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► To cite this version:

Simone Anzellini, Marion Louvel, Francesca Miozzi, Angelika D Rosa, Carla Tiraboschi. Editorial: Advances in the study of fluids and melts under extreme conditions. *Frontiers in Earth Science*, 2023, 11, 10.3389/feart.2023.1187340 . insu-04141842

HAL Id: insu-04141842

<https://insu.hal.science/insu-04141842v1>

Submitted on 26 Jun 2023

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RECEIVED 15 March 2023

ACCEPTED 12 April 2023

PUBLISHED 21 April 2023

CITATION

Anzellini S, Louvel M, Miozzi F, Rosa AD and Tiraboschi C (2023), Editorial: Advances in the study of fluids and melts under extreme conditions. *Front. Earth Sci.* 11:1187340. doi: 10.3389/feart.2023.1187340

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Editorial: Advances in the study of fluids and melts under extreme conditions

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KEYWORDS

fluids, melts, extreme conditions, geodynamic, geochemistry

Editorial on the Research Topic

[Advances in the study of fluids and melts under extreme conditions](#)

Fluids and melts are key vectors of mass and heat transfer between the deep Earth and surficial reservoirs. Consequently, they play a critical role in its structural and chemical evolution over geological times. Their underlying properties control the nature of global geochemical, geophysical and geodynamical processes and are thus of key relevance to understand, for example, the properties of Earth's liquid core dynamo, the differentiation of the core and Earth's mantle, the distribution of major and trace elements between the different reservoirs, the occurrence of deep earthquakes or the variability of volcanism and its bearing on the Earth's atmosphere.

A detailed knowledge of the physico-chemical properties of aqueous fluids and silicate, carbonate, or metallic melts under high to extreme pressure and temperature conditions is therefore essential to many research domains in Earth and Planetary sciences.

The new technical advances achieved in the past decades are enhancing detailed characterization of geologically relevant material under extreme condition of Pressure (P) and Temperature (T). In particular the P - T domain now accessible statically using diamond anvil cells (DAC) has been extended to the Tbar regime with T in excess of 6,000 K, respectively. At the same time, advances in both *in situ* and *ex situ* analytical methods (e.g., micro and nano-probes or time-resolved analyses at synchrotron sources), as well as the design of new high-speed clusters for computational studies, have opened new avenues to gain such knowledge even at Earth's inner core conditions.

This Research Topic collect four original contributions that advance our knowledge on a large range of key topics in Earth sciences, including: i) The mobilization of organic carbon via aqueous fluids in subduction zone forearcs, with implications on shallow carbon leaching but also on deep carbon transport; ii) P -induced effects on boron coordination in silicate melts with important insights on its distributional behavior during slab dehydration and melting thus, the interpretation

of boron geochemistry in natural rock samples; iii) the transport capacity of aqueous magmatic fluids for H, C and N and consequently, the information on their back-recycling efficiency to the Earth's surface, iv) a detailed analysis of the light elements incorporation in liquid iron at Earth's core conditions. Providing important information on their density variations and potential immiscibilities thus, on the composition and dynamics of the Earth's outer core.

In the first work of this Research Topic, [Drewitt and Bromiley](#) addressed the important open question of pressure induced boron coordination changes in silicate melts and its effect on its isotopic fractionation and elemental partitioning between solid and liquid phases (melts/fluids). Because of the high incompatibility of boron, its elemental abundances and isotopic variations present key markers in geochemistry used to elucidate the extent of fluid or melt mediated processes in subduction zones. It is well known that T has a profound effect on B fractionation and partitioning. However, the effect of P variations on the later are less constrained despite the well known drastic P -induced structural changes in silicate melts, that in turn should also affect the incorporation mechanism of trace elements. In order to determine the incorporation mechanism of boron (B) as a function of P in a haplobasalt melt, [Drewitt and Bromiley](#) performed detailed *ab initio* molecular dynamics simulations based on density functional theory (DFT) up to 8 GPa and 1,800 K. The authors found that, while at ambient P boron is predominantly incorporated as trigonal planar BO_3 units, with increasing P , the proportion of tetrahedral BO_4 increases markedly in parallel with increases in the coordination of other cations in silicate liquids. For example, over the P range of 0–3 GPa the fraction of BO_4 increases from 5% to 20%. This finding implies that with increasing pressure/depth of melting, magmas should inherit an increasingly isotopically light boron isotopic signature. Therefore, the ability of melts to record isotopic signatures from subduction-derived fluids may vary not only with T but also with P . These findings have important implications for the interpretation of boron isotope geochemistry of natural samples from volcanic arcs and will permit to elucidate in more detail the extend of fluid-mediated processes within Earth's mantle, and thus volatile transport and release within subduction zones.

Light elements (LE) such as H, C, O, Si and S are expected to exist in the Earth's core due to a 10% density deficit with respect to the one of pure Fe core at the same P - T conditions. However, the presence of LE, does not affect only the density of the Earth's core, but has also a strong influence on the structural and transport properties of liquid Fe. For these reasons, [Ohmura et al.](#) performed *ab initio* molecular dynamic simulations to characterize the P -induced evolution of the structural and bonding properties of liquid iron-LE-oxygen ternary systems (Fe-H-O, Fe-C-O, Fe-Si-O and Fe-S-O). From these calculations, the authors found that H, C and O are incorporated interstitially in the liquid iron-LE-O ternary system, whereas for Si and S, the incorporation happens substitutionally. Concerning the interactions between LE, C-C, Si-Si and Si-O keep a covalent bond for the entire range of simulated P in liquid Fe-C-O and Fe-Si-O. It was also found that the Si-O covalent bond causes a shift in the atomic charge of Si to a more positive one. The authors think that this might be related to the phase separation between Fe-Si-O and Fe-Si domains in liquid Fe-Si-O.

Aqueous magmatic fluids are essential to the transport of H, C and N from the mantle to the surface. However, their speciation and intermolecular isotopic fractionation can be affected by the changes in P - T conditions encountered during this journey. In the article by [Dalou et al.](#) the authors performed a series of hydrothermal diamond anvil cell experiments to evaluate the evolution of the speciation and intermolecular isotopic fractionation of H and N during decompression and cooling of aqueous fluids from 780 MPa to 800 °C down to 150 MPa and 200 °C. In particular, they used Raman spectroscopy to investigate the distribution and exchange reactions of H and N isotopologues between water, methane, ammonia and di-nitrogen molecules under changing physico-chemical conditions. The obtained results support large hydrogen and nitrogen isotopic fractionations between water, methane and ammonia species at high P - T conditions in aqueous fluids. They also observed how the N_2/NH_3 ratio is reduced with the decreasing P - T conditions. This is also accompanied by a decreasing N isotopic fractionation between NH_3 and N_2 and an increasing fractionation between NH_4^+ and N_2 . The obtained results provide important information for understanding the geochemical cycling of H and N. In particular, as C and N-bearing aqueous fluids ascend throughout the crust to the Earth's surface, they will degas D-rich methane and ^{15}N -rich N_2 , depleting the residual aqueous fluid in D and ^{15}N .

Finally, in the last original work by [Toffolo et al.](#) the authors investigated the dissolution of biogenic carbonaceous materials (CM) in water at 1 GPa and 550 °C. These materials are the main carrier of organic carbon in subduction zones, contributing to COH fluid production and volcanic arc gaseous emissions. Here, redox controlled high P - T experiments on different CM analogues were performed, and analyzed with a combination of micro-Raman spectroscopy, transmission electron microscopy (TEM) and *in situ* X-ray photoelectron Spectroscopy (XPS). The authors found out that the P - T induced solubility of carbonaceous material arises not only from its crystallinity but also from its surface properties, such as the proportion of sp^2 and sp^3 -hybridized carbon, the presence of active sites, the amount of oxygen heteroatoms and the quantity and type of functional groups. The kinetic effects that these factors introduce can lead to significant deviations from the COH fluid speciation predicted by thermodynamic models and show a strong dependence from the redox state of the system.

These four contributions underline the importance of volatiles (C, O, H, N, S, B) in shaping the Earth as we know it, both when existing as independent phases or when present as high P - T fluids, silicate melts and metallic melts. They also emphasize that a better understanding of fluids and melts under extreme conditions not only relies on pushing the experimental limits to ever increasing P - T conditions but rather requires to develop and combine complementary analytical and numerical approaches to improve the chemical and structural characterization of these thus far elusive phases. In this process, empirical and numerical studies progress hand in hand, providing confirmation of results and inspiration for future work.

Author contributions

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

Funding

SA thanks the Generalitat Valenciana for the CIDEGENT grant no. CIDEXG/2022/6. CT acknowledges funding from the German Research Foundation (grant TI 1078/2-1).

Conflict of interest

The author SA was employed by Diamond Light Source Ltd.

The remaining authors declare that the research was conducted in the absence of any commercial or financial

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