Machine learning prediction of initial values of elastic constants in resonant ultrasound spectroscopy

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1. Introduction

Elastic constants are one of the most basic physical quantities in material science and solid-state physics because they reflect the atomic bonding of the material and are essential parameters in designing structures. Resonant ultrasound spectroscopy (RUS) has been recognized as a method for measuring elastic constants [1-3]. In principle, it allows us to measure all independent elastic constants with a single small specimen, which is an advantage over other methods requiring multiple specimens according to crystal symmetry, such as the pulse-echo method. In the RUS analysis, we first calculate the theoretical resonant frequencies with the initial guess for elastic constants and compare them to the measured resonant frequencies. We then inversely determine the set of the elastic constants that minimizes the difference between calculated and measured resonant frequencies. To perform the inverse calculation appropriately, we need to find a good initial set of elastic constants, otherwise we will fail to make the correct mode identification and the resultant elastic constants will be physically meaningless. However, this task is never straightforward and requires many trial and error calculations. This is a serious and unsolved problem with the RUS method.

In this study, we propose a strategy to predict the initial values using machine learning, especially deep learning, which has achieved outstanding performance in the field of image recognition [3]. We utilize this image recognition accuracy of deep learning for predicting the initial values in RUS.

2. Method

2.1) Dataset

We convert resonance frequencies into monochrome images for utilizing convolutional neural network image analysis. **Figure 1** shows the schematic of the imaging process we originally developed. The product of the square of the resonance frequency and the mass density corresponds to the eigenvalue of the free vibrational eigenstate of the specimen, and this value reflects the elastic constants of the material. Therefore, we use this value to create the image. We typically use ~100 resonance frequencies to inversely determine the elastic constants in the actual RUS experiment. Therefore, we use the first 100 eigenmodes for making the dataset images. However, it is difficult to measure all 100 resonant modes without any lack because of the noise of the experimental system. To consider this, we randomly involved the missing resonant modes up to three in the dataset images. The imaging procedure takes the following process.

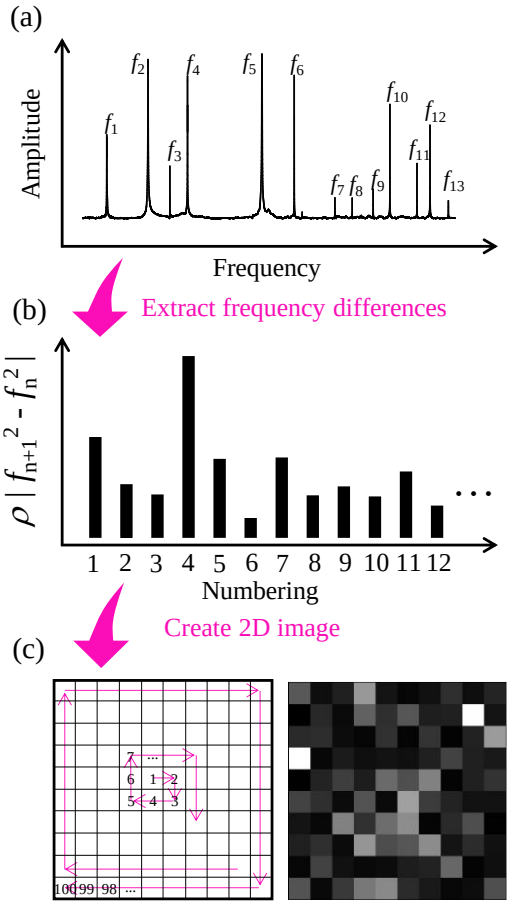

Fig. 1 Schematic diagram of creating the monochrome dataset image from resonance frequencies of a material. (a) Resonance frequency spectrum. f_n denotes the n-th resonance mode. (b) Differences of squares of adjacent resonance frequencies multiplied by the mass density ρ. (c) Arrange them in a spiral manner and create a 10×10 pixels image.

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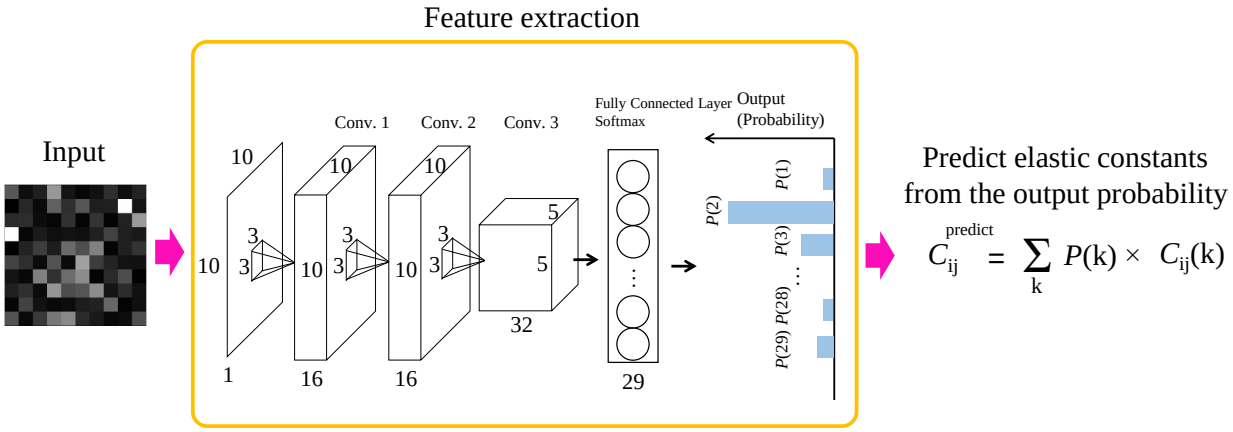

Fig. 2 Deep learning network architecture and prediction method for the elastic constants.

First, we take the differences between each eigenvalue. Second, we arrange them in a spiral manner and create a 100-pixels, 16-bit monochrome image. We here only consider cubic symmetry materials in the training dataset for simplicity. We used 29 materials for training the network. We fixed the specimen dimensions to be $3\times4\times5$ mm^3 in this study. We computed resonance frequencies using the Ritz method with basis functions consisting of the product of normalized Legendre polynomials with the maximum orders of 24.

2.2) Network architecture and prediction method

Figure 2 shows the schematic diagram of the network architecture developed in this study. Sixteen filters of size 3×3 are used for the first two convolution layers, and thirty-two filters of size 3×3 with a stride of 2 are used for the third convolution layer. The batch normalization layer and rectified linear unit layer follow each convolution layer. Finally, the classification probabilities are output by inserting the fully connected layer and the softmax layer.

We predict the elastic constants by multiplying each class probability and corresponding elastic constants and taking a summation.

3. Results and discussion

To check the reliability of our proposed method, we made test images generated by elastic constants as shown in **Table 1**, which we did not include in the dataset, and predicted their elastic constants by the method. We included missing modes in the test image. The image with no missing mode showed the smallest deviation, and all elastic constants, except for C_{44}, and the Poisson ratio were within 2% of the true value. The accuracy of the predictions deteriorated with increasing the number of missing modes. These deviations result from the training data mismatch due to increased missing combinations. However, the Poisson ratio was close to the true value in all missing numbers.

Table 1 The upper rows show elastic constants C_{ij} (GPa), Young's modulus E (GPa), Bulk modulus B (GPa), and Poisson ratio ν. The lower rows show the error with the true value (percent).

	missing	C_{11}	C_{12}	C_{44}	E	B	ν
True		240	130	30	149	167	0.35
Predict	0	238	129	34	147	165	0.35
		−1	−1	13	−1	−1	0
	1	231	124	32	145	160	0.35
		−4	−5	7	−3	−4	0
	2	226	121	33	142	156	0.35
		−6	−7	10	−5	−7	0
	3	227	121	32	142	156	0.35
		−5	−7	7	−5	−7	0

4. Conclusion

We proposed the strategy to predict the initial values of elastic constants for the inverse calculation in RUS analysis using deep learning. First, we prepared the dataset by converting the resonant frequencies of various materials into monochrome images and trained the network. Then, we predicted the elastic constants using images we did not include in the dataset. The predicted values of the image with no missing mode were close to the true values and predicted deviations deteriorated with increasing the missing number. We further investigate to improve the prediction accuracy.

References

1. I. Ohno: Phys. Chem. Miner. **17** (1990) 371.
2. A. Migliori *et al.*: Physica B: 183, (1993) 1.
3. H. Ogi *et al.*: J. Acoust. Soc. Am. 112 (2002) 2553.
4. A. Krizhevsky *et al*. ACM **60** (2017) 84.