CALCULATIONS OF NANOCRYSTALLINE DIAMOND-COVERED WAVEGUIDES BASED ON AMORPHOUS SILICON

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Abstract

Nanocrystalline diamond (NCD) thin films are suitable biointerfaces having excellent stability due to their hardness and chemical inertness. NCD coatings on planar waveguides (WG) in the IR region allow to design optical sensors sensitive to absorbers like proteins or other biomolecules. In this contribution, we present a 2D model of a multi-layer WG developed under FEM (finite element method) simulation software Comsol Multiphysics. The model is based on the modified wave equation solved in the frequency domain and includes optical absorption. Prior to these simulations, calculations of optical modes were performed in order to design a suitable single-mode planar optical WG with the NCD/a-Si:H/glass heterostructure. It was found that for the single-mode WG working in the narrow region of 1550-2000 nm the silicon thickness must be 150-320 nm. Shorter wavelengths are excluded due to the optical absorption of both amorphous silicon and diamond. It was found that in order to keep a reasonable signal attenuation, the NCD film must be prepared with the optical absorption coefficient lower than 10 cm^{-1}, being a rather challenging task. Dependencies of the signal attenuation on the NCD film thickness, absorbing layer height, its absorption coefficient and exciting wavelengths are presented.

Keywords: nanocrystalline diamond, amorphous silicon, optical waveguides, FEM

1. INTRODUCTION

Conventional photonics IR materials such as ZnS, ZnSe and Ge, suffer from the disadvantage of being brittle, easily damaged and having low chemical resistance. On the other hand, nanocrystalline diamond (NCD) thin films are now of interest in photonics and micro/nanophotonics structures because of their low absorption and scattering in the IR region, combined with unique properties like high thermal conductivity, large Young's modulus and high stability under extreme operating conditions and harsh environments [1-3]. In addition, strength of the chemical or electrostatic bonds at the diamond/organic interfaces provides a substantial advantage over other materials [3].

Recent advances in fabrication processes of diamond films by MW-enhanced chemical vapour deposition of nanocrystalline and/or ultrananocrystalline (UNCD) structures [4] enabled to prepare acceptably smooth surfaces with good optical properties [5]. Homogeneous initial surface termination, covalent and non-covalent immobilization of different functional moieties as well as the subsequent grafting of larger (bio)molecules onto previously functionalized nanodiamond have been successfully established [6].

Although waveguiding capabilities of NCD films were recently experimentally confirmed [1], the high optical absorption and optical scattering is still not favourable to use the NCD as a waveguiding material, especially in the visible region. However, a suitable planar optical waveguide (PWG) with low optical absorption, low optical scattering and sufficiently high index of refraction coated by NCD film could be used as a (bio)-chemical sensor. After exposition to the organic vapours or liquid solutions, the adsorbate layer of, e.g., proteins and other biomolecules may result in light attenuation in the PWG.

In this paper, we present a theoretical model of light propagation in a multi-layer PWG based on the NCD/a-Si:H/glass heterostructure. Here, hydrogenated amorphous silicon (a-Si:H) is considered as a waveguiding material, deposited on a glass substrate and coated by NCD film as a functional layer. NCD has sufficiently lower refractive index (~2.34) than a-Si:H (~3.64) in the optical region of interest that it will not affect the waveguide mode structure, although it will affect light attenuation. After designing basic geometrical dimensions by simpler calculations, a 2D model in Comsol Multiphysics software was used to calculate light propagation in the suggested heterostructure.

2. WAVEGUIDE STRUCTURE AND COMPUTATIONAL DETAILS

The suggested waveguide structure is schematically depicted in **Fig. 1**.

Fig. 1 Structure of NCD/a-Si:H/glass optical waveguide with adsorbate layer (red colour).

A non-absorbing glass with the index of refraction 1.5 was considered in calculations as a substrate. Onto this substrate, hydrogenated amorphous silicon and nanocrystalline diamond film are deposited, respectively.

The modified dispersion equation

$$\frac{2\pi h_f}{\lambda_0}\sqrt{n_f^2 - n_{eff}^2} = \arctan\left(p_{fs}\sqrt{\frac{n_{eff}^2 - n_s^2}{n_f^2 - n_{eff}^2}}\right) + \arctan\left(p_{fc}\sqrt{\frac{n_{eff}^2 - n_c^2}{n_f^2 - n_{eff}^2}}\right) + m\pi \tag{1}$$

with

$$p_{fs} = \frac{n_f^2}{n_s^2}, \qquad p_{fc} = \frac{n_f^2}{n_c^2}, \tag{2}$$

was used for calculations of guided optical modes and the estimation of silicon thickness for single-mode PWG. The indices *s*, *f*, and *c* in the equations (1,2) and **Fig.1** state for the substrate (glass), waveguiding core (silicon) and cover (NCD).

Light propagation through the single-mode waveguide structure was simulated by the finite-element method (FEM) in Comsol Multiphysics, under the RF module. Under the assumption of non-magnetic media and time-harmonic waves

$$\mathbf{E}(x, y, z, t) = \tilde{\mathbf{E}}(x, y, z)\cos(\omega t + \varphi) \tag{3}$$

the electric field phasor $\tilde{\mathbf{E}}$ can be solved using the equation

$$\nabla \times (\nabla \times \tilde{\mathbf{E}}) - k_0 \varepsilon_r \tilde{\mathbf{E}} = 0 \tag{4}$$

where $k_0 = \sqrt{(\omega\varepsilon_0\mu_0)}$ is the wavenumber of free space, $\varepsilon_r = (n-ik)^2$ is the relative permittivity specific for the particular material; *n* and *k* are the real and imaginary parts of its complex refractive index . The model is constructed in 2 dimensions (*x, y*), *x* being the propagation direction, but the z-components of both electric and magnetic fields come from the solution as well, since it is assumed that

$$\tilde{\mathbf{E}}(x, y, z) = \tilde{\mathbf{E}}(x, y)\exp(-ik_z z) \qquad (5)$$

where k_z is the out-of-plane wavenumber.

In order to precisely calculate propagation of the electromagnetic wave, a 1 µm–thick air layer was added above the NCD film. The glass substrate had also the thickness of 1 µm. It was confirmed that increasing the thickness of these two layers did not change calculation results. The free triangular computational mesh contained 200-300 000 elements.

Boundary conditions on the top and bottom of the PWG were set as “Perfect electric conductor”, which sets the tangential electric field to zero. The boundary type “Port-numeric” was set at the left-hand side (excited port) and the right-hand side (output port) of the structure. Prior to solving for the electromagnetic field in the PWG, mode analysis was done on both ports in order to calculate the effective mode index and corresponding out-of-plane wavenumber. Then, the equation (4) was solved for the TE_0 mode. Attenuation of the optical signal in the waveguide was calculated from the 21 component of the S-matrix (provided by Comsol) as

$$A = 20\log S_{21} \qquad (6)$$

where S_{21} is defined as

$$S_{21} = \sqrt{\frac{\text{Power delivered to output Port}}{\text{Power incident on input Port}}} \qquad (7)$$

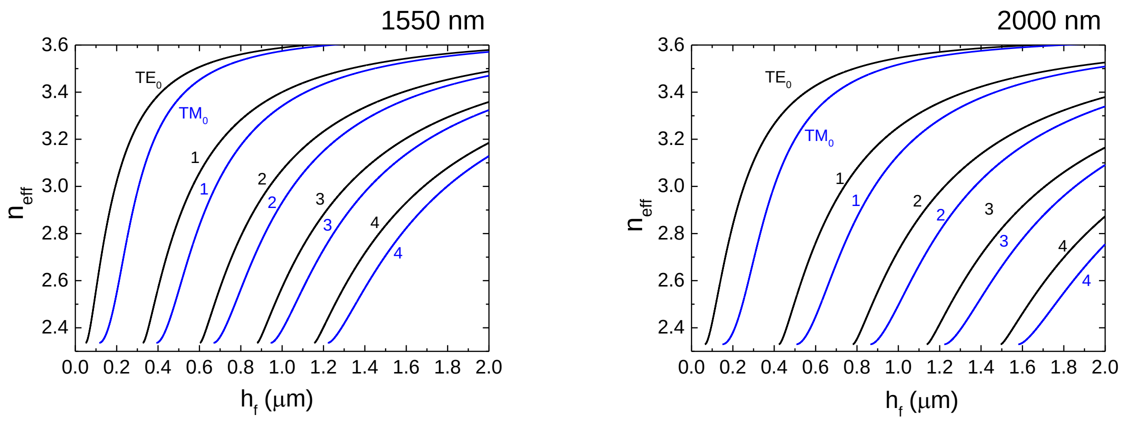
Both solutions of the equations (1,2) and FEM simulations used the optical properties as listed in **Table 1.** The refractive index for 2000 nm was extrapolated from the evaluated wavelength dependence of the absorption coefficient from PDS measurements [7,8].

Table 1. Real (n) and imaginary part (k) of refractive index and corresponding absorption coefficient of considered materials.

material	n	k	α,cm^{-1}	Ref.
λ = 1550 nm				
a-Si:H	3.650	6×10^{-6}	0.49	[7]
NCD	2.336	7.5×10^{-4}	47.1	[5]
λ = 2000 nm				
a-Si:H	3.640	1.5×10^{-6}	0.094	[7,8]
NCD	2.330	1×10^{-4}	6.28	[5]

3. RESULTS

Calculations of guided modes for two wavelengths are shown in **Fig. 2**.



a) b)

Fig. 2 Effective index of refraction (n_{eff}) for individual guided transverse electric (TE) and transverse magnetic (TM) optical modes in dependence on the silicon layer height (h_f) for the excitation wavelength 1550 nm (a) and 2000 nm (b).

The calculated silicon layer thickness for single-mode propagation is 150-320 nm. For the subsequent FEM simulations, the thickness was fixed to 280 nm, fulfilling the single mode propagation for both wavelengths, while the NCD thickness and adsorbate properties varied.

Contours of electric field phasor transverse component for the TE_0 mode and 50 nm thick NCD film are shown in **Fig. 3.**

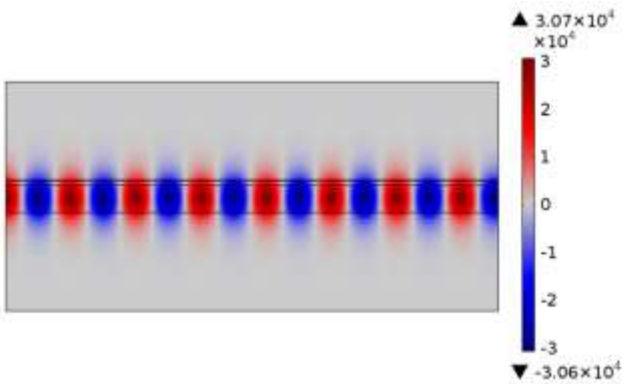


Fig. 3 Contours of electric field phasor $\tilde{\mathbf{E}}_z$ component for TE_0 mode (n_{eff} = 3.025) calculated by FEM. h_f = 280 nm, h_c = 50 nm, λ = 2000 nm.

The propagation of the EM field into glass and air is apparent. Simultaneously, this fact enables to realize the optical sensor for substances adsorbed onto the NCD film. However, the signal attenuation of the PWG itself, especially due to the optical absorption of the NCD film, must be assessed first.

The dependence of signal attenuation on the NCD thickness is asymptotic, as can be seen from **Fig. 4.**

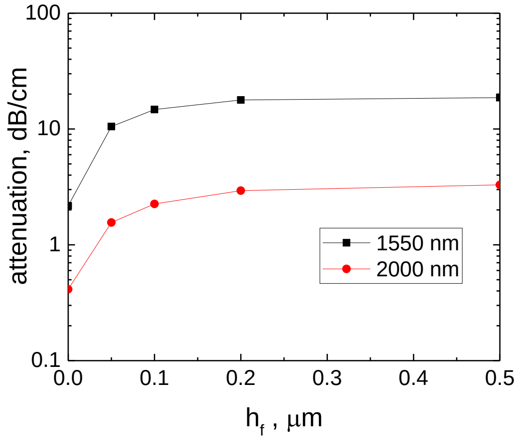


Fig. 4 Dependence of signal attenuation in PWG on the thickness of NCD film (h_c) for λ = 1550 nm and 2000 nm.

While the attenuation for 2000 nm excitation wavelength is acceptable (0.4-3.3 dB/cm), it is quite large for 1550 nm (2-19 dB/cm), as obviously given by the increasing absorption coefficient of NCD for lower wavelengths.

Last, the sensing properties were calculated after placing the adsorbate layer of varied absorption coefficient (the imaginary part of refractive index) and height on the NCD film. The real part of refractive index of the adsorbate was arbitrarily set to 1.5. It was found that its variation in the range 1.5-2 did not change substantially the calculation results. The calculated attenuations for the excitation wavelength of 2000 nm are shown in **Figs. 5,6**.

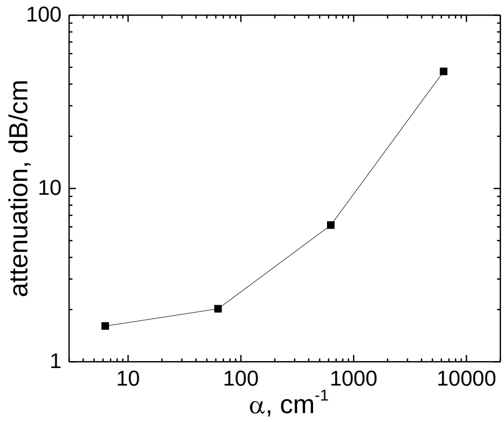


Fig. 5 Dependence of signal attenuation in PWG on the absorption coefficient of the adsorbate with the height of 5 nm. h_f = 280 nm, h_c = 50 nm, λ = 2000 nm.

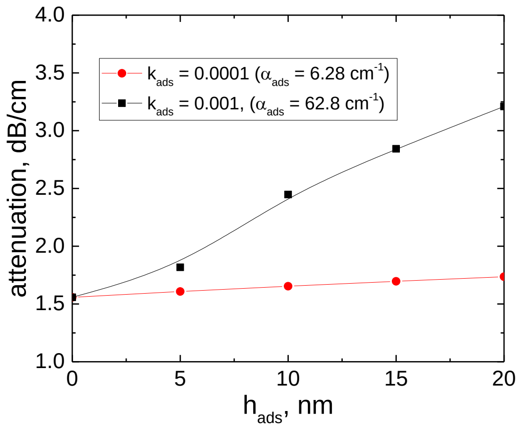


Fig. 6 Dependence of signal attenuation in PWG on the adsorbate layer height (h_{ads}) for two values of its absorption coefficient. h_f = 280 nm, h_c = 50 nm, λ = 2000 nm.

As expected, for the 10 times lower height (5 nm) of the adsorbate layer in comparison with the NCD height (50 nm), the attenuation becomes sensitive to the adsorbate when its absorption coefficient is larger than absorption of NCD by at least an order of magnitude. The attenuation is < 10 dB/cm when the adsorbate absorption coefficient is < 1000 cm^{-1}. The response to the adsorbate layer height is almost linear, as can be seen in **Fig. 6.** The linear fit produces the slopes 0.0089 dB/cm/(nm adsorbate) and 0.083 dB/cm/(nm adsorbate) for the absorption coefficients 6.28 cm^{-1} and 62.8 cm^{-1}, respectively. It means that the slope is directly proportional to the absorption coefficient.

For the very thin NCD films with low absorption coefficient, optical scattering on the randomly rough NCD surface (individual grains) should be taken into account in simulations. This will be solved in future work.

4. CONCLUSIONS

The FEM simulations in Comsol Multiphysics were found a useful tool for designing a multi-layered planar optical waveguide – an optical sensor. The simulations can be used to design not only planar waveguide-based sensors, but also 3D structures of any shape. The planar optical waveguide with an optical channel of 280 nm-thick layer of amorphous silicon and a cover/sensing 50 nm–thick nanocrystalline diamond film operating at the wavelengths of 1550-2000 nm has been suggested. It is concluded that the NCD film must be of good optical quality, with the absorption coefficient < 10 cm^{-1}. The calculated signal attenuation of an arbitrary adsorbate on the top NCD film has nearly linear response to the adsorbate layer height in the range of 0-20 nm. The slope of this response is directly proportional to the adsorbate absorption coefficient.

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