

COMPUTATIONAL MINERAL PHYSICS

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PI: Renata M. Wentzcovitch¹

Collaborators: Tao Sun², Dong-Bo Zhang³, Han Hsu⁴, Mehmet Topsakal¹, Gaurav Shukla¹, Kanchan Sarkar¹, Michel Marcondes¹

¹University of Minnesota, Twin Cities

²University of Chinese Academy of Sciences

³Computational Science Research Center, Chinese Academy of Engineering Physics, Beijing

⁴National Central University, Taiwan

EXECUTIVE SUMMARY:

Mineral physics is one of three branches of geophysics (the others being geodynamics and seismology). Geophysics advances by close cooperation between these fields. Thus, mineral physics focuses on mineral properties that are needed to interpret seismic data or are essential for geodynamics simulations. To be useful, mineral properties must be investigated across a wide range of pressure, temperature, and chemical composition. Chemical composition is complex, encompassing at least five major oxide components and tens of solid phases. Today, first-principles computations address these challenges. Minerals' properties are fundamental to elucidate a planet's state, and atomistic studies of these complex materials are fundamental to understanding their properties. We will use Blue Waters to perform first-principles calculations of unprecedented magnitude and scope in mineral physics.

INTRODUCTION

The goal of high pressure mineral physics is to increase our knowledge of the materials that make up the Earth and other planets [1]. For many problems, first-principles theory [e.g., 2–6] is the only practical method of investigation available. First-principles methods have been addressing materials problems important to understanding the present state and evolution of the Earth and other planets [4,7–14]. However, computation of full thermal elastic anomalies caused by spin crossovers at high temperatures and pressures has not been realized.

Today's first-principles calculations need databases of equilibrium thermal elastic properties of minerals and their assemblages to model Earth and other planets [1]. The challenge to computations is to perform these highly demanding calculations efficiently in a large number of phases with variable compositions. For example, the chemical composition of the terrestrial mantle includes at least five major oxide components (MgO, SiO₂, Al₂O₃, FeO, CaO) and tens of solid phases (fig. 1).

Our work is motivated and informed by central questions in Earth and planetary sciences. It focuses on building highly realistic models that account for all physical and chemical variations in the system (e.g., chemical composition, pressure, temperature, etc.).

We perform calculations on tens of mantle phases using primarily quasi-harmonic (QHA) computations. However, molecular dynamics (MD) or hybrid QHA/MD calculations are performed in the case of anharmonic phases or at temperatures near melting. As far as elasticity is concerned, a rigorous treatment of solid solutions is unnecessary for mineral aggregates. These results will address questions such as:

- What is the seismic signature in the deep mantle produced by the sinking lithospheric plates made of mid-ocean ridge basalt (MORB), harzburgite, and peridotite? Conversely, to what extent can mantle heterogeneities be attributed to seismic contrasts between these assemblages and "normal" pyrolite mantle [19]?
- What are the temperatures, chemistries, and mineral assemblages of the two large, low-shear velocity provinces in the deep mantle [21]? Did they result of accumulation of MORB enriched material?
- What seismic signature do spin changes produce in iron in lower mantle minerals [e.g., 10,16–17]?
- What are the phase boundary and velocity contrast produced by the post-perovskite transition [8,11,20] in MORB, harzburgite, peridotite, and pyrolite? This information must be available before one can interpret seismic observations of the D'' region, the ~300 km above the CMB.

METHODS & RESULTS

We used standard and extended/hybrid density functional theory (DFT)-based methods as implemented in the Quantum ESPRESSO software [e.g., 2–6]. These DFT calculations combined QHA and MD to address thermal elastic properties.

Thermodynamics methods

Thermodynamic states were investigated using QHA [22] and MD. QHA and MD are complementary approaches, the former from low to intermediate temperatures ($T < \sim 2/3 T_{\text{melting}}$) and the latter from intermediate to T_{melting} and beyond. Both methods are CPU intensive because they involve statistical sampling of phase space. In MD this translates into large supercells

and long runs. By contrast, the QHA used in conjunction with first principles vibrational density of states [3,5] is much more efficient for calculations corresponding to very large numbers of atoms.

We routinely performed calculations corresponding to 10⁴ atoms [4,7,9,15]. However, these were high throughput calculations requiring typically 10² to 10³ medium-size calculations with ~10² atoms. In particular, thermoelastic constants, $c_{ijkl}^T(P, T)$, a central topic in our project, was one of the most CPU intensive calculations we performed. These jobs could be executed concurrently in single or distributed compute nodes. Ref. [6] summarizes a few of these calculations [4,7,15,18]. They were

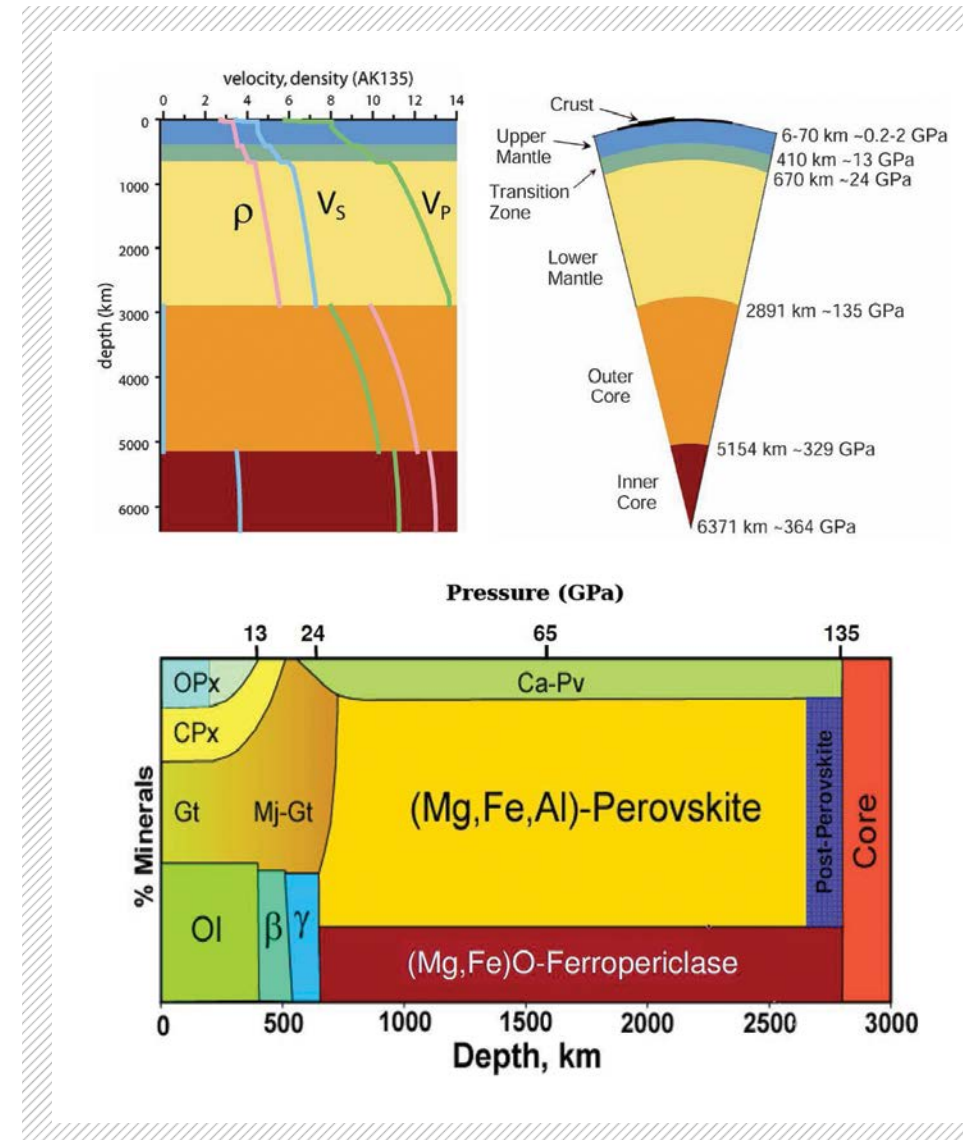


FIGURE 1: Earth's seismic discontinuities (top) [59] and mantle mineralogy (bottom; e.g., [50]).

carried out by submitting bag-of-task (BoT) [14] type jobs to single or distributed systems using the VLab service-oriented cyberinfrastructure [12–14].

On Blue Waters, these calculations were performed using BoTs or MPI directives, “image” parallelization (1st level of parallelization). For a typical system with 20 atoms (e.g., MgSiO₃ perovskite or post-perovskite [7,15]), the best performance was achieved with 128 cores per job. Thus, a full thermodynamic calculation could be performed in less than one minute, or a calculation of thermoelastic constants could be performed in a couple of minutes.

multiple configurations (~10¹–10²) need to be explored in each of up to ~10⁴ calculations.

We have essentially investigated all major end-member phases and simple versions of the main mineral solid solutions of the mantle using only a few atomic configurations. While elastic properties of crystalline aggregates are well described by using few atomic configurations, phase diagrams containing binary (or multi-phase) loops need accurate free energies, which can only be achieved through careful sampling of atomic configurations. An example of this problem can be seen in fig. 1, where OPx and CPx phases “dissolve” into Gt (garnet) within a broad pressure range (i.e. 5 GPa < P < 18 GPa). A detailed description of this phenomenon requires a considerably larger number of (smarter) calculations.

WHY BLUE WATERS?

The major reason for using Blue Waters is the number of cores available. We developed wrappers around several modules of the Quantum ESPRESSO software that allow us to use the system for high-throughput calculations. As explained above, phase space sampling for thermodynamics calculations is intrinsically a high-throughput problem.

A future Track-1 system will allow us to expand the dimension of phase space currently sampled. Minerals are solid solutions and a full investigation of phase equilibrium in these solids involves sampling of atomic configurations. We have just started addressing this issue. We are exploring techniques to do maximally efficient sampling of atomic configurations. Nevertheless,

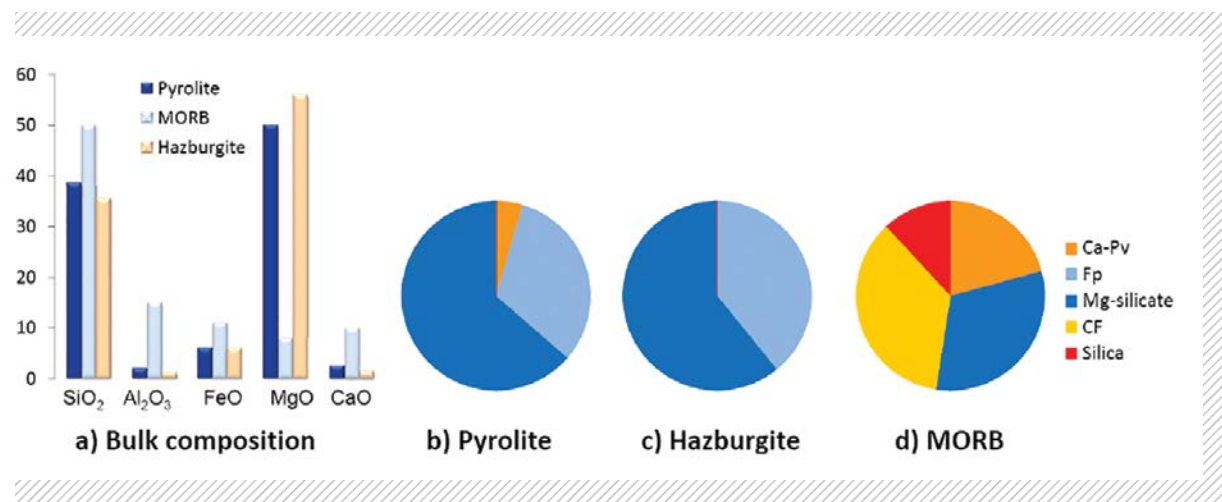
PUBLICATIONS

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FIGURE 2: (a) Chemical compositions of mantle rocks [85–87]. Mineralogy (in mol%) of (b) pyrolite [88], (c) harzburgite, and (d) basalt [89] in the lowermost mantle. Mg-Silicate: MgSiO₃ perovskite and/or post-perovskite, Fp: ferropericlase, Ca-Pv: CaSiO₃ perovskite, and CF: calcium-ferrite-type phase.



USING PETASCALE COMPUTING CAPABILITIES TO ADDRESS CLIMATE CHANGE UNCERTAINTIES

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PI: Donald J. Wuebbles¹

Co-PIs: Zachary Zobel¹, Warren Washington², Thomas Bettge², Julio Bacmeister², Kevin Reed², Xin-Zhong Liang³, Chao Sun³

¹University of Illinois at Urbana–Champaign

²National Center for Atmospheric Research

³University of Maryland, College Park

EXECUTIVE SUMMARY:

This collaborative research between the University of Illinois, the National Center for Atmospheric Research (NCAR), and the University of Maryland uses Blue Waters to address key uncertainties in numerically modeling the Earth’s climate system and accuracy in analyses of past and projected future changes in climate at a level that would be impossible without petascale computing. Our studies used the latest, most advanced versions of the Community Earth System Model (CESM) and two versions of NCAR’s Weather Research and Forecasting Model (WRF and CWRF) for high-resolution regional climate analyses. These model runs put us on the pathway for major international leadership in high-resolution climate modeling studies.

INTRODUCTION

This collaborative research used Blue Waters to address key uncertainties in numerically modeling the Earth’s climate system and accuracy in analyses of past and projected future changes in climate. Our studies used the latest versions of the Community Earth System Model (CESM), the Weather Research and Forecasting model (WRF), and the Climate-WRF (CWRF).

We explored the effect of external forcings (e.g., concentrations of greenhouse gases) on globally averaged temperature, focusing on uncertainties associated with the representation of processes and interactions between clouds, aerosols, and radiative transfer in the models and how these uncertainties influence the climate sensitivity.

Our second objective aimed to evaluate CESM with different model dynamical cores and the

effects of much higher horizontal (10–30 km) and vertical resolution. There is considerable evidence that increased resolution leads to better simulations of both transient small-scale activity (e.g., eddies and waves) and large-scale features of the mean climate.

We expect that results from our studies will be an integral part of the scientific analysis of climate change for the major international climate assessments (e.g., the follow-on to the Assessment Report 5, AR5, 2014) of the Intergovernmental Panel on Climate Change (IPCC), which will likely influence U.S. and international policies regarding the effects of human activities on the Earth’s climate, and provide supplementary data for use in various climate impact assessments at regional to local scales.

METHODS AND RESULTS

CESM

After tuning the physics and testing model settings of (the atmospheric portion of) CESM, we began a series of simulations that will support studies for the next Climate Model Intercomparison Project 6 (CMIP6), which is important to the next IPCC assessment of climate change.

Recent results from simulations that ran 1979 to the present suggested that the global number of tropical storms and hurricanes per year will decrease in a warming climate. However, the maximum intensity seemed to increase, meaning more major hurricanes (category 4 and 5). In the North Atlantic basin the RCP8.5 scenario showed a decrease in the number of tropical cyclones and hurricanes. The selection of a dynamical core can have a significant impact on tropical cyclone intensity and frequency even in the presence of similar climatology and large-scale environments [1]. For example, CAM5 with the spectral element (SE) core produced stronger cyclones, and therefore more hurricanes and major hurricanes per year, than CAM5 with the finite volume (FV) core (figs. 1–2). The exact causes for these differences is an area of continued work.

Compared to the out-of-box model, we improved the performance of CAM5 from 1.3 years/day to 2.5 years/day. Pat Worley (ORNL) and Ryan Mokos (NCSA) helped remove bottlenecks in MPI calls, while John Truesdale