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Single phonon diode operating on a metagrating surface

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Asymmetric transmissions have a number of significant applications in a variety of fields, including communication and sensing systems. In this study, we present the numerical simulations of a single phonon diode model comprising a metagrating and a superlattice structure. By breaking the spatial inversion symmetry, the unidirectional transmission of a single phonon can be achieved in the proposed setup. This unidirectional phenomenon can be attributed to the occurrence of distinct mode transitions at two sides of the diode. Moreover, we demonstrate that the precise control of energy flow partition passing through the metagrating can be achieved by optimizing the metagrating parameters via machine learning, resulting in a significant contrast between the energy transmission in two directions, up to two orders of magnitude. The physical mechanisms to achieve enhanced rectification efficiency are discussed in detail. This work therefore paves a feasible pathway in designing functional phononic devices based on stylized metagrating structures.

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I. INTRODUCTION

Asymmetric transmission, whereby an incident wave exhibits a preferred direction of transmission, has attracted considerable interest due to its intricate physical principles and diverse potential applications [1–5]. Inspired by the rectification capabilities of electronic diodes, considerable efforts have been dedicated to achieving asymmetric transmission via various forms of energy fluxes, such as optical diodes [6,7], thermal diodes [8–12], and acoustic diodes [13,14]. Such unidirectional propagation typically requires breaking either time reversal symmetry or spatial inversion symmetry in the design [15,16]. Furthermore, extremely asymmetric transport can be achieved at exceptional points by introducing losses [17,18], or through unbalanced excitation of evanescent waves along the metasurface [19].

Phonons are quasiparticles in solids that exhibit both wave-like and particle-like characteristics [20,21]. The particle-like aspect can be understood through the incoherent scattering picture, extensively studied in diffusive transport theory and can be controlled by various scattering sources [22–24]. In recent years, the importance of wave-like or coherent phonons has been increasingly recognized [25–28]. Additionally, the wave-like nature of phonons impacts important applications in many fields such as material damage detection [29], phonon scanning probe microscopy [30], and phonon lasers [31], to name but a few. Notably, these studies predominantly focus on the wave-like nature of a single phonon mode at low temperature, where the phonon anharmonicity is suppressed in order to maintain the coherence. Such exploration on the single phonon wave property at low temperature is essential for advancing both fundamental physics and practical applications

in emerging quantum technologies, particularly in quantum computation [32–34], quantum sensing [35,36], and energy-efficient signal processing [37–39].

Here, we present a single phonon diode operation that makes use of the wave-like characteristic of phonons. Asymmetric phonon transmission is achieved by breaking spatial inversion symmetry through a combination of a metagrating and a superlattice structure. Furthermore, we demonstrate via numerical simulations that the efficiency of asymmetric phonon transport can be enhanced by optimizing the metagrating parameters through the use of the machine learning technique. Our work thus provides physical insights into the regulation and control of asymmetric lattice wave transport via metagrating structures.

II. MODEL AND METHODS

We start out by illustrating the working principle of our single phonon diode concept which is based on a heterostructure composed of a phononic metagrating and an integrated superlattice, as depicted in Fig. 1(a). The heterostructure is sandwiched between the incidence and transmission regions, which are set as the homogeneous background media. The metagrating is periodically arranged in the y direction, while the superlattice is periodically arranged in the x direction. The designed superlattice has a unique feature of anisotropic phonon dispersion as shown in Fig. S1(d) in the Supplemental Material [40]. It possesses a finite phononic band gap for the normal incidence along the $[1, 0, 0]$ (x) direction, while the same band gap is absent for the oblique incidence along the $[\cos \theta, \sin \theta, 0]$ direction. Therefore, for a phonon mode with frequency ω_0 inside the band gap that is incident normally to the superlattice from the right side, it undergoes a total reflection so that no phonon mode can be transmitted towards the left side.

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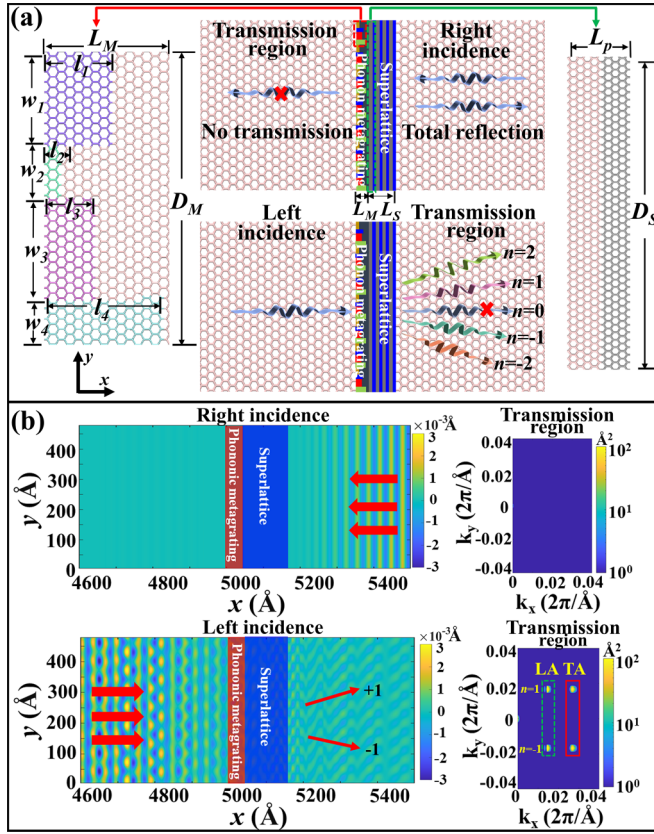


FIG. 1. (a) Working principle for a single phonon diode based on phononic metagrating and superlattice. The left and right sides show the unit cell of the metagrating and superlattice, respectively. (b) Simulated atomic displacement distribution u_y when the phonon is incident from the right side (top panel) or left side (bottom panel). The 2D FFT results for the corresponding transmission regions are displayed on the right side, with the sidebar color representing the amplitude of mode energy in the unit of $\text{\AA}^2$. The parameters here are set as $D_M = 24a_2$, $l_1 = 12a_2$, $l_2 = l_3 = l_4 = 0$, $w_1 = 6a_1$, $w_2 = w_3 = w_4 = 2a_1$, $m_1 = 20$ g/mol, and $m_2 = m_3 = m_4 = 12$ g/mol.

In contrast, when the same phonon mode is incident normally from the left side, the metagrating structure with a periodic width of D_M alters its propagation direction according to the generalized Snell's law [41]

$$k_0 \sin \theta_t = k_0 \sin \theta_i + G_n, \quad (1)$$

where k_0 is the incident wave vector, θ_i is the incident angle, θ_t is the transmission angle, $G_n = 2\pi n/D_M$ represents the reciprocal lattice vector, and n represents the diffraction order. Except for the zeroth-order diffraction mode, the rest of the diffraction modes are allowed to propagate across the superlattice structure, due to the absence of a band gap for oblique incidence, thereby leading to a nonvanishing phonon transmission towards the right side.

To validate the aforementioned single phonon diode model, we use single-layer graphene as the background medium, and construct the metagrating and superlattice structures based on carbon isotopes. We monitor the individual mode propagation via the phonon wave-packet simulations [42–44], with a spatial width of 249.2 $\text{\AA}$. The LAMMPS package [45] with

the optimized Tersoff potential [46] for graphene is used. Accordingly, the lattice constants for the conventional cell of graphene are set as $a_1 = 4.31$ $\text{\AA}$ and $a_2 = 2.49$ $\text{\AA}$. The time step is set as 0.5 fs, and periodic boundary conditions are applied in all directions, with a vacuum layer of 4 nm added in the thickness (z) direction. More details about wave-packet simulations can be found in Sec. S1 of the Supplemental Material [40].

The top panel of Fig. 1(a) depicts the unit cell for the metagrating (left) and superlattice (right), respectively. The unit cell for metagrating has the length L_M and periodic width D_M , and is constructed by four distinct carbon isotopes. Each segment i has length l_i , width w_i , and mass m_i .

Furthermore, the unit cell for the superlattice is formed by ^{12}C and ^{40}C , with a periodic length L_P and total width D_S . In this work, we fix the parameters of the superlattice as $L_P = 5a_1$, $L_S = 10L_P$, and $D_S = 192a_2$. This gives rise to a phononic band gap between 4.48 and 5.25 THz along the $[1, 0, 0]$ direction. For the metagrating, the length of metagrating is set as $L_M = 12a_1$, and the geometric parameters can be tuned within the size of the unit cell. The mass of the carbon isotopes varies from 1 to 50 g/mol.

III. RESULTS AND DISCUSSION

As a specific example, we examine the asymmetric phonon propagation by launching a transverse acoustic (TA) phonon with $\omega_0 = 4.77$ THz inside the band gap. For simplicity, we limit the highest diffraction order in metagrating only to the first order by setting $D_M = 24a_2$, which is above the fundamental limit of $2\pi/k_0$. The metagrating parameters are detailed in the caption of Fig. 1, which hereafter is referred to as the nonoptimized case. As shown in Fig. 1(b), a negligible transmission occurs for the right incident direction. However, when the same phonon is launched from the left side, a notable atomic displacement field emerges in the transmission region, where an obvious oblique transmission pattern is observed.

To obtain the mode distribution in the transmission region, the two-dimensional (2D) fast Fourier transform (FFT) of the atomic displacement in the transmission region is depicted in the right side of Fig. 1(b). No mode emerges in the transmission region when phonons are incident from the right side, while four discrete modes appear for the left incident direction. In addition to two TA modes (solid box), another two longitudinal acoustic (LA) modes (dashed box) also appear in the FFT result, due to the unique mode conversion phenomenon in the lattice system [41]. The number of diffraction orders and transmission angles aligns well with the prediction given by Eq. (1). It is worth noting that the zeroth-order TA mode does not appear in the transmission region because it remains within the band gap in the $[1, 0, 0]$ direction. We have verified that other phonon polarizations show similar results [40]. Furthermore, we have also demonstrated the validity of this single phonon diode in a three-dimensional system with realistic materials and mass (see Sec. S6 of the Supplemental Material [40] and Refs. [47,48] therein). Up to this point, the single phonon diode effect is clearly demonstrated both in real and reciprocal spaces.

In this nonoptimized case, the calculated energy transmission coefficients in the left and right incidence

directions are $T_L = 23.5\%$ and $T_R = 0.6\%$. Unlike plane waves, the phonon wave packet has a finite broadening, leading to the finite-size effect in the transmission coefficient [42]. As a result, T_R is not strictly vanishing due to the fixed superlattice size in our simulations, although the frequency of the launched phonon wave packet lies inside the band gap along the $[1, 0, 0]$ direction. Since T_R is already negligibly small ($<1\%$), we will next focus on how to improve the phononic diode efficiency by enhancing T_L . In this regard, we define the rectification coefficient R_c to further quantify the performance of the single phonon diode as

$$R_c = \frac{T_L}{T_R}. \quad (2)$$

A higher R_c value greater than 1 indicates a stronger asymmetric transmission. R_c reaches 39.1 in the nonoptimized case.

In the left incidence direction, phonons first engage with the phononic metagrating, where they are converted into a series of diffraction modes before reaching the superlattice part. To visually demonstrate the impact of the metagrating on T_L , we present the results of phonons passing through the phononic metagrating under the nonoptimized parameters in Sec. S3 of the Supplemental Material [40]. Since the zeroth-order mode (normal incidence) cannot propagate through the superlattice, the weight of the zeroth-order mode in the transmitted energy has a significant impact on T_L . For instance, the zeroth-order TA mode dominates the energy in the transmission region (more than 59%) in the nonoptimized case, as shown in Fig. S3(c) of the Supplemental Material [40].

The period width D_M of metagrating determines the number of diffraction modes and the transmission directions, while other metagrating parameters determine the energy distribution among different diffraction modes. By fine tuning the structural parameters of the metagrating, the energy distribution in the zeroth-order mode can be notably suppressed, which can significantly improve T_L . Meanwhile, T_R is almost independent on the structural parameters of the metagrating, as phonons incident from the right side are already blocked by the phononic superlattice. Therefore, optimizing the metagrating parameters while keeping superlattice parameters fixed is a feasible strategy to further improve the asymmetric transmission ratio.

Although the optimization strategy is clear in principle, lattice systems present key challenges. Unlike the hard boundary in acoustic systems, the atomic structure and interactions at the interface deviate significantly from the bulk medium, giving rise to unique interfacial phonon modes not present in the bulk spectrum [49,50]. In addition, the phononic metagrating subunits interact strongly with each other via covalent bonds and thus the nonlocal effect becomes significant. These factors make it difficult to analytically track the evolution of lattice waves as they pass through the engineered structure, highlighting the distinct nature of lattice systems compared to acoustic systems.

Machine learning techniques play a crucial role in the structural design and optimization of thermal transport properties [51]. Among a variety of machine learning methods [52–56], the tandem neural network [56] is used in this work to tackle the challenges of high-dimensional nature and the nonunique response-to-design mapping. As shown in

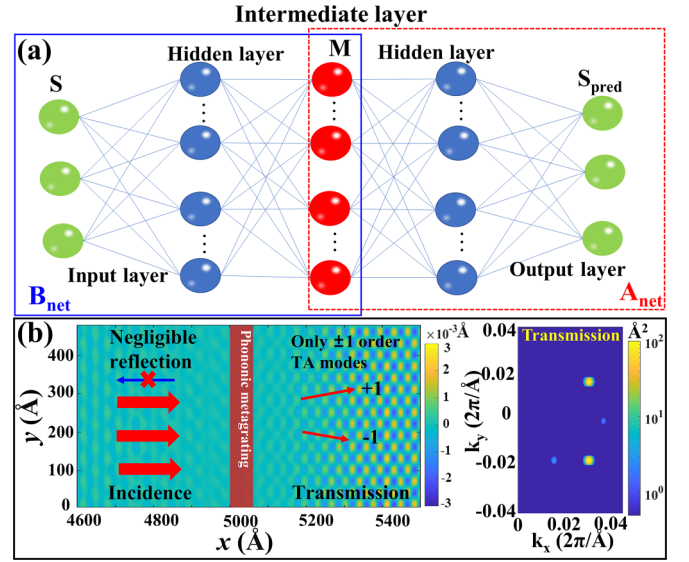


FIG. 2. (a) Schematic representation of the tandem network. This network is composed of a pretrained forward network A_{net} (in the red dotted box) and inverse network B_{net} (in the blue solid box). (b) Simulated atomic displacement in the y -direction mappings with the phonon incident from the left side with optimized metagrating parameters. Red arrows indicate the propagation directions. The sidebar color coding represents the amplitude of atomic displacement in the unit of $\text{\AA}$. The 2D FFT results for the corresponding transmission regions are displayed on the right side. The sidebar color coding represents the amplitude of mode energy in the unit of $\text{\AA}^2$.

Fig. 2(a), the tandem network model consists of two networks A_{net} and B_{net} , sharing the same intermediate layer $\mathbf{M}$. When using the tandem network for inverse design, a desired energy distribution among diffraction modes $\mathbf{S}$ is taken as the input. The intermediate layer $\mathbf{M}$ contains the designed structural parameters, and the output of the tandem network $\mathbf{S}_{\text{pred}}$ is the response predicted from the designed structure. This tandem network overcomes the nonunique issue through spectrum-to-spectrum training ($\mathbf{S}$ and $\mathbf{S}_{\text{pred}}$), and can further extract the desired structural parameters via the intermediate layer $\mathbf{M}$.

For simplicity, we fix the periodic width of metagrating as $D_M = 24a_2$ and redistribute the transmitted energy on the $\pm$ first-order TA modes to demonstrate the general strategy for enhancing T_L . We establish a dataset and introduce a vector $\mathbf{M} = [w_1, w_2, w_3, w_4, l_1, l_2, l_3, l_4, m_1, m_2, m_3, m_4]^T$ to describe the structural parameters of the metagrating. The transmitted energy distribution is expressed by the state vector $\mathbf{S} = [S_{\text{TA}}, S_{\text{LA}}, S_{\text{mix}}]^T$, where $S_{\text{TA}} = S_{\text{TA}}^{+1} + S_{\text{TA}}^{-1}$, $S_{\text{LA}} = S_{\text{LA}}^{+1} + S_{\text{LA}}^{-1}$, and $S_{\text{mix}} = S_{\text{TA}}^0 + S_{\text{LA}}^0$. The state vector component S_p^n of each transmitted diffraction mode is computed as

$$S_p^n = \frac{E_p^n}{E_t}, \quad (3)$$

where E_p^n represents the energy of the transmitted diffraction modes with polarization p and diffraction order n , and E_t represents the total energy of incident phonon.

The dataset for the metagrating consists of many arrays $\{\mathbf{M}, \mathbf{S}\}$, comprising 270 000 training samples and 30 000 test samples. We randomly generate various sets of $\mathbf{M}$ and calculate their corresponding $\mathbf{S}$ through molecular dynamics (MD)

simulations. Clearly, there is a correspondence between these two vectors, $\mathbf{S}_{\text{pred}} = A_{\text{net}}(\mathbf{M})$ and $\mathbf{M} = B_{\text{net}}(\mathbf{S})$, where A_{net} is the forward deep-learning network, and B_{net} is the inverse neural network. More details about machine learning technique can be found in Sec. S4 of the Supplemental Material [40] (see also Ref. [57] therein).

After the successful training of the tandem network model, the optimized metagrating structure can be predicted quickly and intelligently by the use of the inverse neural network. As an example, here we set the state vector as $\mathbf{S} = [1, 0, 0]^T$, indicating that the entire energy is concentrated on the transmitted $\pm$ first-order TA mode. Following this reverse prediction by the aforementioned neural network, we obtain the optimized structural parameters of metagrating as $\mathbf{M} = [2a_2, 4a_2, 2a_2, 16a_2, 1a_1, 8a_1, 5a_1, 1a_1, 33, 33, 23, 18]^T$, and then conduct molecular dynamics simulations using this set of optimized parameters. Figure 2(b) shows the atomic displacement distribution after the incident wave packet passes through the optimized metagrating, where negligible reflection is observed on the left side. Importantly, more than 96% of the transmission energy is concentrated on the $\pm$ first-order mode of the transmitted TA modes, while the other transmitted modes only account for a tiny fraction of the transmission energy (less than 4%) as shown in the right side of Fig. 2(b). These results confirm that the machine learning approach successfully achieves our targeted state vector $\mathbf{S} = [1, 0, 0]^T$, overcoming the challenges arising from the high complexity of both interfacial modes in atomic systems and strong nonlinear effects [41].

We then combine this optimized single phonon metagrating with the superlattice, and launch a phonon wave packet from the left side to test the overall performance. Figure 3(a) shows the atomic displacement distribution after the incident phonon passes through the optimized diode model. Compared to the nonoptimized case in the bottom panel of Fig. 1(b), the atomic displacement field in the transmission region is significantly higher for the optimized case, directly demonstrating the validity of our optimization strategy. Correspondingly, T_L for the optimized case reaches 58.97%, more than twice that for the nonoptimized case. As a result, the rectification coefficient R_c is 96.7 for the optimized case, which means a nearly two-orders-of-magnitude difference in two directions. In addition, the spatial width of the phonon wave packet has no impact on the rectification mechanism, but can affect the rectification coefficient (see Sec. S5 of the Supplemental Material [40]).

Next, we evaluate the frequency response of this optimized metagrating structure. Although we only launch a single-frequency ($\omega_0 = 4.77$ THz) phonon to train the machine learning model, the transmission coefficients of the phonons passing through the metagrating remain very high for various frequencies within the band gap [circles in the gray region of Fig. 3(b)]. However, the transmission coefficient T_L drops with increasing frequency after passing through the superlattice, due to the angle-dependent transmission coefficient in superlattices associated with different frequencies. Despite this variation, the rectification coefficient R_c is still above 15 within the band gap for this optimized design.

In this study, we utilize a simplified model to illustrate the operational principle of a phonon diode and its accompa-

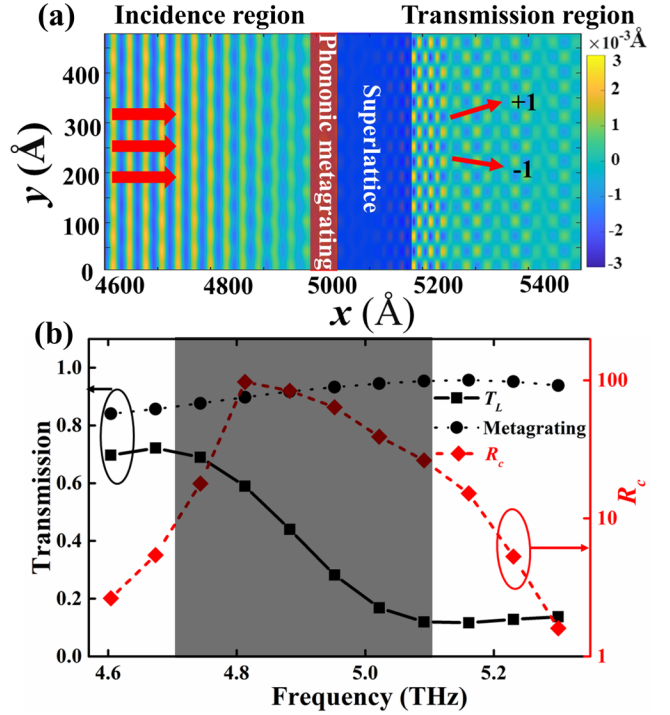


FIG. 3. (a) Simulated atomic displacement in the y -direction mappings with the phonons incident from the left side using the optimized metagrating. The atomic displacement field in the transmission region is significantly higher than that of the nonoptimized structure shown in the bottom panel of Fig. 1(c). (b) The left axis shows the transmission of the optimized metagrating (circles) and the combined diode structure (squares), and the right axis shows the corresponding rectification coefficient (diamonds). The gray area represents the band-gap region of the superlattice.

nying optimization strategy, yet further improvements to the diode performance may be achieved by enhancing the model complexity. Firstly, the utilization of additional training data encompassing different frequencies within the band gap can facilitate the attainment of a broadband response. Second, the period width of the metagrating D_M can be adjusted to generate additional higher-order diffraction modes, thereby creating additional pathways for the redistribution of transmitted energy across the superlattice. Finally, both the metagrating and superlattice can be trained and optimized collectively as a single entity within the machine learning model, which may overcome the decline in T_L observed in Fig. 3(b), although this approach introduces a considerable degree of complexity.

IV. CONCLUSION

In conclusion, we have put forth a theoretical setup of a single phonon diode comprising a metagrating and superlattice, and have subsequently demonstrated its functionality via a thorough numerical analysis. By breaking the spatial inversion symmetry, it is evident that unidirectional transmission of individual phonons occurs. Furthermore, it is demonstrated that the energy flow pattern transmitted through the phonon diode can be precisely regulated by optimizing the parameters of the phononic metagrating via an integrated reverse machine learning algorithm. This optimization strategy has the potential to

significantly enhance the rectification ratio, achieving a nearly two-orders-of-magnitude difference in two directions. In comparison to previous acoustic and optical diode models that employ nonlinearities or losses, our phononic diode model operates entirely linearly and additionally is independent of mode polarization. This offers advantages such as broadband operation, high conversion efficiency, and significantly lower power consumption. Since the manipulation of a coherent phonon wave packet is already accessible in experiment [58], this work offers an intriguing perspective on the manipulation of phonon transport through the modulation of coherent wave properties, thereby paving the way for the development of cutting-edge phononic devices.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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