Hexagonal Boron Nitride Phononic Crystal Waveguides

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Supporting Information

ABSTRACT: Hexagonal boron nitride (h-BN), one of the hallmark van der Waals (vdW) layered crystals with an ensemble of attractive physical properties, is playing increasingly important roles in exploring two-dimensional (2D) electronics, photonics, mechanics, and emerging quantum engineering. Here, we report on the demonstration of h-BN phononic crystal waveguides with designed pass and stop bands in the radio frequency (RF) range and controllable wave propagation and transmission, by harnessing arrays of coupled h-BN nanomechanical resonators with engineerable coupling strength. Experimental measurements validate that these phononic crystal waveguides confine and support 15–24 megahertz (MHz) wave propagation over 1.2 millimeters. Analogous to solid-state atomic crystal lattices, phononic bandgaps and dispersive behaviors have been observed and systematically investigated in the h-BN phononic waveguides. Guiding and manipulating acoustic waves on such additively integratable h-BN platform may facilitate multiphysical coupling and information transduction, and open up new opportunities for coherent on-chip signal processing and communication via emerging h-BN photonic and phononic devices.

KEYWORDS: hexagonal boron nitride (h-BN), phononic crystal waveguide, acoustic wave, nanoelectromechanical systems (NEMS), radio frequency (RF), integrated phonics

The considerable research effort on exploring the unconventional properties of van der Waals (vdW) layered materials has already led to exciting breakthroughs across a variety of disciplines from fundamental science to device engineering. Among families of vdW crystals, hexagonal boron nitride (h-BN), having prevailed as gate dielectric and passivation layers in two-dimensional (2D) electronics and optoelectronics, is emerging as an attractive material platform for nanophotonics and quantum optics. The ultrawide bandgap (5.9 eV) of h-BN is beneficial not only for providing excellent electrical insulation, but also for hosting robust single photon emitters (SPEs) even at room temperature. These defect-related quantum emitters exhibit large Debye-Waller (DW) factors and megahertz (MHz) photon count rates among the brightest SPEs reported so far. The layered structure of h-BN also endorses new and unparalleled flexibility in additive, back-end-of-line, and hybrid device integration free from lattice matching constraints, making it an excellent candidate for implementing on-chip quantum information processing and sensing functions.

Development of future quantum circuitries will require on-chip integration of multiple physical components in a way that the combined advantages of the hybrid system mitigate the weaknesses of individual constituents. In parallel with photonic components, such as photonic crystal cavities and optical resonators, which have been preliminarily demonstrated in h-BN crystals, phononic wave devices also play crucial roles in such hybrid schemes. Traveling at significantly slower speeds than the luminal speed of photons, phonons—the quanta of mechanical vibrations—have been suggested as better carriers allowing information to be stored, filtered and delayed over comparatively small length-scales but with high fidelity. It has been widely demonstrated that mechanical motion can mediate energy/information transduction among different physical domains, as well as bridge the classical and quantum regimes. For instance, the conversion between electrical signal and mechanical vibration has been well established in micro/nanoelectromechanical systems (M/NEMS), which are the backbones of today’s state-of-the-art commercial timing and inertial sensing devices, and the most sensitive probes in exploring fundamental science and limits of measurement.

Coherent photon-phonon interactions can be achieved via radiation pressure forces in optomechanical cavities. In the quantum regime, mechanical resonators can be coupled to artificial atoms embodied as charge qubits or spin qubits through Coulomb interactions or magnetic dipole forces, respectively.

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Specifically and intriguingly, spin-mechanical coupling schemes have been recently proposed and theoretically investigated based on the h-BN quantum emitters.\textsuperscript{27,28}

Thanks to the layered structure of its crystals, h-BN renders a unique combination of mechanical properties with very high in-plane stiffness and strength but low flexural rigidity (especially for monolayer and few-layer structures). It is predicted and validated as an excellent structural material, with a theoretical Young’s modulus \( E_\text{Y} \approx 780 \text{ GPa} \) and a breaking \( \varepsilon \) strain limit up to \( \varepsilon \approx 20\% \).\textsuperscript{29–31} The fundamental mechanical properties have been explored in suspended h-BN structures\textsuperscript{30,32} however, only very few experimental demonstrations of mechanical devices have been reported to date.\textsuperscript{31,33,34} To address the aforementioned needs and challenges for future integrated hybrid systems, it is desirable to explore new h-BN nanomechanical devices, especially ones capable of manipulating waves coherently.

In this work, we take an initiative to experimentally demonstrate one type of building blocks essential for future on-chip phononic integration, namely phononic crystal waveguides, in h-BN crystals. Distinct from individual nanomechanical resonators reported previously,\textsuperscript{33,34} phononic crystal waveguides comprise periodic arrays of coupled mechanical structures with architected unit cells (Figure 1). For individual nanomechanical resonators, the vibrational motion is restricted to the stationary eigenmodes. Whereas, vibration can propagate through coupled resonators, resulting in either constructive or destructive phonon transmission. Hence, by assembling coupled resonators into long-range periodic structures, we can create phononic crystal structures and consequential phononic bands similar to the atomic lattices in crystalline solids and photonic crystal lattices, and their associated band structures. Such devices not only enable fundamental exploration of lattice-based solid-state phenomena including dispersive relation, energy transport, nonlinear dynamics, and topological states in the phononic domain, but also facilitate device functionalities, such as on-chip routing and filtering of radio frequency (RF) acoustic waves.\textsuperscript{35,36}

The basic concept in Figure 1 is enabled and reinforced by the agile, additive features in device nanofabrication in the h-BN platform, evading conventional lithographic patterning and its associated chemical resist and contamination. As illustrated in Figures 1 and S1, the periodic structures are defined on the commonly used oxidized silicon (290 nm SiO\(_2\) on Si) supporting substrates, taking advantage of the well-established patterning and etching techniques with high spatial precision (see Supporting Information). Then, a suite of specially engineered, completely dry exfoliation and stamp-transfer techniques are employed to create large-area suspended h-BN structures.\textsuperscript{31,33,34} In as-fabricated devices, sizable elastic impedance mismatch is created between the suspended and supported regions of h-BN, thereby the acoustic energy can be efficiently confined within the suspended waveguides. The periodic elastic energy potential profile results in the formation of phononic band structure. This device fabrication approach can also help preserve the quantum signatures of emitters in h-BN free from any wet chemistry or surface contamination,\textsuperscript{38} favorable for developing future hybrid quantum devices.

Figure 2 presents the quantitative designs of the devices with modeling results. Quasi-1D chain of edge clamped circular resonators are designed to be overlapped with the neighboring ones to achieve strong mechanical coupling. The effective unit cell can be simplified as a near oval shape highlighted in Figures 2a and S1. The period of the lattice is set to be \( a = 8.25\) μm.\textsuperscript{32,35}
Figure 3. Frequency-domain characterization of h-BN phononic waveguide. (a) Measurement scheme of frequency-domain characterization. The waveguide is photothermally excited by an amplitude-modulated 405 nm laser at one end (near the leftmost cell in panel a) and the resultant phonon propagation is detected via a 633 nm laser interferometry system at the other end (rightmost cell in panel a). In real experiments, the 405 and 633 nm lasers are focused through the same 50× objective with tunable spatial separation up to ~200 μm. Optical microscopy image and simulated mode displacement profile at the excitation frequency ƒ = 14 MHz are embedded in the schematic illustration. (b) Measured frequency responses of the waveguide over a broad range, with the dashed line showing the response corrected according to position dependent detection efficiency (|u_experimental/|u_model| ≈ 6.81) and right axis showing the estimated displacement. (c) Zoom-in spectrum of the frequency range highlighted in light orange shade in panel b, and each peak is fitted with finite-Q harmonic resonance function.

μm and the width of the cell is w = 12 μm, owing to the predicted frequency dispersion with prominent bandgap lying in the MHz range (Figures S2 and S3). According to the finite element method (FEM) simulations (COMSOL Multiphysics), the thickness of h-BN layers is chosen to be larger than 50 nm to ensure the fabricated nanomechanical structures follow the plate model (detailed discussion in the Supporting Information) and immune to local strain inhomogeneity. The experimental and simulation results presented in the main text are attained based on the aforementioned cell geometry settings with a thickness of h-BN being 120 nm, without additional notation. Additional devices with varied unit cell dimensions are showcased in the Supporting Information (Figures S1 and S6).

The phononic band structure of the designed waveguide is revealed as the simulated phonon dispersion relation curves shown in Figure 2b, along with the mode shapes of the unit cell for the first and second lowest eigenfrequency branches at the wavenumber k = 0 and π/a points, respectively. The frequency spectrum is divided into multiple regions. The frequency range below the first phonon band is called stop band, in which no mechanical mode can be supported by the waveguide. Analogous to electron transport in atomic lattices of crystalline semiconductors, bandgaps form between transmission bands, within which phonon propagation is also suppressed. At higher frequencies, neighboring phonon bands start merging and mode crossing/anticrossing occur, related to the phenomenon of strong mode coupling, which can result in the mode type transformation and energy exchange between different phonon branches.

It is worth mentioning that such band structure simulation is fulfilled with Floquet-Bloch periodicity conditions u(x + a) = e^{iα}u(x), where u(x) is the displacement at position x, a is the lattice period, and k is the wavenumber (0 ≤ k ≤ π/a), assuming the number of cells as infinite. However, for device fabrication, we need to balance between the waveguide performance and the device footprint to determine a practical number of cells. Therefore, we also study the influence of the constituent cell numbers (N = 10, 20, 40) numerically, as summarized in Figure 2c. The relative amplitude in frequency-domain simulations, or transmission $T_{N=1} = 20 \log(|u_{n0}|/|u_1|)$ in dB, is defined as the ratio between the areal averaged displacement magnitude ($|u_{n0}| = \int_{\text{Area}} |u(x,y)| dx dy/A_{\text{Cell}}$) of the first and the last cells (note in analysis and simulation of individual cells, $u = u(x,y)$, no longer quasi-1D), with excitation force loaded at the first one. Reliant on the constructive or destructive interference conditions, the displacement amplitude of the last cell can exceed (>0 dB) or fall short (<0 dB) from the amplitude of the first cell. Agreeing with the band structure simulation, clear stop bands (~15 MHz) can be observed with displacement ratio lower than ~90 dB for all the presented cases. Conversely, there is no noticeable relative amplitude decline at the predicted bandgap frequencies (24−27 MHz) for the lattice with $N = 10$. For $N = 20$ and 40 cases, attenuation of ~30 and ~90 dB can be achieved, respectively. Considering the difficulty in obtaining h-BN flakes with very large uniform areas, the number of cells is set around 20 for device fabrication.

To investigate the frequency-domain characteristics of the h-BN phononic waveguides experimentally, we employ a customized ultrasensitive laser interferometry system (Figures 3a and S4). The conventional vibration excitation techniques relying on electromechanical coupling are not readily applicable to the insulating h-BN crystals. Also, the piezoelectric effect in h-BN only becomes accessible when the flake is thinned down to few layers. All-optical actuation and detection scheme is thus suitable for the characterization of these phononic devices, in which the suspended h-BN crystal and the patterned SiOx/Si substrate form an interferometer. The system is equipped with an amplitude-modulated 405 nm blue laser as the driving beam and a continuous-wave 633 nm red laser as the detecting beam. Both beams are focused onto
the devices through the same 50X long-working-distance objective, while the position of the focused laser spots can be individually controlled by a set of mirrors and beam splitters with spatial separation up to \( \sim 200 \) μm. Flexural motion of the suspended h-BN waveguide is photothermally actuated by the modulated 405 nm laser at one end. The acoustic waves with frequencies in the transmission bands can propagate through the waveguide and alter the interferometry condition of 633 nm laser at the other end of the waveguide. Hence, the mechanical displacement of the device can be transduced into the intensity variation of the reflected 633 nm laser beam and read out by a photodetector with frequency swept by a network analyzer.

Measured frequency-domain responses are shown in Figures 3 and 4 (and more data from additional devices in Supporting Information). As predicted, closely packed resonance modes develop into continuous transmission bands with well-defined phononic stop band and bandgap features. In terms of characteristic frequencies, the measured spectrum shows excellent agreement with the simulated one and the dispersive curves (Figure 4c–4f). The first phonon band spans from 15 to 24 MHz, and the second phonon band is from 27 to 40 MHz, separated by a prominent bandgap of \( \sim 3 \) MHz. The amplitude measured from the second phonon band is noticeably smaller than the one from the first band, because the detecting 633 nm laser spot is still parked at the center of the cell (no. 21), but this is now on the node lines of the unit-cell mode shapes \( \odot \) and \( \odot \) illustrated in Figure 2b. The lower branches are replotted in Figure S7 for the analysis and computation of the position-dependent displacement detection efficiency within any unit cell, to obtain the correction coefficient \( \frac{\text{int}_{\text{amplitude}}}{\text{int}_{\text{node}}} \approx 6.81 \) for the second phonon band based on a combination of measurements and simulations with practical laser spot size (1.5 μm) on the device (see Supporting Information). The amplitude-corrected response of the second phonon band is plotted as a dashed line in Figure 3b, which corresponds to the actual displacement at the last cell (no. 21) in this band. The corrected response in the second band can be higher than that in the first band, consistent with simulation results in Figures 2c and 4d. The ratio of displacement amplitude between the bandgap and the first transmission band is approximately \( 10^{-2} \), corresponding to an attenuation of \( \sim 33.5 \) dB, also agreeing with the simulation (Figure 4d–4f).

Figure 4a depicts a system diagram that facilitates analyzing the signal transduction chain and gaining quantitative understanding of the intrinsic characteristics of the waveguide device. The measured raw data (amplitude plot in rms voltage, Figure 3, and transmission plot in dB, Figure 4e) include extrinsic responses and contributions from the peripheral transducers necessary for interfacing with and measuring the device, including the upstream photothermal actuation, the downstream motion detection modules, and their inner components (Figure 4a). Combining multistage signal transduction gain analysis and calibration measurement by replacing the waveguide device with a single h-BN drumhead resonator with dimensions similar to a unit cell and operating within the first phonon band (15–24 MHz), we can obtain a relation that allows us to subtract the extrinsic contributions from the measured data (see Supporting Information). Upon application to the transmission data in Figure 4e, this yields the measured intrinsic transmission of the waveguide, shown in Figure 4f (without repeating the second band amplitude correction dashed line shown in Figure 3b), in very good quantitative agreement with the simulation results in Figure 4d.

In addition, with the analysis and calibration of displacement-to-voltage transduction in the motion detection module (Figure 4a), the corresponding displacement-domain data is...
The displacement of the mechanical wave packet is probed through the phononic waveguide until it relaxes to below the periodic gradually intensified function generator. The pulse train (in each burst actuation signal with 15 cycles by enabling the RF burst mode function generator. We introduce a single-frequency sinusoidal drive signal of the modulated 405 nm laser is shaped by a.

The measured amplitude response shown in Figure 3b, exhibiting ~50 to 400 pm vibrations probed at cell 21 in the first and second phonon bands (refer to the right vertical axis of Figure 3b). The phonon propagation behaviors can be directly visualized in the mode displacement analysis (Figure 4b). When one end of the waveguide is excited at a stop band frequency of 14 MHz, the mechanical motion is restricted to the excitation spot without propagation along the waveguide. When the excitation frequency escalates and reaches the first phonon band, propagating phonons with long wavelengths can be supported by the waveguide (@16.5 MHz in Figure 4b). As the frequency keeps rising, the wavelength of acoustic wave gradually decreases (@20 MHz in Figure 4b). When the half wavelength of the standing wave is in proximity to the same length scale of the unit cell, destructive interference among the reflected waves inside the waveguide leads to suppression of the mechanical motion. Therefore, at a bandgap frequency of 25 MHz, the excited vibration cannot travel through the waveguide (Figure 4b).

To further understand the phonon propagation dynamics in the h-BN phononic waveguide, temporal measurements are performed as well. To monitor the mechanical wave propagation in time domain, we build the time-domain measurement apparatus, as illustrated in Figures 5a and S10. The drive signal of the modulated 405 nm laser is shaped by a function generator. We introduce a single-frequency sinusoidal actuation signal with 15 cycles by enabling the RF burst mode of the function generator. The pulse train (in each burst period) gradually intensifies the mechanical motion of the device, and then the generated acoustic wave propagates through the phononic waveguide until it relaxes to below the thermal noise limit due to the dissipation during propagation. The displacement of the mechanical wave packet is probed at the end of the waveguide by the same 633 nm laser interferometry. But the electrical signal from the photodetector is filtered by a set of bandpass (BP) filters with 10–30 MHz bandwidth and then recorded using an oscilloscope. The results are averaged over 512 times by synchronizing the time-domain signals using the trigger from the function generator. The period of the burst signals is set as 10 ms to ensure the time interval between each excitation pulse train is long enough compared to the ring-down time of the mechanical motion so that the acoustic wave can propagate back and forth inside the waveguide for multiple cycles.

The measured temporal responses in the transmission band contain several displacement wave packets (Figures 5c and S10), which originate from the reflections of the propagating acoustic wave at the ends of the waveguide. Meanwhile, at the stop band or bandgap frequencies, the mechanical displacement is below the noise floor of the system. Color map in Figure 5b is attained by measuring the time-of-flight (ToF) traces as a function of frequency across the first phonon band. Fringes rising from the multiple reflections can be resolved as well. Since the period of these fringes corresponds to the time that acoustic wave travels a round trip inside the waveguide ($\Delta t$), it can be utilized to deduce the experimental group velocity ($v_g$) of the acoustic wave packet, using the equation $\Delta t = 2L/v_g$ (where $L$ is the total length of the waveguide). Likewise, the separation between adjacent peaks ($f_{int}$) in the frequency-domain measurements and simulations is defined as $f_{int} = v_g/(2L)$. The round-trip traveling time $\Delta t$ calculated from the frequency-domain simulation is marked in Figure 5b as yellow squares and dash lines, which align perfectly with the measurement results. Frequency-dependent group velocities can be quantitatively extracted from Figures 5b and S11. At the frequencies adjacent to the stop band, the group velocities are one order smaller than the ones at the center frequencies of the

Figure 5. Temporal dynamics of phonon propagation. (a) Measurement scheme of time-domain characterization. Distinct from the frequency-domain measurement, the excitation laser is modulated by sinusoidal burst signals from a function generator (number of cycles $n = 15$, burst period $p = 10$ ms, pulse train shown in Figure S10a) and these burst signals are also synced to the oscilloscope as references. A set of bandpass (BP) filters are inserted in the detection circuit, which only allow the waves with frequencies of 10–30 MHz passing through. Optical microscopy image and simulated mode displacement at the excitation frequency $f = 18$ MHz are embedded in the schematic illustration. (b) The color map represents the measured time-domain amplitude responses by sweeping the excitation frequency across the first phononic band. $\Delta t$ defines the time of the acoustic wave propagating a round trip along the waveguide. The yellow squares and dash lines mark the round-trip traveling time calculated from the eigenfrequency simulation and the frequency-domain simulation shown in Figure S11. (c) Selected traces of time-domain measurement from panel b at varied frequencies $f = 14, 16.6, 18.2, 20, 22, 25$ MHz.
If only the propagation loss is considered, the effective loss at the clamped end. In this measurement, the acoustic wave undergoes propagation loss. The quasi-1D h-BN waveguide demonstrated here exhibits a prominently higher first band frequency (15–24 MHz) and wider bandgap opening (3 MHz), compared to its counterparts made from conventional materials, such as silicon nitride (Si₃N₄), with similar geometry design. These favorable properties for high frequency (3–30 MHz) RF applications originate from the high Young’s modulus and low mass density of h-BN, which bestow enhancement in mode-coupling nonlinearity of the resonators as well. Moreover, the ultrahigh breaking strain limit of these 2D crystals allows them to be stretched much more significantly and offer wider operation bandwidth, which is unachievable by employing traditional materials with much lower breaking or fracturing strain limits. According to our further simulations (Figure 6), the operation frequency of h-BN phononic waveguides can be easily expanded from high frequency (HF, 3–30 MHz) to very high frequency (VHF, 30–300 MHz) bands, by incorporating strain-engineered thin h-BN layers that follow the membrane model. Especially when monolayer or odd-number layers (<10 layers) of h-BN thin flakes are employed, the piezoelectric effect may be expected to facilitate additional tunability and active devices may also be realized.

Besides the desirable features for classical RF signal routing and processing, the intriguing essential applications of the h-BN phononic waveguides lie in the quantum regime. On the basis of this prototypical demonstration of quasi-1D phononic waveguides, other functional devices, such as photonic-phonon crystals and optomechanical cavities, can be realized by further designing and engineering the periodic elastic energy potential of these vdW layered crystals. Embedding h-BN quantum emitters into such phononic waveguides creates an exceptional platform for exploring spin-qubit interaction and coherent information via photonic-phonon pathways.

In conclusion, we have designed and developed the first phononic crystal waveguides in engineered h-BN nanomechanical structures. Taking advantage of the layered crystal structure, the challenges in nanofabrication of long-range-ordered phononic crystal lattices have been circumvented through a facile integration approach and elastic environment engineering. As-fabricated h-BN devices exhibit strong phonon dispersion relation with prominently higher first transmission
band frequency and wider bandgap opening, compared to their counterparts made from conventional 3D crystalline materials with similar geometric designs. We have experimentally demonstrated that such h-BN waveguides are capable of supporting RF acoustic wave propagation over an effective length of 1.2 mm with a group velocity as high as 250 m/s at the first transmission band, while attenuating the transmission at the stop band and bandgap by over 30 dB. We envision by combining the unique piezoelectric properties of h-BN, such phononic structures can empower dynamically tunable devices for RF signal processing and open a new avenue toward building future integrated phononic and hybrid quantum circuitry. As the final remarks, the phononic crystal design and methodology developed in this work are directly transferable to other layered crystals beyond h-BN, such as the semimetal graphene and semiconducting transition metal dichalcogenides (TMDCs) and their heterostructures. The van der Waals integration of 2D materials also grants the applicability to produce such phononic devices onto any additive nanofabrication-compatible substrates (rigid, curved, and flexible), thereby empowering versatile functionalities.

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