

# Design and investigation of properties of nanocrystalline diamond optical planar waveguides

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**Abstract:** Diamond thin films have remarkable properties comparable with natural diamond. Because of these properties it is a very promising material for many various applications (sensors, heat sink, optical mirrors, chemical and radiation wear, cold cathodes, tissue engineering, etc.) In this paper we report about design, deposition and measurement of properties of optical planar waveguides fabricated from nanocrystalline diamond thin films. The nanocrystalline diamond planar waveguide was deposited by microwave plasma enhanced chemical vapor deposition and the structure of the deposited film was studied by scanning electron microscopy and Raman spectroscopy. The design of the presented planar waveguides was realized on the bases of modified dispersion equation and was schemed for 632.8 nm, 964 nm, 1 310 nm and 1 550 nm wavelengths. Waveguiding properties were examined by prism coupling technique and it was found that the diamond based planar optical element guided one fundamental mode for all measured wavelengths. Values of the refractive indices of our NCD thin film measured at various wavelengths were almost the same as those of natural diamond.

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## 1. Introduction

Nanocrystalline diamond (NCD) thin films are of special interest in photonics and micro/nanophotonics structures because of their unique properties as low absorption and scattering in wide spectral range, high thermal conductivity, high density, large Young's modulus and high stability under extreme operating conditions [1–3]. The table value of the diamond refractive index is approximately 2.3876 at  $\lambda = 1\ 311\ \text{nm}$ . Refractive index of synthetically prepared NCD film usually has lower value but NCD deposited on silica on silicon substrate has still high index contrast. The waveguides created this way are known as high index contrast (HIC) waveguides and have much higher index contrast than common photonic materials (polymers, optical glasses and crystals) [4]. Useful HIC waveguides can be used for small bending radius structures or compact and ultra dense photonics integrated circuits. Because of the combination of high chemical stability and thermal conductivity with attractive optical properties diamond is beginning to find applications in optical components (especially those for IR region) suitable for using in harsh environments [5]. Conventional IR materials such as ZnS, ZnSe and Ge, suffer from the disadvantage of being brittle, easily damaged and having low chemical resistance.

Deposition of thin single-crystalline diamond film has not been up to now fully successful. Recently, fabrication processes of diamond films having NCD and/or ultrananocrystalline (UNCD) structures were presented [6]. Such structures made by an approach based on microwave plasma enhanced chemical vapor deposition (MW PECVD), however only a few of the deposited diamond films had acceptable waveguiding properties.

Here we are going to present NCD planar waveguides, which we proved to support fundamental TE/TM modes in the wavelength range from 473 nm to 1 552 nm. The design of the presented planar waveguides was done on the base of modified dispersion equation and then, an actual NCD film was deposited by microwave plasma enhanced chemical vapor deposition (MW PECVD). This is going to be an approach, different of those already published [7, 8], which will lead to deposition of such diamond layers that would be very close to genuine diamond.

## 2. Experimental

Before the diamond deposition the surface of silicon substrate ( $10 \times 10\ \text{mm}^2$ ) was processed by thermal oxidation and 1 420 nm thick silica film was formed. Prepared silica-silicon arrangement was mechanically seeded in an ultrasonic bath in deionized water/UDD (Ultra Dispersed Diamond) powder solution [9]. The NCD deposition was done from a gas mixture of methane and hydrogen (hydrogen gas flow of 400 sccm, methane gas flow of 2 sccm) in a MW PECVD reactor using an ellipsoidal cavity resonator [10]. The deposition was performed

at the total gas pressure of 5 kPa, microwave power of 2 500 W, and the substrate temperature was 990 °C.

The surface morphology and grain size of deposited diamond film were measured by scanning electron microscopy (SEM, e LiNE writer, Raith GmbH) and the diamond character of the films was studied by Raman spectrometer (Renishaw InVia Reflex) with the excitation wavelength of 325 nm.

The TE polarized reflectance spectra were measured under variable angle of incidence in the spectral range of 600-1 200 nm using a prototype spectrometer. The measurement setup uses a halogen lamp as a light source, monochromator with grating blazed at 750 nm, NIR polarizer in rotary mount, simple rotary sample stage with 1° precision and Si photodiode as a detector.

Waveguiding properties of NCD film were examined by using Metricon 2010 prism-coupler system. The apparatus works on a principle of dark mode spectroscopy [11] (see Fig. 1). The measured NCD sample is brought into contact with the base of a couple prisms by means of a pneumatically-operated coupling head. A small air gap between the waveguide film and the prism is formed. A laser beam strikes the base of the prism and is totally reflected at the prism base onto a photodetector. At certain discrete values of the incident angle  $\Theta$ , called mode angles, photons can tunnel across the air gap into the waveguide film and enter into a guided optical propagation mode, causing a sharp drop of the intensity of light reaching the detector.

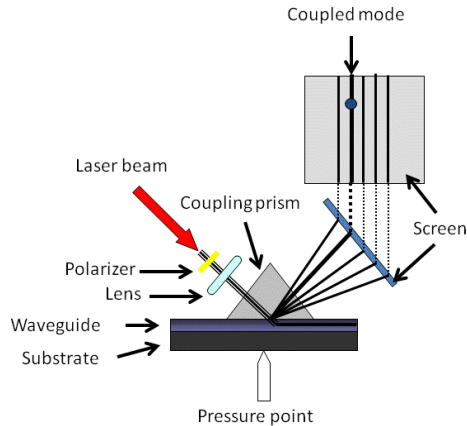


Fig. 1. Schematic view of the dark mode spectroscopy measurement.

### 3. Results and discussions

#### 3.1 Modeling of the nanocrystalline diamond optical planar waveguides

The dimensions of the waveguides were calculated by using modification dispersion equation [12, 13]. The cross-section view of the design waveguide structure is shown in Fig. 2. Before the deposition, dimensions of the NCD waveguides were designed with help of the refractive index values listed in the tables presented in Table 1.



Fig. 2. Schematic view of the optical planar NCD waveguide structure.

**Table 1. Tabular Refractive Indices of the Silicon (Si), Silica (SiO<sub>2</sub>) and Natural Diamond (D) Used for Modeling [14, 15]**

Wavelength (nm)	Refractive index		
	Si [14] $n_{Si}$	SiO <sub>2</sub> [15] $n_{SiO_2}$	D [15] $n_D$
473	4.4676	1.4639	2.4383
632.8	3.8816	1.4570	2.4122
850	3.6621	1.4525	2.3978
964	3.6089	1.4509	2.3939
1260	3.5128	1.4474	2.3882
1311	3.5073	1.4468	2.3876
1552	3.4762	1.4440	2.3855
1625	3.4693	1.4431	2.3851

For the waveguide structure described above, the mode calculations performed for operating wavelengths of 632.8 nm, 964 nm, 1 310 nm and 1 550 nm for TE as well TM polarization are shown in Fig. 3.

From the calculations it follows, e.g., that if we want the deposited film to guide one single mode, the thickness of the diamond film ( $h_{NCD}$ ) should not exceed 200 nm at 632.8 nm (see Fig. 3(a)) and for the 1 550 nm the diamond film ( $h_{NCD}$ ) should not be thicker than approx. 450 nm (see Fig. 3(d)). The thickness of the buffer SiO<sub>2</sub> film ( $h_{SiO_2}$ ) was set according to the calculated one, which ensures that the out-coupled energy of the evanescent wave would be less than 1% (This calculation procedure has been already described in [12, 13]). Calculations made clear that to ensure the above-mentioned conditions the thickness of the silica film should not be less than 900 nm for all considered wavelength. Therefore we used silica-on-silicon substrate with thickness of the silica film to be around 1 420 nm, which is fully sufficient.

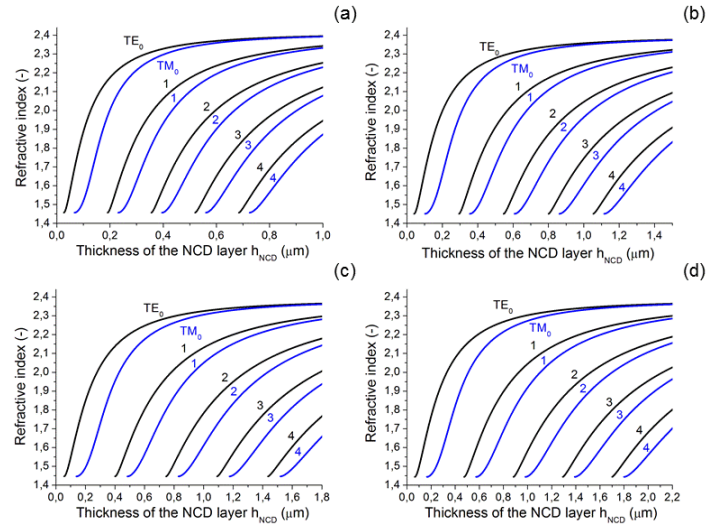


Fig. 3. Mode calculations of the diamond optical planar waveguides, (a)  $\lambda = 632.8$  nm, (b)  $\lambda = 964$  nm, (c)  $\lambda = 1310$  nm and (d)  $\lambda = 1550$  nm.

### 3.2 Morphology, thickness and optical properties of NCD

Top view SEM image is shown in Fig. 4(a) and the appropriate Raman spectrum in Fig. 4(b). Raman spectrum exhibits two sharp peaks, first one is centered at  $521\text{ cm}^{-1}$  and it is assigned to the silicon substrate; the second one centered at  $1332\text{ cm}^{-1}$  is well known as the so called diamond peak and it is related to  $sp^3$  bonds. The wide band located at  $1580\text{ cm}^{-1}$  is known as the G-band (“graphite-band”) and is related to the  $sp^2$  phases (i.e. amorphous phases) preferentially localized at grain boundaries [16].

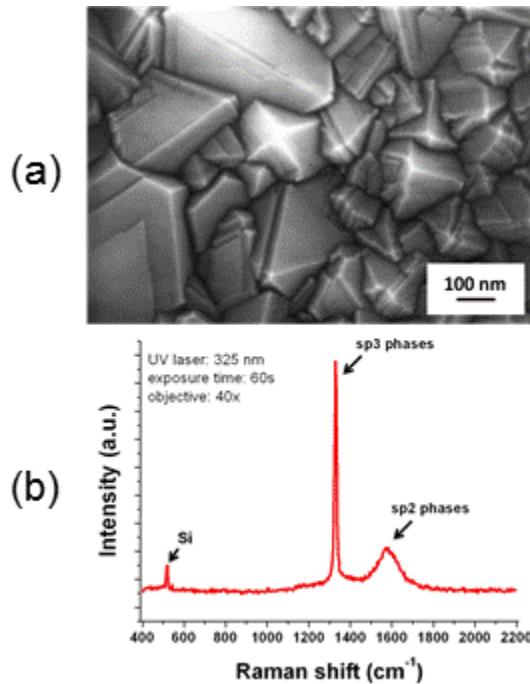


Fig. 4. (a) Top view SEM image and (b) Raman spectrum of the deposited NCD film.

In Fig. 5 we compare the measured and calculated TE reflectance spectra of thin NCD film deposited on silica/silicon substrate. The spectra were measured using TE polarized light under different angles of the incidence. The interferences shift to lower wavelengths with the increasing angle of incidence because of the increased optical path in thin films. Theoretical spectra were calculated with the optical parameters interpolated from Table 1 using commercial software (*Film Wizard*) for advanced modeling of the optical spectra of thin film multilayers. For calculations the effective medium approximation (EMA) was applied [17], to describe the index of refraction of the NCD film supposing that NCD film consists of crystalline diamond with the index of refraction  $n_D$  given by Table 1 and the  $sp^2$  phases with the complex index of refraction  $n_{nonD}$  of the highly absorbing non-diamond phase at grain boundaries. The unknown Cauchy parameters of the  $n_{nonD}$  were found by the fitting procedure:

$$n_{NCD} = \left\{ (1-\xi) \sqrt[3]{n_D} + \xi \sqrt[3]{n_{nonD}} \right\}^3 \quad (1)$$

Here  $\xi \in (0,1)$  is a fraction of the  $sp^2$  phase in the NCD film. The index of refraction  $n_{surf}$  related to the surface film was modeled within the EMA with the index of refraction given by the formula:

$$n_{surf} = (1 + \sqrt[3]{n_{NCD}})^3 / 8 \quad (2)$$

The thickness of the  $SiO_2$  (1 420 nm), NCD (380 nm) and the surface film (42 nm) as well as the complex index refraction of non-diamond phase and its volume fraction  $\xi$  (2%) were optimized during the fitting process. The reflectance spectra measured at angles  $20^\circ$  and  $25^\circ$  were fitted simultaneously. The good agreement between the calculated and measured spectra is shown in Fig. 5 for both angles and it proves the validity of the estimated thickness and the refraction index shown in Fig. 7. The calculated thickness of the surface film (42 nm) suggests the surface rms roughness to be about 21 nm [18].

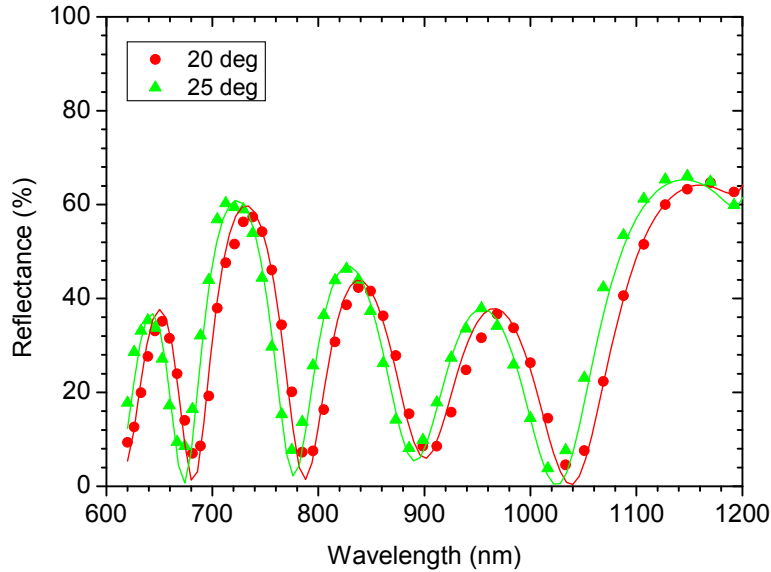


Fig. 5. Measured (scattered points) and calculated (solid curves) TE reflectance spectra of NCD film (calculated thickness 380 nm, surface rms roughness 21 nm) on Si substrate coated by the  $SiO_2$  film (calculated thickness of 1 420 nm) under the angle of incidence of 20 and 25 degrees.

### 3.3 Waveguiding properties of the NCD film

Waveguiding properties of the NCD films were measured by prism-coupling system at five wavelengths: 473 nm, 632.8 nm, 964 nm, 1 311 nm and 1 552 nm. The obtained data are summarized in Table 2.

Waveguiding measurements of the mode spectra for both polarizations (TE and TM) proved that values of the refractive indices for TE and TM modes are almost identical. Based on this observation, further we present only TE modes. Figure 6 shows TE guided mode spectra for four longer wavelengths.

**Table 2. Waveguiding Properties of the Deposited NCD Film: Angle of Incidence of the TE Modes**

Wavelength (nm)	473	632.8	964	1 311	1 552
Angle of incidence (degree)	-26°42'	-14°28'	-14°31'	-20°58'	-25°16'

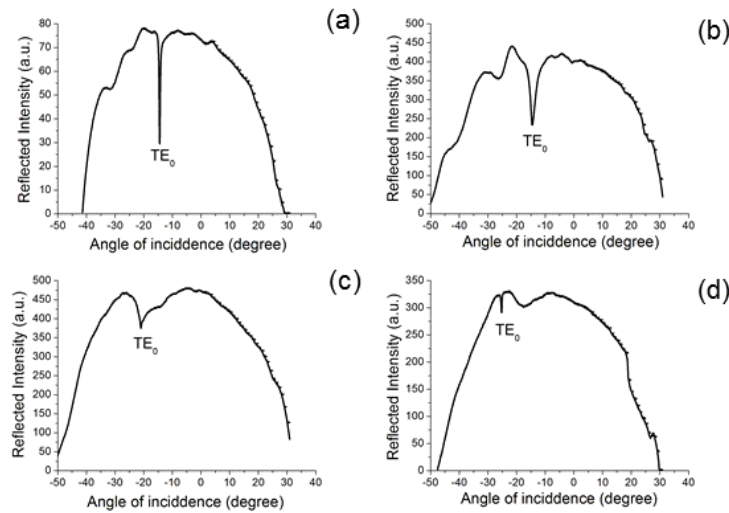


Fig. 6. TE guided mode spectrum for the NCD film at (a) 632.8 nm, (b) 964 nm, (c) 1 311 nm and (d) 1 552 nm.

From results shown in Fig. 6 and summarized in Table 2 it is clearly evident that the NCD films exhibit waveguiding properties. Refractive indices of the deposited films were calculated using the angles given in the Fig. 6(a)-6(d), the wavelengths of the measurement and, if needed, the thickness of the waveguiding films (380 nm). Figure 7 plots refractive indices of the measured NCD film used in this study and data presented in the previously mentioned works [7, 8] are added to compare them with those of the natural diamond [15].

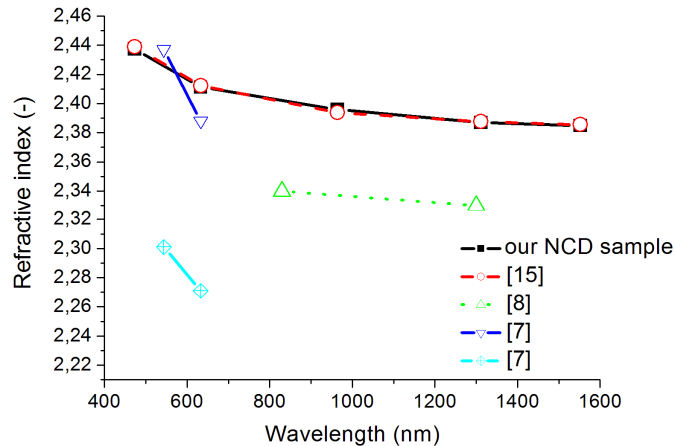


Fig. 7. Comparison of refractive indices of genuine diamond waveguide, our thin film and the films reported in [7, 8, 15]. The indices of our thin film (full line) coincide with those of genuine diamond (dash curve)

According to the calculation mentioned above it was expected that the deposited NCD film having a thickness of 380 nm will support 2 TE modes at the wavelengths of 964 nm and shorter. At the longer wavelengths there would be noticeable one TE mode only. However, the measurement showed that the deposited films actually supported always just one mode at all applied wavelengths.

Optical properties of the NCD films examined by prism coupling technique have been reported only by a limited number of works [7, 8]. Sharda et al. [8] reported about refractive index measurements at two wavelengths, 830 nm and 1300 nm for the microcrystalline and nanocrystalline diamond films, with thickness ranging from 883 to 4100 nm that were deposited on silicon substrate. They found the refractive indices of 2.34 and 2.33 at the wavelengths of 830 and 1300 nm, respectively [8]. Djemia et al. [7] reported about refractive index measurements at two wavelengths, 543.5 nm and 632.8 nm, for the polycrystalline and smooth fine-grained diamond films deposited on a titanium alloy by a two-step microwave CVD with 2  $\mu\text{m}$  and 5  $\mu\text{m}$  thicknesses of the diamond films. Their polycrystalline films had the refractive indices of 2.437 and 2.388 at 543.5 and 632.8 nm, respectively. For the smooth fine-grained diamond films they found the values of the refractive indices 2.301 and 2.271 at 543.5 and 632.8 nm, respectively.

In comparison with presented works [7, 8] our thin film was grown on the Si-SiO<sub>2</sub> substrate. This approach allows for using a wider range of wavelengths for waveguiding, as well as IR spectra measurement. This is of particular interest for sensoric applications. Moreover, in both papers [7, 8] the NCD films were deposited on optically non-transparent substrates, which are rather mirrors and from the text in [7] it is not clear if the conditions for waveguiding properties are fulfilled. What concerns the NCD films deposited on Si [8] there could be found a planar waveguide by the dark mode spectroscopy, however that waveguide cannot be in principle of any practical use. Moreover, our NCD film much more resembles the natural diamond refractive indices than the films reported in [7] and [8], what gives an evidence of its high optical quality.

#### 4. Conclusion

In this paper we presented a modified approach to deposit diamond thin layers. The waveguiding structure of our deposited layers was calculated for various operating wavelengths for TE as well as TM polarization by using modified dispersion equation and



actual waveguiding properties of the deposited Si/SiO<sub>2</sub>/NCD planar optical element were confirmed by prism-coupling technique. Even though that our diamond film was thin (380 nm) and consisted of small grains, a high optical quality of diamond film was confirmed. This was in a good agreement with Raman measurements which detected a sharp diamond characteristic line centered at Raman values 1332 cm<sup>-1</sup>. Our Si/SiO<sub>2</sub>/NCD planar optical element revealed only one fundamental mode for all the measured wavelengths (473 nm, 632.8 nm, 964 nm, 1311 nm and 1552 nm). The comparison with cited references [7, 8] shows the merit of our work, as refractive index of our diamond is very close to the genuine one in spite of the reference above (see Fig. 7). Moreover, we also found that our NCD had a surface conductivity, which makes it potentially interesting for application as new sensors family based on functionalized diamond.

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