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Mechanism of the body-centered cubic iron stabilization under the Earth core conditions ANATOLY BELONOSHKO, KTH Royal Inst of Technology, Stockholm, Sweden — The Earth solid inner core is mostly iron, therefore, the question – what is the structure of iron in the Earth inner core – is central to our understanding of the Core. However, the stable phase of iron in the Core is still unknown. Currently, two major candidates are considered – hexagonal close-packed (hcp) and body centered cubic (bcc) structures. Neither of these structures received unanimous support. We demonstrate stability of the bcc phase under conditions in the center of the Core by performing constant pressure-temperature ab initio molecular dynamics simulations with varying shape and volume of the computational cell. The bcc phase is stabilized by the discovered unique diffusion mechanism that originates in the low temperature dynamical instability of the bcc phase. It appears that the bcc phase has already been observed in the recent experiments, however, the experimental data was misinterpreted. The diffusion of iron atoms in solid state is quite unique and might allow us to explain both the anisotropy and the low shear modulus of the inner Core.

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