

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