

Development of Anharmonic Phonon Property Database using First-Principles Calculation

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1. Project Purpose

In this project, we aimed to accelerate the calculation of anharmonic phonon properties by utilizing machine learning interatomic potentials (MLIPs). While first-principles calculations provide high accuracy, they are computationally expensive, especially for large supercells and high-throughput studies.

Therefore, we investigated the applicability of existing MLIPs for phonon property analysis and explored transfer learning approaches using first-principles datasets generated in our previous and this studies. The goal was to achieve both computational efficiency and reasonable accuracy for large-scale phonon calculations.

2. Results

Phonon property calculations using the MACE potential [NeurIPS 2022] demonstrated that existing MLIPs can reproduce first-principles results to a certain extent. This confirms the potential of MLIPs for accelerating phonon simulations.

However, the accuracy was not yet sufficient for quantitative prediction of thermal properties. The results indicate that further improvement is necessary through expansion of first-principles datasets and refinement of MLIPs via transfer learning.

In particular, transfer learning using first-principles data for supercell calculations enabled systematic improvement of the MACE potential, although the accuracy still depends strongly on the quality and diversity of the training data.

3. Roles of the MCRP and its significance

The GPU-based supercomputing system played a critical role in this project. The allocated resources (approximately 20,000 CPU node-hours and 40,000 GPU node-hours) were effectively utilized for both large-scale simulations and machine learning tasks.

The GPU architecture significantly accelerated MLIP-based simulations, allowing efficient phonon calculations that would otherwise require extensive CPU resources. In addition, transfer learning of the MACE potential using large first-

principles datasets required substantial computational power, which was made feasible by the GPU system.

Thus, the supercomputer enabled both high-speed MLIP simulations and large-scale machine learning, providing a practical pathway toward combining first-principles accuracy with computational efficiency.

4. Future plan

Future work will focus on improving the accuracy and applicability of MLIPs for anharmonic phonon analysis. In particular, we plan to expand the first-principles database and incorporate higher-order anharmonic effects including phonon renormalization (temperature-dependence of effective harmonic phonon properties) and four-phonon scattering effect.

We will also further develop transfer learning techniques using first-principles data to enhance MLIP accuracy. In addition, high-throughput calculations using improved MLIPs will be performed to significantly increase the size of the phonon property dataset. These efforts will contribute to establishing a scalable framework for fast and accurate phonon property prediction.

5. Publications and conference presentations

(1) Journal papers

- Masato Ohnishi, Tianqi Deng, Pol Torres, Zhihao Xu, Terumasa Tadano, Haoming Zhang, Wei Nong, Masatoshi Hanai, Zhiting Tian, Ming Hu, Xiulin Ruan, Ryo Yoshida, Toyotaro Suzumura, Lucas Lindsay, Alan J. H. McGaughey, Tengfei Luo, Kedar Hippalgaonkar, Junichiro Shiomi, "Database and deep-learning scalability of anharmonic phonon properties by automated brute-force first-principles calculations," *npj Comp. Mater.* accepted (2026). 10.1038/s41524-026-02033-w.

(2) Presentations

- Masato Ohnishi, "Anharmonic Phonon Property Database Based on Brute-Force First-Principles Calculations" Materials Research Meeting 2025, Yokohama, Japan, December 8-13th, 2025. (invited talk)
- 大西正人, 塩見淳一郎, "Anharmonic phonon property database based on first-principles calculations," 第9回フォノンエンジニアリング研究会, 宮古, 日本, 2025年5月18-19日.
- M. Ohnishi, K. Kitai, Y. Yoshimoto, Y. Hayashi, R. Yoshida, and J. Shiomi, "Prediction of high-frequency dielectric properties of polymers using molecular dynamics simulations," 2025 MRS Spring Meeting & Exhibit, MT02.09.03, Seattle, USA, April 7-11th, 2025.

(3) Others

- Software for automated first-principles phonon calculation (auto-kappa): <https://github.com/phonix-db/auto-kappa>
- Database for anharmonic phonon database (Phonix): <https://phonix-db.org>

Supercomputer	Use	Allocated resources*		
		Initial resources	Transferred resources**	Purchased resources
Pegasus	<input checked="" type="checkbox"/> Yes/No	14,400		0
Miyabi-G	<input checked="" type="checkbox"/> Yes/No	40,500	0	0
Miyabi-C	<input checked="" type="checkbox"/> Yes/No	5,760	0	0
	*in units of node-hour product			
	** If the budget transfer was performed, fill in here, such as "+2000" and "-1000".			