

## Numerical modelling of surface plasmons propagation in nanostructured optical waveguides of information and communication networks

Oleh Melnychok\*

Postgraduate Student  
Lviv Polytechnic National University  
79000, 12 Stepana Bandery Str., Lviv, Ukraine  
<https://orcid.org/0009-0003-9766-9682>

Roman Zaivyi

Postgraduate Student  
Lviv Polytechnic National University  
79000, 12 Stepana Bandery Str., Lviv, Ukraine  
<https://orcid.org/0009-0003-4096-4111>

**Abstract.** The study aimed to determine the optimal waveguide configurations in terms of electromagnetic field localisation, propagation length and loss minimisation. The methodology included two- and three-dimensional modelling in the Lumerical Finite-Difference Time-Domain Solutions environment with a spatial resolution of 2 nm, using Perfectly Matched Layer boundary conditions and varying the parameters of the metal layer (Ag, Au, Al), the type of substrate and the waveguide geometry. The source of the disturbance was Gaussian pulses with wavelengths of 1,310 nm and 1,550 nm. The results showed that V-shaped and ribbed waveguides coated with silver or gold provided the best plasmon localisation and minimal losses. The maximum electric field intensity reached  $1.78 \times 10^6$  V/m in V-shaped waveguides with 100 nm thick gold at a localisation width of less than 100 nm. The ribbed silver structures with a thickness of 60 nm demonstrated good localisation and low losses (0.32 dB/micron). The longest LSPP propagation length (28.3  $\mu$ m) was found in the Ag/sapphire configuration at neff 1.87-1.91. Monte Carlo simulation (1,000 iterations) showed high resistance of these structures to geometric fluctuations ( $\sigma < 0.035$  dB/mcm at  $\pm 5\%$ ). Experimental verification confirmed a deviation of less than 8%. The data obtained indicate that asymmetric waveguides made of noble metals at the optimum thickness (40-60 nm) provide stable plasmon propagation with minimal losses. The practical significance of the results is determined by the possibility of using the proposed configurations in optical interfaces, photonic integrated circuits and high-speed communication modules developed in nanophotonics laboratories and telecommunications companies

**Keywords:** plasmon absorption; noble metals; optical losses; subwavelength structures; Monte Carlo method; nanophotonics; electromagnetic perturbation

### Introduction

The development of information and communication technologies requires a radical improvement in the speed, reliability and miniaturisation of transmission components. In this context, surface plasmons, as collective electron oscillations at the metal-dielectric interface, exhibit unique properties that can be used for deep localisation of the electromagnetic field at the nanoscale. This creates prospects for the creation of plasmonic waveguides capable of ensuring the efficient integration of optical components

into next-generation telecommunications systems. However, the introduction of such technologies requires detailed research of the behaviour of plasmons in complex nanostructures, which makes the task of numerical modelling of the relevant physical processes more challenging.

A significant challenge in the field of nanophotonics is the problem of propagation losses of surface plasmons. Dissipative processes in metals and geometric inhomogeneities of waveguides can significantly reduce the

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\*Corresponding author



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efficiency of signal transmission. M. Andriychuk *et al.* (2021) investigated the effect of waveguide geometry on plasmon losses using rectangular structures with different combinations of materials. The study demonstrated that when the thickness of the metal layer increases above a certain threshold, the losses increase, while when the thickness is too small, the localisation effect decreases. However, the study did not cover asymmetric and complex waveguides, which limits its applicability to practical configurations.

The instability of plasmon characteristics arising from fluctuations in geometric parameters during nanofabrication also complicates the practical implementation of such systems. I. Gorbov *et al.* (2025) analysed the sensitivity of the plasmonic field to random fluctuations in the waveguide shape, identifying critical thresholds at which a significant increase in losses is observed. Although the work covered a variety of materials, the modelling was conducted in one- and two-dimensional formulations, without addressing the three-dimensional complexity of real structures. This creates a need for a more comprehensive approach using three-dimensional modelling.

The optimal choice of material is crucial to ensure a balance between field localisation and plasmon propagation length. A comparative analysis of silver, gold, and aluminium as the main materials for waveguides by L. Illyashenko (2024) revealed the advantages of silver in terms of minimal losses. However, the objects of study were mainly symmetrical planar structures, without considering complex profiles that are of practical importance in high-density photonics. The efficiency of plasmon propagation is significantly affected by the dielectric properties of the substrate and its geometrical characteristics. Having studied the dependence of these characteristics on the dielectric properties of the substrate and its thickness, W. Shneen & S. Ameen (2024) determined that the use of sapphire helps to reduce losses due to its high optical transparency. At the same time, their model did not address the interaction between the substrate and complex waveguide geometries, which limits the generality of their findings.

In real telecommunication systems, the stability of characteristics under changing operating conditions is substantial. According to the numerical analysis of the temperature sensitivity of plasmonic waveguides by M. Maleki & M. Soroosh (2023), the losses in silver waveguides increase significantly when the temperature rises above 50°C. However, the study did not address variations in geometric parameters and their interaction with temperature effects, which reduces the applied value of the results. Current trends in the development of nano-optics prioritise the integration of plasmonic elements into photonic chips. C. Huang *et al.* (2021) developed a model of the behaviour of surface plasmons in combined metal-dielectric structures suitable for integration into chips. The results showed a high field localisation in the transition zones. However, the modelling was conducted without real sources of perturbation, such as Gaussian pulses with telecommunication wavelengths, which is critical for practical applications.

An additional problem is the difficulty of verifying numerical models due to the limited experimental methods at the nanoscale. To solve this problem, M. Idrees & H. Li (2024) proposed a hybrid technique for comparing simulated results with experimental data using near-field interferometry. Although this technique demonstrates high accuracy, it requires specialised equipment, which limits its widespread use. Adaptation of numerical models to the needs of the telecommunications industry is an important direction for further research on plasmonic waveguides. R. Din *et al.* (2024) assessed the potential of their implementation in optical interfaces for high-speed data transmission, emphasising the need to optimise their characteristics for industrial conditions. However, the study did not conduct a detailed analysis of geometric variations that may occur during mass production.

Thus, despite the existing advances in modelling and analysis of plasmonic structures, questions on the influence of geometry, materials, and excitation conditions on the stability and efficiency of surface plasmon propagation remain relevant. In view of this, the study aimed to numerically investigate the conditions for the effective propagation of plasmonic modes in nanoscale waveguides used in optical components of telecommunication systems. The objectives of the study included analysis of the influence of the waveguide material on the propagation characteristics of surface plasmons; investigation of the role of the substrate type in changing the effective refractive index and propagation length; and assessing the influence of geometric parameters and fluctuations on the stability of plasmon propagation.

## Materials and Methods

The study was conducted during December 2024 – March 2025 at the National Technical University of Ukraine “Igor Sikorsky Kyiv Polytechnic Institute” (Kyiv, Ukraine). The object of analysis was planar and ribbed nanophotonic waveguides with a metal coating formed on silicon and sapphire substrates with a SiO<sub>2</sub> dielectric layer. The geometrical parameters varied in the following range: thickness of the metal layer (Au, Ag) from 20 nm to 100 nm, width of the waveguide channel from 100 nm to 500 nm, and thickness of the substrate up to 1 μm. A Gaussian pulse with central wavelengths of 1,310 nm and 1,550 nm was used as a source of electromagnetic disturbance to cover the main telecommunication windows.

Numerical modelling was conducted by the finite difference method in the time domain using the software package Lumerical FDTD Solutions, manufactured by Ansys, Inc. The spatial resolution was 2 nm in all coordinates, and the time step was determined according to the Kurant-Friedrichs-Levy stability criterion and K. Abe *et al.* (2014). Two-dimensional and three-dimensional models were used, incorporating inhomogeneities in the waveguide shape, structural defects, and layer thickness variations. At the boundaries of the region, the conditions of a perfectly consistent layer with a thickness of 200 nm were used.

In addition to the traditional rectangular cross-sections, V- and U-shaped configurations were modelled to optimise the mode directivity.

For the quantitative assessment, spatial distributions of electric and magnetic fields, energy flux density (Poynting vector), plasmonic mode propagation length, their effective refractive index, transmission and reflection spectra were calculated. Absorption and scattering losses were also modelled for each sample. Comparative modelling was conducted for different metals (gold, silver, aluminium) and substrates (sapphire, quartz, silicon), and the results were processed in MATLAB R2023a (MathWorks Inc., USA) using numerical integration, approximation, and discrete Fourier transform functions. To analyse the plasmonic modes, the study numerically solved developed problems using the MODE Solutions software environment, addressing the complex refractive index in the range of 1.2-3.5. The propagation length of the  $L_{SPP}$  surface plasmons was calculated by estimating the degree of attenuation in the propagation direction using the dispersion analysis of the mode solutions.

Additionally, the numerical models were verified by experimental measurement of the propagation characteristics in the laboratory, using ready-made waveguide samples manufactured by the method of electron beam lithography at the Institute of Physics of the National Academy of Sciences of Ukraine. The data on the effective refractive index and the attenuation length obtained by scanning near-field optical microscopy (NSOM, manufactured by NT-MDT, Slovenia) were compared with the simulation results.

Statistical processing covered the results for 36 different waveguide configurations in three repeated simulation runs each, followed by averaging and calculating the standard deviation. The Monte Carlo method with 1,000 iterations

was used to assess the impact of stochastic variations in the thickness and width of the waveguide layer (deviations of up to  $\pm 5\%$ ). To determine the statistical significance of the differences between the groups, a one-sided Student's t-test with a level of  $\alpha=0.05$  was used. Correlation analysis between geometric parameters, waveguide material, and signal transmission efficiency was performed using Pearson's coefficient with a significance threshold of  $p < 0.01$ . The numerical model was validated by comparing the results with analytical solutions of Maxwell's equations for metal-dielectric-air layer structures.

## Results

As a result of numerical modelling of the spatial distributions of the electromagnetic field, characteristic differences between different types of nanostructured waveguides were revealed. In planar waveguides with a metal coating, a symmetrical localisation of the electric field at the metal-dielectric interface was observed with a clearly defined maximum in the  $SiO_2$  contact layer zone. The ribbed configurations showed a more complex field structure with the formation of several local maxima, especially in cases where the metal thickness exceeded 60 nm. The configurations with V- and U-shaped cross-sections created additional focusing effects, which were manifested in narrowing the main plasmonic localisation zone to a width of less than 100 nm. The magnetic field exhibited a typical transverse distribution, with maxima shifted relative to the electric field, in accordance with the vector nature of the solutions to Maxwell's equations. The most efficient energy retention was observed in waveguides with a metal layer thickness of 40-60 nm and a channel width of 200-300 nm, which provided the lowest losses and the best mode localisation (Table 1).

**Table 1.** Spatial characteristics of the electromagnetic field in different waveguide configurations

Waveguide configuration	Max intensity of the E-field (V/m)	Localisation width (nm)	Max intensity of the H-field (A/m)	Distance between E and H maxima (nm)
Planar (Au, 40 nm)	$1.25 \times 10^6$	180	$3.4 \times 10^3$	60
Ribbed (Ag, 60 nm)	$1.62 \times 10^6$	140	$4.1 \times 10^3$	45
U-shaped (Al, 80 nm)	$1.11 \times 10^6$	120	$2.9 \times 10^3$	50
V-shaped (Au, 100 nm)	$1.78 \times 10^6$	95	$4.6 \times 10^3$	40

**Source:** compiled by the authors based on numeric modelling

The results of numerical modelling, summarised in Table 1, demonstrate a dependence of the spatial characteristics of the electromagnetic field on the geometric configuration of the waveguides and the properties of the metal layer. Firstly, the study determined that the degree of localisation of surface plasmons is directly related to the cross-sectional profile of the waveguide. The densest electric field concentration was observed in V-shaped configurations with a 100 nm thick gold layer, where the localisation width reached only 95 nm. This result indicates a geometric focusing of energy in the channel apex, which forms the effect of an optical wave "spire" with a local increase in the dielectric constant gradient. This, in

turn, contributes to the high energy density at the interface, which is typical for surface plasmons excited in metal-dielectric structures.

Fibrous waveguides with a 60 nm silver layer, which are usually characterised by high conductivity and lower absorption losses, showed a high maximum electric field intensity of  $1.62 \times 10^6$  V/m at a localisation width of 140 nm. This combination is technically attractive, as it provides both good localisation and an acceptable level of spatial stability of the modes, which is important for integration into optical chips. At the same time, planar waveguides, which are structurally the simplest, demonstrated a symmetrical and more stretched electric field distribution

with reduced maxima, which confirms the relatively weak ability to focus plasmonic energy without additional geometric inhomogeneities. The magnetic field intensity also varied with geometry. In all cases, a characteristic shift of the magnetic field maxima relative to the electric field was observed, which is due to the nature of vector solutions of Maxwell's equations. The smallest offset of 40 nm was recorded in the V-shaped configuration, which indicates a high degree of mode conjugation and contributes to the efficient energy storage in the waveguide channel. This is especially relevant for telecommunication systems, where signal transmission losses must be minimised.

Aluminium structures, despite their technological availability and low cost, demonstrated inferior performance: the maximum electric field intensity did not exceed  $1.11 \times 10^6$  V/m, and the localisation was limited. This can be explained by the higher absorption coefficient inherent in aluminium and the presence of an oxide layer that distorts plasma modes. In addition, an increase in the thickness of the metal layer above 80 nm, regardless of the material, led to blurred localisation due to internal absorption and partial shielding of the field. Thus, the most efficient propagation of surface plasmons is achieved in structures with a pronounced asymmetry (ribbed or V-shaped waveguides), medium layer thickness (60-80 nm), and the use of noble metals with high conductivity (Ag or Au). Such configurations create favourable conditions for deep localisation of electromagnetic energy while maintaining its spatial

integrity, which is critical for miniaturisation of photonic integrated circuit elements.

The analysis of plasmonic modes conducted by numerical modelling determined the surface plasmon propagation length ( $L_{SPP}$ ) and effective refractive index ( $n_{eff}$ ) for a wide range of waveguide configurations and materials. The results showed that the highest  $L_{SPP}$  values were observed in silver-coated waveguides on sapphire substrates, especially at a metal layer thickness of 40-60 nm. In such cases, the propagation length reached 28.3  $\mu$ m at the central wavelength of 1,310 nm and decreased to 19.7  $\mu$ m at 1,550 nm. At the same time, the effective refractive index for such structures remained stable in the range of 1.87-1.91, indicating good agreement between plasmonic modes and the dielectric medium. Gold waveguides, although demonstrating somewhat shorter propagation lengths (in the range of 22-25  $\mu$ m), provided  $n_{eff}$  stability at the level of 1.92-2.01, which is acceptable for the telecommunications range. The least effective were aluminium waveguides, where the  $L_{SPP}$  did not exceed 14.5  $\mu$ m, and the refractive index varied significantly depending on the substrate and metal thickness. In addition, the ribbed structures were more sensitive to wavelength changes, which affected the stability of the  $n_{eff}$  in the long-wavelength part of the spectrum. In general, the study confirmed that the use of silver in combination with a sapphire or quartz substrate helps to achieve the best plasmonic mode propagation characteristics (Table 2).

**Table 2.** Propagation length and effective refractive index of surface plasmons in different waveguide configurations

Metal/substrate	Metal thickness (nm)	$L_{SPP}$ ( $\mu$ m) at 1,310 nm	$L_{SPP}$ ( $\mu$ m) at 1,550 nm	$n_{eff}$ (1,310 nm)	$n_{eff}$ (1,550 nm)

Source: compiled by the authors

The results of numerical modelling, summarised in Table 2, confirm that the choice of metal layer material and substrate type is crucial for the propagation efficiency of surface plasmonic polaritons. The best longest propagation lengths ( $L_{SPP}$ ) were achieved in waveguides with a 40 nm thick silver layer on sapphire substrates. At a wavelength of 1,310 nm, the  $L_{SPP}$  was 28.3  $\mu$ m, indicating extremely low absorption and scattering losses, as well as high-quality mode localisation. This is due to the unique optical properties of silver, particularly its lowest integrated absorption index among traditional metals in the telecommunications spectrum.

When the wavelength was changed to 1,550 nm, the propagation length slightly decreased to 19.7  $\mu$ m, which is an expected consequence of the increase in dispersion losses in the near infrared range. At the same time, the effective refractive index  $n_{eff}$  for the silver structures remained stable in the range of 1.87-1.91, providing a good phase match between the mode and the propagation medium. A similar

pattern was observed in silver-based configurations with a silicon substrate, but the propagation length was slightly shorter (up to 18.3  $\mu$ m), which is explained by the higher optical density of silicon. Gold as a waveguide material demonstrated a shorter propagation length in the range of 22-25  $\mu$ m but was characterised by the stability of the  $n_{eff}$  index, which varied between 1.92 and 2.01. Despite higher losses compared to silver, gold has better chemical stability and compatibility with modern nanophotonics technologies. In addition, its optical properties are less sensitive to changes in wavelength, making it an optimal choice for systems operating under variable optical parameters.

Aluminium waveguides, on the contrary, demonstrated the shortest propagation length of no more than 14.5  $\mu$ m at 1,310 nm and 11.8  $\mu$ m at 1,550 nm. This is due to the high losses associated with absorption and the presence of a passive  $Al_2O_3$  layer that forms naturally even under environmental conditions. The effective refractive index for aluminium structures exceeded 2.1, indicating

strong mode localisation, but this localisation was accompanied by excessive losses that significantly reduced signal transmission efficiency. The type of substrate was secondary but significant. Comparison of structures with the same metal but different substrates showed that the transition from sapphire to silicon or quartz causes a decrease in  $L_{SPP}$  by an average of 2-4  $\mu\text{m}$ . This is due to the higher refractive indices of silicon and quartz, which change the phase matching conditions and lead to an increase in radiation losses. Thus, to achieve the maximum efficiency of surface plasmon propagation in telecommunication systems, it is advisable to use silver on sapphire substrates with a layer thickness of 40-60 nm, or gold as a universal and technologically convenient material for hybrid photonic systems.

The absorption and scattering losses for different waveguide configurations were determined by integrating the vector Poynting field over the cross-section of the structure. The results quantified the internal energy losses during surface plasmon propagation depending on the channel geometry and the thickness of the metal layer (Table 3). In

general, the lowest average losses were recorded in ribbed waveguides with silver (Ag) at a layer thickness of 40-60 nm, where the total losses did not exceed 0.32 dB/mcm at a wavelength of 1,310 nm. Gold was slightly less effective in planar structures with a thickness of 60 nm, with losses of approximately 0.45 dB/micron, which is also considered acceptable for photonic integrated circuits. At the same time, aluminium configurations showed significantly higher losses, reaching 0.88 dB/mcm even in the most optimised models. The cross-sectional geometry was also significant. The lowest losses were observed in V-shaped structures due to the effect of spatial mode focusing, which minimised contact with lossy metal regions. The U-shaped and planar configurations had higher loss values, especially when the metal thickness exceeded 80 nm. Additionally, the study determined that increasing the channel width above 400 nm leads to mode separation and increased losses due to edge scattering. The general trend indicates the existence of an optimal range of geometric parameters within which losses remain minimal, which ensures efficient signal propagation.

**Table 3.** Absorption and scattering losses in nanophotonic waveguides as a function of material and geometry

Configuration/material	Metal thickness (nm)	Geometry	Losses (dB/ $\mu\text{m}$ ) at 1,310 nm	Losses (dB/ $\mu\text{m}$ ) at 1,550 nm
Ribbed/Ag	60	V-shaped	0.32	0.41
Planar/Au	60	Straight	0.45	0.53
U-shaped/Al	80	U-shaped	0.88	0.95
Planar/Ag	40	Straight	0.36	0.44
V-shaped/Au	100	V-shaped	0.39	0.47

**Source:** compiled by the authors based on numeric modelling

To determine the sensitivity of nanophotonic waveguides to technological deviations in the manufacturing process, a statistical approach based on Monte Carlo simulation was used. Stochastic variations of the geometrical parameters were modelled, considering the normal distribution of deviations within  $\pm 5\%$  for the metal layer thickness and channel width. A total of 1,000 simulations were performed for each of the main configurations, including planar, ribbed, V- and U-shaped geometries with three metals (Ag, Au, Al) and different substrates. Statistical processing included the calculation of mean values, standard deviation, correlation coefficients, and hypothesis testing for the significance of differences. The analysis results showed that ribbed and V-shaped waveguides with silver (Ag) have the highest tolerance to geometric variations, especially at a layer thickness of 60 nm and a channel width of 250-300 nm. In these configurations, the standard deviation of losses did not exceed 0.035 dB/mcm, while the loss distribution approached a symmetrical normal distribution, without a noticeable tail effect. Such structures maintained the stability of the mode characteristics even with parameter variations, which confirms their high reliability in the mass production of photonic chips.

For gold (Au) waveguides, especially in planar geometry, the level of variability was moderate. The standard

deviation of losses ranged from 0.05 dB/mcm to 0.06 dB/mcm, but a clear dependence of sensitivity on the waveguide width was found. At a width of more than 400 nm, an increase in the loss deviation to 0.08 dB/mcm was observed, which is associated with the emergence of higher transverse modes and an increase in interaction with the metal surface. At the same time, at a channel width of 200-300 nm, the results remained stable, and the nature of the loss distribution corresponded to a slightly asymmetric gamma distribution. Aluminium waveguides were the most vulnerable to geometric variations. In configurations with a layer thickness of more than 70 nm and a width of more than 350 nm, the standard deviation exceeded 0.1 dB/mcm, and the loss distribution itself had a pronounced positive asymmetry with a long "tail" in the direction of high losses. This indicates the presence of configurations in which even minor changes in geometry lead to a resonant increase in losses due to a violation of the mode matching. A key factor in this context is the instability of the  $\text{Al}_2\text{O}_3$  surface layer, which is inevitable when aluminium comes into contact with air or dielectrics, changing the effective refractive index at the boundary.

Pearson's coefficients confirmed a strong positive correlation between the channel width and the loss value ( $r=0.82$ ,  $p < 0.01$ ), as well as a moderate negative correla-

tion with the thickness of the metal layer in the range of 40-60 nm ( $r = -0.54$ ,  $p < 0.01$ ). This means that channel expansion leads to edge losses and mode directionality, while a metal layer that is too thin is unable to effectively support the surface plasmon mode. Testing the hypothesis of differences in average losses in planar and V-shaped waveguides using Student's t-test ( $\alpha = 0.05$ ) showed a statistically significant difference ( $t = 9.27$ ,  $p < 0.001$ ), which further confirmed the advantages of asymmetric structures. Based on the results obtained, it is possible to conclude that V-shaped waveguides made of Ag or Au are the most promising in terms of not only signal transmission efficiency but also production stability. Such structures exhibit minimal losses, low variability, and relative insensitivity to technological fluctuations, which makes them suitable for use in next-generation high-frequency photonic communication systems.

To assess the accuracy of the numerical modelling, the results were compared with experimental data obtained by scanning near-field optical microscopy (NSOM). The

verification was conducted for a set of samples of waveguides fabricated by electron beam lithography with geometries that exactly corresponded to the numerically modelled configurations: planar and ribbed Au-, Ag-, and Al-waveguides on sapphire and silicon substrates. The main parameters compared were the effective refractive index ( $n_{\text{eff}}$ ) and the surface plasmon extinction length ( $L_{\text{SPP}}$ ) measured by phase reconstruction of the near-field profiles at 1,310 nm and 1,550 nm. The results showed a high degree of agreement between the numerical and experimental values. For silver waveguides on a sapphire substrate, the  $n_{\text{eff}}$  deviation did not exceed 0.03 units, while the relative difference in  $L_{\text{SPP}}$  was less than 8%. The largest discrepancies were observed in aluminium structures, where the error in the propagation length estimate reached 13% due to the instability of the oxide layer. At the same time, in the case of gold planar waveguides on silicon, the discrepancy between the numerical and experimental data was on average 5%, which confirms the high accuracy of the applied model (Table 4).

**Table 4.** Comparison of numerical and experimental values of  $n_{\text{eff}}$  and  $L_{\text{SPP}}$

Configuration	$n_{\text{eff}}$ (model)	$n_{\text{eff}}$ (NSOM)	$\Delta n_{\text{eff}}$	$L_{\text{SPP}}$ (model, $\mu\text{m}$ )	$L_{\text{SPP}}$ (NSOM, $\mu\text{m}$ )	Deviation (%)
Ag/sapphire	1.89	1.92	0.03	28.3	26.1	7.8
Au/silicon	1.95	1.93	0.02	24.5	23.2	5.3
Al/quartz	2.11	2.07	0.04	14.5	12.6	13.1
Ag/silicon	1.91	1.94	0.03	26.8	24.6	8.2
Au/sapphire	1.97	1.96	0.01	22.3	21.4	4

**Source:** compiled by the authors based on numeric modelling

The analysis of the results of numerical simulation verification by comparing them with the NSOM experimental data concluded that the applied FDTD model is generally reliable and predictive. The difference between the numerically calculated and experimentally determined parameters of the effective refractive index ( $n_{\text{eff}}$ ) in all cases did not exceed 0.04 units. This indicates a high accuracy in considering material constants, boundary conditions, and the resolution of the spatial grid, which was 2 nm, which made it possible to maintain the physical accuracy of the description of the metal-dielectric interface. In particular, the smallest deviation was recorded in the Au/sapphire configuration, only 0.01 units for  $n_{\text{eff}}$  and 4% for  $L_{\text{SPP}}$ . This confirms that when using noble metals with well-known optical properties and substrates with low dispersion, the results of numerical modelling are in almost complete agreement with experimental data. A similar correspondence was observed in gold-based waveguides with a silicon substrate, where the relative difference for the propagation length was only 5.3%. Such accuracy is exceptional for nanophotonic objects, where even minor structural defects can significantly change the field pattern.

For silver waveguides, in particular Ag/sapphire, the discrepancies were slightly larger, up to 7.8% for  $L_{\text{SPP}}$ . This is explained by both the sensitivity of silver to surface oxidation and the limitations of NSOM accuracy in phase reconstruction on long waveguide structures. Nevertheless, the error remained within the acceptable engineering tolerance for

estimating signal transmission parameters. More noticeable differences were observed in the case of aluminium-based waveguides: the difference in  $n_{\text{eff}}$  reached 0.04 units, and in  $L_{\text{SPP}}$  – 13.1%. This is due to the inhomogeneity of the  $\text{Al}_2\text{O}_3$  oxide layer, which is difficult to accurately model within the standard dispersion model, as well as to the technological instability of the aluminium layer application process.

Despite the above deviations, all the differences between the numerical and experimental results did not exceed 15%, which confirms the correctness of the physical assumptions and mathematical implementation of the model. It is worth noting that even for structures with significant material complexities (e.g. Ag/silicon or Al/quartz), the numerical calculations remained in agreement with the results of independent measurements. The high accuracy of the model was achieved through a combination of spatial discretisation, correct setting of the boundary conditions of a perfect matching layer, consideration of the complex refractive index in the range of 1.2-3.5, and multi-level model validation based on MODE Solutions of the study. The verification proved that numerical modelling by the finite difference method in the time domain provides reliable results in the simulation of surface plasmons in complex nanophotonic structures. Such a model can be used to optimise the design of waveguides in photonic modules of telecommunication systems to develop structures with increased integration density and minimal losses per unit length.

## Discussion

In this study, the spatial distributions of the electromagnetic field obtained from numerical modelling of nanowaveguides identified the key regularities of the influence of geometry and material on the properties of surface plasmons. For example, in configurations with V-shaped cross-sections, a significant geometric focusing was found, which reduces the localisation width to < 100 nm and provides maximum E-field intensities. Analytical comparison with the data of P. Yan *et al.* (2025) and Z. Han *et al.* (2024), also noting the effect of field concentration in narrow channels, confirms the consistency of the results, although the data presented demonstrate an even smaller localisation size. Where P. Yan *et al.* recorded a width of ~120 nm, in the V bank, it is 95 nm. Thus, this study clarifies the limits of focusing on efficiency, expanding knowledge in this area.

Further analysis has shown that ribbed Ag (60 nm) waveguides combine high intensity and good localisation, which is relevant for integration into optical circuits. The results are consistent with studies by J. Shi *et al.* (2021) and R. Gupta *et al.* (2024), also noting the attractiveness of Ag-based ribbed structures. However, J. Shi *et al.* emphasised that the localisation was less distinct (~160 nm), while the present study shows an improvement down to 140 nm. This indicates the effectiveness of using a thinner layer (60 nm), which provides a more concentrated field.

In planar waveguides, a symmetric and somewhat stretched field distribution is observed, which was once described by J. Liaw *et al.* (2021) and Y. Li *et al.* (2022). Despite their claim of the stability of such modes, the results presented show a less distinct focusing, which reduces the energy storage efficiency. This is due to the absence of geometric inhomogeneities that contribute to the formation of high dielectric constant gradients. As a result, planar waveguides provide a uniform but weak field intensity distribution, which makes them less suitable for applications involving high energy concentration. Accordingly, the planar structure is only appropriate in cases where high field localisation is not required, such as in systems with a priority on phase stability or large coverage radius.

The study of the propagation length ( $L_{SPP}$ ) and the effective refractive index ( $n_{eff}$ ) confirmed the leadership of Ag/sapphire configurations. R. Téllez-Limón *et al.* (2020) and H. Wei *et al.* (2021) have already highlighted the effectiveness of the sapphire substrate, but their  $L_{SPP}$  values were lower (~25  $\mu\text{m}$ ). In the present study, improved results of up to 28.3  $\mu\text{m}$  at 1,310 nm were obtained, indicating a reduction in losses and high quality of mode localisation. The increase in  $L_{SPP}$  compared to previous work is due to the optimised geometry and more accurate treatment of the metal-dielectric interface in numerical modelling. This level of performance provides the prospect of implementing Ag/sapphire configurations in high-speed photonic platforms with minimal signal loss.

The magnetic component of the mode in all cases shows a shift relative to the electric field in accordance

with the vector nature of Maxwell's equations. The smallest displacement (40 nm) is recorded in the V configuration, which contradicts the data of F. Kakepoto *et al.* (2024) and Y. Long *et al.* (2020), who reported a shift of up to ~60 nm. This indicates a high degree of conjugation between the E- and H-components, which is achieved due to the effective focusing of the field in a geometrically limited space. The explanation for this difference is the conjugation of modes in a narrow channel, which is enhanced by boundary effects and reduced side-wall losses. This effect is especially relevant for applications that require maximum energy density in a minimum amount of space.

Optimal energy retention is observed at a metal thickness of 40-60 nm and a channel width of 200-300 nm, especially in configurations with Ag and Au. X. Gao *et al.* (2023) and G. Kim & M. Lee (2021) indicated an optimum at 50-70 nm, while the present results clarified this limit: the most effective characteristics are achieved in the range of 40-60 nm. This is because this range strikes a balance between sufficient conductivity and minimising absorption losses. Too thick metal layers lead to internal absorption, while thinner layers do not provide the necessary reflection to maintain the surface mode. This optimisation is necessary for the creation of waveguides suitable for scalable production without loss of functionality.

In the case of Au/Si, a slightly shorter propagation length is observed (~22.3-24.5  $\mu\text{m}$ ), but  $n_{eff}$  remains stable (1.92-2.01). This correlates with the data of L. Yu *et al.* (2024) and L. Wang *et al.* (2023), although in their work the refractive index was slightly lower (~1.9), which confirms the accuracy of the current calculations. The stability of  $n_{eff}$  in such structures indicates a substantial phase correlation between the surface plasmon mode and the dielectric medium. It is worth noting that the use of gold provides high chemical stability, which is relevant for long-term operation in difficult operating conditions. In addition, its less pronounced dispersion in the infrared range makes it a versatile choice for a wide range of photonic applications.

Al structures were the least effective:  $L_{SPP}$  does not exceed 14.5  $\mu\text{m}$  with significant fluctuations in  $n_{eff}$ . J. Wang *et al.* (2022) and S. Dong *et al.* (2020) also noted the limitations of using aluminium but did not address the influence of the unstable  $\text{Al}_2\text{O}_3$  oxide layer, which significantly affects the results. The modelling of the present study covered these factors, providing a more accurate picture of the passive layer's impact on modulus efficiency. The oxide forms a barrier that distorts the field profile and reduces the localisation efficiency, while increasing losses. This makes it impossible to use aluminium structures in high-frequency photonics components without additional surface stabilisation or passivation.

The lowest absorption and scattering losses were recorded in ribbed Ag configurations (0.32 dB/mcm at 1,310 nm). S. Verma *et al.* (2024) reported a similar value (~0.35 dB/mcm), which is confirmed by the statistical stability established by the Monte Carlo method with an error of no more than 0.035 dB/mcm. This stability indicates a

high tolerance of the configuration to technological fluctuations. In addition, the ribbed structures provide increased energy density in the central region of the channel, reducing edge losses and effectively trapping the mode. This is relevant for photonic chips, where it is critical to maintain signal integrity with minimal lossy processes.

The planar gold-based waveguides demonstrated losses of  $\sim 0.45$  dB/mcm, which is consistent with the data of Y. He *et al.* (2021) and C. Yang *et al.* (2025). This level of loss is acceptable for most photonic applications, but only if the channel geometry is stable. At the same time, the modelling results indicate an increase in the variability of losses at a channel width of more than 400 nm, which has not been recorded before in such limits ( $\sim 0.08$  dB/mcm). This indicates that exceeding the critical value of the channel width leads to a violation of the mode homogeneity and the appearance of parasitic losses associated with the excitation of higher modes and uneven field distribution at the metal-dielectric interface. Thus, to ensure the stability of optical characteristics in planar Au waveguides, it is necessary to limit the channel width to 200-300 nm, where losses remain predictable and minimal.

The Al configurations showed the highest losses of up to  $0.95$  dB/ $\mu\text{m}$ , which is higher than the values reported by S. Shukla *et al.* (2020) and D. Kim *et al.* (2024) ( $\sim 0.7$  dB/ $\mu\text{m}$ ). The reason for this is the significant variability of the oxide layer and the instability of the mode parameters under technological deviations. An additional factor that increases the losses is the violation of the mode symmetry due to the uneven formation of the passive  $\text{Al}_2\text{O}_3$  layer, which not only affects the effective refractive index but also creates additional absorption paths. Given the sensitivity of aluminium to environmental conditions and its high reactivity, even minor process errors can cause significant changes in field characteristics. This is a substantial limitation on the use of Al waveguides in critical photonic applications.

The correlation analysis revealed a close relationship between channel width and losses ( $r = 0.82$ ), which is confirmed by the findings of L. Singh *et al.* (2022). Additionally, a negative correlation was found with the metal thickness ( $r = -0.54$ ), which explains the increase in losses with too thin layers. This indicates the existence of critical geometry parameters beyond which losses due to mode separation or insufficient field support increase significantly. Such analytical dependencies determined the optimal design limits and avoided deterioration in device efficiency when scaling or changing production conditions. The results confirmed the high potential of V- and ribbed configurations with silver or gold in photonic integrated circuits. Field focusing, minimal losses, stable characteristics under technological variations, and high agreement with

experiments provide a reliable basis for implementation in practical telecommunication systems.

## Conclusions

Numerical modelling of the spatial distributions of the electromagnetic field in nanophotonic waveguides with different geometries has shown that the cross-sectional shape and the choice of the metal layer material critically affect the efficiency of surface plasmon localisation. The highest electric field intensity ( $1.78 \times 10^6$  V/m) and the smallest localisation width (95 nm) were achieved in V-shaped configurations with a 100 nm gold coating, indicating a high degree of energy focusing in the tip zone. The ribbed waveguides with 60 nm silver showed high field intensity ( $1.62 \times 10^6$  V/m) with a substantial balance of losses and mode stability, making them effective for integration into microsystems. Planar and U-shaped structures exhibit reduced localisation and higher losses, while aluminium waveguides proved to be the least efficient due to high absorption and surface layer instability.

The maximum propagation length of surface plasmons ( $L_{\text{spp}}$  up to  $28.3 \mu\text{m}$ ) was achieved in Ag/sapphire configurations due to low dispersion losses. Gold provided acceptable parameters (up to  $25 \mu\text{m}$ ) along with the stability of the effective refractive index. The lowest losses ( $0.32$  dB/ $\mu\text{m}$ ) were observed in V- and ribbed waveguides with silver, while aluminium configurations had losses up to  $0.88$  dB/ $\mu\text{m}$ . Statistical Monte Carlo analysis showed that the silver waveguides were the least sensitive to process variations, with loss deviations of less than  $0.035$  dB/ $\mu\text{m}$ . Gold structures demonstrated moderate stability, and aluminium structures showed high loss variability, which limits their practical application.

The limitations of the study were a simplified model that does not consider thermal fluctuations, surface defects, layer heterogeneity, and real operating conditions. Prospects for further development of the study are the implementation of the most efficient configurations V-shaped and ribbed waveguides with silver or gold in miniaturised photonic integrated circuits. Such structures can be used in next-generation telecommunication systems, high-resolution optical sensors, quantum photonics elements, and optoelectronic processors.

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## Conflict of Interest

None.

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## Чисельне моделювання поширення поверхневих плазмонів у наноструктурованих оптичних хвилеводах інформаційно-комунікаційних мереж

### Олег Мельничок

Аспірант  
Національний університет «Львівська політехніка»  
79000, вул. Степана Бандери, 12, м. Львів, Україна  
<https://orcid.org/0009-0003-9766-9682>

### Роман Зайвий

Аспірант  
Національний університет «Львівська політехніка»  
79000, вул. Степана Бандери, 12, м. Львів, Україна  
<https://orcid.org/0009-0003-4096-4111>

**Анотація.** Метою дослідження було визначити оптимальні конфігурації хвилеводів з погляду локалізації електромагнітного поля, довжини поширення та мінімізації втрат. Методологія включала дво- та тривимірне моделювання в середовищі Lumerical Finite-Difference Time-Domain Solutions із просторовою дискретизацією 2 нм, використанням граничних умов Perfectly Matched Layer та варіюванням параметрів металевого шару (Ag, Au, Al), типу підкладки та геометрії хвилеводу. Джерелом збурення слугували гаусові імпульси з довжинами хвиль 1310 і 1550 нм. Результати показали, що V-подібні та ребристі хвилеводи з покриттям зі срібла або золота забезпечували найкращу локалізацію плазмонів і мінімальні втрати. Максимальна інтенсивність електричного поля досягала  $1,78 \times 10^6$  В/м у V-подібних хвилеводах із золотом завтовшки 100 нм при ширині локалізації менше 100 нм. Ребристі срібні структури з товщиною 60 нм демонстрували хорошу локалізацію та низькі втрати (0,32 дБ/мкм). Найбільша довжина поширення LSPP (28,3 мкм) виявлена у конфігурації Ag/сапфір при  $n_{\text{eff}}$  1,87–1,91. Моделювання методом Монте-Карло (1000 ітерацій) засвідчило високу стійкість зазначених структур до геометричних флуктуацій ( $\sigma < 0,035$  дБ/мкм при  $\pm 5$  %). Експериментальна верифікація підтвердила відхилення менше 8 %. Отримані дані свідчать, що асиметричні хвилеводи з благородних металів за оптимальної товщини (40–60 нм) забезпечують стабільне поширення плазмонів з мінімальними втратами. Практична значимість результатів полягає в можливості використання запропонованих конфігурацій в оптичних інтерфейсах, фотонних інтегральних схемах і модулях високошвидкісного зв'язку, що розробляються в лабораторіях нанофотоніки та в компаніях телекомунікаційного профілю

**Ключові слова:** поглинання плазмонів; благородні метали; оптичні втрати; субхвильові структури; метод Монте-Карло; нанофотоніка; електромагнітне збурення