Effects of Oxygen Vacancies on the Thermoelasticity of Al-bearing Bridgmanite

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Introduction

- **Mantle transition zone (MTZ)**
A key region to understand mass and heat transport in Earth's mantle

- **Seismic velocity discrepancy**
experimental results
↕ **discrepancy**
seismic obserbations

temperature effect?
compositional effect?

- **Bridgmanite**
A main mineral of the lower mantle
Account for high volume ratio (>70%)
Predicted to have point defects through Al substitution

- **Point defects in bridgmanite**

{ **OV** (oxygen vacancy) abundant at 700-900 km depth
CC (charge coupling) abundant at 900- km depth

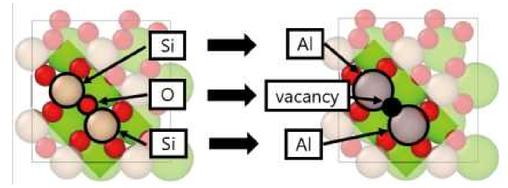
OV is predicted to **reduce seismic velocities**

Not quantified

→ **new factor** for considering the discrepancy

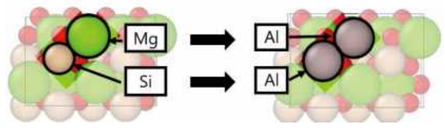
OV

$2MgSiO_3 + 2Al^{3+} = 2MgSiO_{2.5} + 2Si^{4+} + O^{2-}$



CC

$MgSiO_3 + 2Al^{3+} = 2Al_2O_3 + Mg^{2+} + Si^{4+}$



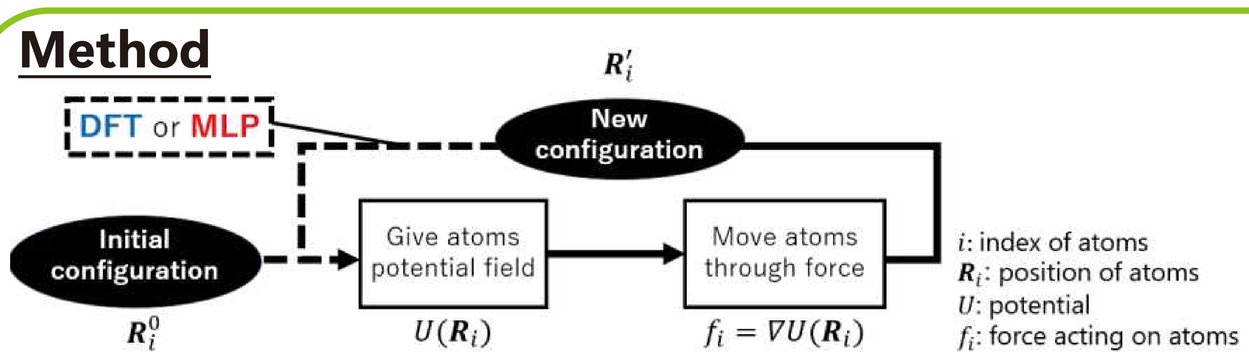
- **Limitation of previous computational researches**

1. Concentration of **point defects** is too high　2. No **OV**'s seismic velocity data with thermal effect

→ Investigating **thermoelasticity with Larger systems** is needed

→ More **efficient** calculation

Method



DFT (density functional theory)
- High accuracy
- High computational cost

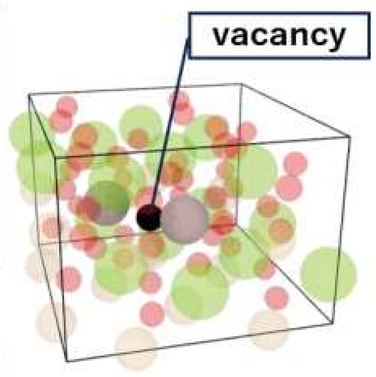
→ structure, energy, force, stress →

MLP (machine learning potential)
- Generated via **DFT data**
- High accuracy
- Low computational cost

- **MD (molecular dynamics)**
Simulation of moving atoms through equation of motion
Various physical properties with thermal effect are obtained

DFTMD data sampling
- **System:** OV (79 atoms), pure $MgSiO_3$ (80 atoms)
- **Pressure**: 0-50 GPa, **Temperature**: 300-2000 K
- **Software**: Quantum ESPRESSO (Giannozzi+, 2009)
- **Pseudopotential**: PAW, **Xc-potential**: PBEsol (GGA)
- **Wave cutoff**: 80 Ry, **Rho cutoff**: 400 Ry, **K-point**: 1*1*1
- **Thermostat**: Nosé-Hoover (Nosé, 1984)

MLP training
- **Pretrained potential :** MatterSim-v1.0.0-1M (Yang+, 2024)
- **Additional training dataset :** DFT data
- **Train : Validation : Test** = 8:1:1

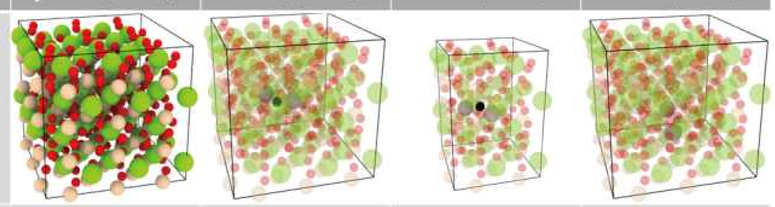


OV (79 atoms)
$14(MgSiO_3)2(MgAlO_{2.5})$

- **Setting of MLPMD**

Pressure : 25, 35, 45 GPa (700-1150 km)
Temperature : 2000 K

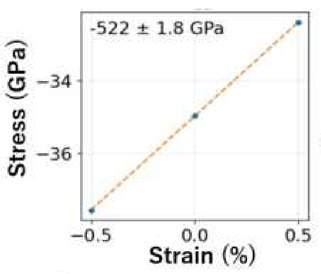
Mg Si O Al vacancy

System (atoms)	pure(360)	OV (359)	OV (159)	CC (360)
				
concentration	0%	2.78%	6.25%	2.78%

- **Determination of elastic constants**

First step MD
Determination of stable structure at each (P, T)

Second step MD
Estimation of the **stress** of **strained** and **unstrained** cells



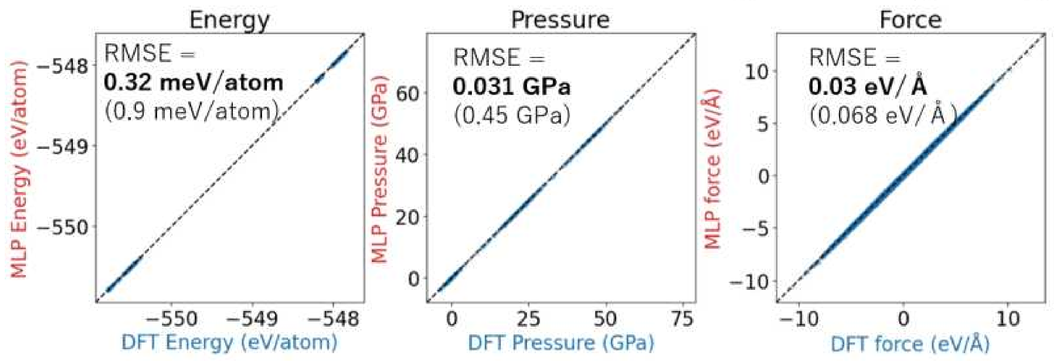
$\sigma_\alpha = C_{\alpha\beta}\,\epsilon_\beta$

Elastic constants are calculated using **stress** and **strain** from MD

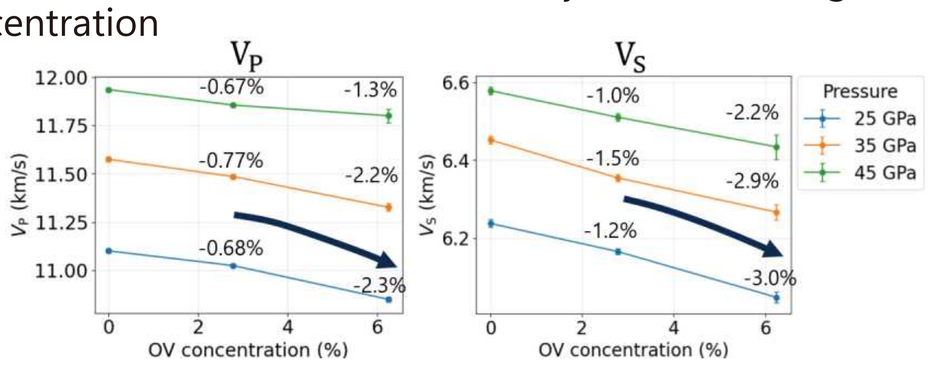
Results

- **Accuracy of MLP**
Sufficient to reproduce physical properties

RMSE =
this study
(previous study Wan+ (2024))



- **Reduction in seismic velocities**
Seismic velocities decrease nonlinearly with increasing **OV** concentration



Disscussion

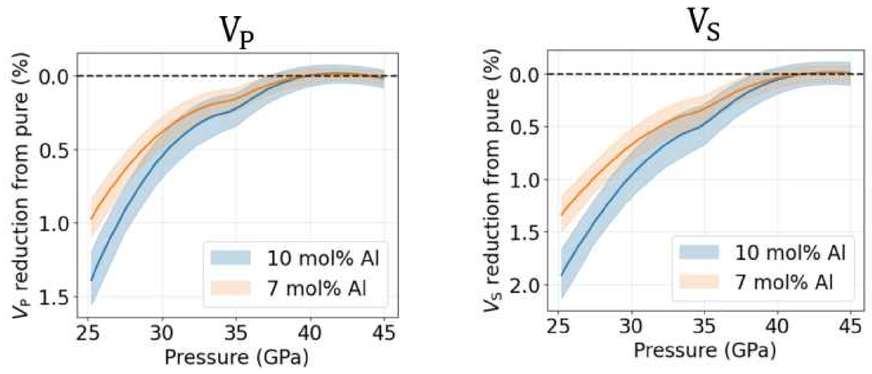
- **Comparison with CC component**

	OV at 25 GPa, 2000 K	CC at 25 GPa, 2000 K
concentration	2.78%	2.78%
V_P	-0.68 ± 0.12%	+0.01 ± 0.16%
V_S	-1.15 ± 0.19%	-0.35 ± 0.25%

The **OV**'s effect on seismic reduction is significant
OV can be dominant factor rather than **CC**

- **The effect of OV on the seismic velocity profile**

We use **OV** concentration depth profile of Criniti+ (2024) scaling with pyrolite model



OV showed significant reduction of V_P (0.6-1.0%) and V_S (1.0-1.5%) at 25-27 GPa

This effect is comparative to thermal and compositional effects.

Reference

- Criniti, G., Boffa Ballaran, T., Kurnosov, A., Liu, Z., Glazyrin, K., Merlini, M., et al. (2024). Thermal equation of state and structural evolution of Al-Bearing bridgmanite. Journal of Geophysical Research: Solid Earth, 129(1), e2023JB026879. https://doi.org/10.1029/2023JB026879
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- Yang, H., C. Hu, Y. Zhou, X. Liu, Y. Shi, J. Li, et al. (2024). MatterSim: A deep learning atomistic model across elements, temperatures and pressures, arXiv e-prints, arXiv:2405.04967, https://doi.org/10.48550/arXiv.2405.04967