Research plan at Institute for Study of the Earth's Interior (ISEI), Okayama University, Japan

Research Theme: Effect of temperature, pressure, Fe content and oxygen fugacity on the electrical conductivity of orthopyroxene

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2016.1.22

Content

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Speciality

Geophysics

Research Interest

Electrical properties of minerals; Shear deformation; Diffusion

Education

Sep., 2004 – Dec., 2009 : Ph.D., University of Science and Technology of China (USTC).

Sep., 1998 – July, 2002 : B.S., Department of Physics, Northwest University

Professional Record

July, 2002 –Dec., 2007 : Assistant, Hefei University of Technology, China

Jan., 2008 – Mar., 2011: Lecturer, Hefei University of Technology, China

Apr., 2011 – June, 2014: Postdoc, Institute for Study of the Earth's Interior (ISEI), Okayama University, Japan

July, 2014 – : Professor, "1000Plan Program for Young Talents" of Chinese government
Institute of Geochemistry, Chinese Academy of Sciences, P. R. China

Research Project

1. Jan., 2015—Dec., 2017: A thermodynamic approach for calculating the diffusion coefficients in mantle minerals and rocks and its applications in geoscience, **Natural Sciences Foundation of China (NSFC), No. 41303048.** **(Principal)**
2. Jan., 2016—Dec., 2018: 1000Plan Program for Young Talents, **Department of Organization of the People's Republic of China.** **(Principal)**

Honors and Awards

2014 Excellent Doctoral Dissertation Award of Anhui Province

2008 ZhuLiYueHua Award for Graduate Student of Chinese Academy of Sciences (CAS)

List of Publications (selected)

1. Zhang B.H., Shan S.M., Wu X.P., 2016. Modeling H, Na, and K diffusion in plagioclase feldspar by relating point defect parameters to bulk properties, *Physics and Chemistry of Minerals*, in press, doi: 10.1007/s00269-015-0782-5.
2. Zhang B.H., Shan S.M., 2015. Application of the cBΩ model to the calculation of diffusion parameters of Si in silicates, *Geochemistry Geophysics Geosystems* 16, 705-718. doi:10.1002/2014GC005551.
3. Zhang B.H., Shan S.M., 2015. Thermodynamic calculations of Fe–Mg interdiffusion in $(Mg,Fe)_2SiO_4$ polymorphs and perovskite, *Journal of Applied Physics* 117(5), 054906.
4. Zhang B.H., Yoshino T., Yamazaki D., Manthilake G., Katsura T., 2014. Electrical conductivity anisotropy of partially molten peridotite under shear deformation, *Earth and Planetary Science Letters* 405, 98-109.
5. Zhang B.H., 2014. Calculation of self-diffusion coefficients in iron, *AIP Advances* 4(1), 017128.
6. Zhang B.H., Wu X.P., 2013. Diffusion of aluminum in MgO: A thermodynamic approach, *Chinese Physics B* 22(5), 056601.
7. Zhang B.H., Yoshino T., Wu X.P., Matsuzaki T., Shan S.M., Katsura T., 2012. Electrical conductivity of enstatite as a function of water content: Implications for the electrical structure in the upper mantle, *Earth and Planetary Science Letters* 357-358, 11-20.
8. Zhang B.H., Wu X.P., 2012. Calculation of self-diffusion coefficients in diamond, *Applied Physics Letters* 100(5), 051901.
9. Zhang B.H., Wu X.P., Zhou R.L., 2011. Calculation of oxygen self-diffusion coefficients in Mg_2SiO_4 polymorphs and $MgSiO_3$ perovskite based on the compensation law, *Solid State Ionics* 186(1), 20-28.
10. Zhang B.H., Wu X.P., 2011. Prediction of self-diffusion and heterodiffusion coefficients in zircon, *Journal of Asian Earth Sciences* 42(1-2), 134-141.
11. Zhang B.H., Wu X.P., Xu J.S., Katsura T., Yoshino T., 2010. Electrical conductivity of enstatite up to 20 GPa and 1600 K, *Chinese Journal of Geophysics* 53(3), 760-764
12. Zhang B.H., Wu X.P., Xu J.S., Zhou R.L., 2010. Application of the cBΩ model for the calculation of oxygen self-diffusion coefficients in minerals, *Journal of Applied Physics* 108(5), 053505.

Research report for Zhang Baohua in 2015

In 2015, my research is mainly concentrated on understanding the highly anisotropic conductivity revealed by magnetotelluric (MT) investigations in the upper mantle, and predicting the diffusion coefficient of mantle minerals by means of a thermodynamic model. Thus the details of these two contents are described as following:

I. Electrical conductivity measurement of partially molten peridotite under shear deformation

Partial melting hypothesis is considered as the most reasonable interpretation on a high-conductivity layer (HCL) with high anisotropy characterized by higher conductivity in the direction parallel to plate motion revealed by ocean floor magnetotelluric (MT) investigations in the oceanic upper mantle (Evans et al., 2005; Naif et al., 2013). In order to verify this issue, I have conducted electrical conductivity measurement of partially molten peridotite under shear deformation during the period of my postdoctoral fellow in Misasa (from April 1st of 2011 to April 1st of 2014). Our experimental results demonstrated that horizontal electrical conductivity anisotropy revealed by magnetotelluric surveys in the oceanic asthenosphere can be well explained by the realignment of partial melt induced by shear stress (Zhang et al., 2014).

Although recent experimental findings are exciting and important, however, some problems in our previous project and others are still needed to be clarified further. For instance, the effect of melt fraction on the electrical conductivity of partial molten peridotite is unclear. The minimum volume fraction for melt to produce the anisotropic conductivity in the upper mantle still remains poorly constrained. In addition, melt distribution also would vary with melt fraction under shear deformation. To solve these difficulties, I visited ISEI again (from August 2st of 2015 to September 15st of 2015), and performed in situ 3D electrical conductivity of partially molten KLB-1 peridotite during deformation in simple shear at 1 GPa in a DIA type apparatus. The conductivity measurements were performed simultaneously in two directions of three principal axes: parallel and normal to the shear direction on the shear plane, and perpendicular to the shear plane, by using impedance spectroscopy at temperature ranges of 1483-1548 K in a frequency range from 0.1 Hz to 1 MHz. Our results show that the melt fraction, the absolute conductivity values, and the degree of electrical anisotropy of partially molten KLB-1 peridotite systematically increases with temperature. Microstructural observations of the recovered samples suggest that the development of conductivity anisotropy was caused by the realignment of partial melt parallel to the shear direction. Our experiments were very successful and the corresponding papers are now in preparation or in review:

(1)Zhang B.H., Yoshino T., 2016. New constrains on the melt fraction in the oceanic upper mantle inferred from in-situ 3D conductivity measurements, Manuscript in preparation.

(2)Zhang B.H., Yoshino T., 2016. Effect of graphite on the electrical conductivity of the lithospheric mantle. Physics of the Earth and Planetary Interiors, in review.

II. Thermodynamic calculation of diffusion coefficient in minerals

On the basis of a thermodynamical model, termed the cBΩ model, we develop a new approach to predict the various elements diffusion coefficients in minerals. Our results show that the absolute Si, Fe-Mg, H, Na, K, Cl diffusion rates derived from the cBΩ model are in agreement with experimental data in a variety of rock-forming minerals including $(Mg,Fe)_2SiO_4$ polymorphs, perovskite, feldspar and NaCl.

(1) Zhang B.H., Shan S.M., 2015. Application of the cBΩ model to the calculation of diffusion parameters of Si in silicates. Geochemistry Geophysics Geosystems, 16(3), 705-718, doi:10.1002/2014GC005551

(2)Zhang B.H., Shan S.M., 2015. Thermodynamic calculations of Fe–Mg interdiffusion in $(Mg,Fe)_2SiO_4$ polymorphs and perovskite. Journal of Applied Physics, 117(5), 054906, doi: 10.1063/1.4907576

(3)Zhang B.H., Shan S.M., Wu X.P., 2016. Modeling H, Na, and K diffusion in plagioclase feldspar by relating point defect parameters to bulk properties. Physics and Chemistry of Minerals, in press, doi: 10.1007/s00269-015-0782-5

(4)Zhang B.H., Li C.B., Shan S.M., 2016. Thermodynamic calculation of self-diffusion in sodium chloride. Physics and Chemistry of Minerals, accepted

Research plan at Institute for Study of the Earth's Interior (ISEI), Okayama University, Japan

1. Research Theme:

Effect of temperature, pressure, Fe content and oxygen fugacity on the electrical conductivity of orthopyroxene

2. Background for Research Theme:

Electrical conductivity is a physical parameter that can be characterized, along with electromagnetic surveys and seismic wave velocities, from measurements at the Earth's surface. A comparison of geophysical models with mineral properties would provide important constraints for mineralogical and compositional models of the Earth's mantle, as well as that of other planets. Therefore, in situ laboratory measurements of the electrical conductivity of the major mantle phases under HP-HT and controlled thermodynamic conditions are very important for our construction of the conductivity-depth profile and interpretation of the recent electrical anisotropy observations by MT in the upper mantle (Evans et al., 2005; Naif et al., 2013).

Electrical properties of minerals and rocks are highly sensitive to many factors such as temperature, pressure, oxygen fugacity (fO_2), Fe content, water (H_2O) content, electronic spin-state transitions, melting, and so on. To evaluate the influence of these factors on the electrical conductivity quantitatively, careful laboratory investigation and novel experimental design are required to distinguish each of them. Although temperature dependence of the electrical conductivity of mantle minerals has been determined precisely, pressure dependence has not been studied in detail. Due to wide pressure range for stability of the major silicate minerals, such as olivine, pyroxene, garnet, bridgmanite, knowledge of the pressure dependence of the electrical conductivity of mantle minerals is also important for the construction of a reference conductivity-depth profile. The electrical conduction mechanisms of the main iron-bearing mantle minerals are considered to be hopping of small polarons associated with the charge transfer between Fe^{2+} and Fe^{3+}. Many workers (Xu et al., 2000; Yoshino, 2010) have shown that hopping conduction is characterized by a low activation energy (1–1.8 eV), but their activation volumes have opposite signs. For example, Yoshino et al. (2012) observed a negative activation volume (-0.3~-0.7 cm^3/mol) for olivine, whereas a positive one (+0.6 cm^3/mol) was reported by Xu et al.

(2000) and Dai et al. (2010). Thus, at present we have no reasonable consensus for the pressure dependence of the electrical conductivity of ferromagnesian minerals. In order to obtain a better understanding of the electrical conductivity of ferromagnesian minerals, we need further studies on the pressure dependence of the electrical conductivity, especially for orthopyroxene.

Iron is the most abundant transition metal in the Earth. The upper mantle, which is mainly composed of $(Fe,Mg)_2SiO_4$ olivine and $(Fe,Mg,Al)_2(Si,Al)O_3$ pyroxene, constitutes more than 80% of the Earth upper mantle's volume and plays an important role in the evolution and dynamics of the mantle. Generally, the electrical conductivity is depended on the number of charge carriers and its mobility. In the case of Fe-bearing silicate minerals, the density of charge carriers is related to Fe content (i.e., $Fe^{3+}/\sum Fe$). As the concentration of $Fe^{3+}/\sum Fe$ is controlled by oxygen fugacity, consequently, the conductivity of iron-bearing silicate minerals should be strongly controlled by the total Fe content and $Fe^{3+}/\sum Fe$ (i.e., oxygen fugacity) (Yoshino et al., 2012).

Oxygen fugacity, fO_2, is another important factor affecting the experimental results of electrical conductivity measurements of minerals and rocks that contain valence variable elements. Oxygen fugacity not only drives redox reactions, element partitioning, and structural phase transitions, but also controls certain transport electrical properties and rheological properties, especially in minerals such as silicates and oxides in which oxygen vacancies play a major role in these processes. Currently, the ability to adjust the oxygen fugacity in multi-anvil apparatuses has become a hotspot of high pressure research. For most traditional conductivity experiments, it is often difficult to control fO_2 during high-pressure processes due to a number of prohibitive restrictions, including the selected buffer pairs have a limited adjustment range of oxygen fugacity and the difficulty of implementing control in an actual high-pressure apparatus. Nevertheless, little is known about the relationship between the electrical conductivity of orthopyroxene and oxygen fugacity at high pressure, as well as Fe content.

Orthopyroxene is the second abundant constituent mineral of the shallow upper mantle, which constitutes about 20-40% of the minerals in the upper mantle. Thus, knowledge of how its electrical properties vary as a function of pressure, temperature, oxygen fugacity and chemical composition can be important in interpreting the mantle's electrical conductivity profile. However, electrical conductivities of the orthopyroxene system have not been studied as thoroughly as the olivine system. Most previous measurements of the electrical conductivity of orthopyroxene only considered the effect of chemical composition (Seifert et al., 1982) and water content (Dai and Karato, 2009; Yang et al., 2012, Zhang et al., 2012). Until now, no systematic data have been reported on the conductivity of orthopyroxene as a function of temperature, pressure, Fe content and oxygen fugacity. Such precise conductivity data obtained in the laboratory are essential for interpreting the field results obtained by geomagnetic depth sounding and magnetotelluric surveys, and also can provide constraints on the mineralogy, chemical composition, thermal structure, thermodynamic state, water distribution, and partial melting of the Earth's interior.

In this study, we will measure the electrical conductivity of anhydrous orthopyroxene with various iron contents (X_{Fe}=0, 0.1, 0.2, 0.3, 0.5, 0.7, 1.0) over a wide range of pressure (P), and temperature (T) and oxygen fugacity (fO_2) covering the stability field of orthopyroxene. Our results are important to understand the conduction mechanism and the origin of the mantle high conductivity layer, and also to provide some constraints on temperature, oxygen fugacity, chemistry and the conductivity-depth profile in the Earth's upper mantle. My research plan is as follows.

3. Proposed Plan:

1) Synthesis of anhydrous orthopyroxene with different Fe content (X_{Fe}=0, 0.1, 0.2, 0.3, 0.5, 0.7, 1.0)
2) In situ conductivity measurements under high pressure and high temperature
   (a) Impedance measurements on the orthopyroxene as a function of T and P;
   (b) Impedance measurements on the orthopyroxene as a function of fO_2;
3) Post-experimental analysis

   The orthopyroxene samples is analyzed using backscatter electron imaging, X-ray diffraction, electron microprobe analyzer (EPMA) and FT-IR before and after the conductivity measurements.

4. Expected Results and Impacts:

In situ laboratory measurements of the electrical conductivity of orthopyroxene as a function of temperature, pressure, Fe content and oxygen fugacity in conjunction with conductivity depth profiles of the mantle derived from electromagnetic data can provide important constraints on mineralogy, chemistry, thermal structure, thermodynamic state, water distribution, redox state, and partial melting of the Earth's interior. Therefore, the present project must not be important only for the electrical conductivity world but must be significant for all the solid geophysics.

5. A proposed research plan that includes what type of facilities is required:

High pressure facilities:

KAWAI-type multi-anvil high-pressure apparatus; Piston cylinder apparatus

Measurement and analysis facilities:

Solartron 1260 impedance/Gain-Phase Analyzer, Solartron 1296 interface;

Optical microscopy; Scanning electron microscopy (SEM); Infrared absorption spectroscopy (FT-IR); X-ray diffraction; electron microprobe analyses (EPMA); and so on.

6. Desired stay period

May to June 2016.

Reference:

Dai L.D., Karato S., 2009. Electrical conductivity of orthopyroxene: implications for the water content of the asthenosphere. Proc. Jpn. Acad. Ser. B 85, 466–475.

Dai L.D., Li H.P., Liu C., Hu H.Y., Shan S.M., 2010. The electrical conductivity of dry polycrystalline olivine compacts at high temperatures and pressures. Mineral. Mag. 74, 849–857.

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Naif S., Key K., Constable S., Evans R.L., 2013. Melt-rich channel observed at the lithosphere–asthenosphere boundary. Nature 495, 356–359.

Seifert K.F., Will G., Voigt R., 1982. Electrical conductivity measurements on synthetic pyroxenes $MgSiO_3$-$FeSiO_3$ at high pressures and temperatures under defined thermodynamic conditions, in High-pressure Researches in Geoscience, edited by W. Schreyer, pp. 419–432, Schweizerbart'sche, Stuttgart, Germany.

Xu Y.S., Shankland T.J., Duba A.G., 2000. Pressure effect on electrical conductivity of mantle olivine. Phys. Earth Planet. Int. 118, 149–161.

Yang X.Z., Keppler H., McCammon C., Ni H.W., 2012. Electrical conductivity of orthopyroxene and plagioclase in the lower crust. Contrib. Mineral. Petrol. 163, 33–48.

Yoshino T., 2010. Laboratory electrical conductivity measurement of mantle minerals. Surv. Geophys. 31, 163–206.

Yoshino T., Shimojuku A., Shan S.M., Guo X.Z., Yamazaki D., Ito E., Higo Y., Funakoshi K., 2012. Effect of temperature, pressure and iron content on the electrical conductivity of olivine and its high-pressure polymorphs. J. Geophys.

Res. 117, B08205.
Zhang B.H., Yoshino T., Wu X.P., Matsuzaki T., Shan S.M., Katsura T., 2012. Electrical conductivity of enstatite as a function of water content: Implications for the electrical structure in the upper mantle. Earth Planet. Sci. Lett. 357–358, 11–20.