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Ab-initio calculations for the search for stable structures for iron-phosphorus and nickel-phosphorus systems

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Abstract. The study of the internal structure of our planet is one of the most relevant topics in fundamental research. In particular, the analysis of the phase ratios of iron and nickelcompounds with light elements at high pressures is an important task for determining the composition and structure of the core of our planet. Due to the complexity of conducting experiments at such high pressures (in the Earth's core ~365 GPa), ab-initio calculations become a useful method for conducting such studies.

With the advent of new algorithms for searching for crystal structures, such as USPEX, AIRSS and CALYPSO, the number of studies and available data on compounds of iron-nickel-containing systems with light elements has increased significantly. These tools have significantly expanded our capabilities in studying the internal processes in planets, creating broader prospects for further research and understanding the evolution of planetary bodies. The integration of these advanced computational methods makes it possible to accurately predict stable and metastable phases of iron compounds under extreme conditions, providing invaluable data on the behavior of materials in the conditions of the Earth's core.

Key words: high pressure physics, ab-initio calculations, quantum chemical modeling, fundamental research, crystal structures.

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Introduction

The inner core of the Earth consists of pure iron and its alloy with nickel, as well as impurities of light elements such as hydrogen, carbon, nitrogen, oxygen, silicon, phosphorus and sulfur [1].

Under conditions of high pressure and temperature of the Earth's inner core, iron can undergo phase changes, forming various structures that affect the properties of the core. In addition, the simulation results [2] show that in an iron-phosphorus alloy in the Earth's core, Ni can significantly affect the structure and formation of a solid inner core. The study of the composition and properties of the Earth's core, including the role of an iron-nickel alloy with an admixture of phosphorus, is the key to understanding the dynamics and evolution of our planet [3].

At atmospheric pressure, three intermediate compounds are known in the Fe–P system – FeP, Fe_2P and Fe_3P [4]. At atmospheric pressure, FeP has an MnP-type structure, characterized by a *Pnma* spatial group. Gu et al. [5] used the method of X-ray powder diffraction and Mossbauer spectroscopy to study FeP up to 15.6 GPa. This experiment showed that FeP remains in the MnP type structure throughout the considered range.

It was believed that at atmospheric pressure Fe_2P is represented in the structure of barringerite ($P\bar{6}2m$) [6]. However, recent results of an experimental study by Litasov et al. [7] have shown that allabogdanite is a thermodynamically stable polymorphic modification of Fe_2P at atmospheric pressure.

At atmospheric pressure, Fe_3P has a schreibersite ($I\bar{4}$) structure. At high pressures, the structure of schreibersite undergoes changes. Thus, Scott et al. [8, 9] conducted experiments in a diamond cell up to 30 GPa. The authors showed that the schreibersite structure undergoes significant compaction above 8 GPa, and peaks of unidentified structure are observed on the X-ray between 17 and 30 GPa. In addition, according to recent data [10], Fe_3P showed thermodynamic stability up to 40 GPa at high pressure and crystallizes into a tetragonal structure.

At atmospheric pressure, the Ni-P system is characterized by the presence of many phases with different crystal structures [11]: Ni_3P, Ni_8P_3, $Ni_{12}P_5$, Ni_2P, Ni_5P_4, NiP, NiP_2 and NiP_3.

However, at high pressures, the amount of data on compounds in the Ni-P system is limited. Dera et al. [12] investigated the behavior of synthetic Ni_2P in a diamond cell with laser heating at high pressures up to 50 GPa. Under normal conditions, Ni_2P has a hexagonal structure with $P\bar{6}2m$symmetry (trans jordan mineral). When compressed without heating, Ni_2P remains in the $P\bar{6}2m$structure up to at least 50 GPa. Chornkrathok et al. [13] investigated Ni_3P in a diamond cell up to pressures of 50 GPa. During the experiments, it was shown that Ni_3P does not undergo structural phase transitions in the studied pressure range.

The data obtained during such calculations are important for further investigation of the triple Fe–Ni–P system. Therefore, it is important to conduct such studies to establish phase ratios in the Fe-P and Ni-P system at high pressures.

Methods

Quantum chemistry is a powerful tool for studying the properties of molecules, crystals, nanostructures and chemical reactions, which is very useful for many fields of science and technology. Modern methods of quantum chemistry provide an opportunity to describe various chemical and physical characteristics of molecules, as well as the electronic and spatial structure of molecules in solids in their ground state with an accuracy comparable to the data obtained by experimental methods [14].

Quantum chemistry methods allow us to obtain information about the properties of substances that are sometimes unavailable for experimental analysis, especially when it comes to substances under extreme external conditions, such as high temperatures and/or pressures. In such situations, first principles calculation methods, also called ab initio, can be useful. Ab initio methods are based solely on the principles of quantum mechanics and seek to solve the electronic Schrodinger equation, taking into account the position of the nuclei and the number of electrons, in order to obtain the necessary data such as electron density, energy and other properties of the system [15].

Due to the difficulty of conducting an experiment at pressures characteristic of the Earth's core – up to ~ 365 GPa, quantum chemical basic calculations are an effective tool for such studies. Examples of the application of basic calculations are a large number of studies, including data on compounds of iron-nickel alloy with light elements has increased significantly. In particular, calculations were performed to search for intermediate compositions and structures in Fe-C and Fe-H [16], Fe-S [17], Fe-N [18], Ni-S [19], Ni-C [20] systems at high pressures.

Studies of the electronic structure were carried out using density functional theory using the VASP software package [21-23]. The exchange-correlation interaction was taken into account using the generalized gradient approximation, presented in the form of the Purdue-Burke-Ernzerhof (PBE) functional [24]. All calculations included consideration of spin polarization.

For a more efficient search for crystal structures, the USPEX software package [25] was used, which divides calculations into two stages. At the first stage, the search for stable intermediate stoichiometries was carried out, which led to the construction of thermodynamic convex hulls. At the second stage, a search was performed for each fixed stoichiometry represented on the convex hull.

The search for crystal structures was carried out at 0, 100, 200, 300 and 400 GPa. In all calculations for the search for crystal structures, optimization was carried out within the framework of density functional theory using the conjugate gradient algorithm. The calculated parameters were as follows: the cutting energy of plane waves – 400 eV; the density of the Monkhorst-Pack k–point grid [26] – 0.5 $Å^{-1}$; electronic blur – according to the Methfessel – Paxton scheme [27]; smoothing parameter $\sigma = 0.2$ eV. Further, the most energetically advantageous structures were optimized at different pressures with higher accuracy, namely, the cutting energy was increased to 600 eV, the density of k-points was 0.2 $Å^{-1}$ and the smoothing parameter $\sigma = 0.1$ eV.

Results

To assess the stability of the phases with respect to decomposition into an isochemical mixture, we used the method of constructing a «convex hull» diagram. To create this diagram, it was necessary to know the stable modifications of pure iron and phosphorus, as well as their enthalpies. Within the pressure range from 0 to 13 GPa, our calculations revealed the well-known BCC modification of pure iron as the phase with the lowest enthalpy. In the pressure range above 13 GPa and up to 400 GPa, the phase with the lowest enthalpy turned out to be GPU-Fe (see Figure 1). This result corresponds well to the experimental data [28-31].

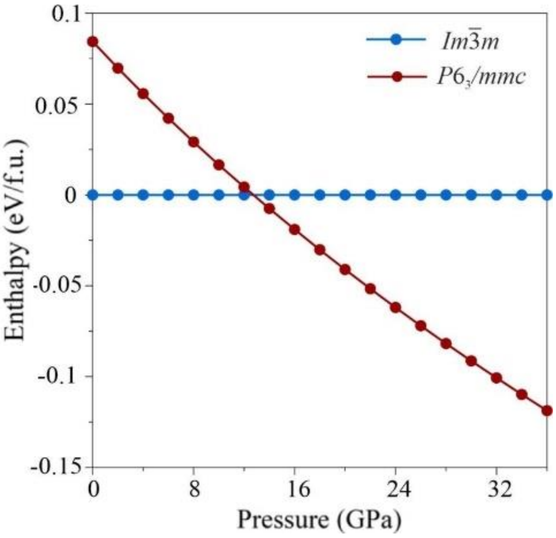


Figure 1 – Dependence of enthalpy on pressure of iron modifications

Note – The results are given with respect to the enthalpy of GPU-Fe

In the case of phosphorus, according to the available experimental data, several structural phase transitions under pressure are observed. The most stable form at atmospheric pressure is the so-called black phosphorus, which is characterized by *Cmca*symmetry and has the structural designation A17 [32]. According to the calculations, the *Cmca*structure transitions into a trigonal structure with R3¯m symmetry at 7 GPa (experimental value of 5 GPa [33]) and then into a simple cubic Pm3¯m at 15 GPa (experiment – 11 GPa [34]). In addition, a phase transition from a simple cubic Pm3¯mto a simple hexagonal (P6) structure is observed through the intermediate *Cmcm* phase in the pressure range 110-127 GPa (experiment – 107-137 GPa [35]). The *Cmcm* structure is an approximated commensurate model of a disproportionately modulated experimental phase, which is characterized by a four–dimensional supergroup*Cmmm*(00γ)s00 [36, 37]. At a pressure of 205 GPa, the P6 structure transforms into a BCC structure (*I*m3¯m). Above 299 GPa, the Im3¯mstructure transforms into *I*4¯3d [38], which is a superstructure of the BCC lattice with small deformations. The I4¯3dstructure is stable up to 308 GPa, above which the GPU structure is stabilized, which retains its stability to at least 400 GPa. The result obtained is in good agreement with the available experimental studies (Figure 2).

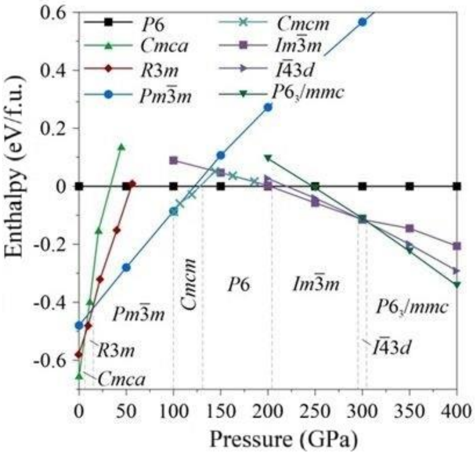
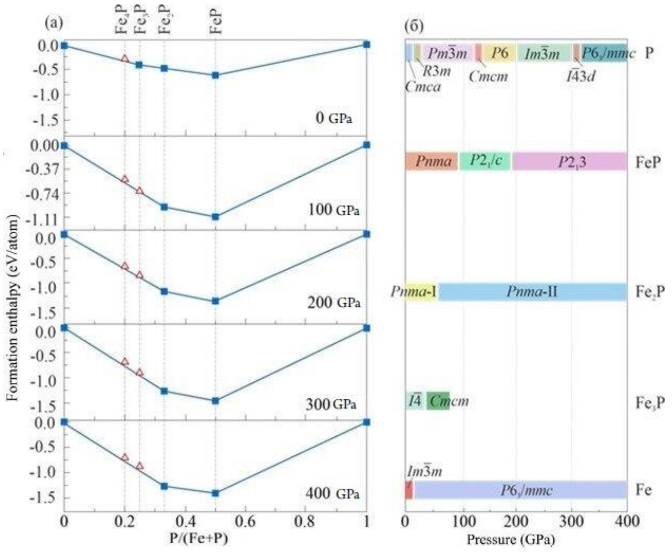


Figure 2 – Enthalpy dependence on pressure of phosphorus modifications

Note – All dependencies are shown relative to the enthalpy of modification P6

At atmospheric pressure, three intermediate compounds are known in the Fe-P system – FeP, Fe_2P and Fe_3P [39, 40]. Similar phases are observed in experiments and at higher pressures of the order of 23 GPa.

The predicted structures of intermediate compounds in the Fe-P system were used to estimate the enthalpy of formation relative to elementary Fe and P. Figure 3 shows convex hulls constructed in accordance with the structures of iron phosphides found. In the pressure range of 0-400 GPa, three intermediate compounds are stable – FeP, Fe_2P and Fe_3P.



a – convex hulls for the Fe–P system at various pressures; b – calculated phase diagram composition-pressure

Figure 3 – Phase stability diagrams in the Fe-P system

Note – Stable structures are indicated by filled blue squares, metastable structures by empty red triangles

FeP undergoes one *Pnma* →$P2_1/c$ phase transition at 75 GPa. Above 200 GPa, the enthalpy of *FeP*-$P2_1/c$ becomes higher than that of *FeP*-$P2_13$ (Figure 4). However, up to 400 GPa, the enthalpy difference between these two phases is on average 3-4 meV/f.u. and is within the accuracy of the method (5 meV/f.u.). Thus, it can be said that above 200 *GPaFeP*-$P2_13$ and *FeP*-$P2_1/c$ are equally stable, i.e.they can coexist with each other.

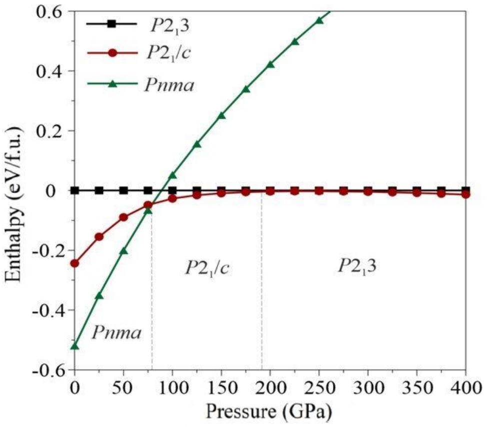


Figure 4 – Enthalpy dependence on pressure of FeP modifications

Note – All dependencies are shown relative to the enthalpy of FeP-P2^{1}3

Iron phosphide Fe_2P, according to the calculations carried out, undergoes one phase transition in the studied pressure range. According to our calculations, the structure of barringerite (P6¯2m) does not have a stability field in the entire studied pressure range, and the stable modification at atmospheric pressure is the structure of allabogdanite, which is characterized by the *Pnma* spatial group (Figure 5). Above 45 GPa, the structure of allabogdanite transitions into a structure that is also characterized by *Pnma* symmetry. Further, we will designate the low-bar modification with the structure of allabogdanite as Fe_2P-*Pnma-I*, and the high-bar modification as Fe_2P-Pnma-II. Fe_2P-Pnma-II is energetically stable up to 400 GPa. It is worth noting that Fe_2P-*Pnma*-I spontaneously transforms into Fe_2P-Pnma-II during optimization above 80 GPa. This indicates the structural similarity of these modifications.

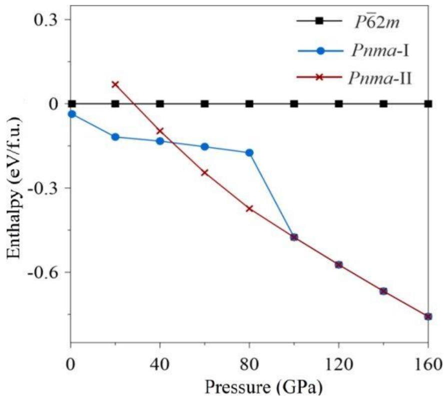


Figure 5 – Enthalpy dependence on pressure of Fe_2P modifications

Note – All dependencies are shown relative to the enthalpy of Fe_2P-P6¯2m

In the case of Fe_3P, the stable modification at atmospheric pressure is the structure of schreibersite with $I\bar{4}$ symmetry. Above 30 GPa, Fe_3P-$I\bar{4}$ passes into a structure characterized by rhombic symmetry Cmcm (Figure 6).

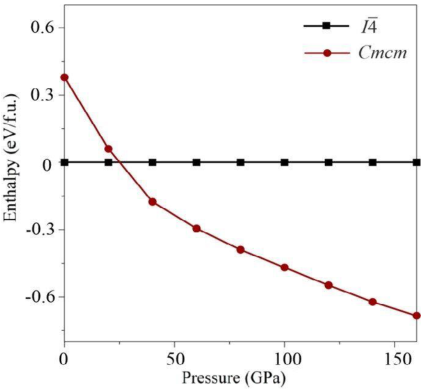


Figure 6 – Enthalpy dependence on pressure of Fe_3P modifications

Note – All dependencies are shown relative to the enthalpy of Fe_3P-$I\bar{4}$

At pressures above 65 GPa, Fe_3P becomes unstable relative to the decomposition reaction $Fe_3P = Fe + Fe_2P$ (Figure 7). Iron phosphide Fe_4P is unstable throughout the studied pressure range (Figure 3).

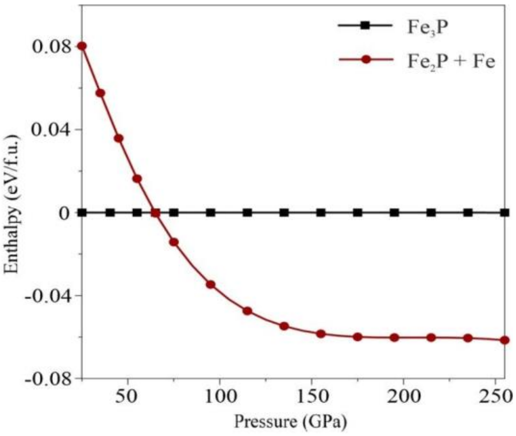


Figure 7 – Dependence of the enthalpy of Fe^3P on the decomposition into Fe_2P and Fe

Nickel does not undergo first-order phase transitions within the pressure range under consideration, and the fcc structure has been identified as a stable modification. This result is consistent with experimental data [41]. In contrast, phosphorus, as demonstrated in Figure 2, goes through a series of phase transitions (see Figure 2).

Both predicted and already known structures were used to estimate the enthalpy of formation relative to elementary Ni and P. To assess the stability of intermediate compounds in the Ni–P system at various pressures, «convex hull»diagrams were constructed in previous work [42]. A number of stable compounds have been identified in thepressure range under consideration.

Nickel phosphides $Ni_{14}P$, $Ni_{12}P$, $Ni_{10}P$, Ni_8P, Ni_7P and Ni_8P_3 are stable over the entire pressure range of 100-400 GPa and do not undergo phase transitions. Ni5P, like the aforementioned phosphides, has no phase transitions. At 100 GPa, Ni_5P is a metastable phase (ΔH =35 meV/atom).The stability field of this phosphide relative to the isochemical mixture Ni_7P + Ni_3P begins at a pressure of 142 GPa and persists up to 400 GPa (Figure 8).

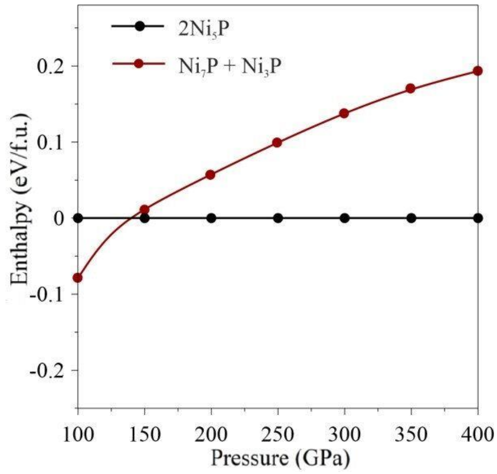


Figure 8 – Dependence of the enthalpy of Ni_5P on the decomposition reaction to Ni_7P and Ni_3P

In the case of Ni_3P, at 100 GPa, the structure of schreibersite (I$\bar{4}$), which is stable at atmospheric pressure, has an enthalpy higher than the newly found structure, which is characterized by Cmca symmetry. The transition from the Ni_3P-I$\bar{4}$structure to Ni_3P-Cmcaoccurs at a pressure of 64 GPa (Figure 9).

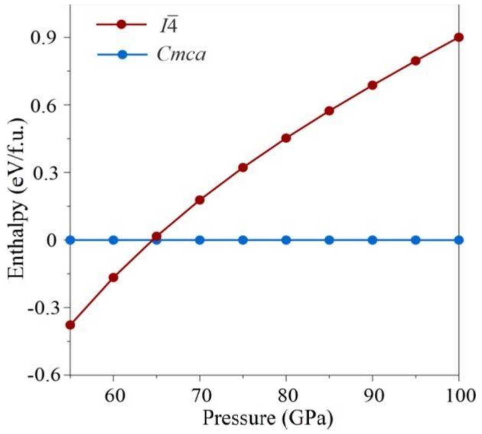


Figure 9 – Enthalpy dependence on pressure of Ni_3P modifications

Note – All dependencies are shown relative to the Ni_3P-Cmca enthalpy

It is worth noting that at a pressure of 100 GPa, Ni_3P-*Cmca* is a metastable phase. Ni_3P-*Cmca* stabilizes above 230 GPa relative to the isochemical mixture Ni5P + Ni_8P_3(Figure 10).

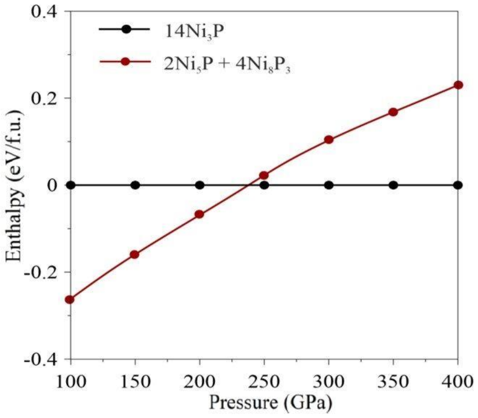


Figure 10 – Dependence of the Ni_3P enthalpy on the decomposition into $Ni_5P + Ni_8P_3$

In the pressure range of 100-400 GPa, Ni_2P is represented as a structure characterized by Pnma symmetry. It is well known that the structure of transjordanite ($P\bar{6}2m$) is more stable at low pressures [43]. Experimental and theoretical studies conducted at pressures up to 50 GPa have not shown the existence of a structural phase transition [12, p. 3205]. According to our calculations, Ni_2P-$P\bar{6}2m$ passes into the found Ni_2P-*Pnma*phase at pressures above 85 GPa (Figure 11), which does not contradict experimental data.

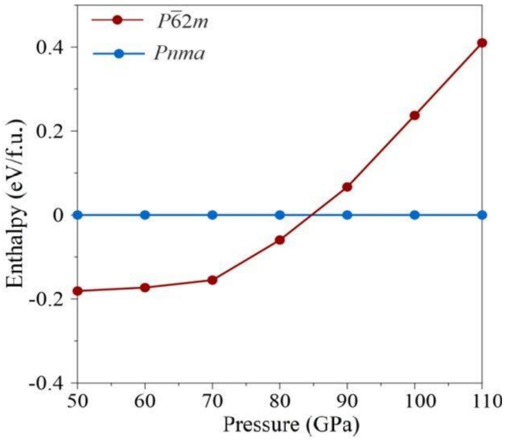


Figure 11 – Enthalpy dependence on pressure of Ni^{2}P modifications

Note – The dependencies are shown relative to the Ni_2P-*Pnma* enthalpy

At pressures up to 223 GPa, the Ni_2P-*Pnma* phase is metastable with respect to the decomposition reaction $13Ni_2P = 3Ni_8P_3 + 2NiP_2$. Above this pressure and up to 400 GPa, this phase is thermodynamically stable (Figure 12).

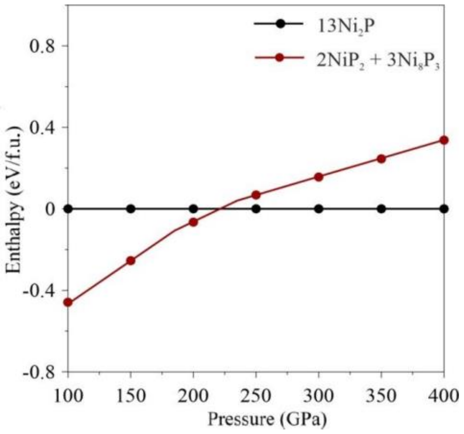


Figure 12 – Dependence of the Ni$_2$P enthalpy on decomposition into NiP$_2$ and Ni$_8$P$_3$

During the search for stable structures, no new structures were identified for the NiP$_2$ compound. The experimentally obtained monoclinic structure of NiP$_2$-C2/cremains stable even at high pressures up to 330 GPa. Above this pressure, NiP$_2$-C2/cdecays into Ni$_2$P-*Pnma* and P-P6$_3$/*mmc*(Figure 13).

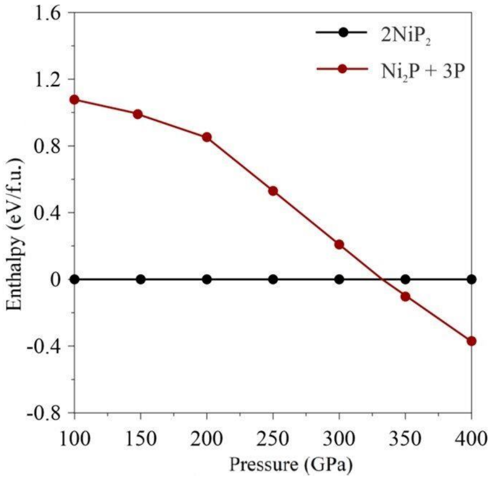


Figure 13 – Dependence of NiP$_2$ enthalpy on decomposition into Ni$_2$P and P

All predicted structures are dynamically stable. This is evidenced by the dispersion curves of phonons calculated by us (Figure 14), which have only real frequencies, which indicates the dynamic stability of these structures.

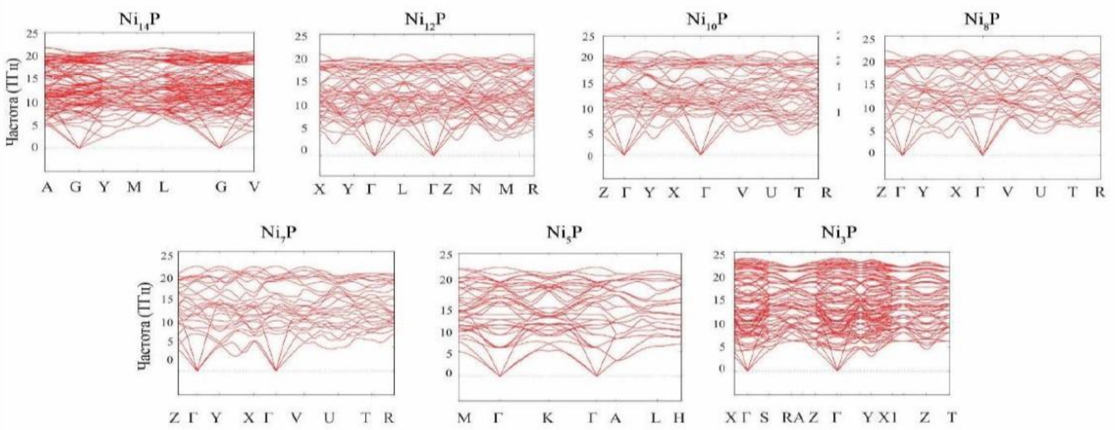


Figure 14 – Dispersion curves of phonons of predicted nickel phosphides

The structures $Ni_{14}P$, $Ni_{12}P$, $Ni_{10}P$, Ni_8P, Ni_7P, Ni_5P and Ni_3P are characterized by fcc packing, with Ni atoms partially replaced by P atoms [44, p. 1980]. The structure of pure Ni is also characterized by fcc packing up to 400 GPa. Thus, the proposed structures can be considered as a series of «ordered» (model) solid solutions (Ni, P). This type of isomorphism between a d-metal and a light element is atypical at atmospheric pressure. At high pressures, where elements that are typical nonmetals, such as sulfur, acquire metallic properties [45], this isomorphism becomes widespread [46,47]. An example is the isomorphic substitution of iron with sulfur, silicon and carbon in GPU and BCC structures [48]. Phosphorus atoms in the structures of model solid solutions tend to be evenly distributed over the structure without clustering or forming groups. It is worth noting that structures with a phosphorus content above ~ 15 wt.% (25 mol.%), i.e. Ni_2P, Ni_8P_3 and NiP_2 cannot be described by fcc packing.

For example, the Ni_2P-*Pnma*nickel phosphide found is characterized by a Co_2Si type structure. Nickel atoms have two unequal positions in the structure. In both positions, the Ni atoms are surrounded by five P. atoms. Phosphorus has one nonequivalent position. It is surrounded by ten Ni atoms, forming PNi_{10}-two-lobed cubes that are interconnected along the edges and along the edges (Figure 15).

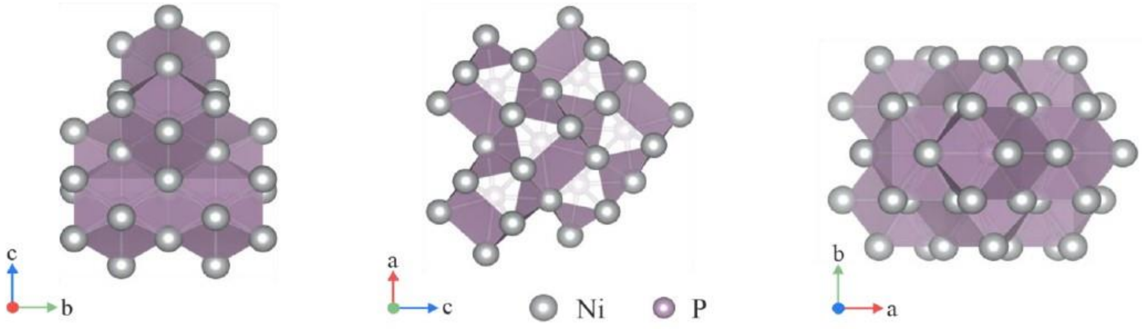


Figure 15 – Ni_2P-*Pnma*structure

Thus, according to the results obtained, it can be assumed that at pressures of the Earth's core 9.5 wt.% of phosphorus can be dissolved in the nickel structure without lattice deformation, and the limit of phosphorus solubility in solid Ni is ~ 15 wt.%. Despite the fact that Fe and Ni have similar chemical characteristics, structures with isomorphic iron substitution in the Fe-P system have not been found. This phenomenon lies in the fact that the solubility of phosphorus in iron is much lower than in nickel, and is approximately 2.6 wt.% at atmospheric pressure [49] and 4 wt.% at a pressure of 23 GPa [50]. In addition, we believe that the high solubility of phosphorus in nickel compared to the solubility of iron will lead to the fact that the solubility of P in the alloy (Fe, Ni) will be higher than in pure Fe.

Conclusion

As a result, calculations were carried out in this study to search for stable crystal structures in Fe-P and Ni-P systems in the pressure range of 100-400 GPa. Using the VASP software package and the USPEX algorithm, we were able to determine the stability fields for the found FexPyandNixPystructures.

A recent experimental study has shown that Fe_2P-Pnma-I is a stable phase under normal conditions, and barringerite is a high-temperature modification. Our DFT calculations are in good agreement with this study and confirm that Fe_2P-Pnma-I is a stable modification at 0 GPa.

There are some discrepancies in the experimental studies on the search for the high-pressure phase of Fe_3P. In [9, p. 377], the transition from Fe3P-$I\bar{4}$to a new phase occurs in the pressure range of 17-30 GPa. The existence of a new phase was later confirmed in experiments by Guet al.[51]. In this work, the transition was observed at a higher pressure equal to 64 GPa. However, it should be noted that in a special experiment with a long exposure at 30 GPa, in addition to the peaks of the Fe_3P-$I\bar{4}$structure, new peaks were observed on the X-ray. The authors assumed that the new peaks correspond to the Fe_2P + Fe association. However, due to the small number of new peaks, the identification of phases was ambiguous, and it is impossible to exclude the correspondence of these new peaks to the new phase of Fe_3P. This interpretation is consistent with our calculations for Fe_3P. According to our data, the transition from Fe_3P-$I\bar{4}$to Fe_3P-*Cmcm* occurs at 30 GPa. In this case, the new phase observed in the experiments of Gu et al. [51, p. 300] corresponds to Fe_3P-*Cmcm.*

The Fe-P system is characterized by two intermediate compounds Fe_2P and FeP under the condition of an internal core. A more jelly-like phosphidem content under this condition appears Fe_2P. All these results are very important for the study of the Fe–P system as a whole.

The Ni-P system is typical for individual plants and three intermediate components Ni8P3, Ni_2P and NiP_2 at 100-400 GPa. The Ni-P system is characterized by the following interactions $Ni_{14}P$, $Ni_{12}P$, $Ni_{10}P$, Ni_8P, Ni7P, Ni_5P, Ni_3P, Ni_8P_3 and Ni_2P under the condition of the Earth's inner core. The most nickel-containing phosphide under this condition appears $Ni_{14}P$.

The trend of phase stability for Ni–P compounds at atmospheric pressure is presented as follows: Ni_5P_4> Ni_2P > $Ni_{12}P_5$>NiP> Ni_8P_3> Ni_3P > NiP_2> NiP_3[52]. With increasing pressure, this sequence changes. At the pressures of the inner core, structures with a low phosphorus content are ordered as follows: $Ni_8P_3 < Ni_3P < Ni_2P < Ni_5P < Ni_7P < Ni_8P < Ni_{10}P < Ni_{12}P < Ni_{14}P$. Among the experimentally known nickel phosphides, Ni_8P_3, $Ni12P_5$, Ni_5P_4, Ni_2P, NiP_2 and NiP_3, only Ni_8P_3 and NiP_2 are stable at high pressures.

The results obtained in the course of this study are fundamental and important for further investigation of the structure and composition of the cores of the Earth and planets. The data obtained will also help identify priority areas for future research.Obtaining accurate information about the composition and structure of the Earth's inner core would contribute to a deeper understanding of the internal structure and dynamics of our planet as a whole. In addition, it is of fundamental importance for the development of models describing the processes of formation, differentiation and evolution of the Earth.

The behavior of phosphorus in Fe-Ni alloys has attracted the attention of researchers, since both elements are potentially important components of the Earth's core. In this regard, understanding the characteristics of Fe-P, Ni-P compounds at high pressures is key for subsequent research.

The contribution of the authors:

A.B.Bazarbek – corresponding authorand has made a significant contribution to the development of the research concept and to the design of the structure of the article. He supervised the work of all co-authors, coordinated their activities and ensured timely completion of all stages of the work;

A.D. Akylbekova – the author was responsible for setting the main objectives of the study,she also took part in writing the text and agreed on the final version of the article for publication;

G.D. Kabdrakhimova – The author was engaged in collecting experimental and theoretical data and conducting analytical calculations. She was responsible for developing the calculation methodology and interpreting the results;

A.Sh. Omarkhan – She made a key contribution to the calculations on the program, and data collection. She was responsible for formulating conclusions based on the results from theoretical calculations;

A.A. Nogai – the author was engaged in the analysis and processing of numerical data. He completed the tasks of interpreting the results and wrote the section of the article related to the results.

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Темір-фосфор және никель-фосфор жүйелері үшін тұрақты құрылымдарды табудың ab-initio есептеулері

Аңдатпа. Біздің планетамыздың ішкі құрылымын зерттеу іргелі зерттеулердегі ең өзекті тақырыптардың бірі болып табылады. Атап айтқанда, темір мен никель қосылыстарының жоғары қысымдағы жеңіл элементтермен фазалық қатынасын талдау біздің планетамыздың ядросының құрамы мен құрылымын анықтаудың маңызды міндеті болып табылады. Осындай жоғары қысымда эксперименттер жүргізудің қиындығына байланысты (Жер ядросында ~365 ГПа) Ab-initio есептеулері осындай зерттеулерді жүргізудің пайдалы әдісіне айналады.

USPEX, AIRS және CALYPSO сияқты кристалды құрылымдарды іздеудің жаңа алгоритмдерінің пайда болуымен жеңіл элементтері бар темір-никель жүйелерінің қосылыстары туралы зерттеулер мен қол жетімді деректер айтарлықтай өсті. Бұл құралдар планеталардағы ішкі процестерді зерттеудегі мүмкіндіктерімізді едәуір кеңейтіп, планеталық денелердің эволюциясын одан әрі зерттеу мен түсінудің кең перспективаларын жасады.Осы озық есептеу әдістерінің интеграциясы Жер ядросындағы материалдардың сипаттамасы туралы баға жетпес деректерді қамтамасыз ете отырып, экстремалды жағдайларда темір қосылыстарының тұрақты және метастабильді фазаларын дәл болжауға мүмкіндік береді.

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Расчеты ab-initio для поиска стабильных структур для систем железо-фосфор и никель-фосфор

Аннотация. Изучение внутреннего строения нашей планеты является одной из наиболее актуальных тем фундаментальных исследований. В частности, анализ фазовых соотношений соединений железа и никеля с легкими элементами при высоких давлениях является важной задачей для определения состава и структуры ядра нашей планеты. Из-за сложности проведения экспериментов при таких высоких давлениях (в ядре Земли ~365 ГПа) расчеты ab-initio становятся полезным методом проведения таких исследований.

С появлением новых алгоритмов поиска кристаллических структур, таких, как USPEX, AIRS и CALYPSO, количество исследований и доступных данных о соединениях железо-никельсодержащих систем с легкими элементами значительно возросло. Эти инструменты значительно расширили наши возможности в изучении внутренних процессов на планетах, создав более широкие перспективы для дальнейших исследований и понимания эволюции планетных тел. Интеграция этих передовых вычислительных методов позволяет точно прогнозировать стабильные и метастабильные фазы соединений железа в экстремальных условиях, предоставляя бесценные данные о поведении материалов в условиях ядра Земли.

Ключевые слова: физика высокого давления, расчеты Ab-initio, квантово-химическое моделирование, фундаментальные исследования, кристаллические структуры.

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