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Investigation of plasmonic studies on morphology of deposited silver thin films having different thicknesses by soft computing methodologies—A comparative study

Rozalina Zakaria [a], Siti Munirah Che Noh [a], Dalibor Petković [c,*], Shahaboddin Shamshirband [b,d], Richard Penny [a]

[a] Photonics Research Centre, Department of Physics, Faculty of Science, University of Malaya, 50603 Kuala Lumpur, Malaysia
[b] Department of Computer Science, Chalous Branch, Islamic Azad University (IAU), 46615-397 Chalous, Mazandaran, Iran
[c] University of Niš, Faculty of Mechanical Engineering, Deparment for Mechatronics and Control, Aleksandra Medvedeva 14, 18000 Niš, Serbia
[d] Department of Computer System and Technology, Faculty of Computer Science and Information Technology, University of Malaya, 50603 Kuala Lumpur, Malaysia

HIGHLIGHTS

- Soft computing evaluation on surface plasmons resonance in wide wavelength range.
- Estimation of sizes of granular structures formed on top of the wafer.
- An experimentally analysis on the tunable localized plasmon resonance.
- Electron-beam physical vapour deposition.
- Support vector regression methodology application as predictive methodology.

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ABSTRACT

This work presents an experimental analysis on the tunable localized surface plasmon resonance (LSPR), obtained from deposited silver (Ag) thin films of various thicknesses. Silver thin films are prepared using electron-beam deposition and undergo an annealing process at different temperatures to produce distinctive sizes of Ag metal nanoparticles (MNPs). The variability of structure sizes and shapes provides an effective means of tuning the position of the LSPR within a wide wavelength range. In this study, the polynomial and radial basis function (RBF) are applied as the kernel function of Support Vector Regression (SVR) to estimate and predict the LSPR over a broad wavelength range by a process in which the resonance spectra of silver nanoparticles differing in thickness. Instead of minimizing the observed training error, SVR_poly, SVR_rbf and SVR_lin attempt to minimize the generalization error bound to achieve generalized performance. The experimental results show an improvement in predictive accuracy and capability of generalization which can be achieved by the SVR_poly approach in compare to SVR_rbf and SVR_lin methodology. It was found the best testing errors for The SVR_poly approach.

1. Introduction

Many researchers discovered nanometer-sized metals such as gold (Au) and silver (Ag) possess interesting optical characteristics. These characteristics are due to time-varying electric fields exerting a force on the gas of electrons inside a metal, with consequent charge density oscillations, known as localized surface plasmons (LSP), confined to the metal [1,2]. When light, as a particular case of an electric field, is incident on these MNPs at a wavelength where resonance occurs, a resulting strong light scattering and absorption can be perceived by the appearance of an intense surface plasmon (SP) absorption band [3,4]. This SP band can be shifted by numerous factors such as type of material, size, shape, inter-particle distance, particle density, and dielectric materials. Significant plasmonic properties can be exploited in various fields, particularly optoelectronic technologies like photovoltaic, phototransistor [5], LED [6,7] and sensor [8], by means of tuning this SP band from the UV through to IR region of the electromagnetic spectrum. Apart from light scattering and absorption, MNPs also

* Corresponding author. Tel.: +381643283048.
E-mail address: dalibortc@gmail.com (D. Petković).

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can be used to enhance local electromagnetic fields. SP excitation causes charges to be concentrated at the metal-dielectric interface and result in very strong amplification of electric fields [9].

Various ways have been developed to fabricate the nanoparticles via a monolayer of metallic films formed either physically or chemically. Sputtering and vacuum deposition are essentially a process where evaporation of metal placed on a heating element will lead to condensation of atoms and an eventual thin film for well-defined nanoparticle structures [1]. Thin films go through an annealing process at an appropriate temperature in order for dewetting to take place. This annealing process will drive the film toward an equilibrium state, whereupon it agglomerates into metal nanostructures at temperatures well below the melting point of the metal [10,11]. Electron beam lithography is the most popular, albeit costly, technique of fabricating arrays of MNPs in preferred sizes, shapes and inter-particle distances [12,13]. One interesting way to produce MNPs at practical cost is electrochemical deposition of nanoparticles by manipulating Faraday's Law, though deposition occurring at the anode is limited to metallic substrates since the process involves the electrolytic reduction of metal in the presence of appropriate anions [1].

The absorption band in the visible range of EM spectrum obtained experimentally or from theoretical calculation, can characterize these MNPs that underlie the characteristic of plasmonics. Gustave Mie introduced the classical Mie's theory with inherent assumptions that the particles and surrounding medium are both homogeneous and can be described via bulk optical dielectric function [1], although Mie theory is only applicable to non-interacting nanoparticles that are well separated. The optical response of more complex shapes is difficult, and often necessitates numerical practices in order to generate a model of the particle response to an incident EM field. Discrete dipole approximation (DDA) [14,15], finite difference time domain (FDTD) [5], finite element simulations and modal expansion techniques are commonly used to simulate the absorption spectra. This paper reports the experimental analysis from silver thin films of various thicknesses of fabrication on the Si/SiO_2 substrate using an electron beam evaporation technique. The obtained results are used as training and data verification for a soft computing methodology.

This paper describes a process constructed in which the resonance spectra in regard to different silver nanoparticles thicknesses is simulated with support vector regression (SVR) method to estimate the surface plasmons resonance (LSPR) over a wide wavelength range. The SVR methodology is used for estimation of the LSPR over a broad wavelength range by a process in which the resonance spectra of silver nanoparticles differing in thickness. The core idea behind the soft computing methodology is to collect input/output data pairs and to learn the proposed network from these data [16,17].

The basic idea behind the soft computing methodology is to collect input/output data pairs and to learn the proposed network from these data. The key goal of this investigation is to establish an approximated support vector regression (SVR) methodology for forecasting and estimation of the LSPR over a broad wavelength range. An attempt is made to retrieve correlation between different thicknesses of silver nanoparticles in regard to surface plasmon resonance.

There are two main categories to support vector machines: support vector classification (SVC) and support vector regression (SVR). SVM is a learning system using a high dimensional feature space [18,19]. The Support Vector Regression algorithms (SVR) specifically developed for regression problems are appealing algorithms for a large variety of regression problems, since they do not only take into account the error approximation to the data, but also the generalization of the model, i.e., their capability to improve the prediction of the model when new data are evaluated by it [20,21]. SVR is based on statistical learning theory and a structural risk minimization principle, which has been successfully used for nonlinear system modeling [22,23]. The accuracy of a SVM model is largely dependent on the selection of the model parameters. However, structured methods for selecting parameters are lacking. Consequently, some kind of model parameter calibration should be made.

The SVR_rbf and SVR_poly are examined in this paper: the first one is radial basis function and the next is polynomial function. These functions represent kernel functions which are utilized to form qualified function for SVM. Hence, the RBF and polynomial function are applied for estimation of sensor voltage output in this study. An experiment is carried out to extract the training and checking data.

2. Materials and methods

2.1. Experiment

This experiment uses a 20 mm × 15 mm p-type silicon (Si) wafer with 300 nm thickness of thermally grown silicon dioxide (SiO_2). The wafer is purchased from Ossila Ltd, and chosen due to the potential for expanding this experiment in the area of optoelectronics where Si/SiO_2 finds common industrial usage. The wafer is cleaned first using methanol, iso-propanol (IPA) and deionized water in succession, then blow-dried using nitrogen gas. Silver film of a selectable thickness is deposited using an Edwards Auto 306 electron beam physical vapor deposition system and annealed at 250 °C for 1 h in order for a dewetting process to conclude. Following confirmation of the presence of silver nanoparticles on top of the wafer via a model JEOL JSM-7600F field emission scanning electron microscope (FESEM), ImageJ software is used for image processing to obtain nanoparticle size and spacing distribution. Simulations are undertaken at this point onwards to determine characteristics of the plasmonics.

2.2. Input parameters

As a data-driven model, the ability of the SVR to make reasonable estimations is mostly dependent on input parameter selection. Adequate consideration of the factors controlling the system studied is therefore crucial to develop a reliable network. According to the presented experimental analyzing of the plasmon resonance (Fig. 1), the input parameters (annealing temperature

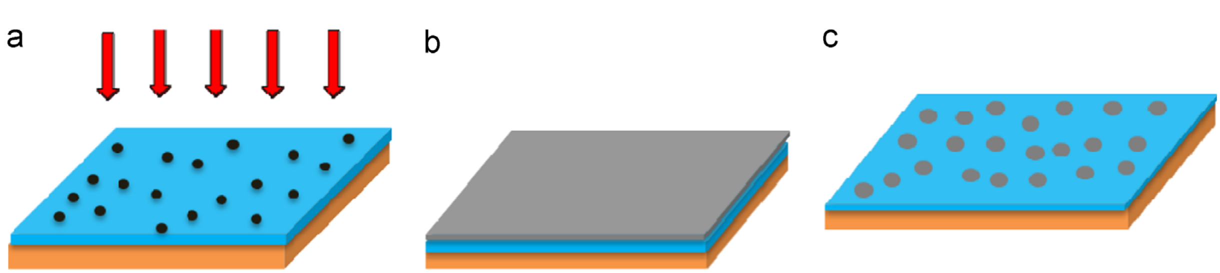

Fig. 1. Schematic procedure of producing Ag nanoparticles on top of Si/SiO_2 substrate (a) Deposition of Ag by electron beam physical vapour deposition system (b) Ag film annealing process at 250 °C for 1 h for dewetting to take place (c) Substrate with agglomerated Ag nanoparticles after dewetting is concluded.