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Photonic band gap in 1D multilayers made by alternating SiO_2 or PMMA with MoS_2 or WS_2 monolayers

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ABSTRACT

Atomically thin molybdenum disulfide (MoS_2) and tungsten disulfide (WS_2) are very interesting two dimensional materials for optics and electronics. In this work we show the possibility to obtain one-dimensional photonic crystals consisting of low-cost and easy processable materials, as silicon dioxide (SiO_2) or poly methyl methacrylate (PMMA), and of MoS_2 or WS_2 monolayers. We have simulated the transmission spectra of the photonic crystals using the transfer matrix method and employing the wavelength dependent refractive indexes of the materials. This study envisages the experimental fabrication of these new types of photonic crystals for photonic and light emission applications.

1. Introduction

The research on atomically thin molybdenum disulfide (MoS_2) and tungsten disulfide (WS_2) is gaining considerable attention, since they are promising for several applications in optics and electronics [1–3]. In literature there are several reports on the optical properties, time resolved photogeneration, and luminescence of few-layers of MoS_2 [4], MoS_2 monolayer [5–7], and WS_2 monolayer [8]. Very recently, the development of population inversion, very useful for laser applications, has been observed in WS_2 [9].

Photonic crystals are composite materials in which two compounds, with a different refractive index, are alternated and the arising periodicity is comparable with the wavelength of light. Such periodicity gives rise to energy regions where the photons are not allowed to propagate in the materials, called photonic band gap [10–12]. Multilayered structures are a particular case of one-dimensional photonic crystals, which are easy to fabricate with several methods [13–15], and can be employed for different applications, as sensors [16], electro-optic switches [17], and lasers [18]. In literature there are interesting reports on one-dimensional photonic crystals containing MoS_2 [19] and on microcavities in which a MoS_2 monolayer is embedded [20,21]. However, a study of the transmission properties of one-dimensional multilayer photonic crystals, where atomically thin layers of different semiconducting transition-metal dichalcogenides are employed in the periodic structures, is still missing.

Here we describe the realization of a one-dimensional photonic crystal that is made with materials that are usually employed for these types of crystals, as silicon dioxide (SiO_2) or poly methyl methacrylate (PMMA), and transition metal dichalcogenides as MoS_2 or WS_2. The photonic crystals consist of multilayers and we have simulated the transmission spectra of the photonic crystals using the transfer matrix method and utilizing the wavelength dependent refractive indexes of the materials. We have found that a photonic band gap arises with atomically thin layers of MoS_2 or WS_2.

2. Methods

We have considered an air/multilayer/glass system. The wavelength dependent refractive index of SiO_2 is taken from Ref. [22], and the corresponding Sellmeier equation is:

$$n_{SiO_2}(\lambda) = \left(1 + \frac{0.6962\lambda^2}{\lambda^2 - 0.0684^2} + \frac{0.4080\lambda^2}{\lambda^2 - 0.1162^2} + \frac{0.8975\lambda^2}{\lambda^2 - 9.8962^2}\right)^{1/2} \quad (1)$$

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Instead, the refractive index of PMMA is taken from Ref. [23] and the Sellmeier equation is:

$$n_{PMMA}(\lambda) = \left(1 + \frac{0.99654\lambda^2}{\lambda^2 - 0.00787} + \frac{0.18964\lambda^2}{\lambda^2 - 0.02191} + \frac{0.00411\lambda^2}{\lambda^2 - 3.85727}\right)^{1/2} \tag{2}$$

The unit for the wavelength in the two Sellmeier equations is micrometer.

The wavelength dependent dielectric function (real and imaginary parts) of MoS_2 is taken from Ref. [24], while the one of WS_2 from Ref. [25], considering the refractive index of MoS_2/WS_2 $n_{MoS_2/WS_2} = \sqrt{\varepsilon_{MoS_2/WS_2}}$.

The simulation of the transmission spectra of the multilayers have been performed by using the transfer matrix method, exhaustively described in Refs. [26–28].

3. Results and discussion

We have simulated the transmission spectra of multilayer photonic crystals in which the layers of SiO_2, or PMMA, are alternated with monolayers of MoS_2, or WS_2. In Fig. 1 we have depicted a sketch of the photonic crystal.

We have carefully taken into account the wavelength dependent refractive index of all the employed materials, in order to give an accurate prediction of the transmission spectra of the photonic crystals. For the MoS_2/SiO_2 multilayer, we have chosen a thickness of the SiO_2 layers of 250 nm, while the thickness of the monolayer of MoS_2 is 0.65 nm [24]. In Fig. 2 we show the transmission spectrum of a MoS_2/SiO_2 photonic crystal made by 15 bilayers.

In the spectrum the transmission valleys at around 450, 605, and 660 nm are related to the absorption of MoS_2 (due to the excitonic resonances [29–31]). The valley at about 720 nm is related to a photonic band gap arising from the periodicity of the refractive index.

For the WS_2/SiO_2 multilayer the thickness of the SiO_2 layers is again 250 nm, and the thickness of the monolayer of WS_2 is 0.65 nm [25]. In Fig. 3 we show the transmission spectrum of a WS_2/SiO_2 photonic crystal made by 15 bilayers. In this multilayer the transmission valleys related to the excitonic resonances of WS_2 [8,29] are at 435 nm, 515 nm, and the very intense one at 618 nm. The photonic band gap is observed at about 720 nm.

We have also simulated the transmission spectra of photonic crystals in which the transition metal dichalcogenide monolayers are alternated with a plastic material as PMMA. For the MoS_2/PMMA multilayer the thickness of the PMMA layers, as for SiO_2, is 250 nm, and its transmission spectrum is shown in Fig. 4.

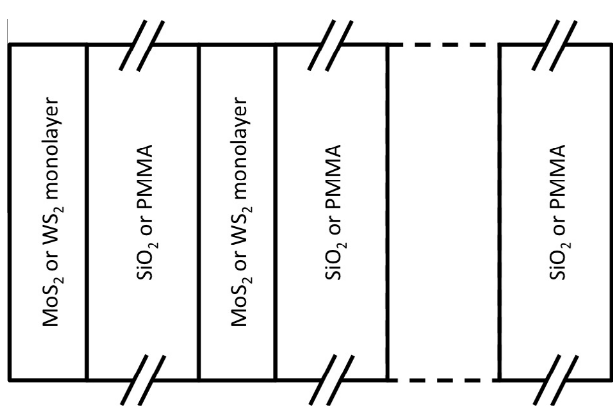

Fig. 1. Schemes of the photonic crystals made by alternating layers of SiO_2 or PMMA with atomically thin layers of MoS_2 or WS_2.

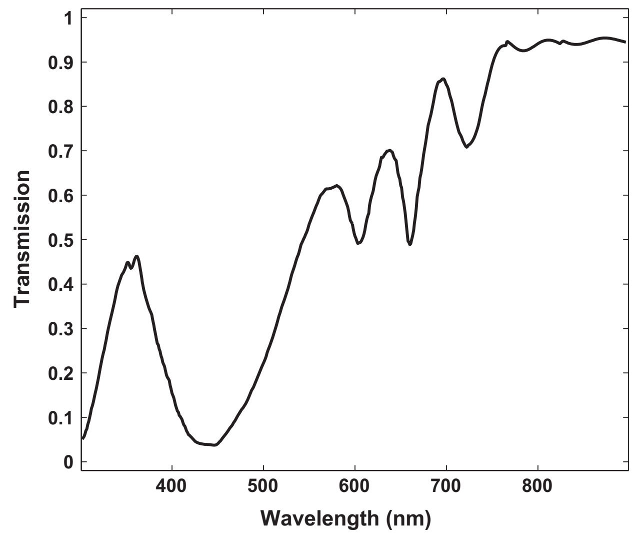

Fig. 2. Transmission spectrum of a one-dimensional photonic crystal made alternating 15 layers of SiO_2 and 15 monolayers of MoS_2.

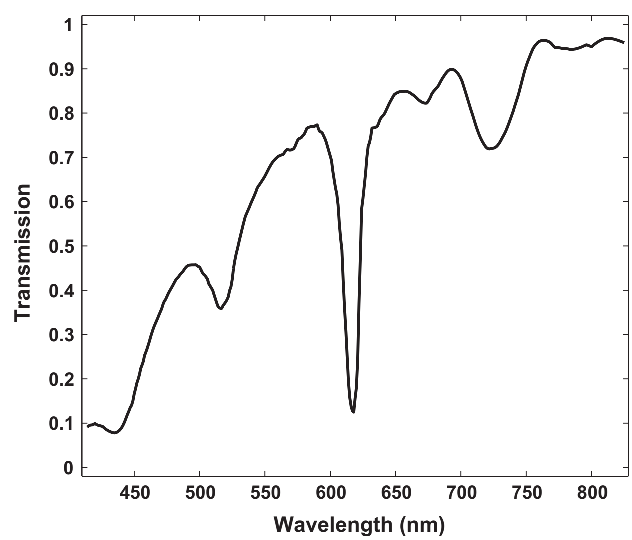

Fig. 3. Transmission spectrum of a one-dimensional photonic crystal made alternating 15 layers of SiO_2 and 15 monolayers of WS_2.

Also in the case of the atomically thin WS_2/PMMA multilayer the thickness of the PMMA layers is 250 nm, and its transmission spectrum is shown in Fig. 5 (1ML, i.e. a monolayer).

It is worth noting the photonic band gaps on the multilayers that we have shown are weak in intensity, with a transmission minimum between 0.7 and 0.8. This is due to the fact the thickness of MoS_2 or WS_2 monolayers is inherently very small (i.e. 0.65 nm). To obtain a more intense photonic band gap a higher number of bilayers is needed. Another possible solution is to increase the thickness of MoS_2 or WS_2 in the multilayer, i.e. from a monolayer to a tetralayer. For example, we have also simulated the transmission spectrum of a multilayer photonic crystal where the WS_2 consists of a tetralayer, with a thickness of 2.6 nm. In this case, because of the larger thickness of WS_2, we have decreased the thickness of PMMA to 245 nm. The transmission spectrum of the photonic crystal is shown in Fig. 5 (4ML). We have observed that the photonic band gap is already very strong with 15 bilayers, reaching a transmission, at about 750 nm, of around 0.1.