

Editorial

Editorial for the Special Issue “Properties of Melt and Minerals at High Pressures and High Temperature”

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This Special Volume sets out to summarize knowledge in the rapidly developing area of the high-pressure and high-temperature properties and structure of silicate melts and minerals.

A silicate melt phase is the essential component of nearly all igneous processes. Silicate melts have acted as transport agents in the chemical and physical differentiation of the earth into core, mantle and crust throughout the Earth since its early beginning. Although near-surface melts are observed directly during volcanic eruptions, the Earth’s interior is not easily accessible, and the quantitative understanding of the high P and T properties of magmas within the Earth must be achieved via the simultaneous development of theory, experiment and simulation. Our understanding of how silicate melts behave at depths of the Earth is vital because of our vulnerability to volcanic activity, as eruptions can vary widely in style, scale, duration and frequency depending on magma behavior.

High-pressure mineralogy studies have recently benefited from extraordinary developments in high-pressure high-temperature techniques. Minerals can now be investigated in the P-T conditions pertaining to the whole Earth, from the near-surface to the inner core, with a precision and accuracy that parallel ambient condition measurements. High-pressure and high-temperature physical and chemical properties of minerals must be properly characterized to understand, from the atomic to global scale, the structure and the dynamic evolution of our “living” planet.

In the last few years, rather fast progress has been made in these areas of science, mostly through an interdisciplinary effort, and it appeared timely to produce a review volume summarizing the current state of the art. Here, we present a collection of papers that significantly improves our understanding of the behavior of the liquid and solid state of silicates at high P and T and provides us with a glimpse of future directions and challenges.

The range of topics we have tried to cover is broad, spanning a wide range of experimental techniques, properties investigated and pressures within the Earth’s mantle, from the core–mantle boundary (CMB) to the upper mantle to more shallower depths pertaining to the volcanic realm.

In the study of Thorne et al. [1], new ultralow-velocity zones (ULVZs) at the core–mantle boundary (CMB) were identified based on the processing of a new collection of 58.155 broadband recordings of the seismic phase SPdKS in the epicentral distance range from 106° to 115°. The authors used a Bayesian approach to identify the regions of the CMB that have the highest probability of containing ULVZs, thereby identifying sixteen new regions of interest. These zones most likely contain partial melt, extremely high iron content ferropericlase, or combinations of both.

The ultralow-velocity zones are formed by the density contrast between the melt and the mantle material [2–6], which controls the migration of the magma during the differentiation process. Depending on the density contrast between silicate melts and the ambient mantle, melts can either migrate upwards or sink into the deep interior, resulting in melt pods, which have been suggested by geophysical observations, at the lithosphere–asthenosphere boundary, atop the 410 and 660 km discontinuities, and, as in [1], in the ultra-low velocity zone above the core–mantle boundary. Knowledge of the density of silicate melts at high pressures is therefore essential to evaluate their gravitational stability in the

mantle as well as to model the solidification of the early magma ocean and the differentiation of the early Earth [7–12].

In the study of Xu et al. [13], the volumetric compression and the density of jadeite melts were obtained at high pressures and high temperatures up to 4.8 GPa and 1955 K by three-dimensional volume imaging using the synchrotron-based X-ray microtomography technique in a rotation-anvil device. Comparison with literature data shows that alkali-rich, polymerized melts are generally more compressible than those that are alkali-poor and depolymerized. The high compressibility of jadeite melt at high pressures implies that polymerized sodium aluminosilicate melts, if generated by low-degree partial melting of mantle peridotite at ~250–400 km depth in the deep upper mantle, are likely denser than surrounding mantle materials, and thus gravitationally stable.

Migration of the magmas upwards or downwards in the deep interior of our Earth strongly depends not only on density but also on the viscosity of magmas. Understanding the viscosity of mantle-derived magmas is therefore needed to model their migration mechanisms and ascent rate from the source rock to the surface [14–22]. The viscosity of volatile-bearing melilititic melts is investigated in the study by Stagno et al. [23], for their importance as plausible carriers of deep carbon in the present day as well as in the early Archaean. In their work, the authors experimentally determined the viscosity of synthetic liquids with ~31 and ~39 wt % SiO₂, 1.60 and 1.42 wt % CO₂ and 5.7 and 1 wt % H₂O, respectively, at pressures from 1 to 4.7 GPa and temperatures between 1265 and 1755 °C, using the falling sphere technique combined with in situ X-ray radiography. The atomic structure of the melt was also determined at high pressure and temperature, using in situ multi-angle energy-dispersive X-ray diffraction supported by ex situ micro-FTIR and micro-Raman spectroscopic measurements. The experimental results, combined with thermal and rheological parameters of mantle rocks, suggest a much slower ascent rate of melilititic melts compared to carbonatitic melts, with important implications for the modeling of CO₂ flux and differentiation processes in the present day and/or in the Archaean mantle.

Another undersaturated system of great interest in igneous petrology for its peculiar origin is represented by the ultrapotassic magma [24–30], object of two different studies in this volume.

The first of these studies by Föster et al. [31], focuses on the origin of such peculiar magmas in the deep interior of the Earth, where, for the first time, extremely K-enriched ultrapotassic melts have been generated experimentally. In this study, this two-stage formation of ultrapotassic magmas was simulated using an experimental approach that involves the re-melting of parts of an experimental product in a second experiment. The two experimental stages are (1) the heating of two-layer charges consisting of carbonate-bearing siliciclastic marine sediment and dunite, resulting in a phlogopite-rich pyroxenite metasomatic reaction layer, and (2) the partial melting of the phlogopite-rich pyroxenite synthesized in the first experiment to generate ultrapotassic (UP) melts with K₂O > 6 wt %. The re-use of the sediment-melt metasomatized dunite confirms that two-stage formation can account for ultrapotassic magmatism with K₂O > 6 wt % involving significant contributions from silicic crustal components, as seen in almost all post-collisional ultrapotassic magmas.

The second study regards the ascent and recharge rate of ultrapotassic melts derived from crystallization kinetics studies of clinopyroxenes at the particularly highly hazardous system of the Campi Flegrei Volcanic district [32]. Bonechi [32] performed time-series experiments using both natural and vitrified starting materials. Experiments were carried out at a pressure of 0.8 GPa, temperatures between 1220 and 1250 °C and dwell times ranging from 0.16 to 12 h. The influence of the starting material and the dwell time and undercooling on the nucleation and growth rates of clinopyroxenes was determined. The combination of the clinopyroxene growth rates with the thermobarometric estimates and crystal size analysis of natural clinopyroxenes from Procida island (CFVD) allowed them to estimate the magma ascent rate and the recharge rate of the deep reservoir, the top of which has been located in the CFVD at about 8 km depth. These data suggest that a deep reservoir of primitive parental magma, similar to that which fed the Campanian Ignimbrite eruption (39 ka), could have

been formed in a time interval ranging from 10^4 to 10^5 years (absence of pre-existing nuclei) or from 10^3 to 10^4 years (presence of pre-existing nuclei).

The study of the corundum-bearing anatectic aluminous rocks exposed in the North Dabie orogen, Central China, with the micro-structural evidence of anatexis by dehydration melting of muscovite [33] serves as an ideal link between magmatic and metamorphic processes investigated in the study of shock metamorphic features of feldspar from the Xiuyan impact crater [34]. The partial melting of high-pressure (HP) and ultra-high-pressure (UHP) metamorphic rocks can profoundly influence the tectonothermal evolution of collisional orogens, the geochemical differentiation of the continental crust and the crust–mantle interaction dynamics within subduction zones [35–38]. Moreover, the partial melting of deeply buried continental crust also has critical effects on weakening rocks and promoting deformation, thus playing an important role in evolutionary processes of continental collision orogens [35–38].

In his paper, Li et al. [33] report the occurrence of corundum-bearing aluminous rocks from the deeply subducted slice of the Dabie orogen, in Central China. Mineral textures and chemical data integrated with phase equilibria modeling indicate that corundum is a product of dehydration melting of muscovite in silica-undersaturated assemblages at $T = 900\text{--}950$ °C, and $P = 9\text{--}14$ kbar.

A wider range of P and T conditions is considered in the study of the shock-metamorphic features of feldspar from Xiuyan Impact Crater. The shock-metamorphic features can provide clues for the search for impact craters on Earth and can also enrich the understanding of the behavior of feldspar under high temperatures and high pressures. In the study of Yin et al. [34], shocked alkali feldspars in the lithic breccia and suevite from Xiuyan Impact Crater were investigated using polarizing optical microscopes, Raman spectroscopy and electron microprobes to better constrain the shock history of this crater. The alkali feldspar had developed a variety of shock-metamorphic features, including irregular fractures, undulatory extinction, PDFs, diaplectic glass, and vesicular glass indicating an impressive shock history of the crater with shock pressure and post-shock temperature varying from ~ 5 to >60 GPa and T from ~ 100 to >1500 °C (shock stage), respectively.

Physical and chemical properties of the Earth's mantle minerals, such as electrical conductivity and density, were investigated in various contributions. High-pressure conduction mechanisms in the Earth's interior were analyzed in two contributions dealing with occupancy in hydrous forsterite by FTIR spectroscopy [39] and fluorine conduction in fluorine-bearing Earth material by means of complex impedance spectroscopy [40].

Water distribution in the deep Earth represents one of the most important topics in the field of geodynamics due to its large impact on the physical and chemical properties of the Earth's mantle, such as electrical conductivity, seismic anisotropy, diffusion, and rheology [41–49].

To constrain the deep-water cycle, the knowledge of the storage capacity and mobility of H_2O in nominally anhydrous minerals (NAMs) in the mantle is a key issue [50–53].

In the study of Del Vecchio et al. [39], in order to quantitatively investigate potential equilibria that might occur between H-bearing defect species present in hydrous forsterite synthesized at 4 GPa, high-temperature FTIR spectroscopy was used to evaluate the evolution of IR spectra as a function of water content and temperature. The seven vibrational bands identified at high frequencies (>3450 cm^{-1}) were assigned to OH stretching vibrations where hydrogen is incorporated into silicon tetrahedral vacancies. The specific contribution of each type of defect was identified by considering their evolution in temperature, up to 500 °C. From these observations, the authors highlight the very low enthalpic contribution due to the topological changes of these defects that could play a role in the electrical behavior of hydrous minerals in addition to higher enthalpy processes such as protonic conduction.

In addition to protons, the electrical conduction of Earth materials, especially silicate minerals, is usually attributed to: the transfer of ions, such as Na^+ occupying crystallographic sites [54,55]; small polarons, due to the hopping of electron holes between ferrous (Fe^{2+}) and ferric (Fe^{3+}) sites in the lattice framework [55–57] and oxygen vacancies, which are related to the transfer of point defects [58].

Recent experimental studies on fluorine-bearing silicate minerals have suggested that fluorine might also be an important charge carrier for electrical conduction of Earth materials at elevated conditions [59,60].

In the investigation by Liu et al. [40], the electrical conductivity of gem-quality natural single crystal fluorite, was determined at 1 GPa and 200–650 °C by complex impedance spectroscopy. The authors show that the electrical property is dominated by a single conduction mechanism from ~350 to 650 °C: the conductivity is very high, reaching ~0.01 S/m at 650 °C, and the activation enthalpy is ~130 kJ/mol. The authors suggest that the conduction is controlled by the transfer of fluoride, and that fluorine conduction may therefore be, in addition to more conventional charge carriers, a novel and important mechanism for the electrical conductivity of Earth materials in the deep crust and mantle.

In addition to electrical conductivity, elastic properties (e.g., bulk and shear modulus) of minerals present in the Earth's interior at high pressures and high temperatures must be properly known to interpret seismological profiles needed to determine the structure and composition of the Earth's interior and in order to understand the formation and evolution of the solid Earth [61]. To do so, accurate knowledge of the evolution of the elastic properties of olivine as a function of pressure and chemical composition is required [62,63].

The study by Pamato et al. [64] reports structural refinements from single-crystal X-ray diffraction data obtained on olivines with composition Fo₁₀₀ (synthetic), Fo₈₀, and Fo₆₂ (natural) collected at room temperature and high pressure up to approximately 8 GPa. The new results, along with data from the literature on Fo₀, are used to discuss and clarify the effect of Mg/Fe substitution on the structural deformation mechanisms occurring along the forsterite–fayalite join, relevant to upper-mantle compositions. In particular, this study discusses which structural mechanisms, on the atomic scale, can cause the very small variations of bulk modulus and its first pressure derivative that have been previously reported.

Finally, a glimpse towards the industrial application of minerals is offered by the study of new high-temperature phases produced during the spontaneous combustion of coal [65]. The occurrence of natural clinkers (calcined clays by coal combustion) associated with coal deposits has recently been described in some areas [66–69].

In the study of Laita et al. [65], natural clinkers from a lower Cretaceous coal outcrop in Ariño (Teruel, NE Spain) were investigated by X-ray diffraction and optical and electron microscopy, in order to describe mineral and textural transformations produced during the spontaneous combustion of coal. The studied natural clinkers are composed of vitreous phase mullite, hematite, hercynite, cristobalite, quartz, pyroxenes, cordierite, gypsum, pyrite, and calcium oxides. These new minerals are also particularly interesting on account of their similarity with those formed during ceramic processes often used in the manufacture of stoneware and ceramic tiles, as well as in refractory ceramics.

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