Numerical simulation of terahertz-wave propagation in photonic crystal waveguide based on sapphire shaped crystal
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Abstract. Terahertz (THz) waveguiding in sapphire shaped single crystal has been studied using the numerical simulations. The numerical finite-difference analysis has been implemented to characterize the dispersion and loss in the photonic crystalline waveguide containing hollow cylindrical channels, which form the hexagonal lattice. Observed results demonstrate the ability to guide the THz-waves in multi-mode regime in wide frequency range with the minimal power extinction coefficient of 0.02 dB/cm at 1.45 THz. This shows the prospectives of the shaped crystals for highly-efficient THz waveguiding.

1. Introduction
Terahertz (THz) technologies attract considerable interest in the recent years [1]. THz-waves offer many scientific and technological applications of THz spectroscopy and imaging [2–4] in many fields, including, medical diagnosis [5–8], material characterization [9–12], remote sensing and non-destructive evaluation [13–15]. Despite the significant progress in THz technology, the problem of low-loss THz waveguiding over long distances remains challenging.

Numerous approaches for THz waveguiding have been introduced. In Refs. [16–18], (i) low-loss waveguiding in metal and meal-dielectric hollow tubes has been studied. In Ref. [19], (ii) waveguides/fibers made of sapphire [20] have been proposed. In Refs. [21–24], (iii) THz-wave propagation in polymer waveguides and photonic crystal (PC) fibers has been considered. In Refs. [25–29], (iv) waveguiding based on plasmonic effects in metal wire, array of wires, or metal ribbons has been discussed. Finally, in Refs. [30–32], (v) combination of the plasmonic waveguiding principle with the polymer PC fibers has been introduced. However, neither metal and metal-polymer tubes and plasmonic waveguides, nor polymer PC fibers can be used to guide
the sub-picosecond THz pulses over a long distance, owing to both the high loss from the finite conductivity of metals, or high absorption of polymer materials, and significant material and waveguide dispersion.

In present paper we consider an alternative approach for THz waveguiding, which is associated with the use of shaped crystals. We apply numerical simulations to study the ability of THz-wave propagation in a PC waveguide based on sapphire multichannel single crystals. Using the numerical finite-difference analysis, we estimate the dispersion and the loss in the sapphire PC waveguide containing hollow cylindrical channels, which form the hexagonal PC lattice. Observed results demonstrate the ability to guide the THz-waves in multi-mode regime in wide frequency range with the minimal power extinction coefficient of 0.02 dB/cm at 1.45 THz. These results show the prospectives of the shaped crystals for highly-efficient THz waveguiding.

2. Results
We apply the numerical finite-difference analysis [33] (Lumerical Mode Solutions [34]) to find waveguiding modes, dispersion and loss of the multichannel PC waveguide based on sapphire shaped crystal.

Figure 1 (a) gives geometrical definition of the waveguide structure. The diameter of the shaped crystal is 12 mm. It has seven cylindrical hollow channels of 2.5 mm in diameter, which form the conventional hexagonal PC lattice with the period of 3 mm. In simulations, we use the well known data on the THz material parameters of sapphire from Ref. [20]. We assume the ordinary THz-wave propagating the crystal, since the optical axis of the waveguide is equal to the $c$-axis of sapphire, and the birefringence effect is observed for the THz-wave propagating perpendicularly to the $c$-axis of the crystal. Described waveguide could be manufacture using

Figure 1. Numerical finite-difference analysis of THz waveguiding in the shaped sapphire single crystal. Panel (a) shows geometrical definition of the PC waveguide structure. Panel (b) visualizes simultaneously the dispersion and loss for various waveguiding modes from A to K. Panel (c) shows the electromagnetic field intensity for the waveguiding modes from A to J.
edge-defined film-fed growth (EFG) [35] technique based on Stepanov method of shaped crystal growth [36]. In the EFG technique, crystals of various cross-sections are grown from a melt film formed on the top of a capillary die [35, 37–41].

Figures 1 (b) and (c) show the simulation results. Panel (b) visualizes simultaneously the dispersion and loss of the PC waveguide. Namely, it plots the THz-wave power extinction coefficient $\alpha$ versus the effective mode index $n_{\text{eff}}$ and the electromagnetic wave frequency $\nu$. Sharp blue stripes in figure 1 illustrate various waveguiding modes, marked with the characters from A to K. Panel (c) plots the intensity of these modes: the A-mode is localized in the cladding channels, while the modes from B to K are localized in the central channel of the shaped crystal. The multichannel sapphire crystal allows guiding the THz-waves in frequency range of 0.85 to 1.55 THz with relatively small loss in range of 1.0 to 1.55 THz. The minimal power extinction coefficient of 0.02 dB/cm corresponds to 1.45 THz, which is close to the advanced results of Refs. [17, 18].

Figure 1 (b) demonstrates the existence of paired modes, i.e., B&C, D&E, F&G, H&I, and J&K. This would lead to the intermodal interference phenomenon [42]. Due to the intermodal interference the coupling and decoupling of THz-waves to the PC waveguide could become rather unstable [42]. Moreover, the intermodal beating might lead to light decoupling into the lossy higher order modes [42]. At the same time, the mode interference could become a basis for development of novel THz sensing techniques based on intermodal interferometry [43, 44]. Description of the proposed waveguide manufacturing, its theoretical study and experimental characterization, is presented in details in Ref. [45].

In conclusion, in the present paper the THz waveguiding in sapphire shaped single crystal has been studied via the numerical simulations based on the numerical finite-difference analysis. The ability to use the multichannel sapphire crystal for broadband THz waveguiding in frequency range of 0.85 to 1.5 THz has been demonstrated with the minimal THz-wave power extinction of 0.02 dB/cm at 1.45 THz. The waveguiding efficiency could be increased by optimizing the PC structure and by substituting the sapphire with the other crystalline media possessing less THz wave absorption, for example, HRFZ-Si or crystalline $\text{SiO}_2$. Observed results show the prospective of the shaped crystal use for THz waveguiding.

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