

Developing a Universal Pressure Scale for High Pressure-Temperature Experiments

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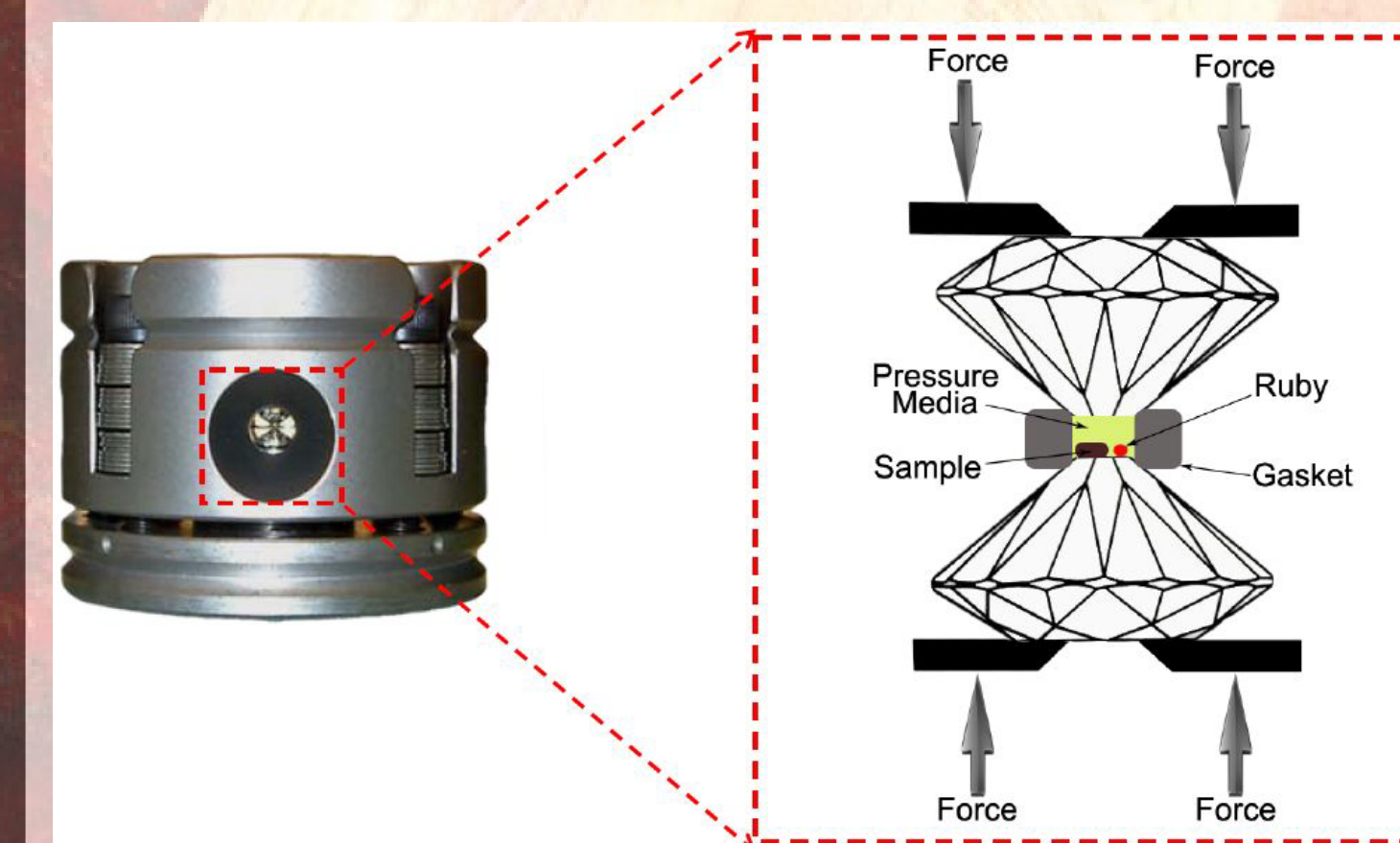


Abstract

Materials within the Earth are subject to high Pressure-Temperature (P-T) conditions, and thus we must be able to accurately determine pressures in high P-T experiments in order to explore the properties of the deep Earth. Numerous high P-T experiments have been conducted using different internal pressure markers such as Au, Pt, MgO, Neon, and NaCl. The data obtained through both static and shock wave experiments are used to construct equations of states that define the pressure scale for each pressure markers. Experiments can often produce conflicting pressure estimates, however, due to the differences in explored pressure-temperature ranges, as revealed by studies including multiple standards. Our research creates a database of both the parameters and data obtained for each experiment by extracting and digitizing data from research journals. We then attempt to fit the experimental data by adjusting parameters in the equations of state, and to compare the model with other existing models. In the long run, this project known as Unified Bayesian Iterative And Systematically Determined Pressure Scale Project, attempts to construct a unified pressure scale where both shock wave and static data results fit well with each other across many materials.

Diamond Anvil Cell

The diamond anvil cell is the apparatus used in conducting high (P-T) experiments. We are able to model the extreme conditions in the deep Earth by subjecting a small (sub-millimeter sized) material sample to very high pressures (> 600 Gpa). Pressure is measured relative to a pressure standard whose behavior under pressure is well-characterized (Pt, Ne, Au, NaCl etc). High temperatures (~>3000 K) can also be achieved at the same time using laser-induced heating.



(image from Yang and Zhui)

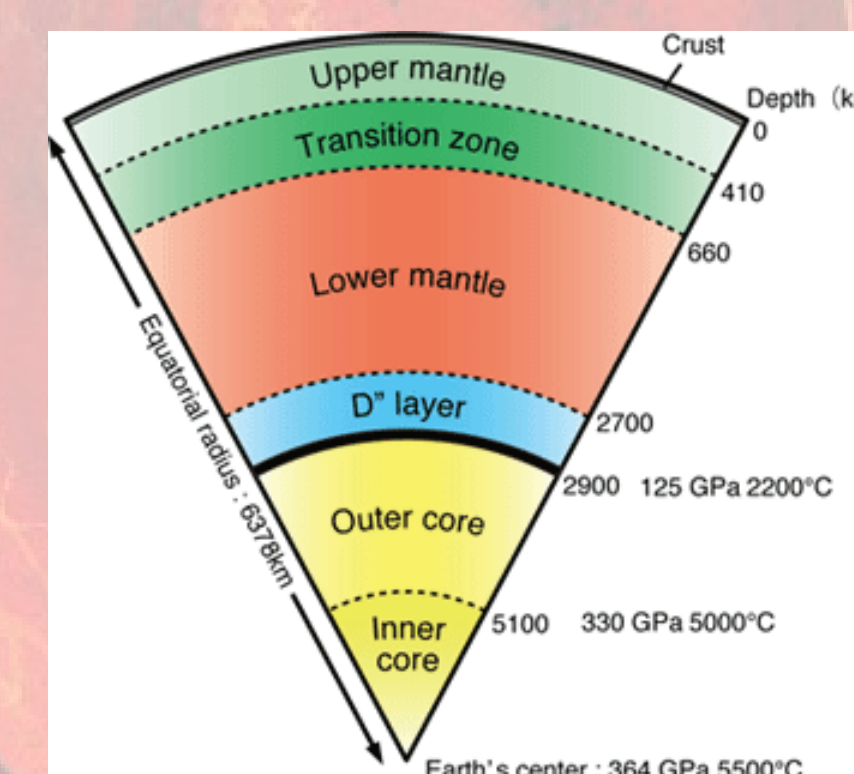
Methods

The goal of the UnBIASeD Pressure Scale Project is to create a universal pressure scale that minimizes the difference between pressure scales across different pressure markers. To achieve this goal:

- We digitize static and shock wave experiment data from numerous articles for various pressure standards (Au, MgO, Pt, Ne, NaCl). The database is accessible to the public at github.com/aswolf/unbiased-pscale
- Using the Vinet and Mie-Gruneisen-Debye Equations of State, we fit the static experimental data to the model data obtained from the equations of state and determine the parameters that would result in the best fit and compare with the reported results.
- We plot the pressure confidence regions, using fitted parameter uncertainties to determine where sparse data coverage strongly impacts model uncertainties.

The Earth Interior

- The Earth's interior holds clues both about how our planet formed and how it evolved to its current state.
- By observing seismic velocity discontinuities, we have been able to identify the boundaries of the Earth layers.
- Materials under the earth behave differently due to variations in pressure and temperature. Unfortunately, we are unable to sample the components of the earth interior as it is impossible to drill holes into the deep Earth and mantle rocks that are brought to the earth surface are rare and highly altered.
- We attempt to study the behavior of materials in the Earth interior by recreating the high P-T conditions in the lab.



(image from Chisato Hata)

Results

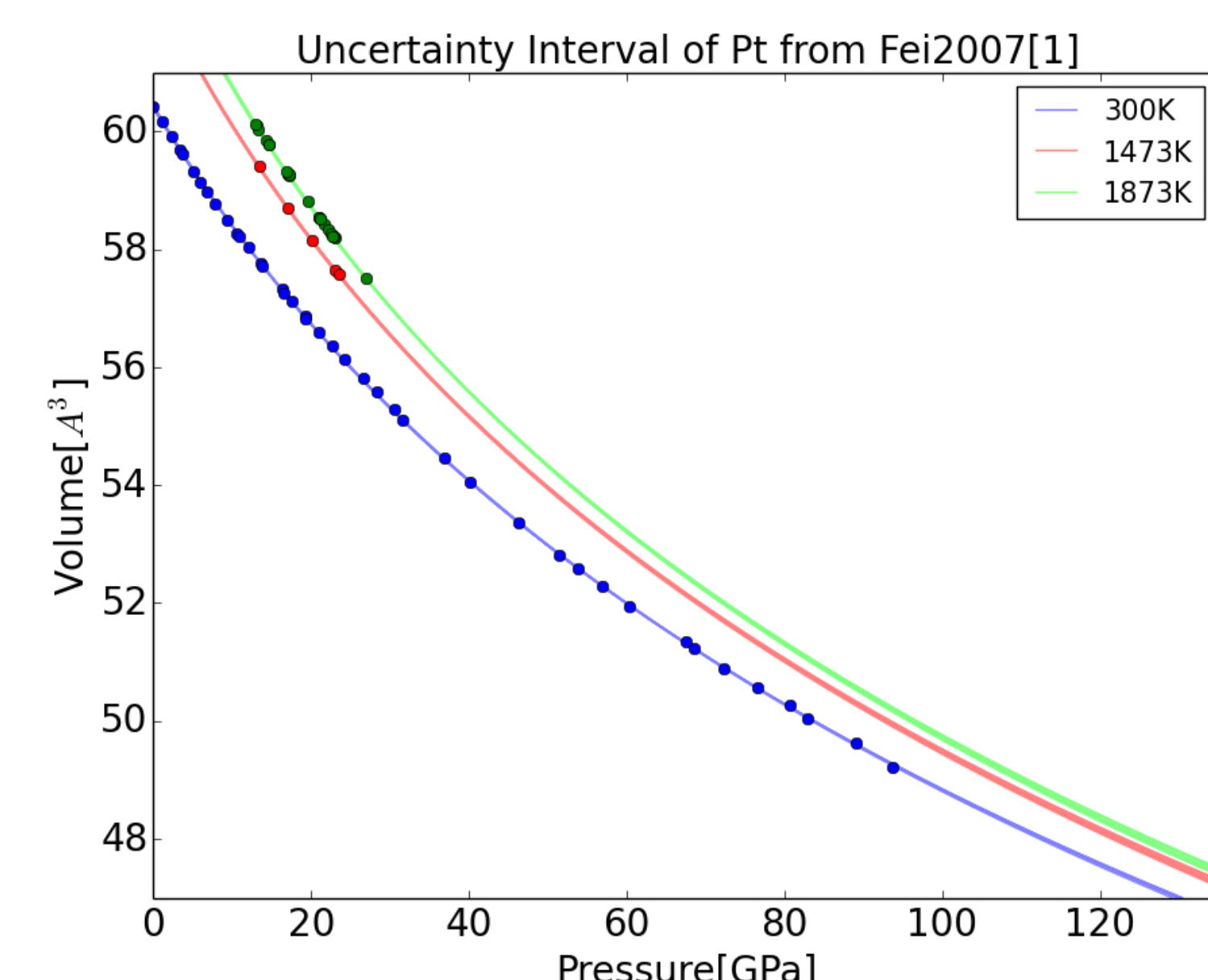


Fig 1. Rough confidence bounds for Pt (analyzing data from Fei, 2007) are shown by plotting 10 representative isotherms computed at 300K, 1473K and 1873K. [2][4]

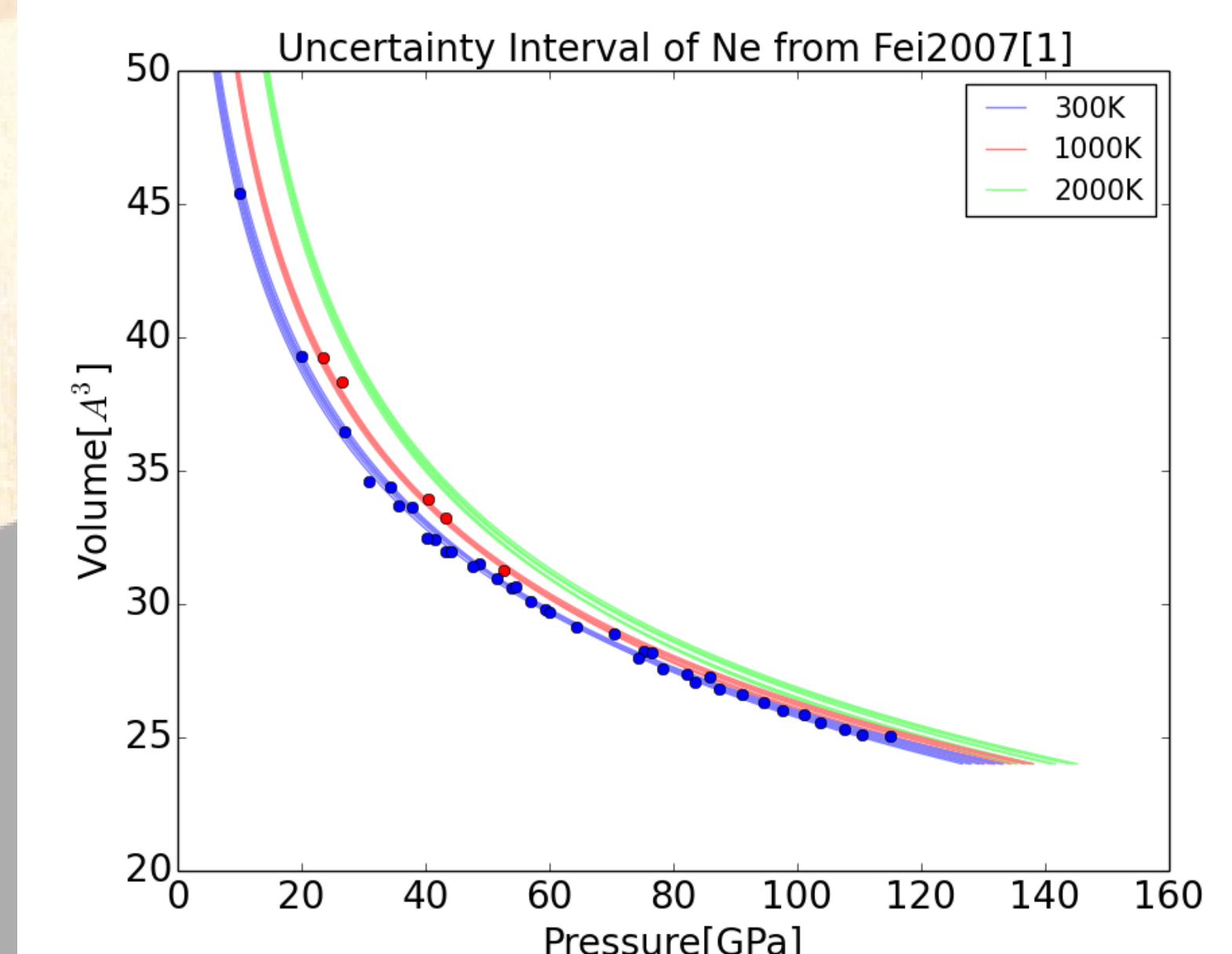
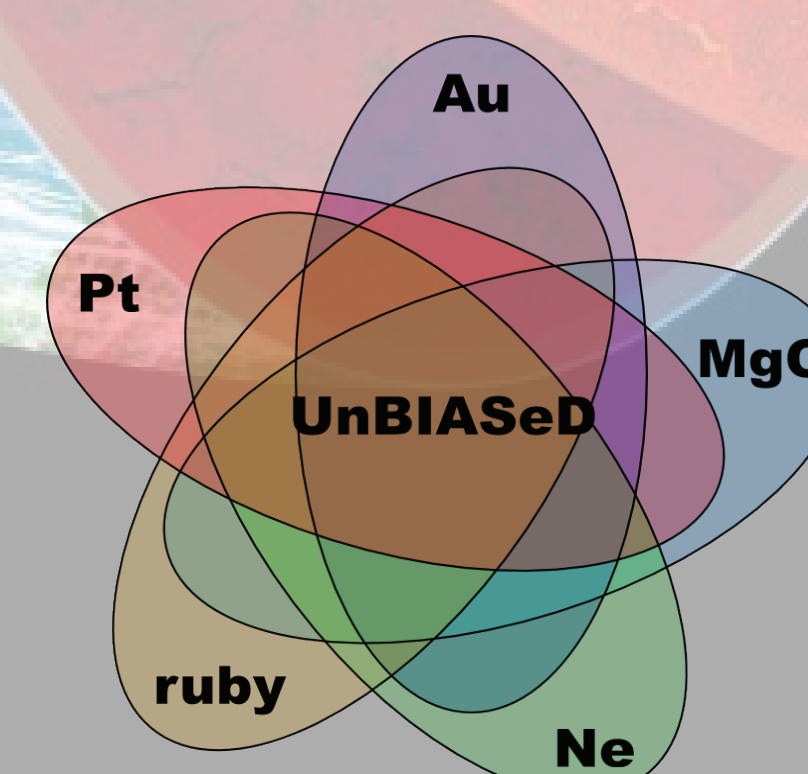


Fig 2. Rough confidence bounds for Ne (analyzing data from Fei, 2007) are shown by plotting 10 representative isotherms computed at 300K, 1000K and 2000K. [3]

Why do we need a unified pressure scale?

- To help us interpret the seismic observations of the Earth, we depend on high P-T experiments to understand the behavior of Earth materials under extreme conditions.
- We rely on a limited set of calibrated pressure markers such as Au, MgO, Ne, Pt and ruby that are highly sensitive to uncertainties in their high P-T properties.
- Due to the different choices of pressure markers in addition to different experimental and analytical techniques used in different experimental laboratories, it is crucial that we have a calibrated unified pressure scale.
- The UnBIASeD (Unified Bayesian Iterative and Systematically Determined) Pressure Scale project attempts to create a unified pressure scale that minimizes the systematic errors in these calibrated pressure scales through a Bayesian analysis of high P-T measurements.



(image from Aaron Wolf)

What Next?

We will apply the above methods to analyze shock wave data, which provide the true pressures for the Au, MgO, Ne, Pt and NaCl pressure markers. Thus, we do not need to rely on any pressure markers as we did when analyzing the static data. We can then attempt to minimize the difference between the best fit parameters for static data and those for shockwave data. This will result in the consistency of the pressure scales for different materials. In this way, future studies of materials under extreme condition can rely on a unified pressure scale providing more accurate estimations of pressures relevant to the deep Earth.

References

- Fei et al. PNAS. 2007, 104, 22.
- Dewaele et al. Physical Review B. 2008, 77, 9.
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- Fei et al. Physics of The Earth and Planetary Interiors. 2004, 143-144.