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Editorial

Editorial for Special Issue "High-Pressure Physical and Chemical Behaviors of Minerals and Rocks"

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The eighth "From Atom to Earth" symposium on high-pressure science and earth science was held at the Key Laboratory of High-temperature and High-pressure Study of the Earth's Interior, Institute of Geochemistry, Chinese Academy of Sciences (IGCAS), the People's Republic of China, from 2 to 5 July 2021. As the conference president, Professor Lidong Dai from the IGCAS Key Laboratory of High-temperature and High-pressure Study of the Earth's Interior was also the conference organizer. Participants from Chinese top colleges and research institutions gathered to communicate some of the most recent progress in the field of the physical and chemical behaviors of minerals and rocks under high-temperature and high-pressure conditions.

This research topic of the high-pressure physical and chemical behaviors of minerals and rocks, as hosted by *Minerals*, sets its root in the eighth "From Atom to Earth" symposium on high-pressure science and earth science in order to provide an opportunity to explicitly display new developments in high-pressure mineral physics. This Special Issue it contains ten original articles and one review paper, which mainly focus on high-pressure experimental studies and the theoretical calculation of results on minerals and rocks in high-temperature and high-pressure conditions.

As we known, the electrical conductivity of minerals and rocks (e.g., olivine, clinopyroxene, wadsleyite, epidote, amphibole, peridotite, etc.) in the deep Earth interior are very sensitive to several factors, including temperature, pressure, water content, titanium content, dehydration effect, oxidation−dehydrogenation effect, crystallographic orientation, structural phase transition, and iron content [1–5]. In their review article, Hu et al. [6] retrospectively examined experimental measurements on the high-temperature and high-pressure electrical conductivity of hydrous minerals and rocks in the deep Earth crust, upper mantle, and subduction zone by means of the multi-anvil high-pressure apparatus and diamond anvil cell. Using the electrochemical alternating impedance spectroscopy method, some recent research progress for several recently reported electrical conductivity on four representative hydrous silicate minerals, including the lower case titanium-bearing and water-bearing synthetic polycrystalline olivine aggregates, single crystal epidote, single crystal amphibole, and as well as polycrystalline kaolinite powder, was summarized and outlined by them under conditions of high temperatures and pressures. Specially noted, five main influential factors, including the titanium content, water content, dehydration effect, oxidation−dehydrogenation effect, and structural phase transition on the high-pressure electrical conductivity for those of hydrous silicate minerals, were deeply explored. Furthermore, some comprehensive remarks on several possible future research aspects have been discussed in detail.

A series of new high-pressure experimental results are here presented for many typical minerals and rocks by means of several different high-pressure equipment, such as autoclave, multi-anvil press, diamond anvil cell, shock wave, etc. In order to measure in situ rock porosity under high-temperature and high-pressure conditions and different isostatic pressure environments, Liu [7] designed and applied an experimental assemblage

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on the base of the high-pressure apparatus of autoclave, located at the Key Laboratory of High-temperature and High-pressure Study of the Earth's Interior, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang, China. In order to test the accuracy and validity of the high-temperature and high-pressure measurement assembly, the effect of experimental parameters, including the initial gas pressure at the inlet, the time needed for the gas to reach equilibrium, and as well as the time needed for vacuuming on the porosity experiment, was fully examined under different isostatic pressures. The cylindrical 304 stainless steel, cylindrical copper samples, and cylindrical sandstone under the high isostatic pressure of up to 200 MPa, as three dominant test samples, the authors believe that it is quantitatively verified at the high interrelation between the degree of rock porosity and its correspondent isostatic pressure. By virtue of YJ-3000t multi-anvil high-pressure apparatus and a Solartron-1260 impedance spectroscopy analyzer, Wang et al. [8] measured the electrical conductivities of the dry hot-pressed sintering gabbro with various mineralogical proportions (Cpx_XPl_{100-X}, X = 0, 10, 20, 30, 40, 50, 60, 70, 80, 90, and 100 vol% (the signals of *Cpx* and *Pl* stand for the single crystals of clinopyroxene and plagioclase, respectively) at temperatures of 773–1073 K and pressures of 1.0–3.0 GPa. The functional relationship between the electrical conductivity of the sample and influential factors (e.g., temperature, pressure, and mineralogical proportion) was deeply established. Furthermore, laboratory-based electrical conductivity–depth profiles for the hot-pressed sintering gabbro with various mineralogical proportions and temperature gradients were successfully constructed. They concluded that, although their acquired electrical conductivity results on the dry hot-pressed sintering gabbro with various mineralogical proportions cannot explain the high conductivity anomaly in the oceanic crust and West African craton, it can provide one reasonable constraint on the mineralogical composition in those of representative gabbro-rich regions. Ren [9] performed the high-pressure phase transition from the α–quartz powder to coesite using YJ-3000t multi-anvil high-pressure apparatus at a temperature range from 500 °C to 700 °C, confining pressures between 1.5 GPa and 1.8 GPa and differential stress conditions. The occurrence of quartz–coesite phase transition was observed under conditions of the specific temperature of 500 °C and high differential stress with a relatively longer reaction time. He believes that the appearance of a recovered coesite phase is highly related to differential stress, reaction time, and reaction temperature, with coesite formation being a multifactorial coupling process. By the hydrothermal diamond anvil cell, Chen et al. [10] investigated the variations in the Raman spectra of pyrite under conditions of temperature ranges from 113 K to 853 K and atmospheric pressure, and as well as temperature ranges from 297 K to 513 K and pressures up to 1.9 GPa. They found that the high-pressure hematite phase began to form at the temperature point of 653 K and, subsequently, the starting material of the pyrite phase was thoroughly transformed into the hematite phase at the temperature point of 688 K, and, finally, the hematite phase would be melted at a temperature higher than 853 K. The formation of the high-pressure phase of pyrite occurred at an increase in temperature at each correspondent initial pressure (group 1: 0.5 GPa, group 2: 1.1 GPa, group 3: 1.7 GPa, group 4: 1.9 GPa), which showed no evidence for the occurrence of a chemical reaction or sample decomposition. Pressure and temperature effects are evident for groups 1 and 2, whereas, for groups 3 and 4, the temperature displayed a relatively larger effect than pressure and resulted in a sharp decrease in A_g and E_g modes. Zhang et al. [11] performed in situ Raman scattering and electrical conductivity experiments on calcite in order to study the phase state and structural stability of the sample during both compressed and decompressed processes using the piston-cylinder and four column-type diamond anvil cells under conditions of temperature ranges from 298 K to 873 K and pressure ranges from 1 atm to 19.7 GPa. They observed the pressure hysteresis and reversible behavior during the process of structural phase transformations from $CaCO_3$-I to $CaCO_3$-II phases, from $CaCO_3$-II to $CaCO_3$-III phases, and as well as from $CaCO_3$-III to $CaCO_3$-VI phases at a room temperature condition. At three representative pressure points (i.e., 10.5 GPa, 12.5 GPa, and 13.8 GPa), the phase transition temperatures between $CaCO_3$-III and $CaCO_3$-VI phases were individually determined. Furthermore,

the pressure–temperature diagram in the phase boundary of calcite was well established at temperature ranges from 298 K to 773 K, pressures up to 16.0 GPa, and a depth up to 480 km, and further, its potential geophysical implications were discussed in detail. Gao et al. [12] performed a series of investigations via high-pressure Raman spectroscopy using the *BX90*-type diamond anvil cell and theoretical calculations, utilizing the density functional theory (DFT), on the structural phase transition from zircon to reidite at temperature ranges from 298 K to 800 K and pressure ranges from 0.6 GPa to 26.0 GPa. Their experimental results indicate that the high-pressure reidite phase becomes thermodynamically more stable in comparison with the starting material of the zircon phase at conditions of the fixed pressure of 8 GPa and atmospheric temperature, and the slope of the phase boundary within the relatively lower temperature ranges of 298–800 K abruptly differs from those of previously reported results at the relatively higher temperature ranges of 1100–1900 K. Further, in comprehensive considerations of their experimentally observed equilibrium phase boundary and theoretical calculations based on the density functional theory (DFT) method, it indicates that the kinetic effect of the zircon–reidite phase transition is obvious, and there exists a sufficiently large energy driving force provided by an overpressure to overcome the activation energy barrier below a critical temperature of approximately 880 K. Sun et al. [13] adopted the laser indirectly driven shock compression for quartz to investigate the sound velocity of quartz at extremely high-pressure ranges from 270 GPa to 870 GPa during the lateral unloadings at the Shenguang-III prototype laser facility (SG-IIIp), located at the Laser Fusion Research Center, Chinese Academy of Engineering Physics, Mianyang, China. On the base of those of obtained shock wave data, they also calculated all of these parameters' values, including the high-pressure shock wave velocity, density, and Grüneisen parameter from sound velocity data. All of these obtained experimental results on the sound velocity of quartz under the laser indirectly driven shock compression can provide a new insight to support the dissociation and metallization for the liquid quartz at extremely high-pressure conditions.

On the other hand, some recently acquired results of theoretical calculations including all of these physical characteristics, including the self-consistent thermal expansion, heat capacity, Grüneisen parameters, equation of state, compressibility, and vibrational properties for the minerals in the regions of the upper mantle and subduction zone at conditions of a high temperature and high pressure are displayed in detail in this Special Issue. Using an iterative numerical approach, Su et al. [14] theoretically calculated a series of self-consistent thermodynamic parameters, including the thermal expansion, heat capacity, and Grüneisen parameters on diopside within relatively wider temperature ranges from 0 K to 2000 K and pressure ranges from 0 GPa to 20 GPa. According to all of these obtained thermodynamic parameters' data on the diopside of major mantle silicate mineral, they extrapolated the adiabatic temperature gradient and geotherm of an eclogitic upper mantle. Furthermore, their theoretical calculating results can reveal that the adiabatic temperature gradient of the eclogitic upper mantle model is lower than the pyrolite model at the same depth, which can result in a relatively slower increase in temperature than that of a pyrolitic upper mantle and lead to a similar adiabatic geotherm for both pyrolitic and eclogitic upper mantle within depth ranges from 200 km to 410 km. By virtue of the atomistic computer simulations with the modified ClayFF classical force field method, Tararushkin [15] theoretically calculated the equation of the state, compressibility, and vibrational properties on the brucite of hydrous hydroxide mineral in the subducting zone at conditions of temperatures up to 873 K and pressures up to 15 GPa. Their theoretically acquired pressure and temperature dependencies of the crystalline lattice constant, unit cell volume, compressibility, bulk elastic modulus, and its corresponding high-order derivative, thermal expansion coefficient, the structural M–O–H bond angle, the structural hydroxyl bond length, the angular distribution of the hydroxyl orientation along the {001} crystallographic plane and spectra of vibrational density of states on brucite were comprehensively compared with a diverse set of available experimental data including X-ray diffraction, neutron scattering, infrared spectroscopy, and Raman spectroscopy. They demonstrate that

ClayFF-MOH, as simple and approximate as it is, can be quite accurate in predicting the physical characterization of brucite, which greatly expands the area of its applicability to the simulations of other hydrous minerals with a much more complex crystalline structure under the subduction zone conditions.

In addition, Liu et al. [16] investigated the geological characteristics of Lvwen stone with the yellow-green carbonate jade gemstone using conventional gemological testing methods and analytical techniques, including X-ray diffraction, Fourier transform infrared spectroscopy, ultraviolet–visible spectroscopy, laser ablation plasma mass spectrometry, and scanning electron microscopy (SEM). They found that the chemical composition of Lvwen stone is mainly composed of Ca element, with lesser amounts of Mg, Mn, Cu, Zn, Fe, and other trace elements with the electronic transition absorption band of iron (III) and copper (II) intra-ions; the mineralogical composition of Lvwen stone is calcite element, and trace-element- and crystal-size-induced colors result in its characteristic of having a banded appearance. They indicate that both the electronic transitions of Fe^{3+} and Cu^{2+} intra-ions give rise to the unique yellow-green color of the material. Lvwen stone is produced by ultra-high-pressure tectonic fluids in a relatively closed, reducing environment, and the green matrix was formed earlier than the white bands.

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