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

EX26306

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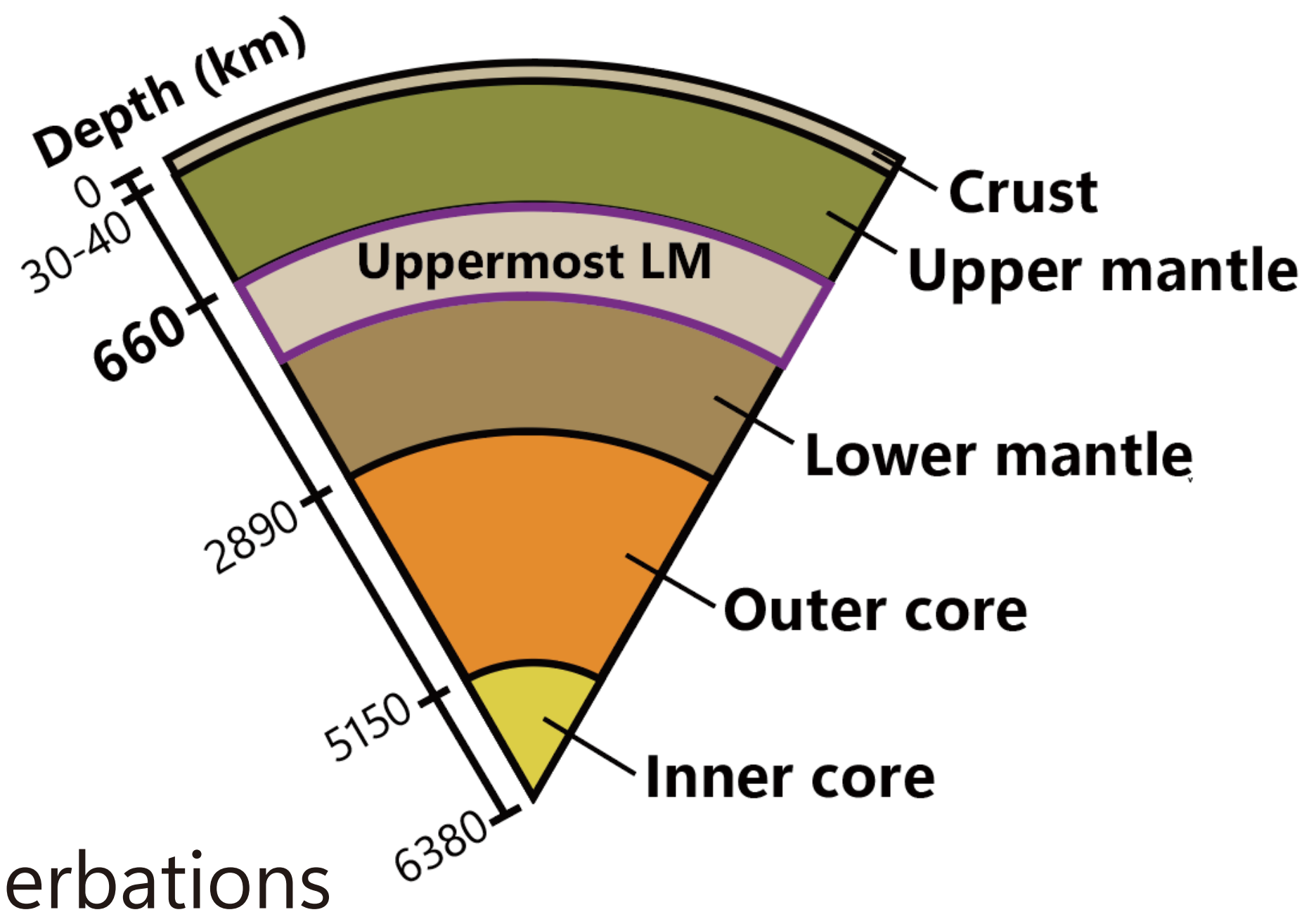
Introduction



- **660-km discontinuity**

A key region to understand mass and heat transport in Earth's mantle

- **Seismic velocity discrepancy at uppermost LM**

experimental results > seismic obserbations

➡ 20-30% global accumulation of oceanic crust (Gréaux+, 2019)

➡ Efficient segregation and accumulation mechanisms are required

- **Point defects in bridgmanite**

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

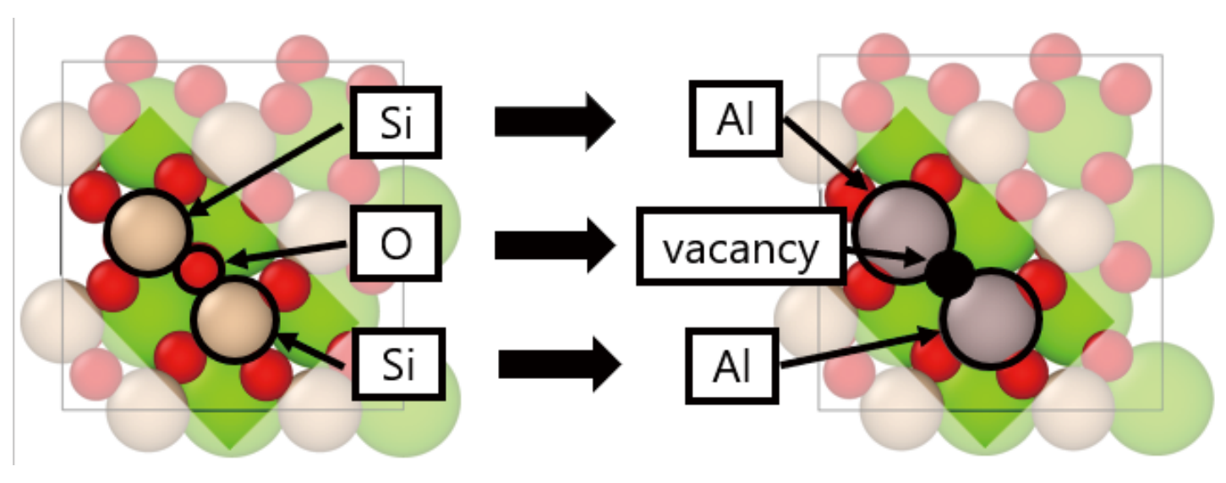
OV is predicted to **reduce seismic velocities**

Not quantified

➡ **new factor** for considering the discrepancy

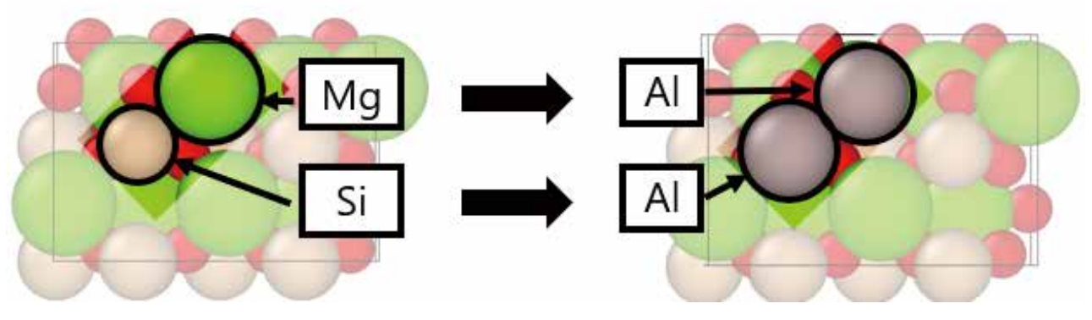
OV

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



CC

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



- **Bridgmanite**

A main mineral of the lower mantle
High volume ratio (>70%)
Predicted to have point defects through Al substitution

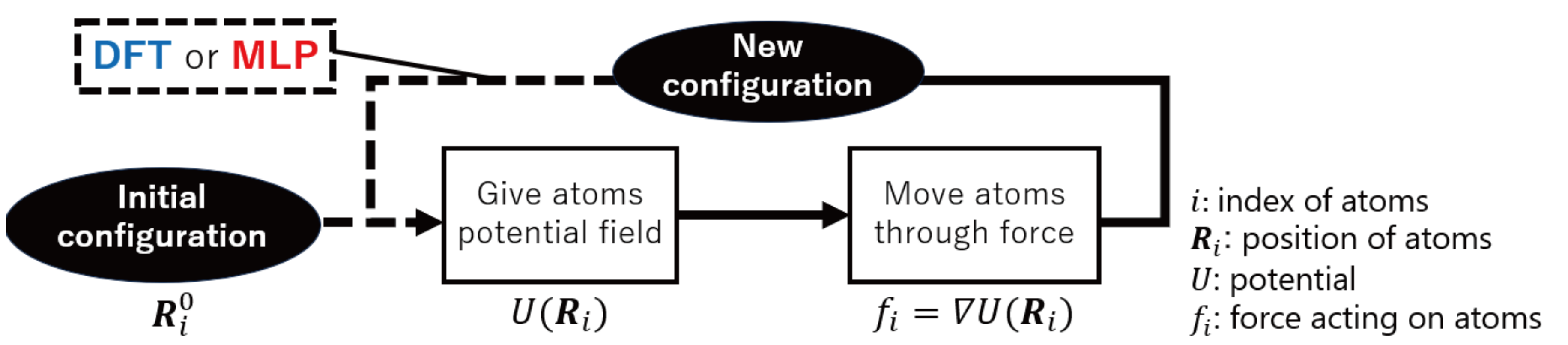
- **Limitation of previous computational researches**

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



i: index of atoms
R_i: position of atoms
U: potential
f_i: force acting on atoms

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

- structure
- energy
- force
- stress

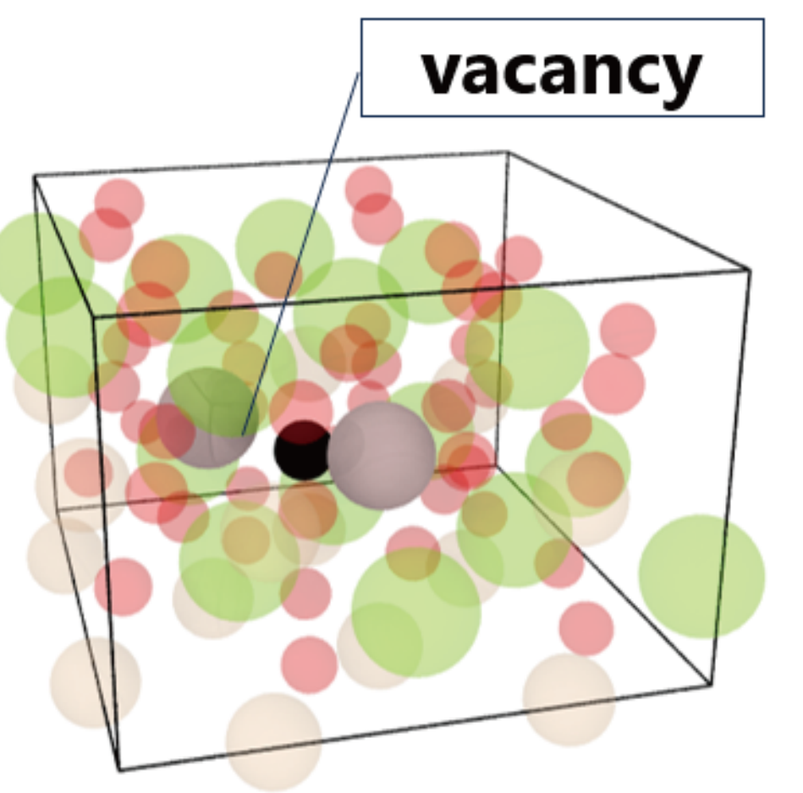
MLP
(machine learning potential)
- Generated via **DFT data**
- High accuracy
- Low computational cost

- **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), CC, $MgSiO_3$ (80 atoms)
- **Pressure**: 0-150 GPa, **Temperature**: 300-5000 K
- **Software**: Quantum ESPRESSO (Giannozzi+, 2009)
- **Pseudopotential**: PAW, **Xc-potential**: PBEsol (GGA)
- **Wave cutoff**: 80 Ry, **Rho cutoff**: 400 Ry, **K-point**: 2*2*1
- **Thermostat**: Nosé-Hoover (Nosé, 1984)



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

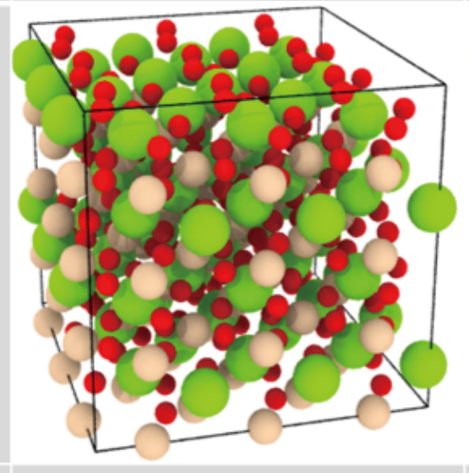
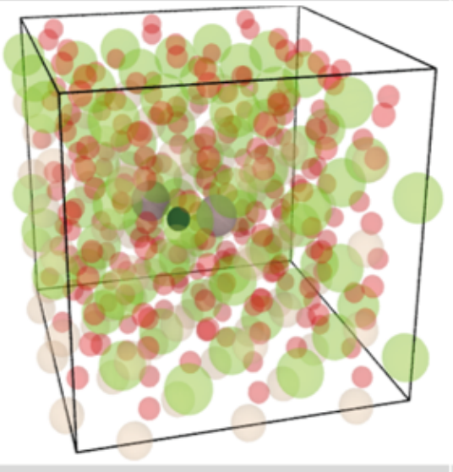
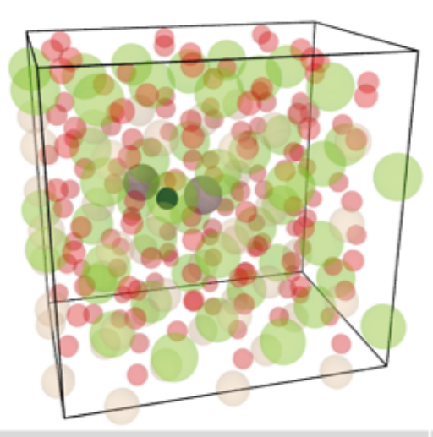
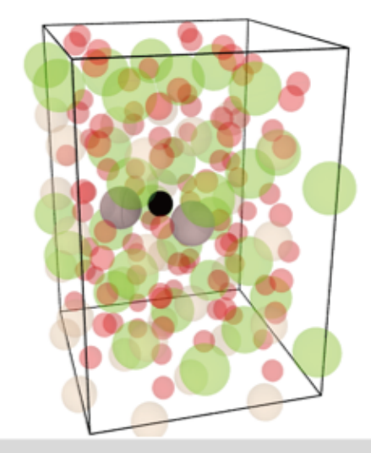
MLP training

- **Pretrained potential: Orb-v3** (Rhodes+, 2025)
- **Additional training dataset: DFT** data
- **Train : Validation : Test** = 8:1:1

- **Setting of MLPMD**

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

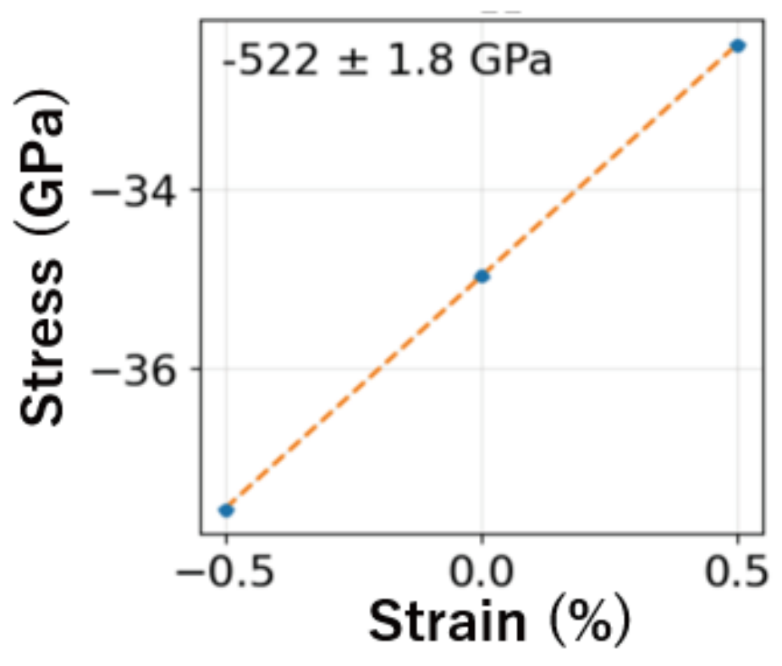
Mg Si O Al vacancy

System	$MgSiO_3$ (360 atoms)	OV (359 atoms)	OV (239 atoms)	OV (159 atoms)
				
Conc.	0%	2.78%	4.17%	6.25%

- **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



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

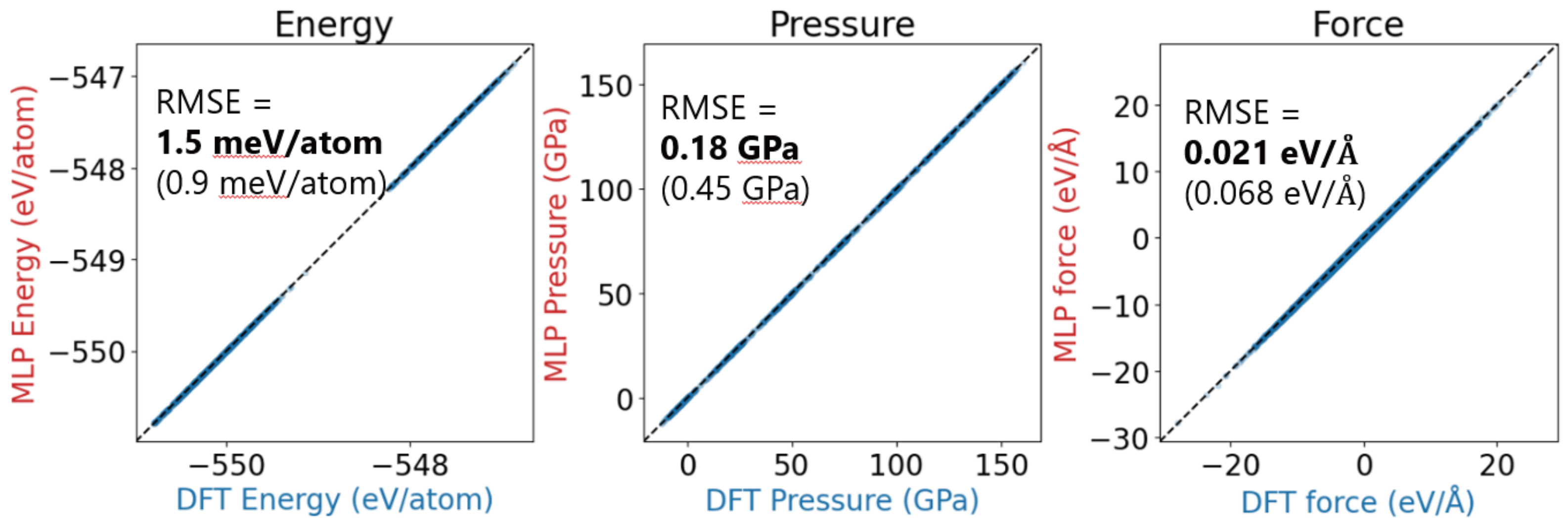
Elastic constants are calculated using **stress** and **strain** from MD

Results

- **Accuracy of MLP**

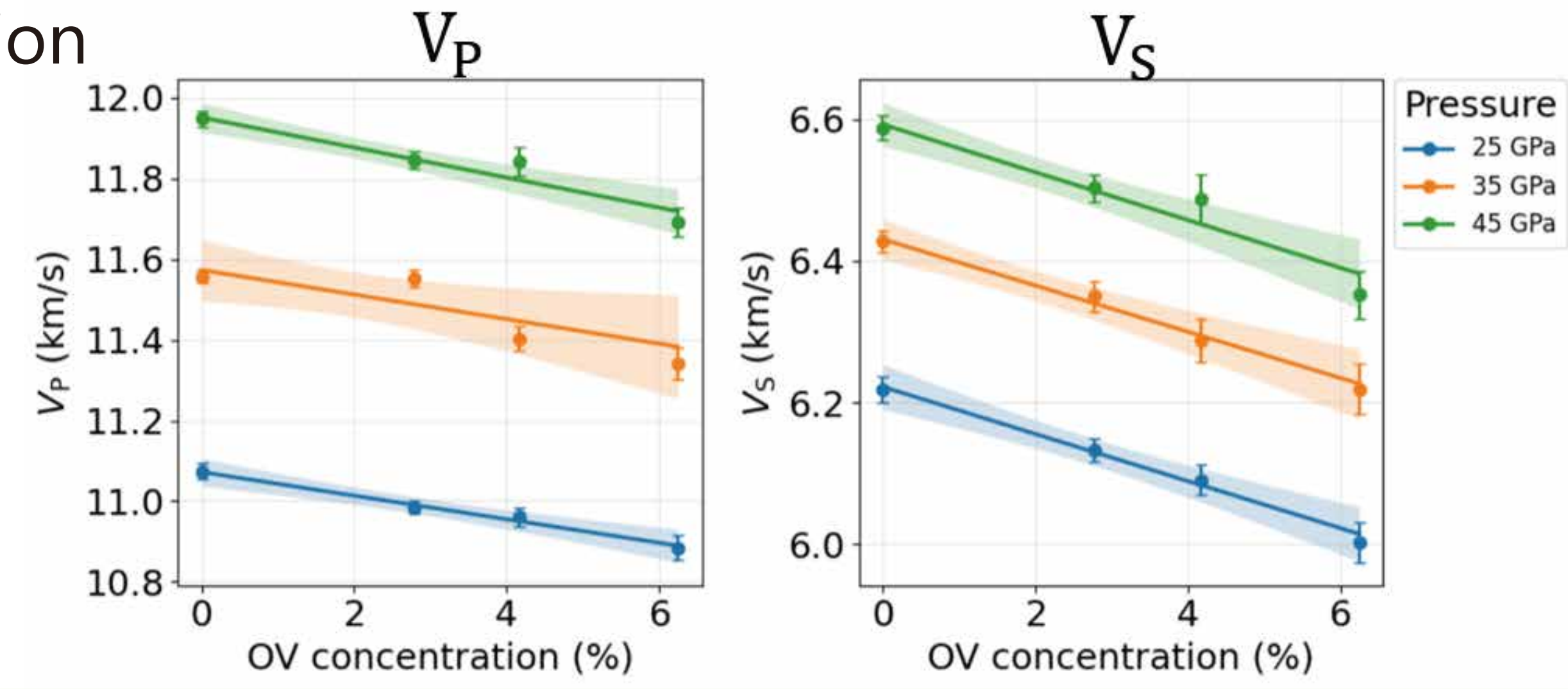
Sufficient to reproduce physical properties

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



- **Reduction in seismic velocities**

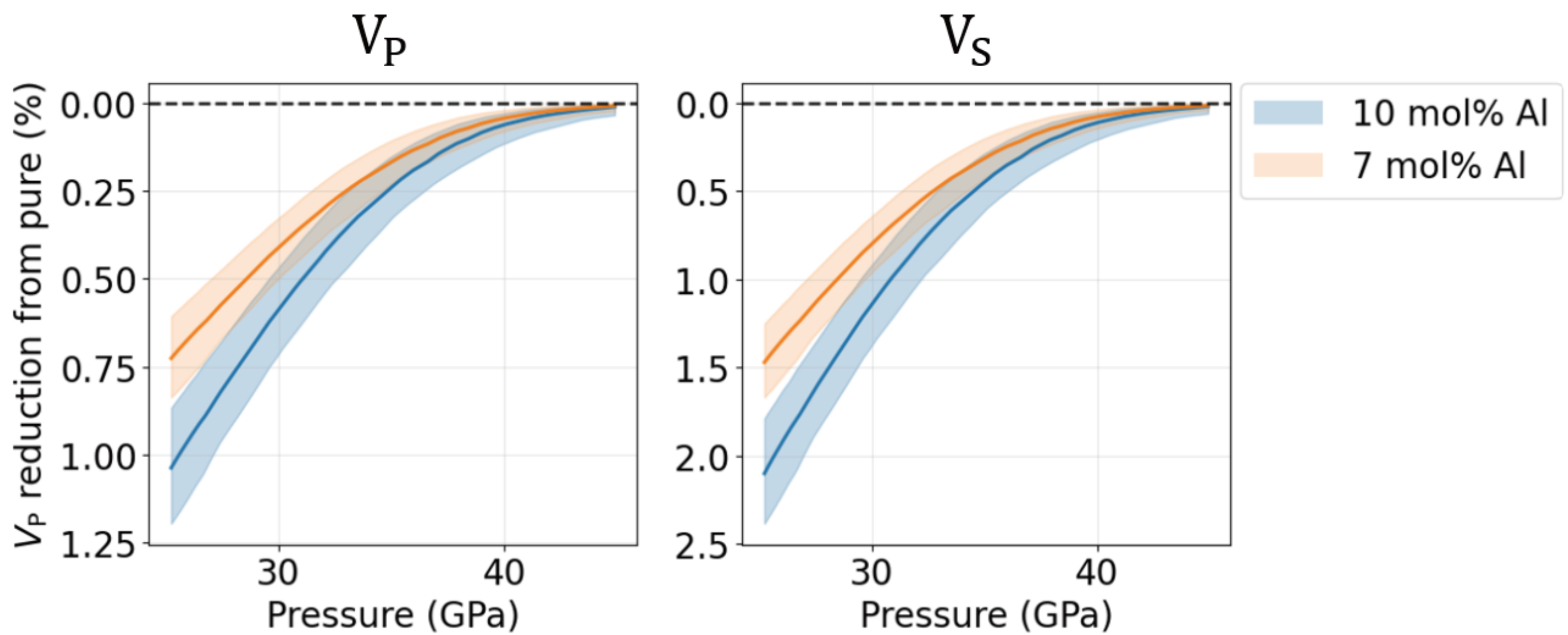
Seismic velocities decrease nonlinearly with increasing **OV** concentration



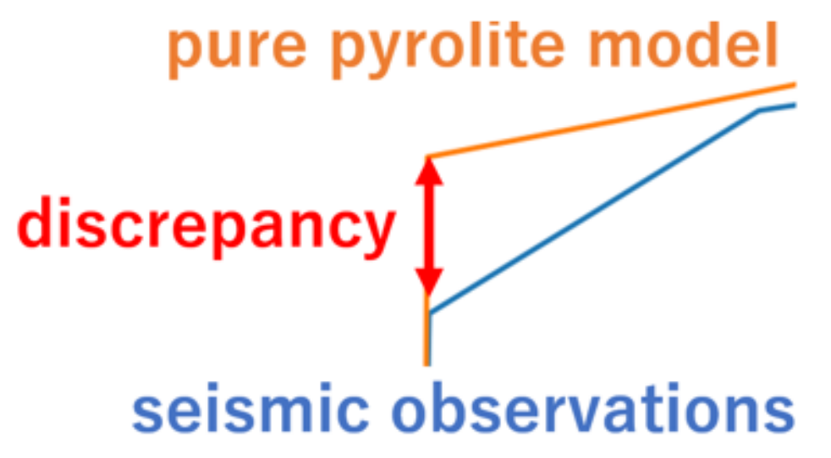
Disscussion

- **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 effect at 25-27 GPa.
V_P (0.6-0.8%), V_S (1.2-1.7%)



	Discrepancy (Gréaux+, 2019)	Compositional effect (MORB 10%)	OV's effect (This study)
V_P	0.3-0.7%	0.8%	0.6-0.8%
V_S	2.4-2.9%	1%	1.2-1.7%

The effect of OV can explain the discrepancy to some extent

➡ **Seismic discrepancy at uppermost LM can be explained without assuming MORB-rich mantle**

Reference

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