Hydrostaticity and Equation of states of NaCl, KCl, KBr up to 70 GPa at room temperature

KAMADA, Seiji[1]* ; MAEDA, Fumiya[2] ; TAKAHATA, Akihiro[2] ; AMAIKE, Yohei[2] ; OHTANI, Eiji[2] ;
HIRAO, Naohisa[3] ; OHISHI, Yasuo[3]

[1]FRIIS, Tohoku Univ., [2]Dept, Earth Sci., Grad. School of Sci. Tohoku Univ., [3]JASRI

Recently, the high pressures and temperatures corresponding to the inner Earth's core have been achieved due to the progress of the experimental techniques (e.g., Tateno et al., 2010). To understand the physical properties of the Earth's core, it is essential to perform high pressure and temperature experiments. Fiquet et al. (2001) reported first results on sound velocities of Fe by an inelastic X-ray measurement over 100 GPa. Antonangeli et al. (2004) and Ohtani et al. (2013) also reported sound velocities of Fe over 100 GPa. Fiquet et al. (2001) reported slow sound velocities above 100 GPa due to preferred orientation of iron. They concluded the preferred orientation was caused by a uniaxial compression using a diamond anvil cell and slow sound velocities propagated along c-axis were observed. Therefore, hydrostatical compression is essential to avoid texturing of the samples and understand physical properties under high pressure.

To produce hydrostatic condition under high pressures, some liquid pressure media have been used, such as 4:1 (in volume ratio) Methanol Ethanol mixture (ME), 16:3:1 (in volume ratio) Methanol Ethanol Water mixture (MEW). Those materials are solidify at around 10 GPa. Therefore, the hydrostatic conditions are limited up to 10 GPa. Noble gases are also used as pressure media. He is solidified at 12 GPa and Ne is solidified at 5 GPa. They show hydrostatic behavior up to 40 and 20 GPa, respectively. Although they are good material to produce hydrostatic compressions, ME and MEW are reactive under high temperature and the noble gases require a special equipment to load them into a sample chamber. In this study, we employed alkali halides (NaCl, KCl, KBr) as pressure media, which are relatively soft and are expected to produce pseudo hydrostatic condition.

A foil made from powdered Au was used as a pressure scale (Fei et al., 2007) and a laser absorber. The foil was embedded between alkali halides pellets which served as pressure media and thermal insulators. A symmetric diamond anvil cell was used to generate high pressure. A double-sided laser heating method using fiber lasers was used for annealing the Au foil under high pressures for 10 min. Experimental pressure was imposed to the sample every a few GPa step and its X-ray diffraction (XRD) patterns were taken at room temperature. At 50 GPa and 70 GPa, the sample was annealed in order to reduce stress in the chamber. XRD patterns were taken before and after annealing. All XRD patterns were taken at BL10XU of SPring-8, Japan (Ohishi et al. 2008). The diameter of the X-ray beam was collimated to be 20 μm. The volume of Au at ambient pressure was measured to be 67.69(5) $\mathring{A}^3$ (a=4.0755(9) $\mathring{A}$) at the BL10XU, SPring-8. The gold volume obtained here was used for V_0 in the equation of state for Au to calculate experimental pressures.

We have obtained XRD patterns from the samples between 1 and 70 GPa and annealed the samples at 2000 K at 50 and 70 GPa. KCl, KBr, and NaCl transformed from B1 to B2 phase at 2.6, 2.8, and 32.6 GPa, respectively. The standard deviations of the pressure distributions in the chamber decreased slightly due to the transformations. The pressure standard deviations increased from 0.1 GPa at 1 GPa to 0.2 GPa at 20 GPa. After further compressions, the pressure distributions of Au in NaCl was almost constant but those in KCl and KBr increased up to 0.8 GPa and 1.2 GPa, respectively. After annealing at 50 GPa, the pressure distributions slightly reduced in KCl and KBr but they increased in NaCl. The compression behaviors of KCl and KBr are in good agreement with Dewaele et al. (2012) and those of NaCl are consistent with Dorfman et al. (2012).

Keywords: equation of state, hydrostatic compression, alkali halides, high pressure

Jadeite in shocked meteorites: various textures and formation processes

OZAWA, Shin[1*] ; MIYAHARA, Masaaki[2] ; OHTANI, Eiji[1] ; ITO, Yoshinori[1] ; SUZUKI, Akio[1] ;
KIMURA, Makoto[3] ; KOROLEVA, Olga N.[4] ; LITASOV, Konstantin[5] ; POKHILENKO, Nikolay P.[5]

[1]Department of Earth Science, Graduate School of Science, Tohoku University, Sendai 980-8578, Japan, [2]Department of Earth and Planetary Systems Science, Graduate School of Science, Hiroshima University,, [3]Faculty of Science, Ibaraki University, Mito 310-8512, Japan, [4]Institute of Mineralogy, UB RAS, Miass, 456317, Russia, [5]V. S. Sobolev Institute of Geology and Mineralogy, SB RAS, Novosibirsk, 630090, Russia

Introduction

Collision of materials is one of the most fundamental processes in planet formation of the early solar system. Heavily-shocked meteorites sometimes contain high-pressure minerals, which provide important constraints on the nature of the impact events. Jadeite is a high-pressure mineral identified in various types of meteorites such as H, L and LL chondrites, and Martian meteorites [1-8]. Here, we show various occurrences of jadeite observed in shocked meteorites, and discuss the conditions and mechanisms of jadeite formation.

Results and Discussions

Heavily-shocked ordinary chondrites (H, L and LL) were mainly observed in our studies. They consist of chondritic host-rock and pervasive shock-induced melt veins (SMVs). Jadeite is usually identified in fragments of the host-rock entrained to the SMVs. Albitic feldspar grains in these fragments have been replaced by jadeite plus amorphous material.

A variety of texture was observed in jadeite-bearing grains of Sahara 98222 L6 chondrite, such as "particle-like" , "stringer-like" , and "polycrystalline-like" phases [4]. Similar textures were also reported in jadeite-bearing grains of other L and H ordinary chondrites [5], and shocked rocks from Ries crater, Germany [7]. Detailed TEM observations by Miyahara et al. [5] clarified that these jadeite-bearing grains consist of massive or network-like assemblages of jadeite crystals and interstitial amorphous (or poorly-crystallized) materials. Bulk chemical compositions of the jadeite-bearing grains are almost identical to that of albitic feldspar in the host-rocks. Therefore, the jadeite described above is considered to have formed by solid-state reactions.

On the other hand, we recently found a new occurrence of jadeite in Chelyabinsk LL5 chondrite [8]. Needle-like or skeletal-rhombic crystals of jadeite coexist with amorphous material. The bulk chemical compositions of the jadeite-bearing grains are different (more K-rich) from that of albitic feldspar in the host-rock. In addition, jadeite-rich part is enriched in Na, whereas the amorphous part is highly enriched in K. The significant element migrations appear to be difficult in solid-state reactions during a short duration of an impact. Thus, jadeite in Chelyabinsk meteorite is considered to have crystallized from feldspathic melt.

It is experimentally revealed that albite dissociate into jadeite plus silica phase over 3 GPa, and jadeite can be stable at 3-19 GPa as a liquidus or subsolidus phase [9-14]. The two types of jadeite formation (from solid or melt) were probably caused by different temperature conditions. For the jadeite formed by solid-state reactions, the temperature is considered to have been lower than at least 1400 ℃, the melting temperature of albite at 3 GPa [10,11]. For the jadeite formed from melt, the temperature could have been higher than 1400 ℃. The different textures and chemical compositions of the jadeite-bearing grains reflect different P-T-t (Pressure-Temperature-time) conditions during the impact events on different parent bodies of the meteorites.

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Keywords: jadeite, meteorite, impact, high-pressure mineral, shock melt vein, formation mechanism

Viscosity and structure of anorthite melt under high pressure and high temperature conditions

SAKAMAKI, Tatsuya[1]* ; KONO, Yoshio[2]

[1]Department of Earth and Planetary Materials Science, Tohoku University, [2]HPCAT, Geophysical Laboratory, Carnegie Institution of Washington

The viscosity and structure of the anorthite ($CaAl_2Si_2O_8$) melt has been measured up to 6.1 GPa and 2173 K using the in-situ falling sphere method with X-ray radiography for viscosity and energy-dispersive X-ray diffraction technique for structure at beamline 16-BM-B of the Advanced Photon Source. The viscosity of the melt decreases with pressure up to 4 GPa, and then increases. The viscosity and its pressure dependence of anorthite melt are smaller than albite melt, which is also fully polymerized melt. Obtained structural information support the difference in viscosity behavior between anorthite and albite melts. Anorthite melt shows a smaller shift of the first sharp diffraction peak (FSDP) in the structure factor, S(Q), to higher-Q with pressure than albite one, indicating the pressure-induced structural shrinkage of an intermediate-range order is small. The radial distribution function, G(r), of anorthite melts exhibits the longer T-O distance, which is the length between tetrahedrally coordinated cations and oxygen. The TO_4 tetrahedra are the most fundamental units in the silicate melts, and the T-O distance reflects strength of the units. Thus, anorthite melt initially shows the low viscosity due to longer T-O distance. On the other hand, a pressure dependence of T-T distance in anorthite melt is smaller than albite one, and T-O-T angle is also small.

Keywords: viscosity, structure, anorthite melt, albite melt, high pressure

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The effect of Ni and C on sound velocity of liquid Fe at high pressure

KUWABARA, Soma[1] ; TERASAKI, Hidenori[1*] ; SHIMOYAMA, Yuta[1] ; NISHIDA, Keisuke[2] ; HIGO, Yuji[3] ;
TAKUBO, Yusaku[1] ; SHIBAZAKI, Yuki[4] ; TAHARA, Masaki[4] ; IGARASHI, Mako[4] ; SAKAMAKI, Tatsuya[4] ;
TANGE, Yoshinori[3] ; KONDO, Tadashi[1]

[1]Department of Earth and Space Science, Osaka University, [2]Department of Earth and Planetary Science, The University of
Tokyo, [3]Japan Synchrotron Radiation Research Institute, [4]Department of Earth and Planetary Materials Science, Tohoku University

Nickel is a highly plausible element in the terrestrial core together with iron. However, the effect of Ni on elastic properties of
liquid Fe at high pressure has not been reported. It is important to study the effect of Ni together with light elements on the sound
velocity of liquid Fe to give a constraint on the liquid core composition of terrestrial planets by comparing with the observed
seismic data. In this study, we focused on the effect of Ni and C on the P-wave velocity and elastic properties of liquid Fe up to
6.5 GPa.

High pressure experiments were carried out using 1500 ton Kawai-type multi-anvil press at BL04B1 beamline, SPring-8
synchrotron facility. P-wave velocity (V_P) was measured using pulse-echo overlap method. Used sample compositions were
Fe-10wt%Ni and Fe-10wt%-4wt%C. The sample pellet was sandwiched by single crystal sapphire buffer rods for the V_P measurement. The experimental pressures and temperatures were determined based on lattice volumes of MgO and BN, which were
used as a pressure marker, combined with their equations of state. The measurements were performed up to 6.5 GPa and 2100 K.

Obtained VP of liquid Fe-Ni is located slightly lower and aligned almost parallel to the V_P curve of liquid Fe as a function
of pressure. This suggests that alloying 10 wt% of Ni into liquid Fe slightly decrease the V_P but little influence on the bulk
modulus and its pressure dependence. Alloying C slightly increases the V_P of liquid Fe and it is also found that the effect of
temperature on the V_P is not negligible. In the presentation, we will compare these results with the reported results of other light
element such as S in the sound velocity-density relation (Birch plot) and discuss a clue to constrain the core composition of small
terrestrial planets.

Keywords: Sound velocity, Fe alloy, Core, High pressure

Melting relationships in the Fe-S-Si system at high pressure and temperature

SAKAIRI, Takanori[1]* ; OHTANI, Eiji[1] ; SAKAI, Takeshi[2] ; KAMADA, Seiji[1] ; SAKAMAKI, Tatsuya[1] ;
HIRAO, Naohisa[3]

[1]Graduate school of Science, Tohoku Univ., [2]Geodynamics Research Center, Ehime Univ., [3]JASRI

It is widely accepted that the Earth's core is mainly composed of iron and contains light elements to account for its density deficit. Alloying with light elements significantly affects the physical properties of iron and depresses its melting temperature. Therefore, the melting relation of the Fe-light elements system is the key to clarify the thermal structure of the Earth's core. Although there are many candidates for light elements in the core, sulfur and silicon are considered to be the major light elements. Some geochemical models predicted that sulfur and silicon could be present not only in the core of the Earth but also in the core of other terrestrial planets such as Mars and Mercury. In spite of the importance of the effect of sulfur and silicon on the physical properties of iron, there are few previous reports and the melting relationships in the Fe-S-Si system at high pressure were not revealed in details. To better understand the properties of the planetary cores, we investigated the melting relationships of the Fe-S-Si system under high-pressure conditions.

Here, we report the phase relationships and melting temperatures in the Fe-S-Si system up to 60 GPa. Melting experiments were performed in the pressure range of 20-60 GPa and the temperature range of 1300-2500 K using a double-sided laser-heated diamond anvil cell combined with X-ray diffraction technique. The sample compositions used in this study were $Fe_{80.1}S_{12.7}Si_{7.2}$ (Fe-8wt.%S-4wt.%Si) and $Fe_{74.4}S_{18.5}Si_{7.1}$ (Fe-12wt.%S-4wt.%Si). In situ X-ray diffraction experiments were conducted at the BL10XU beamline of the SPring-8 facility. The melting detection was based on disappearance of the X-ray diffraction peaks of the sample. On the basis of X-ray diffraction patterns, we confirmed that iron-silicon alloy which hcp and fcc structure and Fe_3S are stable phases under subsolidus conditions. Because of dissolution of silicon into iron, the boundary of fcc and hcp phase of this study shifts towards higher pressure compared to that of pure iron. Both solidus and liquidus temperatures are significantly lower than the melting temperature of pure Fe and increases with pressure in this study. In addition, the present melting curve is lower than the melting temperature of the Fe-Si system reported by Asanuma et al. (2010) and slightly lower than the eutectic temperature of the Fe-Fe_3S system (Kamada et al., 2012) and that of the Fe-O-S system (Terasaki et al., 2011). In order to draw the melting curve as a function of pressure, we fitted the present results using the Simon's equation. The obtained fitting parameters are T_{mR} =1277(6), a=116.1(21) and c=1.06(2) for the solidus and T_{mR} =1582(13), a=127.9(48) and c=1.00(3) for the liquidus. Because sulfur and silicon are the candidates for the light elements in the cores of Earth, Mars, and Mercury (e.g., Malavergne et al., 2007), the present results on the solidus and liquidus temperatures can be applicable to the core formation processes in the Earth, Mars, and Mercury.

Keywords: Core, Melting relationships, Diamond Anvil Cell, Light elements, Fe-S-Si system

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Sound velocity measurements of solid iron under high pressure and high temperature using an ultrasonic method

SHIBAZAKI, Yuki[1]* ; NISHIDA, Keisuke[2] ; HIGO, Yuji[3] ; IGARASHI, Mako[4] ; TAHARA, Masaki[4] ;
SAKAMAKI, Tatsuya[4] ; TERASAKI, Hidenori[5] ; SHIMOYAMA, Yuta[5] ; KUWABARA, Souma[5] ; TAKUBO, Yusaku[5] ;
OHTANI, Eiji[4]

[1]Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, [2]Department of Earth and Planetary Science, The University of Tokyo, [3]Japan Synchrotron Radiation Research Institute, [4]Department of Earth and Planetary Material Sciences, Tohoku University, [5]Department of Earth and Space Science, Osaka University

The Earth's interior has been directly investigated by seismic wave propagation and normal mode oscillation. Based on those observations, the distributions of density and sound velocity of the Earth's interior have been estimated (e.g. PREM). The core, which is located at the center of the Earth, is believed to consist of metallic iron with a certain amount of light elements, such as hydrogen, carbon, oxygen, silicon, and sulfur. A large number of experiments on the compressibility of iron and iron-light element alloys have been carried out in order to constrain the abundances of the light elements in the core. In the past fifteen years, the sound velocities of the iron and iron alloys have also been measured intensively at high pressure. Although the sound velocity consists of longitudinal (V_P) and transverse (V_S) components, most discussions about the core composition have been based on the only V_P data because of the technical issues of the high-pressure experiments. In order to estimate the abundances of the light elements more correctly, the precise measurement of V_S as well as V_P is necessary. In this study, we measured the V_P, V_S, and density of solid iron under high-pressure and high-temperature conditions using an ultrasonic method, and X-ray radiography and diffraction techniques.

Simultaneous ultrasonic measurements, and X-ray radiography and diffraction experiments were carried out at BL04B1 beamline, SPring-8 in Japan. High-pressure and high-temperature were generated using a 1500-ton Kawai type multi-anvil apparatus installed at BL04B1 beamline. The experimental conditions were up to 7 GPa and 800 K (stability field of bcc-Fe). The Fe powder or rod was used as the sample. Ultrasonic V_P and V_S measurements were performed using the pulse reflection method. P- and S-wave signals with a frequency of 57 MHz and 30 MHz, respectively, were generated and received by a 10 degree Y-cut $LiNbO_3$ transducer. The sample was first compressed to the target pressure and heated up to the maximum temperature in each press load in order to reduce the deviatoric stress. Then, we got the ultrasonic data, X-ray radiography image, and X-ray diffractions from the sample and the pressure marker (MgO + hBN) at each about 150-200 K temperature step on decreasing temperature.

Our high-pressure V_P and V_S data are good agreement with the previous ambient-pressure results measured using the same ultrasonic method [Dever, 1972]. In contrast, our V_P data are slightly smaller than the results obtained by high-energy resolution inelastic X-ray scattering (HERIX) technique [Liu et al., 2014]. The values of both V_P and V_S at high temperature are lower than the linear relationship of a velocity-density, i.e., Birch's law, at room temperature, which is the same trend as the previous HERIX result [Liu et al., 2014].

Keywords: high pressure, planetary core, iron, sound velocity

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Synthesis of unsaturated hydrocarbons at the core-mantle boundary

BELONOSHKO, Anatoly[1] ; LITASOV, Konstantin[2]* ; LUKINOV, Timofiy[1] ; ROSENGREN, Anders[1] ; BRYK, Taras[3]

[1]Department of Theoretical Physics, Royal Institute of Technology, Stokholm, Sweden, [2]VS Sobolev Institute of Geology and Mineralogy, Novosibirsk, Russia, [3]Institute for Condensed Matter Physics, Lviv, Ukraine

The origin of life on Earth converges to the problem of the origin of first organic molecules, so called 'blocks of life'. The synthesis of complex organic molecules with C-C bonds is possible under conditions of reduced activity of oxygen or at a surface of catalyst via Fischer-Tropsch reaction (Kenney et al., 2002; Lobanov et al., 2013). It is clear, however, that such conditions should have sustainably existed to provide continuous flow of large quantities of organic material. We found, performing *ab initio* molecular dynamics simulations of the C-O-H-Fe system, that such conditions exist no deeper than at the core-mantle boundary of the Earth. H_2O and CO_2 can be delivered to the CMB by subducting slabs. Indeed, carbon and hydrogen can be also emitted from the core itself. The mixture of H_2O and CO_2 subjected to high pressure (130 GPa) and temperature (around 4000 K) does not lead to synthesis of complex hydrocarbons. However, when metallic Fe is added to the system, C-C bonds emerge. Being lighter than the material in the mantle, the hydrocarbons can rise towards the surface via mantle plumes as a part of fluid or melt component, providing the 'blocks of life' for further synthesis of complex organic molecules. Stability of hydrocarbon molecules and their possible mobility as a light component of the plume was argued in recent study of peridotite and eclogite systems with reduced C-O-H fluid (Litasov et al., 2014).Thus, the iron core not only protects Life on Earth creating the magnetic field, but may also create the Life. This means that search for Life on other planets can also be oriented towards the planets with iron cores.

Keywords: high pressure, core mantle boundary, ab initio molecular dynamics, C-O-H fluid, hydrocarbons, iron