

# MATTER UNDER EXTREME CONDITIONS IN THE EARTH'S INTERIOR: A CHALLENGE FOR PHYSICISTS AND MINERALOGICAL CRYSTALLOGRAPHERS

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The state of matter under the extreme conditions of temperature and pressure supposed to subsist in the inner core of our planet configures a great challenge for physicists. Furthermore, transformations undergone by matter from the interior up to the Earth's crust involve many unresolved questions in the domain of crystal chemistry. Predicting and modelling the behaviour of mineral crystal structures under high pressure and temperature (HP-HT) therefore became a major target for actual mineralogical crystallographers.

Prospective issues susceptible of contributing to the understanding of phase evolution in the Earth's interior [1] –namely, structural compression processes that comply with external pressure– and of clarifying mineral behaviour will be focused, and a suggestion about how carbon may efficiently be hosted deep in the mantle will even be advanced.

Possible geophysical implications of symmetry-breaking transformations by tilting of anion coordination polyhedra and of displacive, symmetry-conserving phase transitions in minerals are revisited, with emphasis on the generation of closest-packed analogs. An abridged revision is presented on the main crystal structure-types amongst minerals having the general formulae  $ABO_3$  (pyroxenes, perovskites and other double oxides like ilmenite) and  $A_2BO_4$  (spineloids and perovskite derivatives) focusing on the structural role played by the geometry of anion coordination polyhedra around cations and on the topology of the bulk array of cations (cationic structural fraction). Such array configures a body-centred lattice in cubic perovskite where the metal-metal environment gathers 8 closer plus 6 slightly further neighbours, a higher coordination comparatively to 12 close neighbours in a cubic closest-packing. Symmetry-breaking transformations of perovskites by processes of octahedral tilting/rotation and cation off-centring through symmetry sub-group relations, keeping either the unit cell or the symmetry class, will be analysed in connection with the topology of the cationic array in Earth's post-perovskite phases. Such analysis emerges as a potential means of interpreting phase sequences from the deep Earth's interior to the crust and of contributing to understand elemental geochemistry and search for metal resources.

In view of recent guesses about a metallic superfluid [2] and once recognized that some metals may accommodate elemental oxygen at normal pressure but high temperature (e.g., -W or  $W_3O$ , A15 structure type, Strukturbericht II, 1937), it is opportune to question the very state of matter under the extreme HP-HT conditions of Earth's core-mantle boundary: are we dealing with elemental metals hosting oxygen atoms instead of metallic ions within an close-packed array of oxygen anions? Contributions will hopefully be provided by the presentation.

[1] T.S. Duffy (2008) Mineralogy at the extremes. *Nature* **451**, 269-270.

[2] E. Babaev, A. Sudbo, N.W. Ashcroft (2005) Observability of a projected new state of matter: a metallic superfluid. *Phys. Rev. Lett.* **95**, 105301, 4 pp.