Inverse design of a topological phononic beam with interface modes

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Abstract

Inspired by the idea of topological mechanics and geometric phase, the topological phononic beam governed by topological invariants has seen growing research interest due to generation of a topologically protected interface state that can be characterized by geometric Zak phase. The interface mode has maximum amount of wave energy concentration at the interface of topologically variant beams with minimal losses and decaying wave energy fields away from it. The present study has developed a deep learning based autoencoder (AE) to inversely design topological phononic beam with invariants. By applying the transfer matrix method, a rigorous analytical model is developed to solve the wave dispersion relation for longitudinal and bending elastic waves. By determining the phase of the reflected wave, the geometric Zak phase is determined. The developed analytical models are used for input data generation to train the AE. Upon successful training, the network prediction is validated by finite element numerical simulations and experimental test on the manufactured prototype. The developed AE successfully predicts the interface modes for the combination of topologically variant phononic beams. The study findings may provide a new perspective for the inverse design of metamaterial beam and plate structures in solid and computational mechanics. The work is a step towards deep learning networks suitable for the inverse design of phononic crystals and metamaterials enabling design optimization and performance enhancements.

Keywords: phononic crystals, metamaterials, deep learning, autoencoder, interface mode

(Some figures may appear in colour only in the online journal)

1. Introduction

Topological physics and mechanics inspired phononic crystals (PnCs) and acoustic metamaterials (AMs) have observed a surge of research studies in unusual control of acoustic and elastic waves. Interface states that are related to topological phase inversion [1] of trivial and non-trivial phases provide robust, lossless, immune to backscattering and sharp edges wave transportation at the interface of topologically distinct PnC and AM [2–5]. Such interface mode provides potential avenues for wave control including wave energy focusing/harvesting [6], vibration and noise control [7, 8], topological insulators [9, 10], higher order corner states/modes [11, 12], and design of other acoustic devices. For a one-dimensional (1D) periodic system, such an interface mode is initially reported in condensed matter physics using Su–Schrieffer–Heeger model [13, 14]. The interface state is observed inside the bandgap (BG) of topologically protected PnC. Later, multiple other studies have reported the interface state generation mechanism, role of geometric phases in the bounding BG edges and procedure to achieve interface modes
in 1D [3, 5, 15], two-dimensional (2D) [16–18] and three-
dimensional [19] periodic structures for both air-born acoustic
and solid-born elastic waves.

While discussing topological mechanics and its application
in PnCs and AM, one cannot negate the importance of topo-
logical/geometric phases [20]. The idea of geometric phase,
also refereed as Pancharatnam–Berry phase is first proposed
by Pancharatnam in 1956 for investigating light propagation
through a series of polarizer. Then this idea is employed by
Berry in 1984 for quantum mechanics [21]. Further details can
be found in a recently reported review articles [20, 22–24].
Chern number is used to characterize the topological invari-
ants for 2D system that is identical to Berry phase enclosing
the first Brillouin zone [24–26]. For a 1D system, Zak
phase (a special type of Berry phase defined along a 1D
bulk band) is employed to determine the topological invari-
ants. In such a system, the presence of nontrivial Zak phase
indicates the birth of interface or edge states. Therefore,
in modern physics topological invariants has a vital role in the
discovery of materials. As described in the prior works [2, 26],
the Zak phase explains the global characteristics of wave
functions throughout a whole band of a 1D system and is
unaffected by local disturbances and disorders, preserving
the system’s symmetry. Ma et al [24] applied this concept
from condensed matter physics to acoustic and mechanical
systems. Hence in the context of topology, Zak phase has a
prime importance in identifying the interface states. The
interface state is generated when the mode transition fre-
quency is common between the trivial and nontrivial phases
bounding the BG edges with symmetric and antisymmetric
eigenmode polarization [2, 15].

In general, the complex structural geometry and wave
responses play a substantial role in the elastic topological
states. The works about topological PnC to date reported are
mostly based on a forward-design approach where first we
precisely define the geometric parameters and subsequently
obtain the wave response such as wave dispersion/frequency
response. In this process, a set of geometric entities are sup-
plied and wave response is calculated based on trial and error
method. Depending upon the complexity of the model, this
approach is computationally expensive and time demanding.
In contrast, an inverse design mechanism can achieve design
parameters from target topological response/wave dispersion
property. An example is recently reported by Li et al [27]
where machine learning (ML) and deep learning (DL) data-
driven methods are employed to inversely design PnC unit
cell structures from a large set of generated database based
on random geometries. Recently, these data-driven approaches
have found a surge of research interest in the field of PnC
and AM due to the fact that metamaterial structural features
determine the wave performance rather than material com-
position and/or chemistry [28]. If one maps the data pattern
between metamaterial geometric features with wave proper-
ties like acoustic/mechanical frequency responses, then by for-
ward and inverse design processes, optimized PnC and AM
can be obtained. Prior to applying it for the complex PnC struc-
tures that would be promising for real-life applications, this
work begins with a simple structure namely a beam model that
has simple and accurate analytical solutions.

Therefore, in this study we develop ML and DL data-driven
models to inversely design a topological phononic beam to
accurately predict topological interface states via both forward
and inverse design approaches. The analytical modelling and
PnC design strategy is based on results reported in Muhammad
et al [2]. Here we extend this study by introducing ML and
DL based forward and inverse design approaches to effectively
design phononic beam with interface states. The transfer ma-
trix method (TMM) is employed to derive the constitutive wave
dispersion relation for longitudinal elastic wave. We employed
Euler–Bernoulli beam theorem with modified TMM to obtain
the dispersion relation for bending elastic waves. These con-
stitutive analytical equations are used to generate a large data-
base for network training. The choice of network is very much
dependent on the input data and desirable output. In this study,
an auto-encoder is developed to optimize the phononic elastic
beam. Here we transform the band structure data from fre-
quency spectrum to binary digits 0, 1 and −1 where 0 shows
passbands and 1 and −1 correspond to BG with different wave
energy polarization determined by analytical calculation of
Zak phase [26, 29]. First by forward design process, for a
set of geometric parameters, the band structure is obtained.
Here we designate the geometric entities with shape function
δ = (2Lb − La) / L where L is length of beam and subscript
shows beam A, B. Then by inverse design process, δ is pre-
dicted for the required topological beam band structure gov-
erning interface states. These network generated results are
validated by FEA based COMSOL Multiphysics and experi-
ment testing on predicted δ values. Overall, an excellent agree-
ment is observed.

The paper is organized as follows. Section 2 briefly explain
the modelling strategy and procedure for deriving the con-
stitutive dispersion relation. The ML and DL network archi-
tecture are explained in section 3. The results are discussed in
section 4. Finally, the conclusion and future prospect of the
developed network for metamaterial research are discussed in
section 5.

2. Modelling strategy and governing equations

In this section the TMM and modified TMM for deriving
the constitutive relation for longitudinal and bending elastic
waves, respectively are briefly discussed. For more details,
one can refer to Muhammad et al [2]. The schematic diagram
of 1D phononic beam is shown in figure 1. The lattice con-
stant of the periodic beam is a = L = 100 mm. The unit cell
of the periodic lattice consists of two topologically distinct
beams with varying length and diameter. The beam B with
length Lb and diameter Db = 8 mm is sandwiching beam A
of length La and diameter dA = 4 mm. The topology of beam
is varied by introducing a shape parameter δ = (2Lb + La) / L.
We consider aluminium rod with young modulus E = 70GPa,
mass density ρ = 2700kg m−3 and Poisson ratio ν = 0.33 for
analytical and numerical modelling, see table 1. Later for
experiment, stainless steel with young modulus $E = 210 \text{ GPa}$, mass density $\rho = 7850 \text{ kg m}^{-3}$ and Poisson ratio $\nu = 0.33$ is used. Such type of periodic beam supports both longitudinal and bending elastic waves. In such elastic medium, longitudinal and bending waves are present in the form of mixed waves that are coupled at the junction of phononic beams. As reported in Muhammad et al. [2, 15], bending eigenmodes are present at a lower frequency region compared to the longitudinal counterpart. In numerical codes, such eigenmodes are present in sequential order and need to be separated by post-processing steps [2, 15]. For beam $B$, the displacement and axial force correlation can be written as

$$u_B(x, t) = A_1 e^{i \omega x c} + A_2 e^{-i \omega x c}.$$  

Likewise, the constitutive equation for the axial force is

$$F(x, t) = ES \frac{\partial u}{\partial x}.$$  

where $F(x, t)$ and $S$ are the axial force and cross-section area of the beam. For beam $B$, the displacement and axial force correlation can be written as

$$
\begin{pmatrix}
    u_B \\
    F_B
\end{pmatrix} =
\begin{pmatrix}
    e^{i \omega x c} \\
    iES_B \frac{\omega}{c} e^{i \omega x c} - iES_B \frac{\omega}{c} e^{-i \omega x c}
\end{pmatrix}\begin{pmatrix}
    A_1 \\
    A_2
\end{pmatrix}.
\tag{4}
$$

According to TMM, the displacement and axial force at the left and right sides of beam $B$ becomes

$$
\begin{pmatrix}
    u_B(0) \\
    F_B(0)
\end{pmatrix} =
\begin{pmatrix}
    1 & 1 \\
    iES_B \frac{\omega}{c} & -iES_B \frac{\omega}{c}
\end{pmatrix}\begin{pmatrix}
    A_1 \\
    A_2
\end{pmatrix}.
\tag{5}
$$
\[
\begin{pmatrix}
  u_B(L_B) \\
  F_B(L_B)
\end{pmatrix} =
\begin{bmatrix}
  e^{i\frac{\omega L_B}{c_L}} & e^{-i\frac{\omega L_B}{c_L}} \\
  i\epsilon \omega B e^{i\frac{\omega L_B}{c_L}} & -i\epsilon \omega B e^{-i\frac{\omega L_B}{c_L}}
\end{bmatrix}
\begin{pmatrix}
  A_1 \\
  A_2
\end{pmatrix}.
\]

(6)

Here \( A_1 \) and \( A_2 \) are unknown displacement fields representing the eigenmodes. From equations (5) and (6), transfer matrix can be expressed as

\[
\begin{pmatrix}
  u_B(L_B) \\
  F_B(L_B)
\end{pmatrix} = T_B\begin{pmatrix}
  u_B(0) \\
  F_B(0)
\end{pmatrix}.
\]

(7)

Likewise, applying the above procedure for beam \( A \), the transfer matrix becomes

\[
\begin{pmatrix}
  u_A(L_A) \\
  F_A(L_A)
\end{pmatrix} = T_A\begin{pmatrix}
  u_A(0) \\
  F_A(0)
\end{pmatrix}.
\]

(8)

See appendix for expression of \( T_A \) and \( T_B \). The boundary condition considered between two sub-beams is

\[
\begin{pmatrix}
  u_A(0) \\
  F_A(0)
\end{pmatrix} = \begin{pmatrix}
  u_B(0) \\
  F_B(0)
\end{pmatrix}.
\]

(9)

Combining equations (7)–(9) leads to

\[
\begin{pmatrix}
  u_A(L_A) \\
  F_A(L_A)
\end{pmatrix} = T\begin{pmatrix}
  u_A(0) \\
  F_A(0)
\end{pmatrix}.
\]

(10)

In order to make the proposed unit cell structure infinitely periodic, Floquet–Bloch condition is applied on equation (10)

\[
\begin{pmatrix}
  u_A(L_A) \\
  F_A(L_A)
\end{pmatrix} = T\begin{pmatrix}
  u_A(0) \\
  F_A(0)
\end{pmatrix} = e^{i\beta L} \begin{pmatrix}
  u_A(0) \\
  F_A(0)
\end{pmatrix}.
\]

(11)

Further simplification of equation (11) gives

\[|T - e^{i\beta L}| = 0\]

(12)

where \( k \) is Bloch wavenumber in 1D system and \( I \) is a \( 2 \times 2 \) identity matrix. The solution of equation (12) gives the constitutive dispersion relation as [2]

\[
\cos(kL) = \cos\left(\frac{2\omega L_B}{c_L}\right) \cos\left(\frac{\omega L_A}{c_L}\right)
- \frac{1}{2} \left(\frac{S_A}{S_B} + \frac{S_B}{S_A}\right) \sin\left(\frac{2\omega L_B}{c_L}\right) \sin\left(\frac{\omega L_A}{c_L}\right).
\]

(13)

Equation (13) is so-called dispersion relation for longitudinal wave where for each \( \omega \), wavenumber \( k \) can be easily calculated. We used equation (13) to develop database for longitudinal wave.

#### 2.2. Analytical solution for bending elastic wave

According to Euler–Bernoulli beam theory, the governing equation of motion for bending elastic wave can be expressed as [2]

\[EI_x \frac{\partial^2 w(x,t)}{\partial x^4} + \rho S \frac{\partial^2 w(x,t)}{\partial t^2} = 0\]

(14)

where \( w(x,t) \) is lateral displacement, \( EI_x, \rho \) and \( S \) are bending rigidity, mass density and the cross-sectional area of beam, respectively.

For harmonic solution of the form \( w(x,t) = w(x)e^{i\omega t} \), the expression for out-of-plane displacement filed can be written as

\[w(x) = AP(kx) + BQ(kx) + CR(kx) + DS(kx)\]

(15)

where \( k = \rho \omega^2 / EI \) is wavenumber for the flexural waves and \( A, B, C, \) and \( D \) are unknown parameters. The expression for angular rotation, shear force and bending moment are \( \varphi(x) = w'(x), V(x) = -Ew''''(x), M(x) = -Ew'''(x) \) respectively where \( w'(x), w''(x) \) and \( w'''(x) \) are the first order, second order and third order derivatives of \( w(x) \) with respect to \( x \). The expression for \( P, Q, R, S \) are the combination of hyperbolic and triangular functions

\[
P(kx) = 0.5[\cosh(kx) + \cos(kx)]
\]

\[
Q(kx) = 0.5[\sinh(kx) + \sin(kx)]
\]

\[
R(kx) = 0.5[\cos(kx) - \cos(kx)]
\]

\[
S(kx) = 0.5[\sin(kx) - \sin(kx)]
\]

(16)

The equation (16) also satisfy following conditions

\[
P'(kx) = kS(kx), P'''(kx) = k^2R(kx), P''''(kx) = k^3Q(kx)
\]

\[
Q'(kx) = kP(kx), Q''(kx) = k^2S(kx), Q''''(kx) = k^3R(kx)
\]

\[
R'(kx) = kQ(kx), R''(kx) = k^2P(kx), R''''(kx) = k^3S(kx)
\]

\[
S'(kx) = kR(kx), S''(kx) = k^2Q(kx), S''''(kx) = k^3P(kx)
\]

(17)

The first, second and third derivatives of \( w(x) \) with respect to \( x \) are

\[
w'(x) = k[AQ(kx) + BR(kx) + CS(kx) + DP(kx)]
\]

\[
w''(x) = k^2[AR(kx) + BS(kx) + CP(kx) + DQ(kx)]
\]

\[
w'''(x) = k^3[AQ(kx) + BR(kx) + CS(kx) + DP(kx)]
\]

(18)

That leads to

\[
w(0) = A, w'(0) = kB, w''(0) = k^2C, w'''(0) = k^3D
\]

(19)

where

\[A = w(0), B = \frac{w'(0)}{k}, C = \frac{w''(0)}{k^2}, D = \frac{w'''(0)}{k^3}.
\]

(20)

Now the unknown parameters \( A, B, C, D \) are in the form of displacement \( w(x) \), angular rotation \( \varphi(x) \), bending moment
$M(x)$ and shear force $V(x)$. The expressions at $x = 0$ are denoted by $w_0$, $\varphi_0$, $M_0$ and $V_0$ that can be expressed as

$$
\begin{bmatrix}
w(x) \\
\varphi(x) \\
M(x) \\
V(x)
\end{bmatrix} =
\begin{bmatrix}
T_{11} & T_{12} & T_{13} & T_{14} \\
T_{21} & T_{22} & T_{23} & T_{24} \\
T_{31} & T_{32} & T_{33} & T_{34} \\
T_{41} & T_{42} & T_{43} & T_{44}
\end{bmatrix}
\begin{bmatrix}
w(0) \\
\varphi(0) \\
M(0) \\
V(0)
\end{bmatrix}.
$$

(21)

Hereafter all the parameters are presented in dimensionless formats. This is required for development of input database. The normalized parameters introduced are

$$
\hat{x} = x/L, \hat{w} = w/L, \hat{\varphi} = \varphi/L, \hat{S} = S/L^2, \hat{\omega} = \omega L \sqrt{\rho A/E_A}, \hat{\rho} = \rho/\rho_A, \hat{I}_L = I_L/L^4, \hat{M} = M/(E_A L^3), \hat{V} = V/(E_A L^2).
$$

(22)

Further modification of equation (21) gives

$$
A(\hat{x}) = \begin{bmatrix} \hat{w}(\hat{x}) & \hat{\varphi}(\hat{x}) & \hat{M}(\hat{x}) & \hat{V}(\hat{x}) \end{bmatrix}^T
$$

and

$$
T_j(\hat{x})^j =
\begin{bmatrix}
T_{11}^j & T_{12}^j & T_{13}^j & T_{14}^j \\
T_{21}^j & T_{22}^j & T_{23}^j & T_{24}^j \\
T_{31}^j & T_{32}^j & T_{33}^j & T_{34}^j \\
T_{41}^j & T_{42}^j & T_{43}^j & T_{44}^j
\end{bmatrix}
$$

(23)

j = 1, 2, ..., n.

Further simplification leads to $q = -\ln (e^{\pi x^2})$ and

$$
p = \frac{1}{L} \arctan \frac{y}{x}, x > 0
$$

$$
p = \frac{1}{L} \left( \pi + \arctan \frac{y}{x} \right), x < 0, y > 0
$$

$$
p = \frac{1}{L} \left( -\pi + \arctan \frac{y}{x} \right), x < 0, y < 0
$$

(24)

over the Brillouin zone $[\pi a, -\pi a]$ where $a = L$ is the lattice constant. By solving the equation (31) based on the conditions defined in equations (22)–(23), the wavenumber is determined for specified frequency range.

2.3. Zak phase

The detailed description and signification of Zak phase is beyond the scope of this work. More details can be found in [26, 29]. Xiao et al. [26] extended the concept of Zak phase to acoustics. For nth Bloch band, the Zak phase can be expressed as

$$
\theta_{n,k}^{\text{Zak}} = \int_{-\pi/a}^{\pi/a} \int_{\text{Unicell}} \frac{1}{2\rho c^2} d\xi_k n(x) \partial \xi_k n(x) dk
$$

(34)

where $\xi_k n(x)$ is the Bloch eigenfunction of a periodic structure for a specified wavenumber $k$. $1/(2\rho c^2)$ is a factor for the weight function of elastic medium. In the nth band of the longitudinal and bending waves, the Bloch eigenfunction is [26]

$$
U_{n,k}(x) \text{ or } W_{n,k}(x) = \xi_{n,k}(x) e^{ikx}
$$

(35)

where $U_{n,k}(x)$ and $W_{n,k}(x)$ denote the longitudinal and bending wave fields, respectively. In this study, the reflection phase
of the associated two BGs is determined to calculate the Zak phase
\[
\text{sgn}(\psi_{n-1}) / \text{sgn}(\psi_n) = -e^{i\theta_n^{2\pi}} \text{ with } \delta \text{Zak} = 0 \text{ or } \pi. \quad (36)
\]

Where \( \psi \in (-\pi, \pi) \) is reflection phase of the \( n \)th BG and it satisfies \( \text{Sgn}[\psi] = -1 \) correspond to \( \psi_n \in (-\pi, 0) \), \( \text{Sgn}[\psi] = 1 \) is associated to \( \psi_n \in (0, \pi) \). Hence, the determined value of Zak phase can be either 0 or \( \pi \). In this study, the unknown displacement fields that represent eigenmodes are determined from equations (4) and (20) for longitudinal and bending Bloch bands respectively. Such information is passed to ML network as binary digits 0, 1 and \(-1\). Further details are given in the preceding sections.

2.4. Numerical modelling

The role of numerical modelling is limited to validation of the network findings. We employed COMSOL Multiphysics finite element codes to confirm the presence of interface states from network predicted \( \delta \) values. The comparison of numerical results with TMM is available in Muhammad et al [2]. The supercell array of topologically predicted \( \delta \) is built inside COMSOL Multiphysics, solid mechanics physics module and by performing frequency response study, the interface state is highlighted. COMSOL built-in fine tetrahedral mesh is applied to obtain the solution.

3. Autoencoder (AE) network architecture

A brief explanation on ML and DL network architecture developed in this study is provided. We developed an AE to train and predict the topological properties of phononic beam. An AE is a data compression neural network comprised of two parts i.e. encoder and decoder. The encoder compresses input data into a low-dimensional representation, termed as the bottleneck. Later, the decoder network reconstructs the original input data from the bottleneck, see figure 2. Generally, encoder and decoder networks are symmetrical. However, this is not necessary and they can be asymmetrical. In either case, the dimension of input layer and output layer are identical. Mathematically, the input \( x \in \mathbb{R}^n \) is multiplied by the weight matrix \( W \) and summed with a bias \( b \) to obtain the output of the fully connected layer as
\[
a^i = f^i(W^i x + b). \quad (37)
\]

Where the superscript \( i \) refers to \( i \)th layer of AE and \( f^i \) is the activation function. Here in this study we have used ReLU activation function, see table 2. The output \( a^i \) from the \( i \)th hidden layer is used as input for \((i+1)\)th hidden layer and this process is continued until the last hidden layer of network to reconstruct the input data at the decoder output. The encoder maps the data from input space to latent space i.e. bottleneck layer \( h \) as
\[
h = \Gamma(x). \quad (38)
\]

While in an inverse process \( \Gamma^{-1} \), the decoder maps the bottleneck back to the input space, see figure 2

The AE is trained in a self-supervised mode, where the network learns to reconstruct its input. The difference between actual input and reconstructed input at the decoder output layer is used to quantify the loss function. This loss function is minimized in order to improve the network performance. Network training is achieved by back-propagating sensitivities (gradient of a loss function with respect to the network parameters) from the output layer of decoder to the input layer of encoder, and subsequently updating the network parameters. Mathematically, the loss function can be defined as
\[
L = \frac{1}{2m} \sum_{i=1}^{m} \left\| x_i - \hat{x}_i \right\|_2^2 \quad (40)
\]

where \( \| . \|_2 \) denotes \( L^2 \) norm and \( m \) is number of training examples. Therefore, the job of encoder \( \Gamma(x) \) is to extract relevant features from a high dimensional input space to a low dimensional latent space. While the decoder \( \Gamma^{-1}(h) \) reconstruct the corresponding input from the feature vector \( h \).

The input data is generated through analytical formulations based on TMM to train and test the AE, see schematic workflow in figure 1. The topology of a beam is linked with shape parameter \(-1 \leq \delta \leq 1\). The \( \delta \) is swept with a step size of 0.005 to generate thousands of data samples. Initially, the generated band structure data is in the form of normalized frequency \( \bar{\omega} \) and wavenumber \( k \). To distinguish the Zak phase for each Bloch band, the band structure is converted into binary digits 0, 1 and \(-1\) where 0 shows passband and 1 and \(-1\) are associated to symmetric and anti-symmetric Bloch bands. The binary digit band structure data is arranged as label vector \( \alpha \) with dimension 200 \times 1 (longitudinal wave) and 500 \times 1 (bending wave). The network training is performed in two steps: first the encoder is trained to map \( \alpha \) to the bottleneck layer which approximates shape parameter \( \delta \). Second, the decoder which is connected to the encoder is trained, while the encoder is frozen and runs in inference mode.

The number of neurons in the input and output layers are same as the dimension of \( \alpha \). The input database is split into
two parts where 80% of data is allocated for network training and 20% data for network performance testing. The network hyperparameters including number of layers, layer size, learning rate, training algorithm etc have been fixed by heuristics and trial and error approaches and is listed in table 2. The hyperparameter optimization is outside the scope of this study. The Python codes utilized in this study will be available in the open access repository after publication.

4. Results and discussions

This section will discuss the results obtained from AE in two parts, separately for longitudinal and bending elastic waves. A brief summary of network performance in the form of $R^2$ and mean square error (MSE) are given in table 3. Overall, excellent agreement is observed that indicate AE is learning well the co-relation between band structure and phononic beam topology defined by $\delta$.

First, we will discuss the training and testing of AE for correctly mapping the band structure and $\delta$ values for longitudinal wave propagating in the phononic beam. Later, same approach is adopted for bending elastic wave. To train the network, TMM and modified TMM based analytical dispersion relation is formulated, see sections 2.1 and 2.2. Using in-house MATLAB code, the $\delta$ is swept from $-1$ to $1$ with step size of 0.005 and associated band structures are obtained. The band structure is in the form of $\omega$ and $k$. By using the analytical formulation based on reflection phase of Bloch band, the geometric Zak phase is identified. Since proposed phononic beam is symmetric with respect to central cross-section plane, therefore the Zak phase can have either 0 or $\pi$ values depending upon symmetry of eigenmodes, see section 2.3. The band structure and Zak phase information is passed to AE input layer in the form of binary digits 0, 1 and $-1$ via label vector $\alpha$. The number of neurons in the input layer is same as dimension of $\alpha$. Figures 3 and 4 show some examples where normalized band structure is transformed into binary digit band structure with distinct geometric phase as 1 (Zak phase is 0 i.e. symmetric) and $-1$ (Zak phase is $\pi$ i.e. anti-symmetric) for longitudinal and bending elastic waves propagating in the phononic beams.

The geometric Zak phase provides useful information about the presence of topologically protected interface states. The interface state is generated when mode transition frequency observed from Dirac cone degeneracy, see Muhammad et al [2] for details, is common in the BG of topologically distinct phononic beams. In order to teach the algorithm about this concept, the Zak phase is presented in the form of 1 and $-1$. Otherwise from normalized band structure obtained from TMM, it is very difficult to distinguish the geometric phase of Bloch bands. The distinction is only possible through theoretical, numerical and experimental [26] means where symmetry type/reflection phase of Bloch band is investigated.

We generated approximately 4000 data samples for longitudinal and bending elastic wave separately to train and test the AE. The AE is developed and networking training and testing performance is quantified by calculating the $R^2$ and MSE. Figure 5 shows the learning curve for encoder and decoder for both types of waves. We have used 2500 epochs for longitudinal wave and 5000 epochs for bending wave. Excellent agreement is observed between training and test data. These curves validate that the AE is learning the correlation between binary band structures and $\delta$ values.

After AE training and testing, the network is assigned the task for making predictions. The prediction is made for $\delta$ values and this newly predicted results were compared with ground truth i.e. $\delta$ values swept in the analytical model to obtain normalized band structures. The predicted and target $\delta$ values comparison is performed for both longitudinal and bending waves as shown in figure 6. To aid understanding, the error histogram is also shown and one can observe with increase in instances, the error tends to move towards zero.

Next, we asked the network for combination of $\delta$ values that has mode transition frequency common in their BGs to predict the interface states. For both longitudinal and bending elastic waves, interestingly the network does output some possible combinations. The obtained $\delta$ values are passed to COMSOL Multiphysics and a supercell phononic beam is constructed. In total 10 unit cell structures with distinct topology are considered to perform the frequency response study. For longitudinal wave, the harmonic excitation is applied at the left

| Table 2. Network specification. |
|---------------------------------|
| **Autoencoder**                |
| **Longitudinal wave**          |
| Architecture                   |
| 200-16-8-4-1-4-8-16-32-64-128-|
| 256-512-200                    |
| Batch size                     |
| 128                            |
| Learning rate                  |
| 0.0001                         |
| Epoch                          |
| 2000                           |
| Hidden activation function     |
| ReLU                           |
| Training algorithm             |
| Adam                           |

| **Bending wave**               |
| 500-16-8-4-1-4-8-16-32-64-128-|
| 128-256-512-500                 |
| 128                            |
| 0.0001                         |
| 5000                           |
| ReLU                           |
| Adam                           |

| Table 3. Training and testing networks performance. |
|---------------------------------------------------|
| **Longitudinal wave**                            |
| **Training**                                      |
| $R^2$                                             |
| 0.9936                                           |
| MSE                                               |
| $2.2 \times 10^{-3}$                             |

| **Bending wave**                                 |
| **Training**                                     |
| $R^2$                                             |
| 0.9992                                           |
| MSE                                               |
| $2.7 \times 10^{-4}$                             |
Figure 3. Normalized and transformed band structures for longitudinal wave with varying δ values. (a), (b) $\delta = -0.2$ (c), (d) $\delta = 0.2$ (e), (f) $\delta = 0$ and (g), (h) $\delta = 0.6$. The transformed band structure plots are presented in the form of target (before AE training) and prediction (after AE training). The distinct geometric Zak phase is presented as 1 and $-1$. 
Figure 4. Normalized and transformed Band structures for bending wave with varying $\delta$ values. (a), (b) $\delta = 0.5$ (c), (d) $\delta = 0.7$ (e), (f) $\delta = 0.2$ and (g), (h) $\delta = 0$. The transformed band structure plots are presented in the form of target (before AE training) and prediction (after AE training). The distinct geometric Zak phase is presented as 1 and $-1$. 
Figure 5. AE learning curve for (a) longitudinal wave (b) bending wave. In total, 2500 and 5000 epochs are used for training and testing of longitudinal wave and bending wave, respectively. The MSE is shown on log-scale and excellent agreement between training and testing data samples can be observed.

end along the in-plane direction of the supercell array i.e. x-direction, see figure 1. The boundary probe is used to record the output displacement field at the right end. As reported in previous studies [2, 5, 26], at the topologically protected interface mode frequency, a sharp transmission peak is observed inside the BG. We observed sharp transmission peak designating topologically protected interface mode frequency inside the BG for predicted combination of $\delta$ values, see figure 7. The displacement field plots corresponding to these frequencies are also shown. In these plots, one can observe the localization of wave energy at the interface and decaying energy fields away from it.

Likewise, the supercell array consisting of 10 unit cell structures are constructed to validate the presence of topologically protected interface mode frequency in the phononic beams upon bending wave excitation. The harmonic out-of-plane excitation along z-direction (see figure 1) is applied at the left end and response in the form of out-of-plane displacement is recorded at the right end of the supercell array. For predicted $\delta$ values, interface state with sharp transmission peak inside the common BG of topologically distinct beam is observed as shown in figure 8. The displacement field plots depicted also show concentration of wave energy at the interface with decaying energy fields away from it. This validates the AE performance for correctly predicting the $\delta$ values that governs topologically protected interface states.

To further corroborate AE findings, we converted a 1 m-long steel rod into topologically protected phononic beam with $\delta_1 = 0.4$ and $\delta_2 = 0.85$. We choose steel for the experiment as the mechanical behaviour is closer to linear elasticity and the material strength also allows the manufacture of the prototype in a single piece. Further, steel produces a better signal to noise ratio and a smooth wave transmission spectrum can be observed. In addition, since the results are presented in the normalized frequency, the choice of aluminium or steel should not make much difference for predicted behaviour of interface modes. The length of each beam are as follows: $L_{A1} = 30$ mm, $L_{B1} = 35$ mm, $L_{A2} = 7.5$ mm, $L_{B2} = 46.25$ mm. The diameter of beam is: $d_A = 4$ mm, $D_B = 8$ mm. The on-site and schematic diagram of experiment setup is shown in figure 9. The out of plane excitation is induced by white noise with frequency range (50–20 000 Hz) using PCB High Frequency Shaker Model 2025E-HF. The shaker is controlled by amplifier (PCB 2100E21-100 Smart Amplifier). The input signal is recorded.
Figure 6. AE target and prediction curves with error histograms for (a), (b) longitudinal wave (c), (d) bending wave. The target is actual data obtained from analytical model and AE correctly predict the ground truth data.

Figure 7. Longitudinal wave frequency response spectrum with topologically protected interface states (highlighted in green) for predicted combination of $\delta$ values. (a) $\delta_1 = 0.2, \delta_2 = -0.2$ (b) $\delta_1 = -0.6, \delta_2 = 0.6$ (c) $\delta_1 = 0, \delta_2 = -0.6$ and (d) $\delta_1 = 0.2, \delta_2 = 0.6$. The displacement field plot corresponding to these frequencies are also shown.
Figure 8. Bending wave frequency response spectrum with topologically protected interface states (highlighted in green) for predicted combination of $\delta$ values. (a) $\delta_1 = 0.5$, $\delta_2 = 0.7$ (b) $\delta_1 = 0.4$, $\delta_2 = 0.85$ (c) $\delta_1 = -0.2$, $\delta_2 = 0$ and (d) $\delta_1 = 0$, $\delta_2 = 0.2$. The displacement field plot corresponding to these frequencies are also shown.

Figure 9. Experiment setup (a) topological phononic beam connected with shaker and accelerometers (b) schematic diagram for developed experiment setup.
Figure 10. Experimental frequency response spectra for $\delta_1 = 0.4$ and $\delta_2 = 0.85$. The sharp wave transmission peaks are observed for interface mode frequencies as highlighted.

by accelerometers (PCB 352A60) in out-of-plane direction. The output signal is captured at the interface of topological beams by a Polytech PDV-100 laser vibrometer. The data is recorded and passed to the computer for post-processing using a NI-USB-4431 24 Bit Data Acquisition USB Module. We used compiled MATLAB programme to postprocess the recorded data.

The obtained experimental result is shown in figure 10. Since the selected beam configuration has two topologically protected interface modes, we observed sharp transmission peaks in response spectrum at 4764 Hz and 11 304 Hz that is indicative of topological protected interface modes. We also scan the beam with laser at multiple points to double check if the selected transmission peaks are interface modes. The obtained signals verify our prediction and selected transmission peaks around noisy signals are observed. This is reasonable and as you move away from the interface, the wave energy decay due to presence of BG. Further, we are not the first who performed an experimental test on topologically protected phononic beams. Prior studies [26, 32, 33] have also reported experimental results and for solid structures, the transmission signal is always noisy due to material anisotropy and the wide range of frequency spectrum considered. The contribution of the present study includes experimental test on phononic beam with topological properties predicted by a deep learning algorithm. Therefore, in terms of wave transmission peak that is an established approach to observe interface mode, the current numerical and experimental results show excellent agreement.

5. Conclusion

In summary, this work proposed the application of deep learning methods for the inverse design of topological phononic beams to predict topologically protected interface modes. To achieve this goal, a rigorous analytical model is established using the TMM for both longitudinal and bending elastic waves. The obtained constitutive equations are used to generate input data for deep learning network training and testing. In order to map a correlation between the beam geometry and band structure, the frequency spectrum data is converted into binary digits. The geometric Zak phase provide useful information about the band inversion and variances in symmetry of Bloch eigenmodes. Bloch bands with distinct Zak phase having mode transition frequency common in the BGs of topologically distinct phononic beams induce topologically protected interface modes, evident from the sharp transmission peak in frequency response spectrum. For the set of generated data, the Zak phase is analytically calculated by determining the reflection phase of Bloch eigenmode. The distinct Zak phase is differentiated as 1 (symmetric eigenmode) and $-1$ (anti-symmetric eigenmode) with reference to central cross-section plane of beam and this information is passed to the autoencoder. The network is trained based on generated data for both longitudinal and bending elastic waves. Upon successful training and testing, the interface mode prediction is made for combination of phononic beams. The network findings are validated by finite element based numerical simulations and experimental test on the manufactured topological beam. Overall, excellent agreement is observed. The study findings may provide a new insight into the application of deep learning methods in solid and computation mechanics for design and optimization of metamaterials based on beam and plate structures. Future studies will focus on applying a more holistic deep learning network for design optimization and performance enhancement of PhCs and metamaterials to control subwavelength acoustic and elastic waves.

Data availability statement

The data generated and/or analysed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request.
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Conflict of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Author contributions

Muhammad: Conceptualization; Data curation; Formal analysis; Funding acquisition; Investigation; Methodology; Project administration; Software; Validation; Visualization; Roles/Writing—original draft; Writing—review & editing. Oluwaseyi Ogun: Investigation; Data curation; Software. John Kennedy: Investigation; Validation; Funding acquisition; Project administration; Resources; Supervision; Writing—review & editing.

Appendix

The expression for transfer matrix for longitudinal and bending elastic waves are as follows

$$T_A = \begin{bmatrix} e^{\frac{-ja}{l}} & e^{-i\frac{aj}{l}} \\ iES_A e^{\frac{a}{l}} & -i\frac{a}{l} ES_A e^{-\frac{a}{l}} \end{bmatrix}$$

$$T_B = \begin{bmatrix} e^{\frac{-ja}{l}} & e^{-i\frac{aj}{l}} \\ iES_B e^{\frac{a}{l}} & -i\frac{a}{l} ES_B e^{-\frac{a}{l}} \end{bmatrix}^{-1}$$

$$T^{ij}_{11} = P\left(k_x L\right), \quad T^{ij}_{12} = \frac{1}{k_y} Q\left(k_x L\right),$$

$$T^{ij}_{13} = \frac{1}{E_j k_y} R\left(k_x L\right), \quad T^{ij}_{14} = \frac{1}{E_j k_y} S\left(k_x L\right),$$

$$T^{ij}_{21} = k_S \left(k_x L\right), \quad T^{ij}_{22} = P\left(k_x L\right),$$

$$T^{ij}_{23} = -\frac{1}{E_j k_y} Q\left(k_x L\right), \quad T^{ij}_{24} = -\frac{1}{E_j k_y} R\left(k_x L\right),$$

$$T^{ij}_{31} = -E_j k_y^2 R\left(k_x L\right), \quad T^{ij}_{32} = -E_j k_y S\left(k_x L\right),$$

$$T^{ij}_{33} = P\left(k_x L\right), \quad T^{ij}_{34} = \frac{1}{k_y} Q\left(k_x L\right),$$

$$T^{ij}_{41} = -E_j k_y^2 Q\left(k_x L\right), \quad T^{ij}_{42} = -E_j k_y^2 R\left(k_x L\right),$$

$$T^{ij}_{43} = k_S \left(k_x L\right), \quad T^{ij}_{44} = P\left(k_x L\right).$$

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