Theoretical study of surface states excitation in one-dimensional photonic crystal by halide perovskite microstructures

A.A. Popkova¹, K.R. Safronov¹, D.I. Markina², A. Pushkarev², S.V. Makarov², V.O. Bessonov¹,³, and A.A. Fedyanin¹
¹ Faculty of Physics, Lomonosov Moscow State University, Moscow 119991, Russia
² Department of Physics and Engineering, ITMO University, St. Petersburg 197101, Russia
³ Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Moscow 119071, Russia
E-mail: popkova@nanolab.phys.msu.ru

Abstract. In this work we develop the concept of integrated light source based on halide perovskite microwires for Bloch surface waves (BSWs) in one-dimensional photonic crystals. We theoretically study modes supported by a CsPbBr₃ microwire placed on the surface of a photonic crystal. The modes with field distribution similar to BSW are observed. We study the coupling of microwire modes with BSWs depending on the geometric parameters of the wire. BSW excitation efficiency exceeding 40% is found for BSW-like modes of microwire. We also examine resonant modes of finite microwire and show that BSW-like modes play a main role in the excitation of BSWs with perovskite radiation. Our research paves the way for the implementation of complete integrated optical setups on the surface of photonic crystals.

1. Introduction
Bloch surface waves (BSW) are promising platform for integrated photonics. Due to a sensitive spectral-angular resonance, localization of the electromagnetic field near the surface and a long propagation length that can reach several millimeters [1]. BSWs are actively used in sensing [2], enhancement of luminescence emission [3] and nonlinear optics [4], micromanipulation [5] and others. The ability to control the excitation wavelength in a wide spectral range (from UV [6] to IR [7]) by changing the structure parameters allows one to combine the BSWs with various existing platforms.

At this moment, the main elements of integrated optics based on BSW, such as waveguides [8], lens [9], resonators [10], interferometers [11] have been demonstrated. However further development of BSW integrated photonics require on-chip BSW sources. Since the wave vector of the BSW is larger than the wave vector of light in vacuum, special schemes are required for BSW excitation [12]. Currently, the most efficient and simple scheme to implement on-chip BSW excitation is a miniaturized grating, which demonstrate the efficiency up to 18% [13]. Increased efficiency can be achieved by using lasing structures, such as perovskite microwires, on top of photonic crystals. Lead-halide perovskites have a high refractive index, a direct band gap and high quantum yield of luminescence at room temperature [14]. Due to relatively simple chemical fabrication methods [15], perovskites are actively employed for creating of solar...
cells [16], photodetectors [17], and light emitting devices [18]. The possibility of fabrication of microresonator structures with good quality on various substrates allows generating stimulated emission in the visible spectral range [19].

In this article, we propose to use of emitting perovskite microstructures to excite BSWs. The modes that can be excited in CsPbBr$_3$ microwires are studied numerically, and the efficiency of radiation coupling with BSWs is estimated. Our research demonstrates the possibility for the implementation of compact BSW sources on the surface of a photonic crystal, which is a new step in creating a complete integrated platform based on BSWs.

2. Results and discussion

Studied system is schematically shown in Fig.1a. The CsPbBr$_3$ microstructure is placed at the surface of one-dimensional photonic crystal (PC). The PC parameters are chosen to sustain TE-polarized BSWs in the spectral range of perovskite luminescence (510-550 nm). The parameters were optimized using the transfer matrix method as well as finite difference in the time domain (FDTD) method in the Lumerical Solutions software. The resulting structure is consisted of 6 pairs of alternating layers of SiO$_2$ ($n = 1.48$) and Ta$_2$O$_5$ ($n = 2.12$) with thicknesses of 143 nm and 101 nm, respectively, deposited on a glass substrate ($n = 1.52$). This number of layers provides high leakage radiation, making BSW to be easily visualized in experiments using leakage radiation microscopy [11].

First, we numerically studied the modes supported by the perovskite film (with $n = 2.5$) with thickness $h$ on the PC surface at $\lambda = 535$ nm. This wavelength corresponds to the center of the CsPbBr$_3$ gain spectral region [20], while $n$ corresponds to refractive index of perovskite over lasing threshold. We used finite difference eigenmode solver realized in Lumerical FDTD. Our analysis (Fig. 1b) shows that, depending on the film thickness, the system may sustain from 1 (as $h$ approaches zero) to 7 (at $h \approx 420$ nm) modes simultaneously. Modes can be divided into 2 classes according to the value of the effective refractive index $n_{eff}$ equal to the ratio of the mode propagation constant and the vacuum wavenumber: high-index modes with $n_{eff} > 1.8$ and low-index modes with $n_{eff} < 1.7$. Range from $n_{eff} = 1.7$ to $n_{eff} = 1.8$ corresponds to transmission region of PC for $\lambda = 535$ nm. High-index modes can be TE- or TM-polarized, while all low-index modes are TE-polarized. As the bare PC supports the excitation of only TE-polarized BSWs, we consider only modes of the same polarization, since coupling between

![Figure 1](image-url)
modes of different polarizations is inefficient. Fig.1c demonstrates the field distribution of TE-polarized modes supported by perovskite film with $h = 300$ nm. High-index modes ($TE_{00}$ and $TE_{01}$) are conventional waveguide modes inside the film. The low-index mode ($TE_{02}^s$) is localized inside the film, like high-index modes, but attenuates inside PC with oscillations similar to those of BSW, so that we classified this mode as surface waveguide mode. Fig.1c also shows the field distribution of BSW on the bare PC surface. The field distribution of the $TE_{02}^s$ surface waveguide mode is quite similar to BSW, while conventional waveguide modes are noticeably different. Thus, BSW should be excited more efficiently with surface waveguide modes.

To study the BSW excitation efficiency we launch a particular mode in a half-infinite wire with particular height $h$. The mode reaches the end of the wire, where it partially reflects, partially scatters, and partially couples to BSW on the bare surface. In order to differentiate scattering and BSW excitation, we calculated the field distribution across PC at a distance of $5 \mu m$ from the wire end and than calculated overlap integral of this field and the field distribution of BSW on the bare PC. So that we estimated BSW coupling efficiency $\eta$ as the ratio of energy transferred to BSW and the energy of the launched mode. Surface waveguide modes demonstrate BSW coupling efficiency of the order of tens of percent in a narrow range of $h$ (Fig.2a), while $\eta$ is less than 0.3 for conventional $TE_{00}$ mode and less than 0.1 for $TE_{01}$ and $TE_{02}$ modes. Thus, conventional waveguide modes excite BSW significantly weaker, since their field distributions differ from BSW field distribution. Fig.2b demonstrates the excitation of BSW with $TE_{02}^s$ mode propagating inside the wire with $h = 250$ nm. We observe the field localization on the PC surface.

Then we consider finite microwire, which acts as Fabry–Perot cavity. In order to study resonant modes, we place a cloud of dipoles with random phases and positions inside microwire. Polarization of all the dipoles was the same (TE or TM). Our calculations confirm that depending on wavelength and polarization, one of the conventional or surface waveguide mode is excited inside the microwire. Quality factors of TE-polarized modes lies in the range from 200 to 500, while for TM-polarized modes, the value is around 200. We also studied BSW coupling efficiency for finite wire. Similar to the case of half-infinite wire, maximum $\eta$ is observed when one of the surface waveguide modes is excited.

Figure 2. a) Dependence of BSW coupling efficiency for modes inside perovskite film on the film thickness $h$ at $\lambda = 535$ nm. b) Excitation of BSW on the PC surface by $TE_{02}^s$ mode inside the wire with $h = 250$ nm.
Conclusion
In this work, we propose integrated light source for BSW, based on halide perovskite microwires. We study the modes supported by microwires and efficiency of BSW excitation by them. The arrangement of the perovskite structure on the PC surface leads to the appearance of new modes that do not exist in the structure on the surface of the glass or ITO. These modes plays a major role in the excitation of BSW on the PC surface. Our research takes a significant step in the development of BSW-based integrated photonics.

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