Analysis of even and odd modes of a two-dimensional photonic crystal at Si/SiO/Cu interface

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We present a careful analysis of field characteristics in two-dimensional photonic crystals with square and hexagonal symmetry designed in a Si/SiO_2/Cu heterostructure. A special attention is devoted to frequencies close to photonic band gap. Following the symmetry classification in odd and even modes, their field characteristics are studied. The material prepared in a dedicated deposition chamber in ultra-high vacuum by annealing the Si/SiO_2 substrate and subsequent deposition of 10Å copper in order to prevent the sample oxidation, allows the study of the photonic characteristics of the copper/silicon oxide/silicon interface. The chemical state of the Cu/SiO/Si system is addressed by photoelectron spectroscopy which allows us to deduce the amount of crystalline Si and amorphous oxide. In this manner a precise estimation of the dielectric constant of the materials is possible. It is expected that at the interface with copper, a strong confinement of radiation should appear due to high reflectivity of copper.

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1. Introduction

The emergence of photonic crystals (PhCs) as novel systems with potential applications in optoelectronics attracted consequently considerable amount of work at both theoretical and experimental level. In order to understand the way their properties can be tailored so that they could be used for microwave, infrared or visible regimes, a rigorous understanding of the light-matter interaction mechanisms applied in these systems is required. This interaction leads to various phenomena appearance: photonic band gaps (PBGs) due to propagation of light in periodic dielectric medium, light localization in waveguides, photon trapping near defects, guiding of light along bent waveguides [1-4]. For example when PhCs are designated as optoelectronic devices (filters, splitters, data transmission systems, microstructured optical fibers [5]) the construction of waveguide is often demanded which will further support modes propagating along it. An effective way of designing a waveguide is by making use of the gapped modes which naturally arise in defective photonic crystals [6-7]. There are several parameters which can be modified in order to tune the properties of the PhCs: dielectric constant, geometry and the properties of the interfaces in layered materials. On the other hand, the effectiveness of the PhCs may be influenced by localized states associated with surface effects.

In this paper we investigate the possibility of confining the light in two dimensional photonic crystals at the interface of the native silicon oxide covering the crystalline Si, capped with an additional 1nm thick Cu layer. A comparative view of PhCs built with square and hexagonal symmetry is given.

The structure of the paper is as follows: Section 2 presents the experimental details on the sample preparation, Section 3 deals with numerical simulations: ab-initio for electronic structure of the interface and frequency-domain time-domain (FDTD) for photonic properties. Section 4 debates on the results obtained from correlated studies of photoelectron spectroscopy and numerical simulations studies, focusing on the difference between PhCs with square and hexagonal symmetry. The last section is devoted to conclusions.

2. Experimental

Sample was prepared by annealing a silicon wafer at about 700^o in an ultra-high vacuum chamber (base pressure $8x10^{-9}$ mbar). On its surface a 1nm thick copper layer was grown. The system was investigated by means of photoelectron spectroscopy and surprisingly, after the Cu deposition, a mixture of crystalline silicon and native oxide was found. This fact was addressed in the next section by means of ab-initio calculations performed in order to establish the configuration of Cu growth at the interface of SiO_2 and the phenomena which appear due to their interaction. XPS spectra were recorded in a dedicated chamber (Specs, Germany), under ultra-high vacuum ($P=1x10^{-10}$ mbar), using as excitation the Al K_α=1486.74 eV monochromatized radiation. The electrons were collected using a hemispherical electron energy analyzer (Phoibos 150) operating with a pass energy of 30 eV. Resolution (in terms of full width at half maximum) of 0.45 eV is achieved with monochromatized Al K_α

radiation. During the measurements, a flood gun operating at 1 eV acceleration energy and 100 μA electron current was used in order to achieve sample neutralization.

3. Calculation details

Electronic structure calculation were performed using SIESTA software [8] which solves self-consistently the Kohn-Sham equations associated with the atomic system under consideration and treats valence electrons by norm conserving pseudopotentials. We used the Generalized Gradient Approximation for the exchange functional [9].

The first thing is to determine the position of Cu atoms on the SiO_2 surface. Despite the native oxide layer is mainly amorphous, over a few lattice constant it can fairly be approximated as crystalline, which justifies our calculations performed on a crystalline SiO_2 rather than amorphous one. In this manner the computational efforts are reduced, the results standing qualitatively similar.

We relaxed the coordinates until a force $<10^{-7}$ eV/atoms was reached, and the difference between the energy calculated in two successive self-consistent iterative cycle was $<10^{-7}$ eV. A *7x7x7* sampling of the Brillouin zone according to Monkhorst and Pack prescription was found enough for assuring the convergence of the calculations [10]. We found that the formation energy of Cu layer on SiO_2 is *-0.21* eV only if the copper atoms "infiltrates" in-between the top-most Si layer. All other cases lead to a positive energy, suggesting that this is the most favorable growth case.

Once the position of Cu atoms relative to oxide layer deduced, the charge analysis was performed and projected density of states straightforwardly obtained.

Fig. 1 depicts the relaxed configuration of the Cu/SiO_2 system and the total charge distribution around the containing atoms. We identify that due the Cu deposition, a charge accumulation occurs at the top-most layer.

It is worth noting that due to copper growth on SiO_2 the electronic density of states changes, and in the otherwise insulating silicon oxide, at the Fermi level at ~ 2eV below it, localized states due especially to Cu but also to oxygen appears. This shows that indeed, at least a few of Si-O bond are affected by Cu deposition, which in turn modifies the surface properties. Additionally, these electronic levels can be excited with radiation belonging to a photonic band gap, leading to localization and enhancement effects due to coupling of radiation with elementary electronic excitations.

Moreover, the down-shift of the valence states can also be noticed which can be associated with the bending of the electronic levels. Their down-shift originating in the bending of the valence bands stands for the down-shift of the Si2p core level as seen in the XPS spectrum depicted in Fig. 4, suggesting that apparently, Si lies in a highly reduced state.

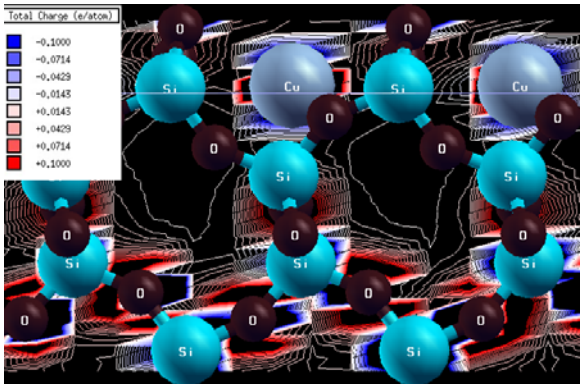


Fig. 1. The relaxed coordinated of Cu layer covering the native silicon oxide layer. In a red-blue scale the charge distribution of the system under study is presented.

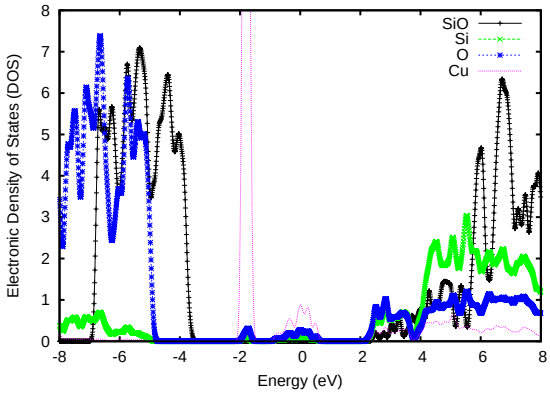


Fig. 2. Projected density of states for SiO_2 layer (black) and the modifications induced by Cu growth on the oxide layer for Si atoms (green), oxygen (blue) and Cu (magenta).

Photonic properties were calculated using the MPB software [11]. **MIT Photonic Bands (MPB)** is a software package to compute definite-frequency eigenstates of Maxwell's equations in periodic dielectric structures. Its primary intended application is the study of **photonic crystals**: periodic dielectric structures exhibiting a band gap in their optical modes, prohibiting propagation of light in that frequency range. However, it could also be easily applied to compute other optical dispersion relations and eigenstates (e.g. for conventional waveguides such as fiber-optic cables).

The simulated structures were two-dimensional photonic crystals consisting in a thick Si layer covered with 3 nm native oxide, capped with a very thin copper film. The modulation of dielectric medium was obtained by piercing the structure with periodic array of air cylinders with different radii as seen in Fig. 3, where a prototypical two dimensional photonic crystal with hexagonal symmetry is presented. The color scale is that red corresponds to the material with the higher dielectric constant and blue to the lowest one. The lattice constant is 1μm and the hole diameter ranges from 600 nm to 920 nm. All length and energy units are normalized at the lattice constant. We were interested in deducing the variations of photonic band gaps magnitude and position depending on the radius of the cylinders and the symmetry of the

structure. The field patterns of the modes lying in the close proximity of the photonic band gaps were analyzed in several high-symmetry points of the Brillouin zone.

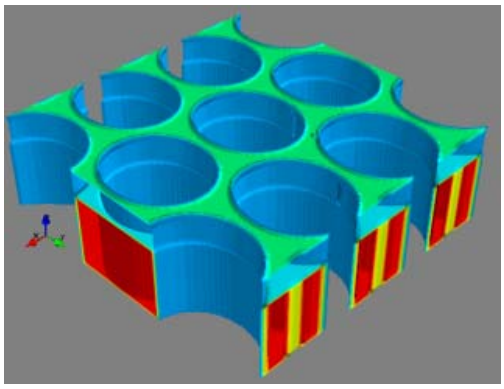


Fig. 3. A two dimensional photonic crystal formed in a Si/SiO/Cu layered system

4. Results and discussion

As a result of the copper deposition, a charge accumulation at the interface SiO_2/Cu appears.

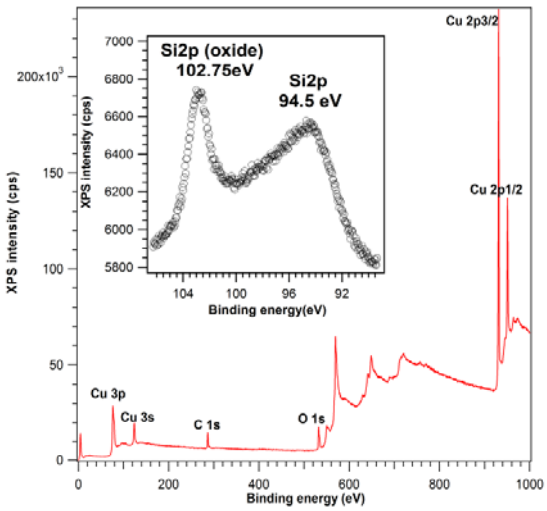


Fig. 4. XPS spectrum of Si/SiO_2/Cu layered system. The inset shows the core level spectrum in Si2p region. The silicon oxide and pure silicon peaks may be observed.

This leads to Si reduction from the oxide, a fact supported by the position of the Si oxide XPS line (102.75eV) belonging to SiO [12] instead of SiO_2. The down-shift is more dramatic for the Si peak which is found at 94.5 eV, way below the usual position (~4 eV) seemingly to a highly reduced state. On the other hand, as seen in Fig. 2, the copper layer leads to localized electronic levels appearance in the vicinity of the Fermi level, originating mainly from Cu, but also from the oxygen in a less extent.

These levels are seen in the XPS spectra at about 4.5 eV, somehow deeper that the results predicted by ab-initio calculations, which suggest that they should be located at ~2.5eV below the Fermi level. Still, the result is consistent since it is known that generally GGA approximation for the exchange-correlation functional underestimates the energies by at least 30% [13]. Applying this correction, we find a satisfactory similarity between XPS results (Fig. 3) and first-principles calculations.

Concerning the photonic crystal based on Si/SiO/Cu pierced with holes with different diameters giving rise to alternating air cylinders in the layered structure, with the dielectric constants of Si (ε_r=11.1-crystalline instead of 11.8 for amorphous silicon), SiO (ε_r=2.4 instead of 3.8 for SiO_2) and Cu (ε_r=5.4), we calculated the photonic band dispersion along high-symmetry lines of square and hexagonal Brillouin zone. The field distribution patterns of the modes lying in the vicinity of the photonic band gaps were compared with those belonging to bands away from the gapped states. The difference is also seen at the level of positioning in different symmetry points (Γ, M, X, K), where generally the group velocity ($v_g=d\omega/dk$) is very high. On the other hand, it is very interesting to notice that bands with low group velocity, also named "slow bands" are suitable for resonators and field coupling with electronic excitation, leading to field amplification and lasing effects.

The band dispersions were calculated for modes with quasi transversal electric and magnetic character and the results are summarized in Table 1 and 2. One can observe that for PhCs designed in triangular lattice, we have a single TE band centered at 0.29 for a hole diameter of 0.6a and a magnitude of 0.07; centered at 0.39 for a hole diameter of 0.8a and a wider magnitude of 0.13. For 2D PhCs with hole diameter of 0.92a, we have two photonic band gaps, the first one centered at 0.43 and a magnitude of 0.12 and the second one centered at 0.617 and narrower, with a width of only 0.02 but still reachable with well monochromatized radiation if guiding effects are in view. The TE-like modes for the square lattice reveal no bands if the diameter is 0.6a and two very narrow ones appearing as the diameter increases.

It is evident from the analysis of the pictures presented in Table 1 and Table 2 that the high frequency modes are rather slow, allowing for trapping effects rather than the low-energy ones. Even if no complete gaps exist for these states, their low dispersion property can be exploited if we select certain incidence angle for the incoming radiation (a well-defined wave vector) which lies in a pseudo-gap (partial gap), so that localization effects may be generated. On the other hand for the TM-like modes, no gaps are obtained for small radius air cylinders. For high diameter ones (0.92a), two bands for hexagonal PhCs and a single, narrow one for the square symmetry are found.

It is clear that depending on the targeted application the convenient structure can be chosen. One the other hand, as far as complete band gaps are concerned (both TE and TM-like), the square structure seems to be the more efficient due to its location in the telecommunication frequency range.

Table 1. Calculated photonic band structure for square and hexagonal 2D PhCs (TE-like polarization)

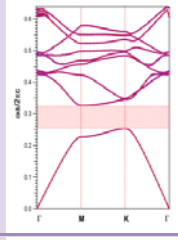
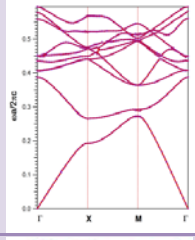
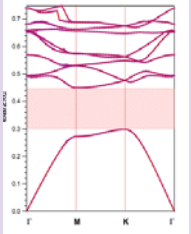
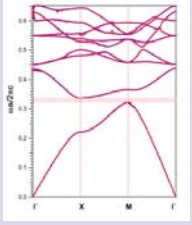
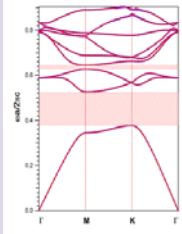
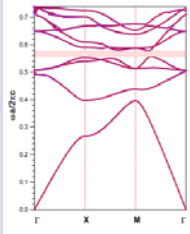
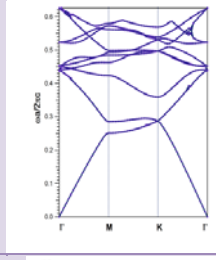
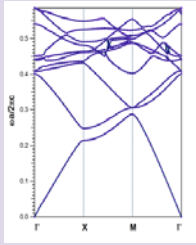
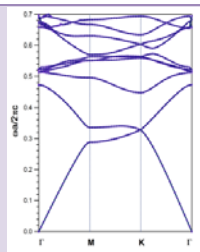
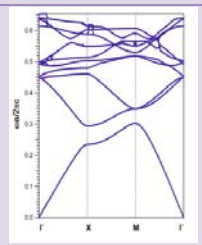
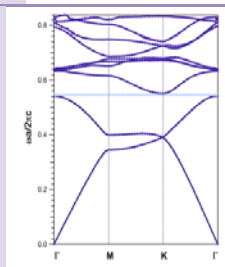
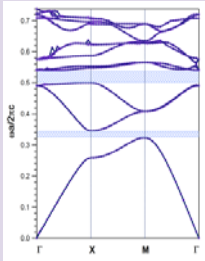
TE-like	Hexagonal symmetry	Square symmetry
R = 0.3a		
r = 0.4a		
r=0.46a		

Table 2.Calculated photonic band structure for square and hexagonal 2D PhCs (TM-like polarization)

TM-like	Hexagonal symmetry	Square symmetry
r= 0.3a		
r= 0.4a		
r= 0.46a		

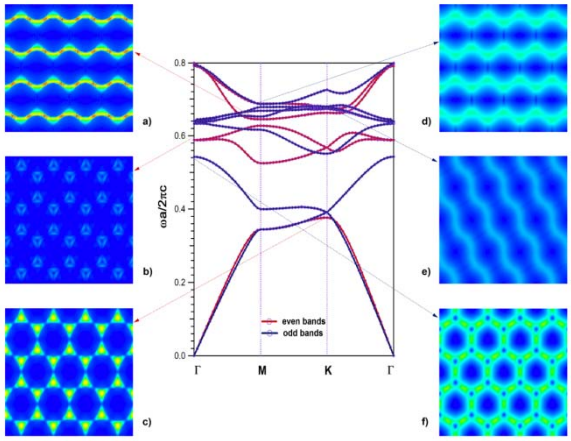


Fig. 5. Field patterns of the triangular lattice for bands near a PBG, for even (TE-like polarization): a) M point and c) K point and for bands away from gaps, b) at Γ point. Figures d), e), f) presents respectively the field patterns for odd modes (TM-like) for states near gap at M point, away from gap at K point and near gap at Γ point

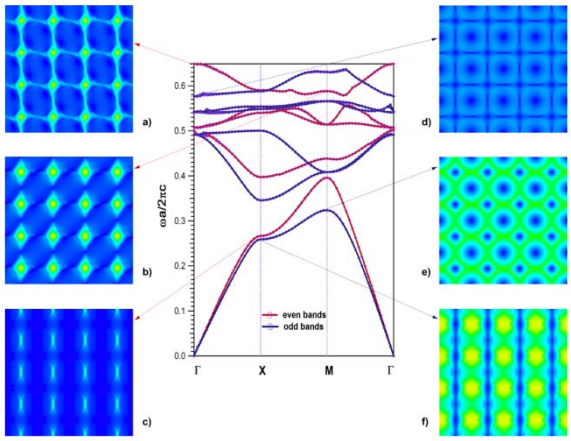


Fig. 6. Field patterns of the square lattice for even modes (TE-like polarization) at a) Γ point, b) M point and c) X point. Figures d), e), f) presents respectively the field patterns for odd modes (TM-like) for states away from the gap at Γ point, near the gap at M point and near gap at X point.

Envisaging these results one can formulate an efficient strategy for selecting the frequency domain desired for application in the optoelectronics field.

They are based on:

a) conveniently choosing the lattice structure so that certain modes are activated;

b) modifying the morphology of the photonic crystal by tuning the hole diameter;

c) tailoring the material properties by employing techniques routinely used in material science laboratories in order to achieve a desired combination of dielectric constants which accordingly may lead to the shift of the photonic gaps towards desired regions of the optical spectrum.

Concerning the symmetry of the modes which belong to definite photonic band, Fig. 5 collects the most

important results for the 2D PhCs in triangular lattice. One can readily observe that closer the concerned band is from the gap, the more localized are the field patterns, suggesting in a general manner which states can be used for guiding the light and which one are more suitable for amplification due to local interactions, field amplification around impurities, trapping or lasing effects. The similar results for the square lattice are presented in figure 6.

Future measurements and experiments will assess the goodness and viability of these samples for photonic crystals applications [14-21].

5. Conclusions

Concluding, we investigated numerically the properties of Si/SiO/Cu thin layer system for photonics applications. The surface composition, addressed by photoelectron spectroscopy reveals a mixture of Si and SiO at the surface. The electronic density of states reveals that due to copper deposition, localized states appear in the energy gap near the Fermi level, which can easily be excited with radiation from a photonic band gap, leading to an enhancement of the electromagnetic field. Depending on the symmetry of the photonic crystal and on the radius of the air cylinders, the magnitude and the position of the photonic band gaps can be tuned so that, depending on the desired application, different frequency regimes can be selected.

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References

[1] J. D. Joannopoulos, R. D. Meade, J.N. Winn, Photonic Crystals: Molding the Flow of Light, Princeton, NJ: Princeton University Press, 1995.
[2] C.C. Cheng, A. Scherer, J. Vac. Sci. Technol. **B 13,** 2696 (1995).
[3] R.D. Meade, A. Devenyi, J.D. Joannopoulos, O.L. Alerhand, D.A. Smith, K. Kash, J. Appl. Phys. **75**, 4753 (1994).
[4] D.G. Popescu, P. Sterian, U.P.B. Sci. Bull., A Series in press (2013)
[5] D.G. Popescu, P. Sterian, U.P.B. Sci. Bull., A Series **75** (2), 205-215 (2013).
[6] D.G. Popescu et al., J. Optoel. Adv. Mater. **14**, 356-362 (2012).
[7] D.G. Popescu, P. Sterian, J. Adv. Research in Phys. **2**, 021105 (2011).
[8] J. M. Soler, E. Artacho, J.D. Gale, A. García, J. Junquera, P. Ordejón, D. Sánchez-Portal, J. Phys. C **14**, 2745 (2002).
[9] J. P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).
[10] H.J. Monkhorst, J.D.Pack, Phys. Rev. **B 13**, 5188 (1976).
[11] S.G. Johnson, J.D Joannoupoulos, Optics Express **8**, 173 (2001).
[12] A. Ermolieff, P. Bernard, S. Marton , J.C. da Costa, J. Appl. Phys. **60**, 3162 (1986).
[13] L. Wang, T. Maxisch, G. Ceder, Phys. Rev. **B 73**, 195107 (2006).
[14] Petrescu, A. et al., ICCSA 2007, Pt 1, 4705450-461.
[15] Stefanescu, E.N. et al., Study of the fermion system coupled by electric dipol interaction with the free electromagnetic field, Vol. 5850, 160-165, Advanced Laser Tehnologies 2004, edited by A. Giardini, V. Konov, V. Pustavoy, (2005), Rome.
[16] Vizireanu, S. et al., Appl. Surf. Sci. **255,** 5378-5381 **(**2009).
[17] A. Sterian, "Computer modeling of the coherent optical amplifier and laser systems", Editor(s): Gervasi,O; Gavrilova, ML., Computational Science and Its Applications - ICCSA 2007, Pt 1, Proceedings 4705436-449, (2007).
[18] N.G. Gheorghe et al., Digest Journal of Nanomaterials and Biostructures 7, 373-384 (2012).
[19] M. Dima, M. Dulea, D. Aranghel et al., Optoelectron. Adv. Mater. – Rapid Commun. **4**(11), 1840 (2010).
[20] C. Iliescu, M. Avram, B. Chen, et al., J. Optoelectron. Adv. Mater. **13**(2-4), 387 (2011).
[21] D. Mihalache,. J. Optoelectron. Adv. Mater. **13**(9), 1055 (2011).

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