Report on Visiting ERI

from Feiwu Zhang (visiting period: 2008/04/11 - 2008/08/10)

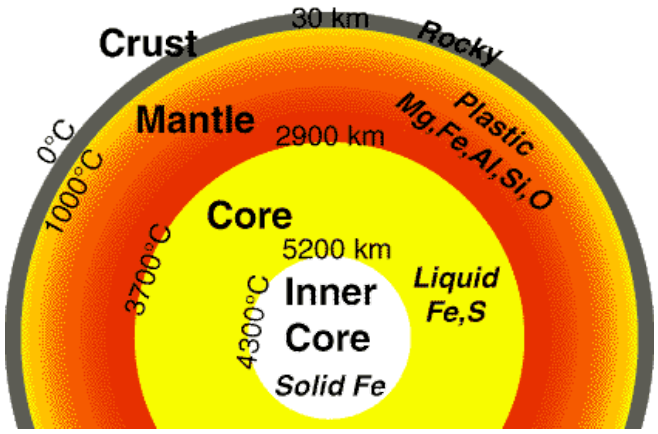
Feiwu Zhang, 2008/08/15

Introduction

I was invited by the office of International Earthquake and Volcano research promotion, ERI, the University of Tokyo (Director: Prof. Teruyuki KATO; Secretary: Tokie WATANABE) to have a research visiting at ERI from April 11 to August 10, 2008. During this period of visiting, I worked with Prof. Sun'ichi NAKAI on the project of "Investigations on core-mantle interaction by quantum-mechanics calculation."

Research background

The interaction at the core-mantle boundary (CMB) may involve disequilibrium chemical reactions and isotopic exchange, which may impart distinct isotopic and chemical signatures to the adjacent mantle. These phenomena are called as core-mantle interaction. Os and W isotope are good tracers of core–mantle interactions. They are used to detect the presence of core materials in the sources of some purported plumes that may have risen from the CMB. Professor Shun'ichi Nakai et al. at ERI experimentally measure W isotope ratio of Oceanic Island Basalt (OIB) of South Polynesia islands and a Hawaii island, Ontong Java Plateau of ODP samples. I will conduct quantum-mechanics calculations to simulate the elements partitioning between earth's outer core and lower mantle and the core-mantle material chemical reactions by sampling such as Os and W bearing minerals.



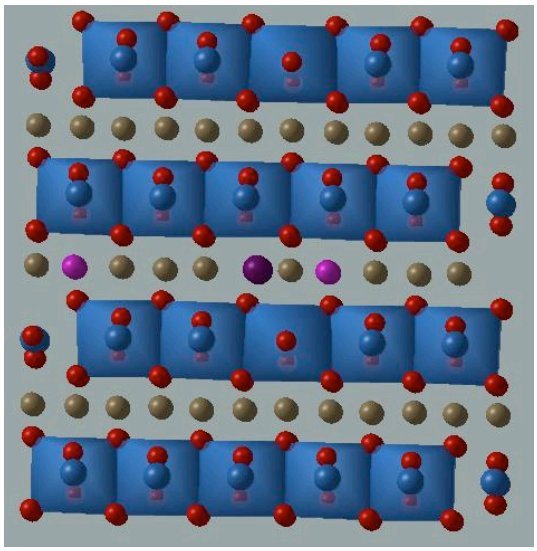
Research Activities

During my visiting period in ERI, I conducted the computer simulation research on the elements partitioning between the earth outer core and the Lower mantle at the

condition of 135 GPa and 3500 K. As compare with the previous work, I also performed the calculation on a modest temperature (2800K) and lower pressure (20 GPa). Most calculations are performed using density functional theory, a revolutionary formulation of quantum mechanics which gave its inventor, W. Kohn, a 1998 Nobel Prize in Chemistry. *Ab initio* molecular dynamics is the most powerful method available for studying highly anharmonic systems such as liquids, solids at high temperatures, dynamically disordered and soft-mode systems. The main tool is the state-of-the-art *ab initio* simulation packages VASP, which allows one to study large systems.

Besides to the daily research work, I had taken part in some scientific activities: such as seminars, laboratory tours, international conferences et al. The details will be shown in the following section.

Research Outcomes:



Based on the calculations on the systems of Co+Fe, Ni+Fe, Co+Ni+Fe, Os+Fe, Os+W+Fe, Pt+W+Fe, W+Fe, W+Co+Ni+Fe and the systems of Co+$MgSiO_3$, Ni+$MgSiO_3$, Co+Ni+$MgSiO_3$, Os+$MgSiO_3$, Os+W+$MgSiO_3$, Pt+W+ $MgSiO_3$, W+$MgSiO_3$, W+Co+Ni+$MgSiO_3$. I got the opportunity to take the insight to the elements behaviors in the Earth outer core and lower mantle. The graph shows the structure of Os and W bearing $MgSiO_3$ post-perovskite. The calculations gave the information about the elements distribution and diffusion within the Fe systems as well as the $MgSiO_3$ systems under the CMB conditions. Further results and discussions are being developed.

I had given (a) seminar talks within ERI work group and at the Whole Solid Earth Colloqium in the department of Earth and Planetary Science; (b) Poster presentation at the international conference on Quantum Simulators and Design 2008 held in Tokyo on May 31 to Jun. 3.

Acknowledgment

I would like to thank the office of International Earthquake and Volcano research promotion, for inviting me visit ERI, the University of Tokyo during the period of April 11 to August 10, 2008. Especially thanks to Prof. Teruyuki Kato and Ms. Tokie Watanabe for their work and help in the paperwork and all the information supplies. Thanks also should come to Prof. Sun'ichi Nakai as my host in ERI for his friendly host and kindly help in Tokyo. I am appreciating to the discussion and work with Prof. Nakai and his group. The life and research environment left me very deep impression. The convenience and the service supplied by the Japanese society made me much easy during my stay in Tokyo. I am looking forward to coming back and visiting ERI again in the near future.

CV of Feiwu Zhang

Feb. 2005 – April. 2008	PhD. Department of Materials, ETH Zurich, Switzerland. Computer simulation studies of minerals in the Earth's deep interior.
April. 2008 - Aug. 2008	Visiting Researcher. ERI. The University of Tokyo. Investigations on core-mantle interaction by quantum-mechanics calculation.
July 2008 – June 2010	Research Fellow, Nanochemistry research Institute. Curtin University of Technology. Perth. Australian. Defects and Deformation in Olivine: From Molecules to Mantle".