The Fe-N system at pressures of the Earth's inner core

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Nitrogen is not included into the list of classic candidates for the light elements in the Earth's core. However, the findings of iron nitrides in iron meteorites and in inclusions in diamonds from kimberlites indicate the possibility of their crystallization in the Earth's mantle and core [1, 2]. In material science, the discovery of the superconducting properties of iron nitrides FeN_2 and FeN_4 at high pressures and their unusual crystal chemistry have attracted attention from crystallography [3, 4] and high-pressure mineral physics [5-7].

Currently available theoretical results on the stability of iron nitrides at high pressures refer to a temperature of 0 K and the high temperature region remains unexplored. Although this area is not of interest from the point of view of superconductivity phenomena, knowledge of phase relations is necessary for the experimental synthesis of the corresponding crystals and for determination the phases stable in the deep interior of the Earth and planets.

In the present work using crystal structure prediction methods (USPEX and AIRSS software packages), we found the crystal structures of iron nitrides Fe_xN_y stable against decomposition.Four new iron-rich structures have been discovered in the Fe-N phase diagram, whose pressure stability is shown in Fig.1. Only one stable intermediate stoichiometry, Fe_4N_3-*Imm*2, was detected in the area of the Fe-FeN diagram at pressures up to 200 GPa. The Fe_3N-*C*2/*m* and Fe_2N-*Pnma* phases are stabilized at pressures of 200-400 GPa. Fe_2N-*Pnma* is isostructural to the corresponding carbide, while Fe_3N-*C*2/*m* has no analogues among carbides. FeN structure changes from orthorhombic modification (*Pnma*) to cubic ($P2_13$) at a pressure above 263 GPa (Fig.2).

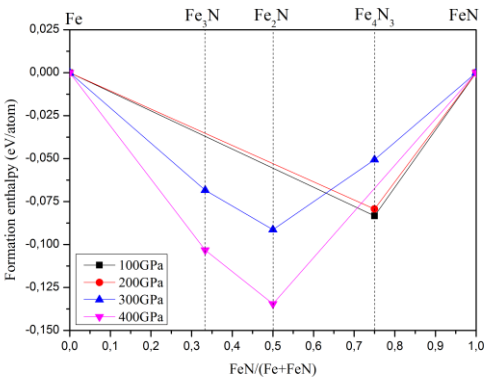

Figure 1. Convex hulls of the Fe–N system at 100-400 GPa

Calculated phase relations in the Fe-FeN system reproduce those previously recorded in experiments and calculations [3, 7]. The described phase relations refer to 0 K. At present, we perform calculations to determine the phase diagrams in the high-temperature region and their results will be presented at the conference.

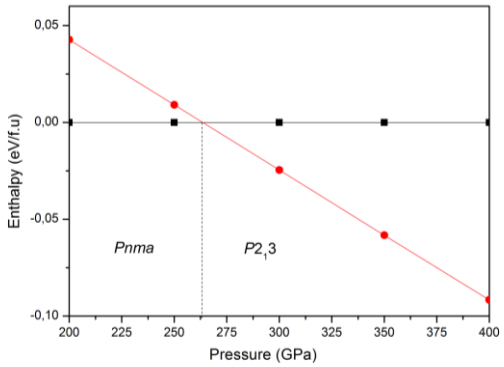

Figure 2. Pressure dependence of the enthalpy for FeN

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