

DESIGN AND MODELLING OF NANOPLASMONIC CHEMICAL SENSORS

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INDIAN INSTITUTE OF TECHNOLOGY DELHI

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DESIGN AND MODELLING OF NANOPLASMONIC CHEMICAL SENSORS

by

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Submitted

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to the



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CERTIFICATE

This is to certify that the thesis entitled “**Design and Modelling of Nanoplasmonic Chemical Sensors**” being submitted by **Mr. Kaleem Ahmed** to the **Indian Institute of Technology Delhi**, for the award of the degree of **Doctor of Philosophy** in the Department of Electrical Engineering, is a record of bonafide research work carried out by him. Mr. Kaleem Ahmed has worked under my guidance and supervision and has fulfilled the requirements for the submission of this thesis, which to my knowledge has reached the requisite standard. The results contained in this thesis have not been submitted in part or in full to any other University or Institute for the award of any degree or diploma.

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ABSTRACT

Devices made from metallic nanostructures and metallic thin films have been extensively studied due to their vast potential in the different fields such as sensing, optical switching, memory devices, photodetectors, solar cells, tunable filters, and photo-thermal therapy. Several advantageous properties stem from plasmon-related effects of the metallic nanoparticles and they are easily adaptable to a vast array of applications. Excitation of surface plasmons in plasmonic nanostructures and thin films through SPR (surface plasmon resonance), LSPR (localized surface plasmon resonance) leads to the high electric-field enhancement which enable SERS (surface-enhanced Raman scattering) based sensors employed for the precise and sensitive identification of targeted chemicals and biological molecules. Moreover, SPR and LSPR based plasmonic sensors are extensively employed to measure variations in refractive indices in the bulk media surrounding the metallic nanostructures or in the close proximity of metallic nanostructures with nanoscale dimensions.

A novel nanostructure consisting of a cross-shaped nanoaperture nanoantenna inside plasmonic nanorings for achieving very large values of electric field enhancement, as well as large theoretical surface-enhanced Raman scattering (SERS) enhancement factor is presented. In this work, we employed Finite-Difference-Time-Domain (FDTD) numerical modelling to simulate the plasmonic (gold) nanostructures present on silica substrates. The electric field enhancements and the resonance wavelengths of nanostructures can be tuned in the visible and the NIR region by modifying the nanostructure dimensions.

Nanostructure based plasmonic sensing platforms have several advantages such as label-free detection of biomolecules in the Visible and IR region. However, to improve their sensing capabilities in the UV spectrum remains a significant challenges. Therefore, we have proposed a

1-D Al plasmonic nanograting sensors for bulk and localized changes of refractive index in the UV region. Rigorous coupled wave analysis (RCWA) and finite difference time domain (FDTD) methods are used for optimization of different grating parameters to get the reflectance spectra in the UV region. Performance characteristics like sensitivity and FOM calculated for bulk and localized sensing of biomolecules. These nanograting have very high sensitivity in the UV wavelength ranges. The proposed nanograting-based SPR sensors can be used for chemical sensing, biosensing, and other medical applications, particularly in UV radiation-induced DNA mutation studies.

We also present a theoretical study and comparison of performance characteristics of different shape plasmonic periodic nanohole arrays in which the optical transmission spectra, near-field intensity enhancements, as well as the plasmon resonance wavelengths lies in the UV and DUV regime. The proposed Al based nanohole arrays are analyzed, and their sensing capability is compared using the FDTD numerical method. We have compared the plasmonic nanostructure nanohole arrays with different geometries of holes like circular, square and triangular shape to obtain the bulk and localised sensitivity in the UV region. The proposed configuration of plasmonic sensors can be directly coupled normally incident radiation to excite surface plasmons without the requirement of the prism.

सार

धातु नैनो संरचनाओं और धातु पतली फिल्मों से बने उपकरणों का विभिन्न क्षेत्रों जैसे संवेदन, ऑप्टिकल स्विचिंग, मेमोरी डिवाइस, फोटो डिटेक्टर, सौर सेल, ट्यूनेबल फिल्टर और फोटो-थर्मल थेरेपी में उनकी विशाल क्षमता के कारण बड़े पैमाने पर अध्ययन किया गया है। धातु नैनोकणों के प्लाज़्मोन-संबंधी प्रभावों से कई लाभकारी गुण उत्पन्न होते हैं और वे अनुप्रयोगों की एक विस्तृत श्रृंखला के लिए आसानी से अनुकूलनीय हैं। एसपीआर (सतह प्लाज़्मोन अनुनाद), एलएसपीआर (स्थानीयकृत सतह प्लाज़्मोन अनुनाद) के माध्यम से प्लाज़्मोनिक नैनोस्ट्रक्चर और पतली फिल्मों में सतह प्लाज़्मोन की उत्तेजना उच्च विद्युत-क्षेत्र वृद्धि की ओर ले जाती है जो लक्षित रसायनों और जैविक अणुओं की सटीक और संवेदनशील पहचान के लिए नियोजित एसईआरएस (सतह-संवर्धित रमन बिखराव) आधारित सेंसर को सक्षम बनाती है। इसके अलावा, एसपीआर और एलएसपीआर आधारित प्लाज़्मोनिक सेंसर का व्यापक रूप से धातु नैनोस्ट्रक्चर के आसपास के बल्क मीडिया में या नैनोस्केल आयामों के साथ धातु नैनोस्ट्रक्चर के निकटवर्ती क्षेत्र में अपवर्तक सूचकांकों में भिन्नता को मापने के लिए उपयोग किया जाता है।

प्लास्मोनिक नैनोरिंग के अंदर एक क्रॉस-आकार के नैनोएपर्चर नैनोएंटेना से युक्त एक नवीन नैनोस्ट्रक्चर प्रस्तुत किया गया है, जो विद्युत क्षेत्र वृद्धि के बहुत बड़े मानों को प्राप्त करने के साथ-साथ बड़े सैद्धांतिक सतह-संवर्धित रमन स्कैटरिंग (एसईआरएस) वृद्धि कारक को भी प्राप्त करता है। इस कार्य में, हमने सिलिका सबस्ट्रेट पर मौजूद प्लास्मोनिक (सोने) नैनोस्ट्रक्चर को अनुकरण करने के लिए परिमित-अंतर-समय-डोमेन (एफडीटीडी) संख्यात्मक मॉडलिंग का उपयोग किया। नैनोस्ट्रक्चर के आयामों को संशोधित करके विद्युत क्षेत्र वृद्धि और नैनोस्ट्रक्चर की अनुनाद तरंगदैर्घ्य को दृश्यमान और निकट अवरक्त क्षेत्र में ट्यून किया जा सकता है।

नैनोस्ट्रक्चर आधारित प्लाज़्मोनिक सेंसिंग प्लेटफ़ॉर्म के कई फ़ायदे हैं जैसे कि दृश्यमान और अवरक्त क्षेत्र में बायोमोलेक्यूल्स का लेबल-मुक्त पता लगाना। हालाँकि, पराबैंगनी स्पेक्ट्रम में उनकी संवेदन

क्षमताओं को बेहतर बनाना एक महत्वपूर्ण चुनौती बनी हुई है। इसलिए, हमने पराबैंगनी क्षेत्र में अपवर्तक सूचकांक के विस्तृत और स्थानीयकृत परिवर्तनों के लिए एक आयामी एल्यूमीनियम प्लाज़्मोनिक नैनोग्रेटिंग सेंसर का प्रस्ताव दिया है। पराबैंगनी क्षेत्र में परावर्तन स्पेक्ट्रम प्राप्त करने के लिए विभिन्न ग्रेटिंग मापदंडों के अनुकूलन के लिए कठोर युग्मित तरंग विश्लेषण (आरसीडब्ल्यूए) और परिमित अंतर समय डोमेन (एफडीटीडी) विधियों का उपयोग किया जाता है। जैव अणुओं के विस्तृत और स्थानीयकृत संवेदन के लिए संवेदनशीलता और योग्यता के आंकड़े जैसी प्रदर्शन विशेषताओं की गणना की जाती है। इन नैनोग्रेटिंग में पराबैंगनी तरंगदैर्घ्य श्रेणियों में बहुत अधिक संवेदनशीलता होती है। प्रस्तावित नैनोग्रेटिंग-आधारित एसपीआर सेंसर का उपयोग रासायनिक संवेदन, बायोसेंसिंग और अन्य चिकित्सा अनुप्रयोगों के लिए किया जा सकता है, विशेष रूप से यूवी विकिरण-प्रेरित डीएनए उत्परिवर्तन अध्ययनों में।

हम विभिन्न आकार के प्लाज़्मोनिक आवधिक नैनोहोल सरणियों की प्रदर्शन विशेषताओं का एक सैद्धांतिक अध्ययन और तुलना भी प्रस्तुत करते हैं जिसमें ऑप्टिकल ट्रांसमिशन स्पेक्ट्रा, निकट-क्षेत्र तीव्रता संवर्द्धन, साथ ही प्लाज़्मोन अनुनाद तरंगदैर्घ्य पराबैंगनी और गहरी पराबैंगनी शासन में निहित हैं। प्रस्तावित एल्यूमीनियम-आधारित नैनोहोल सरणियों का विश्लेषण किया गया है, और उनकी संवेदन क्षमता की तुलना परिमित अंतर समय डोमेन (एफडीटीडी) संख्यात्मक विधि का उपयोग करके की गई है। हमने पराबैंगनी क्षेत्र में विस्तृत और स्थानीयकृत संवेदनशीलता प्राप्त करने के लिए गोलाकार, चौकोर और त्रिकोणीय आकार जैसे छिद्रों की विभिन्न ज्यामितियों के साथ प्लाज़्मोनिक नैनोस्ट्रक्चर नैनोहोल सरणियों की तुलना की है। प्लाज़्मोनिक सेंसर के प्रस्तावित विन्यास को प्रिज्म की आवश्यकता के बिना सतह प्लाज़्मोन को उत्तेजित करने के लिए सामान्य रूप से घटना विकिरण को सीधे जोड़ा जा सकता है।

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List of Abbreviation

EF: Electric field

EM: Electromagnetic

EOT: Extraordinary transmission

FDTD: Finite-difference time-domain

FOM: Figure of Merit

FWHM: Full Width Half Maximum

LSP: Localized surface plasmon

LSPR: Localized surface plasmon resonance

MIM: Metal-Insulator-Metal

PML: Perfectly Matched Layer

PSP: Propagating Surface Plasmon

RCWA: Rigorous Coupled-Wave Analysis

RIU: Refractive Index Unit

SERS: Surface-enhanced Raman scattering

SP: Surface plasmon

SPP: Surface Plasmon Polariton

SPRi: Surface Plasmon Resonance Imaging