Optical modes in perovskite nanowire with shallow bi-periodic grating

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Abstract. In this work, we investigate electromagnetic modes supported by a perovskite CsPbBr₃ nanowire with a shallow periodic grating on top. By creating a domain-wall geometry, we introduce a topological defect into the nanowire and observe a defect-localized lasing state. By tuning the parameters of the structure we ensure that the frequency of the localized state fits the frequency of exciton resonance in perovskite and perform full-wave numerical simulations of the field distribution for such state.

1. Introduction
Currently, there is an active search for new materials for cheap, effective, and compact semiconductor lasers [1]. Semiconductor nanowire lasers, owing to their small sizes, highly localized coherent output, and efficient waveguiding, are a promising designs for integrated nanophotonic and optoelectronic devices [2]. However, typical semiconductor materials, such as CdSe, GaN, or GaAs, do not support strong excitons at room temperature, whereas their gain is not high enough for deeply subwavelength compactization of the lasing designs in the visible and near-infrared domain. In turn, inorganic and hybrid (organic-inorganic) halide perovskites have attracted high attention owing to their easy processability, high optical absorption, broadly tunable luminescence, high gain, strong optical nonlinearity, pronounced excitonic states at room temperature, and sufficiently high dielectric permittivity [3, 4, 5]. High-quality single-crystal perovskite nanowires demonstrate room-temperature lasing with low lasing thresholds, high quality factor and quantum yield, as well as broad spectral tunability [6]. Moreover, the perovskite nanowire lasers can be synthesized chemically in just several minutes [7]. However, one of the main disadvantages is the lack of directivity for the emitted light from the perovskite nanowires, as well as its sensitivity to defects and imperfections.

In this work, to make the operation of perovskite nanowire lasers more robust and directive, we exploit here the concepts of topological photonics [10] which enable a new class of the so-called topological lasers [11, 12]. Topological lasers are able to operate in a single-mode regime despite the presence of defects and imperfections. Recently, such active photonic topological structures were implemented in one- [11] and two-dimensional [12] systems. In this work, we investigate topologically protected lasing from a perovskite nanowire with shallow modulation of nanowire thickness.
2. Results and discussion
As a material of the nanowire we choose CsPbBr$_3$, which allowed for both simple synthesis of high-quality nanowires [7], and also exhibits extremely high gain around the frequencies 560-580 THz at room temperature [8]. The dispersion of CsPbBr$_3$ is taken from the work [9]. The nanowires can serve as a waveguide along the axial direction, whereas the flat facets form a Fabry-Perot resonator. Due to the fact that perovskite is a good amplifying medium, lasing is observed in such nanowires. However, as mentioned above, in this case, light is emitted from facets in all directions. In order to be able to control the output of radiation at certain angles, as well as to make nanowire-based lasers immune to defects, we create various gratings on top of them. Due to the introduced periodicity, the opening of a photonic bandgap is observed. By creating defects on the edge or in the center of the nanowire, it is possible to achieve the presence of a localized state in the bandgap, which allows to develop nanowire-based lasers.

![Band diagram of the perovskite infinite nanowire with shallow biperiodic grating.](image)

**Figure 1.** Band diagram of the perovskite infinite nanowire with shallow biperiodic grating. Black line and black dashed line are the light line in vacuum and substrate, respectively. The inset shows a schematic representation of the biperiodic grating structure.

In order to study the effects associated with the presence of a defective state inside the bandgap, we calculated numerically in COMSOL the band diagrams for a periodic lattice on the surface of a perovskite nanowire. To open the bandgap, we chose a biperiodic lattice consisting of alternating holes of different depths. Figure 1 shows the band diagram for the perovskite layer with height $h_0 = 200$ nm. The depth of the larger and smaller wells was $h_1 = \frac{2}{3} h_0$ and $h_2 = \frac{1}{3} h_0$, respectively, and their width was $w = 24$ nm. The period was 150 nm. As can be seen from Figure 1, a full photonic bandgap opens at frequencies from 565 THz to 580 THz.
The grating parameters were chosen so that the exciton frequency in the CsPbBr$_3$ perovskite (~571 THz) is within the bandgap.

We also carried out the calculation of electromagnetic fields in a nanostructure of finite size with a defect in the center of the nanowire. The nanowire length was 1.5 µm, the height and width were chosen to be 200 nm, the depth of the wells was $h_1 = 2/3 h_0$ and $h_2 = 1/3 h_0$, and their width $w = 24$ nm. Figure 2 shows the patterns of the energy density distribution in a perovskite nanowire at frequencies of 560 THz and 571 THz. Figure 2 (a) presents the energy distribution typical for the standard Fabry-Perot mode. At the same time, Figure 2 (b) shows that at the frequency of 571 THz there is a state localized on the topological defect in the center of the nanowire. The field in this mode is not radiated in the horizontal direction, as is the case with Fabry-Perot mode, but is rather emitted in the vertical direction.

![Figure 2](image)

Figure 2. Energy density in perovskite nanowire with shallow bi-periodic grating at different frequencies: (a) 565THz at a Fabry-Perot mode and (b) 571THz at a topological defect mode.

3. Conclusions

In conclusion, we have investigated electromagnetic modes supported by the perovskite CsPbBr$_3$ nanowire in the presence of shallow bi-periodic modulation of the nanowire thickness. By properly choosing the parameters of the structure, we were able to ensure that the mode localized on a topological defects, appears at frequency corresponding to exciton resonance, and, thus, enabling the lasing from the topological mode.

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