The University of Oxford Department of Earth Sciences

EARTHSCIENCES

UNIVERSITY OF OXFORD

Atomic scale simulations to unlock isotopic fractionation in crystalising magma oceans (NONUNE ERC)

Supervisory Team

- **Dr Andrew Walker (https://www.earth.ox.ac.uk/people/andrew-walker/)**
- **Prof Tim Elliott (University of Bristol)**

Key Words **Deep Earth, mineral physics, geochemistry, mantle dynamics**

N.B. Funding from the European Research Council means that applicants of all nationalities are eligible for this project. Please contact us for further information regarding this funding.

Overview

In this project, you will make use of computer simulations of minerals and melts at the atomic scale to understand isotopic fractionation in the early Earth. As well as providing insights on early Earth history, your results will contribute to a larger multi-institutional research project probing Earth's evolution before plate tectonics.

The Earth's earliest history was punctuated by periods of global melting and the subsequent crystallization of planetary scale oceans of magma. Culminating in the Moon-forming giant impact and including the separation of the metallic core and silica rich crust from the mantle, understanding these early energetic processes is key to resolving the long-term evolution of our home planet including the onset of plate tectonics. These dramatic events are best recorded by isotopic anomalies in rock samples including those returned from lunar exploration and from ancient terrains exposed at the Earth's surface. Improving analytical techniques now make it possible to measure these anomalies with the precision needed to untangle the early history of our planet. However, because many of the fractionation processes leading to the generation of the isotopic anomalies happened at great depth, and at correspondingly high pressures and temperatures beyond those easily amenable to experiment, extracting meaning from these precise measurements is fraught with challenges (e.g. Young et al. 2015). In this project you will develop and make use of atomic scale techniques to simulate equilibrium isotope fractionation in crystallizing magma oceans at high temperature and pressure. You will then use these results to interpret isotopic measurements and constrain where and when the Earth's magma oceans solidified.

The project is fully funded for 4 years by an ERC grant. The successful candidate will be one of a cohort of three students contributing to this project.

Artist's impression of the moon forming giant impact that leading to the formation of a global magma ocean. NASA/JPL-Caltech, Public Domain.

The other students will research the history of continental growth by the analysis of detrital feldspars and numerical models of mantle convection as part of a multi-disciplinary endeavour to determine the onset of plate tectonics on Earth. As well as engaging in their own project, the successful candidate will closely interact with the other students, to help introduce them to atomic scale simulation and to learn from their expertise. This will involve regular meetings and extended exchanges between partners at Bristol (Tim Elliott) and ETH Zurich (Paul Tackley). We are therefore seeking candidates with specific enthusiasm for sophisticated computational modelling of isotope fractionation alongside a broad interest in solid Earth Sciences and motivation to gain a multi-faceted training in the field.

Methodology

The studentship will exploit advances in atomic scale simulation techniques, where the properties of Earth materials are predicted by considering the behaviour of the electrons, and improvement in the power and availability of high-performance computing. We will initially examine the controls on isotope fractionation between crystals at high pressure and temperature (e.g. Huang et al. 2013, 2014; Wu et al. 2015) before developing these approaches further to simulate fractionation between crystals and coexisting melts. The project will involve training in cutting edge atomic scale simulation techniques including density functional theory, lattice and molecular dynamics, as well as the development of scientific software and the use of supercomputers.

Timeline

Year 1: Doctoral training courses (optional), training in the use of density functional theory to simulate minerals at high pressure and temperature. Calculation of isotope fractionation between mantle minerals at high temperature and pressure.

Years 2 and 3: Training in the simulation of melts at high pressure and temperature. Development of a methodology for the determination of isotope fractionation between solids and co-existing melts. Application of this methodology to crystalising magma oceans. Presentation of research at national and international conferences

Year 4: Integration of results with those of other project students. Further data analysis leading to the publication of papers in international journals. Thesis completion. Presentation of results at an international conference.

Training & Skills

The supervisory team are leaders in computational mineral physics and its application to the interpretation of geological and geophysical processes (A. Walker) as well the use of isotope geochemistry to reveal the chemical evolution of the Earth (T. Elliott). The supervisory team undertaken significant collaboration to develop the tools needed to use computational mineral physics to understand the processes leading to isotopic fractionation at high pressure and temperature.

As part of this project you will learn how simulate minerals and melts at the atomic scale using density functional theory. Density functional theory is used extensively across a wide range of applications, from drug discovery and materials design to minerology and solid-state physics. This training will extend beyond the use of density functional theory to the ability to develop new approaches embodied as pieces of software.

As part of an interdisciplinary team, you will also develop the ability to collaborate with scientists with different backgrounds and who use different scientific approaches. You will develop these skills alongside other research students (at the Bristol University and ETH Zurich) and by working with other researchers contributing to the overall project.

References & Further Reading

F. Huang, L. Chen, Z. Wu, and W. Wang, First-principles calculations of equilibrium Mg isotope fractionations between garnet, clinopyroxene, orthopyroxene, and olivine: Implications for Mg isotope thermometry. *Earth and Planetary Science Letters* 367 (2013) 61 – 70

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E. D. Young, C. E. Manning, E. A. Schauble, A. Shahar, and C. A. Macris, High-temperature equilibrium isotope fractionation of non-traditional stable isotopes: Experiments, theory, and applications *Chemical Geology* 395 (2015) 176 – 195

Z. Wu, F. Huang, and S. Huang, Isotope fractionation induced by phase transformation: First-principles investigation for Mg_2SiO_4, *Earth and Planetary Science Letters* 409 (2015) 339 – 347

Further Information

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