https://doi.org/10.52676/1729-7885-2024-2-11-17
УДК 538.94

SEARCH FOR STABLE STRUCTURES FOR THE NICKEL-SULFUR SYSTEM AND COMPARISON WITH THE IRON-SULFUR SYSTEM

A. B. Bazarbek[1], **A. D. Akylbekova**[1], **A. A. Kissabekova**[2], **A. A. Nogai**[3], **A. T. Akilbekov**[1]

[1] L. N. Gumilyov Eurasian National University, Astana, Kazakhstan
[2] Higher School of Natural Science, NJSC "Pavlodar Pedagogical University named after A. Margulan", Pavlodar, Kazakhstan
[3] Kazakh agro-technical research university, Astana, Kazakhstan

**E-mail for contacts: asyl.bazarbek.92@mail.ru*

The core of the Earth consists mainly of iron and nickel, forming an iron-nickel alloy. At the same time, sulfur is one of the potential candidates for the role of a light element in the inner core. To date, many theoretical studies have been conducted by quantum chemical modeling to search for intermediate compositions and structures in systems such as Fe-C, Fe-H, Fe-O, Fe-Si, Fe-S and Fe-P up to pressures of 400 GPa.

Despite extensive research on the iron-light element systems, to date no mineralogical model of the Earth's core has been created that fully corresponds to the observed seismological data. A possible reason for this discrepancy may be insufficient consideration of the influence of the core's key alloying element, nickel. Theoretical studies for the nickel-light element system at high pressures have not been sufficiently carried out. Therefore, it is necessary to conduct more in-depth studies of these binary systems in order to further study and identify possible intermediates in triple Fe-Ni-S systems.

Keywords: *theoretical calculations, phase transition, laser heating, stable modification, high pressure physics.*

INTRODUCTION

The Earth's inner core growth is a key process for understanding Earth's evolution. This process is inherently related to the crystallization properties of the core's constituents, primarily Fe, Ni, and some light elements such as hydrogen (H), carbon (C), nitrogen (N), oxygen (O), silicon (Si), phosphorus (P) and sulfur (S) [1]. The article [2] provides evidence of the strong influence of the second most common element of the core, nickel (Ni), on the crystallization of iron (Fe) under the influence of pressure from the inner core of the Earth. It has been established that the presence of nickel can stabilize the bcc phase and accelerate the process of iron crystallization under pressure conditions characteristic of the core. The results obtained indicate that nickel alloying of iron can contribute to the joint existence of the phases of bcc and gpu of the inner solid core. These findings play an important role in understanding the mechanisms of formation of the inner core and the formation of its complex crystal structure.

In this regard, the behavior of sulfur in Fe-Ni alloys has interested scientists, since both elements are potentially important components of the Earth's core. Given the above understanding of the behavior of Fe-S and Ni-S compounds at high pressures characteristic of the Earth's core, it is important to discuss and limit the properties of planetary nuclei.

The Fe–S system has been the subject of intensive research, both experimental and theoretical. At atmospheric pressure, the enriched part of the system, Fe, forms only one intermediate compound, FeS [3]. When the pressure increases, other intermediates are formed. For example, Fe_3S_2 is formed above 14 GPa [4], and Fe_2S and Fe_3S are formed above 21 GPa [5]. To assess the phase stability of Fe-rich sulfides at Earth's outer core conditions, Fe-rich sulfide compositions were examined to 200 GPa and 3250 K using single-crystal and powder X-ray diffraction techniques in a laser-heated diamond anvil cell. At high temperatures between 120 and 200 GPa, Fe_5S_2 is synthesized in the Ni_5As_2-type structure [6]. Also Oka K. and others [7] examined pressure-induced phase transitions in Fe_2S based on high-pressure and high-temperature X-ray diffraction measurements in a laser-heated diamond-anvil cell. Fe_2S is not stable at ambient pressure but is known to form above 21 GPa with the Fe_2P-type (C22) structurePreviously, it was believed that Fe_3S sulfide is the most enriched Fe compound in the Fe–S system and can contribute to the composition of the Earth's inner core, with iron retention. However, recent theoretical studies using evolutionary methods to predict crystal structures show that thermodynamically stable iron sulfides in the pressure range of 100–400 GPa are Fe_2S, FeS and FeS_2, while Fe_3S is unstable and decays into Fe + Fe_2S [8]. The work of Tateno and colleagues [9] using DAC and laser heating methods confirmed that Fe_2S is the most enriched Fe sulfide above ~250 GPa, while Fe_3S is not stable, which corresponds to the results of theoretical studies.

The Ni–S system has not been studied in as much detail as Fe–S, due to the underestimated interest associated with the relatively low Ni/Fe ratio in the cores of planets. Numerous phases in the Ni-S system were detected at atmospheric pressure. Among them are Ni_3S_2, Ni_7S_6, Ni_9S_8, NiS, Ni_3S_4 and vaesite NiS_2 [10].

At high pressures, data on the Ni–S system is limited. Prewitt et al. [11] investigated Ni_3S_2 at high pressures.

Their experimental study revealed a phase transition to an orthorhombic phase with Cmcm symmetry at 23 GPa and 462 K. This result was later confirmed by theoretical studies based on calculations based on first principles [12]. In [13], calculations were performed in the pressure range of ~0–24 GPa. The calculated crystal structures for nickel sulfides showed that NiS, Ni_3S_2 and Ni_3S_4 are stable at the studied pressure. It should be noted that theoretical data and calculations on the search for stable compositions and structures in the Ni–S system are practically absent. Thus, it is important to conduct such a study as was done for the Fe–S system [8, p. 1027] in order to expand our knowledge about stable phases in the Fe–Ni–S system at pressures of the core of the Earth and other planets.

METHODS

The calculations of the electronic structure were carried out within the density functional theory using the VASP package [14].The exchange–correlation interaction was taken into account in the generalized gradient approximation (GGA) in the form of the Perdew–Burke–Ernzerhof (PAW) functional.

The search for new stable crystal structures of nickel borides, carbides, and nitrides were performed using evolutionary algorithms implemented in the USPEX package [15].

For a more efficient search for crystal structures the calculations were divided into two stages. At the first stage, the search for stable intermediate stoichiometries was carried out, which resulted in the construction of thermodynamic convex hulls. In the second stage, a search was performed for each fixed stoichiometry represented on the convex hull.

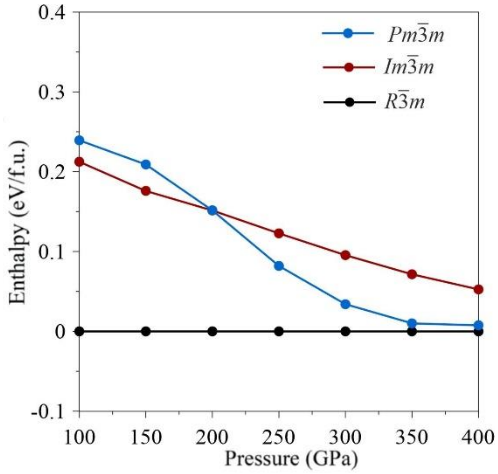
The search for crystal structures was carried out at 100, 200, 300 and 400 GPa with a maximum number of atoms in a cell equal to 32, in the case of calculating a variable composition, and 1–4 formula units in a cell, in the case of calculating a fixed composition. In the first generation, 55 structures were randomly generated. 60% of these structures with the lowest enthalpy were selected after optimization and then used to generate the next generation (35% of all structures of the next generation were generated according to the heredity scheme, 20% according to the atomic mutation scheme, 10% according to the lattice permutation scheme and 35% randomly).

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 is 400 eV; the density of the Monkhorst-Pack k–point grid [16] is 0.5 $Å^{-1}$; electronic blurring is according to the Methfessel–Paxton scheme [17]; 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

This article presents the results of calculations for the search for crystal structures of nickel sulfides and their relative stability at the pressure of the Earth's core.

Nickel in the range of 100-400 GPa under consideration has only one stable modification (fcc structure). This conclusion is consistent with the experimental results [18]. In the case of sulfur, the β-Po (*R-3m*) type structure was stable in our calculations over the entire pressure range (Figure 2). This result is in agreement with the works [19], and differs from what was obtained in the works [20]. According to [21], at pressures above 280 GPa [28, p. 330] (330 GPa [19, p. 1600857]), the β-Po type structure transforms into a simple cubic structure (*Pm-3m*). We associate this transition with the insufficient accuracy of calculations [19, p. 1600857] and the pseudo-potential used [18, p. 342]. At pressures above 350 GPa, the enthalpy difference between the *R-3m* and *Pm-3m* structures decreases to 10 meV/atom, which is almost comparable to the accuracy of calculations (5 meV/atom). This difference can be compensated by the temperature effect. Therefore, the possibility of the existence of a simple cubic structure cannot be excluded.



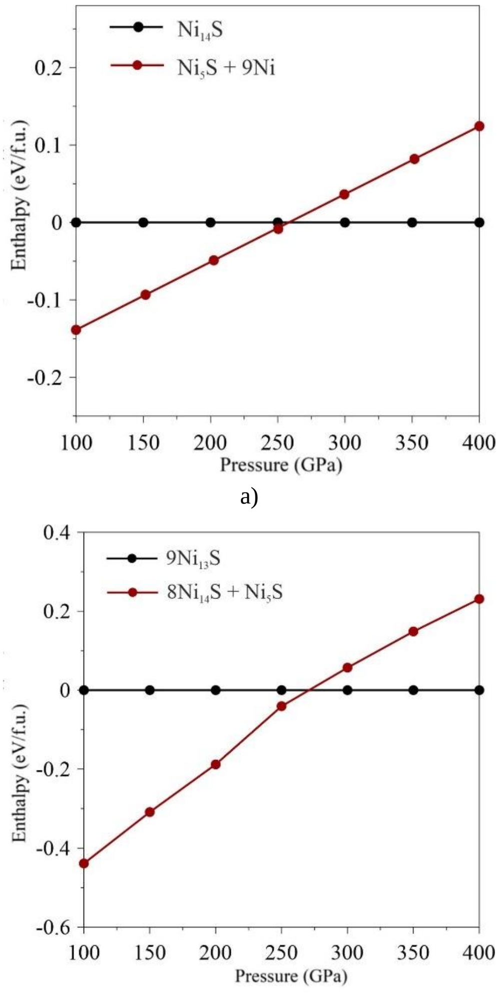
Note – The dependencies are shown relative to the enthalpy of the *R-3m* modification

Figure 1. Enthalpy dependence on pressure of various sulfur modifications

To assess the stability of intermediate compounds in the Ni−S system at various pressures, «convex hull» diagrams were constructed in previous work [22]. The enthalpy of formation relative to elementary Ni and S was calculated earlier for both predicted and known structures. A number of stable compounds have been identified in the pressure range under consideration.

As a result, the equilibrium compounds at 100 and 200 GPa are Ni_5S, Ni_3S, Ni_2S and NiS_3. With increasing pressure, nickel-enriched compounds $Ni_{14}S$, $Ni_{13}S$, $Ni_{12}S$ and Ni_4S are stabilized. Over the entire pressure range, $Ni_{14}S$ has one modification characterized by *C2/m* symmetry. $Ni_{14}S$-*C2/m* becomes stable with respect to the decay reaction to Ni_5S and 9Ni above 255 GPa (Figure 2a).

$Ni_{13}S$ also does not undergo phase transitions in the pressure range under consideration and has a structure with *R-3* symmetry. This sulfide is relative to the decomposition reaction of $9Ni_{13}S = 8Ni_{14}S + Ni_5S$ above a pressure of 274 GPa (Figure 2b).



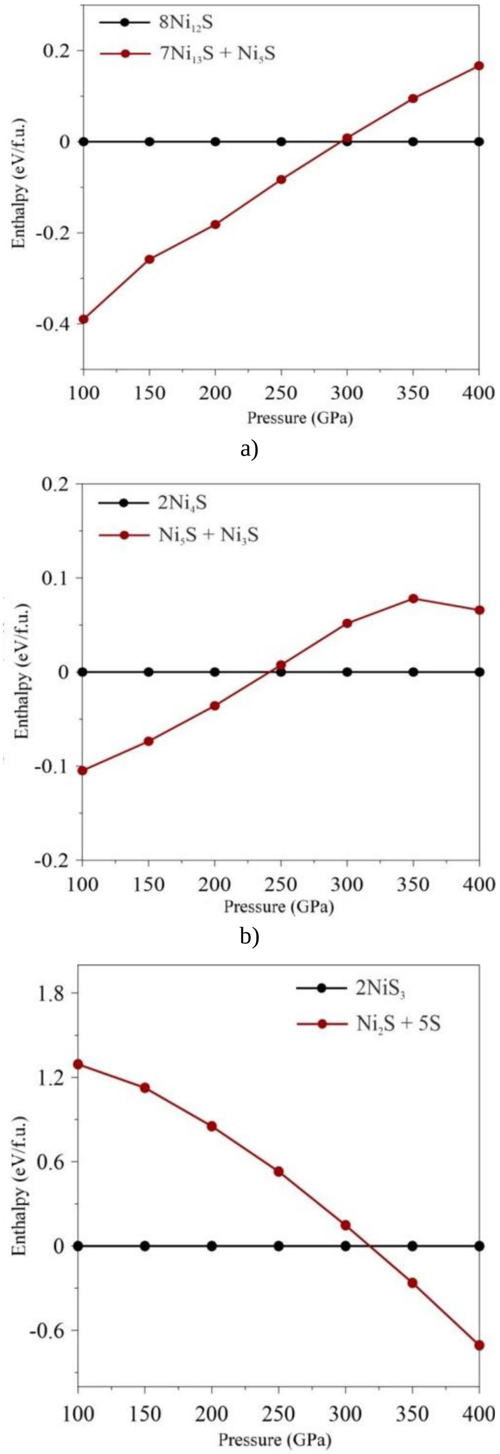
a)

b)

Figure 2. Decomposition into an isochemical mixture:
a) Dependence of the enthalpy of $Ni_{14}S$ on the decomposition reaction to Ni_5S and Ni; b) Dependence of the enthalpy of $Ni_{13}S$ on the decomposition reaction to $Ni_{14}S$ and Ni_5S

$Ni_{12}S$ has an *R-3* structure and becomes energetically advantageous above 296 GPa with respect to the reaction $8Ni_{12}S = 7Ni_{13}S + Ni_5S$ (Figure 3a). Ni_4S stabilizes relative to the reaction $2Ni_4S = Ni_5S + Ni_3S$ above 243 GPa and has a *P-1* structure (Figure 3b). With increasing pressure, NiS_3 becomes unstable above 318 GPa and decays into Ni_2S and S (Figure 3c). Ni_5S, Ni_3S and Ni_2S are stable over the entire pressure range of 100–400 GPa. Thus, the following compounds are stable at 400 GPa: $Ni_{14}S$, $Ni_{13}S$, $Ni_{12}S$, Ni_5S, Ni_4S, Ni_3S and Ni_2S.

In the pressure range under consideration, Ni_5S has one *C2/m* modification, while Ni_2S and Ni_3S undergo one phase transition. For Ni_2S, the phase with *Pmma* symmetry is stable at least above 100 GPa. At 272 GPa, Ni_2S-*Pnma* enters a phase with *P-62m* symmetry (Figure 4a). For Ni_3S, the phase with *I-4* symmetry is stable from at least 100 to 330 GPa, and above this pressure it passes into the phase with *Cmcm* symmetry (Figure 4b).

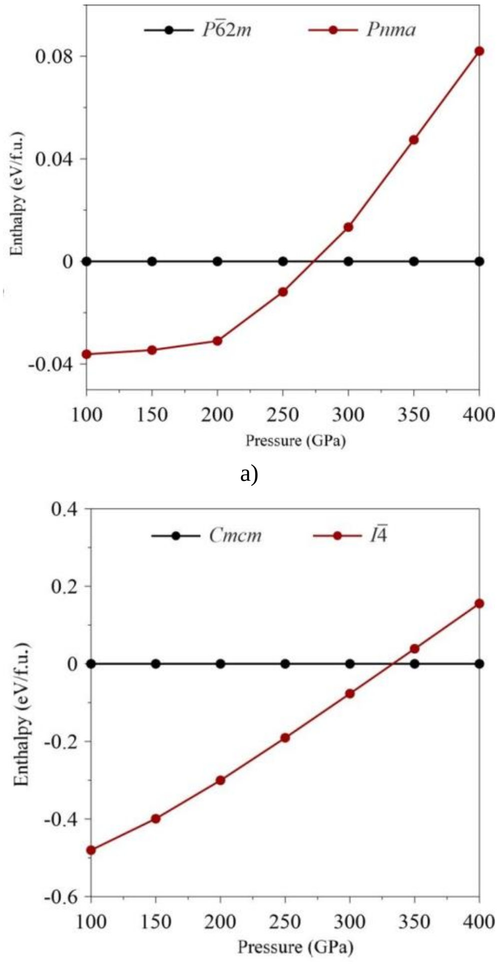


a)

b)

c)

Figure 3. Decomposition into an isochemical mixture:
a) Dependence of the enthalpy of $Ni_{12}S$ on the decomposition reaction to $Ni_{13}S$ and Ni_5S; b) Dependence of the enthalpy of Ni_4S on the decomposition reaction to Ni_5S and Ni_3S;
c) Dependence of the enthalpy of NiS_3 on the decomposition reaction to Ni_2S and S



a)

b)

Figure 4. Decomposition into an isochemical mixture: a) Enthalpy dependence on pressure of Ni_2S *modifications (all dependencies are shown relative to the enthalpy of* Ni_2S*-P-62m); b) Enthalpy dependence on pressure of* Ni_3S *modifications (all dependencies are shown relative to the* Ni_3S*-Cmcm enthalpy)*

In addition to the predicted structures, we also examined experimentally synthesized structures Ni_3S_2, Ni_7S_6, Ni_9S_8, NiS, Ni_3S_4 and NiS_2 at atmospheric pressure. Two known structures of α- and β-NiS were considered for NiS. According to our calculations, in the pressure range from 100 to 400 GPa, the α-phase turned out to be energetically more advantageous than the β-phase. Nevertheless, α-NiS and all other experimentally known compounds turned out to be thermodynamically unstable in the pressure range under consideration.

Extensive studies of the structural and thermodynamic properties of these compounds in a given pressure range provide important information for understanding their behavior under high pressure conditions, which may be significant for geochemistry and physics of the Earth's inner core.

The predicted Ni–S structures can be considered as ordered solid solutions. $Ni_{14}S$, $Ni_{13}S$ and $Ni_{12}S$ are characterized by almost perfect fcc packing. A further increase in the sulfur content leads to sufficient deformation of the ideal fcc structure [22, p. 600].

The low-pressure phase of Ni_3S-*I-4* cannot be characterized by the densest packing of atoms, like the previous phases. This phase is isostructural Ni_3P-*I-4* (schreibersite structure), and is characterized by the 9th S-Ni coordination, forming single-cap square antiprisms connected along edges and faces (Figure 5).

Ni_2S-*Pnma* sulfide is isostructured by Fe_2S-*Pnma*. It is characterized by a 10-fold S-Ni coordination (Figure 6). Ni_2S-*P-62m* is isostructured by δ-Ag_2Ga and is topologically similar to Fe_2P-barringerite.The structure is characterized by 9-fold S-Ni coordination, forming SNi_9-three-lobed trigonal prisms (Figure 7).

Sulfur-enriched nickel sulfide NiS_3 crystallizes in the cubic space group *Im-3m* and consists of NiS_6 octahedra connected by vertices and SNi_2S_4 distorted octahedra connected by edges (Figure 8).

It is important to note that at pressures above 330 GPa, structures containing more than ~15% sulfur by weight, such as Ni_2S and NiS_3, cannot be adequately described by fcc packing. The results obtained suggest that at pressures characteristic of the Earth's core, about 4% of sulfur by weight can be dissolved in solid nickel without deformation of the structure. At the same time, it can be argued that the maximum amount of dissolved sulfur in solid nickel is approximately 15% by weight. These findings provide valuable information about the composition and structure of the Earth's inner core under high pressure conditions.

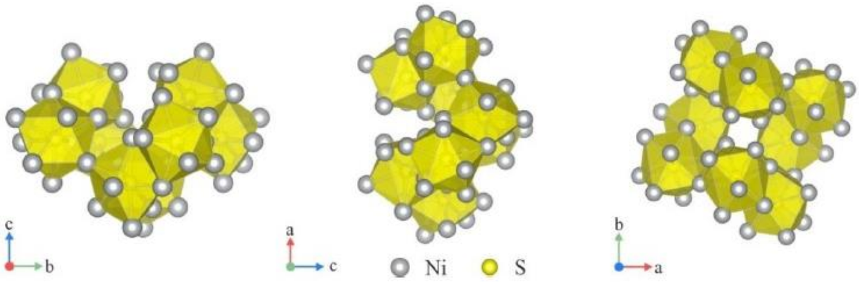


Figure 5. Structure of Ni_3S*-I-4*

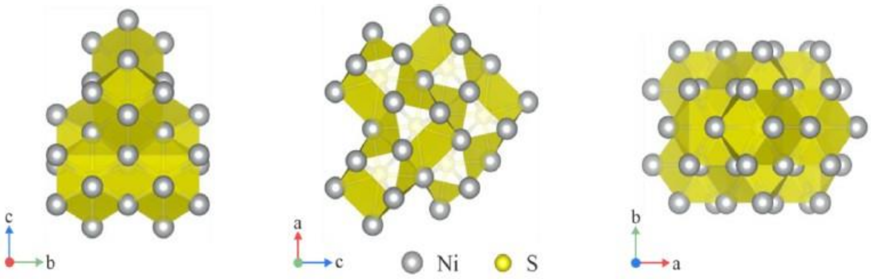


Figure 6. Ni_2S-Pnma Structure

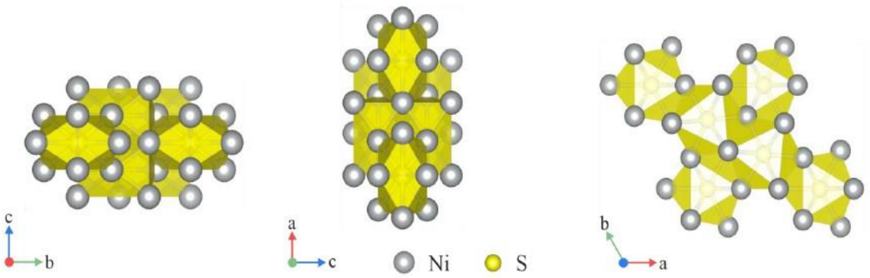


Figure 7. Structure of Ni_2S-P-62m

We also performed first-principle calculations for the Fe-S system, but did not identify any new stable compounds. Our studies using evolutionary methods to predict crystal structures show that thermodynamically stable iron sulfides in the pressure range of 100–400 GPa are the same Fe_2S, FeS and FeS_2. Despite the similar chemical characteristics of Fe and Ni, the only known stable sulfide enriched with iron under pressure conditions in the Earth's core is Fe_2S [8, p. 1029].

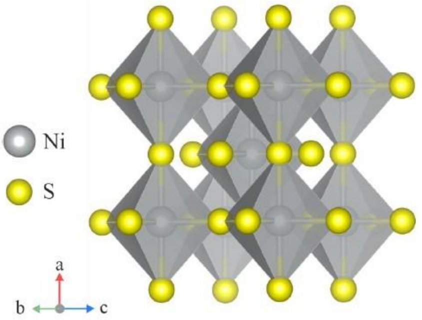


Figure 8. NiS_3-Im-3m structure

CONCLUSION

In conclusion, the studies conducted on the Ni-S system under extreme pressure conditions (100-400 GPa) using the VASP software package and the USPEX algorithm made it possible to identify stable crystal structures and determine stability fields for various Ni_xS_y compounds. The results indicate a wide variety of structural changes and phase transitions depending on pressure.

Our calculations within the framework of density functional theory and evolutionary algorithms showed that in the pressure range of 100–400 GPa, Fe_2S has only one stable structure, which has the space group *Pnma*. Ni_2S undergoes one phase transition. The phase with *Pnma* symmetry is stable above 100 GPa. At 272 GPa it enters a phase with *P-62m* symmetry. At a pressure similar to that in the inner core of the Earth (~365 GPa): Fe_2S-*Pnma*, FeS-*Pnmn*, FeS_2-*C2/m*, Ni_2S-$P\bar{6}2m$, Ni_3S-*Cmcm*, Ni_4S-$P\bar{1}$, Ni_5S-*C2/m*, $Ni_{12}S$-$R\bar{3}$, $Ni_{13}S$-$R\bar{3}$, $Ni_{14}S$-*C2/m*.

Thus, it is important to conduct such a study as was done for the Fe–S system [8, p. 1027] in order to expand our knowledge about stable phases in the Fe–Ni–S system at pressures of the core of the Earth and other planets. These data will also have a significant impact on determining key areas for future research.

These results are important for a better understanding of the composition and structure of the Earth's inner core, especially in the context of nickel's influence on the formation of stable compounds under extreme conditions. The obtained data have an impact on our understanding of geochemical processes in the Earth's crust and mantle, and also provide a basis for further theoretical research and experiments in the field of condensed matter physics.

REFERENCES

1. Sagatov N., Sagatova D., Gavryushkin P. and Litasov K. Fe–N System at High Pressures and Its Relevance to the Earth’s Core Composition // ACS Publications. – 2021. – Vol. 21. – P. 6101–6109.
2. Sun Y., Mendelev M., Zhang F., Ho K. Unveiling the effect of Ni on the formation and structure of Earth’s inner core // Earth, atmospheric, and planetary science. – 2024. – Vol. 121. – P. 121.
3. Thompson S. and others. High-pressure melting experiments of Fe_3S and a thermodynamic model of the Fe–S liquids for the Earth’s core // Journal of Physics:

Condensed Matter. – 2022. – Vol. 34. – Iss. 39. – P. 394003. https://doi.org/10.1088/1361-648X/ac8263

4. Beyer C. and others. High-pressure phase relations in the system Fe–Ni–Cu–S up to 14 GPa: implications for the stability of sulfides in the Earth’s upper mantle. Mineralogy and Petrology. – 2022. – Vol. 177. – P. 1966.
5. Fei Y. et al. Structure type and bulk modulus of Fe_3S, a new iron-sulfur compound // American Mineralogist. – 2000. – Vol. 85. – P. 1830–1833.
6. Zurkowski C. Fe_5S_2 identified as a host of sulfur in Earth and planetary cores // Earth and Planetary Science Letters. – 2022. – V. 593. – P. 117650.
7. Oka K. A cotunnite-type new high-pressure phase of Fe_2S // American Mineralogist. – 2022. – Vol. 107. – P. 7959.
8. Bazhanova Z., Roizen V., OganovA. High-pressure behavior of the Fe–S system and composition of the Earth's inner core // Physics-Uspekhi. – 2017. – Vol. 60. – P. 1025–1032.
9. Tateno S. et al. Fe_2S: The Most Fe-Rich Iron Sulfide at the Earth's Inner Core Pressures // Geophysical Research Letters. – 2019. – Vol. 46. – P. 11944–11949.
10. Urakawa S. Stability and bulk modulus of Ni_3S, a new nickel sulfur compound, and the melting relations of the system Ni-NiS up to 10 GPa // American Mineralogist. – 2011. – Vol. 96. – P. 3578.
11. Prewitt C., Gramsch S., Fei Y. High-pressure crystal chemistry of nickel sulphides // Journal of Physics: Condensed Matter. – 2002. – Vol. 14. –P. 11411–11415.
12. Yu Y., Ross N. Vibrational and thermodynamic properties of Ni_3S_2 polymorphs from first-principles calculations // Physics and Chemistry of Minerals. – 2011. – Vol. 38. – P. 241–249.
13. Znahg Q. and others. First-Principles Study of the Elastic Properties of Nickel Sulfide Minerals under High Pressure // MDPI Minerals. – 2020. – Vol. 10. – P. 737.
14. Kresse G., Furthmuller J. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set // Physical review B. – 1996.– Vol. 54. – P. 11169–11186.
15. Oganov A., Lyakhov A., Valle M. How evolutionary crystal structure prediction works – and why // Accounts of Chemical Research. – 2011. – Vol. 44. – P. 227–237.
16. Monkhorst H., Pack J. Special points for Brillouin-zone integrations // Physical review B. – 1976. – Vol. 13. – P. 5188–5192.
17. Methfessel M., Paxton A. High-precision sampling for Brillouin-zone integration in metals // Physical Review B. – 1989. – Vol. 40. – P. 3616–3621.
18. McMahan A., Albers R. Insulating Nickel at a Pressure of 34 TPa // Physical Review Letters. – 1982. – Vol. 49. – P. 1198–1201.
19. Zakharov O., Cohen M. Theory of structural, electronic, vibrational, and superconducting properties of high-pressure phases of sulfur // Physical Review B. – 1995. – Vol. 52. – P. 12572–12578.
20. Rudin S., Liu A. Predicted simple-cubic phase and superconducting properties for compressed sulfur // Physical review letters. – 1999. – Vol. 83. – P. 3049–3052.
21. Rubin A., Ma C. Meteoritic minerals and their origins // Geochemistry. – 2017. – Vol. 77. – P. 325–385.
22. Sagatov E., Bazarbek A., Inerbaev T. et al. Phase Relations in the Ni−S System at High Pressures from ab InitioComputations // ACS Earth and Space Chemistry. – 2021. – Vol. 5. – P. 596–603.

НИКЕЛЬ-КҮКІРТ ЖҮЙЕСІ ҮШІН ТҰРАҚТЫ ҚҰРЫЛЫМДАРДЫ ТАБУ ЖӘНЕ ТЕМІР-КҮКІРТ ЖҮЙЕСІМЕН САЛЫСТЫРУ

А. Б. Базарбек[1*], **А. Д. Акылбекова**[1], **А. А. Кисабекова**[2], **А. А. Ногай**[3], **А. Т. Акилбеков**[1]

[1] Л.Н. Гумилев атындағы Еуразия ұлттық университеті, Астана, Қазақстан
[2] Жаратылыстану жоғары мектебі, «Ә. Марғұлан атындағы Павлодар педагогикалық университеті» коммерциялық емес акционерлік қоғамы, Павлодар, Қазақстан
[3]Қазақ агротехникалық зерттеу университеті, Астана, Қазақстан

***Байланыс үшін E-mail: asyl.bazarbek.92@mail.ru*

Жердің ядросы негізінен темір мен никельден тұрады, олар темір-никель қорытпасын құрайды. Сонымен қатар, күкірт ішкі ядродағы жеңіл элемент рөліне әлеуетті үміткерлердің бірі болып табылады. Бүгінгі күні кванттық химиялық модельдеу арқылы Fe-C, Fe-H, Fe-O, Fe-Si, Fe-S және Fe-P сияқты жүйелердегі аралық құрамдар мен құрылымдарды 400 ГПа қысымға дейін іздеу үшін көптеген теориялық зерттеулер жүргізілді.

Темір-жеңіл элементтер жүйелерін кеңінен зерттеуге қарамастан, бүгінгі күнге дейін бақыланатын сейсмологиялық мәліметтерге толық сәйкес келетін жер ядросының минералогиялық моделі жасалмаған. Бұл алшақтықтың ықтимал себебі ядроның негізгі легирлеуші элементі – никельдің әсерін жеткіліксіз есепке алу болуы мүмкін. Жоғары қысымда никель-жеңіл элементтер жүйесіне теориялық зерттеулер жеткіліксіз жүргізілді. Сондықтан Fe-Ni-S үштік жүйелеріндегі ықтимал аралық қосылыстарды әрі қарай зерттеу және анықтау мақсатында осы екілік жүйелерге тереңірек зерттеулер жүргізу қажет.

Түйін сөздер: *теориялық есептеулер, фазалық ауысу, лазерлік қыздыру, тұрақты модификация, жоғары қысымды физика.*

ПОИСК СТАБИЛЬНЫХ СТРУКТУР ДЛЯ СИСТЕМЫ НИКЕЛЬ-СЕРА И СРАВНЕНИЕ С СИСТЕМОЙ ЖЕЛЕЗО-СЕРА

А. Б. Базарбек[1]*, А. Д. Акылбекова[1], А. А. Кисабекова[2], А. А. Ногай[3], А. Т. Акилбеков[1]

[1] Евразийский национальный университет им. Л.Н. Гумилева, Астана, Казахстан
[2] Высшая школа Естествознания, НАО «Павлодарский педагогический университет им. Ә. Марғұлан», Павлодар, Казахстан
[3] Казахский агротехнический исследовательский университет, Астана, Казахстан

**E-mail для контактов: asyl.bazarbek.92@mail.ru*

Ядро Земли состоит в основном из железа и никеля, образующих железо-никелевый сплав. В то же время сера является одним из потенциальных кандидатов на роль легкого элемента во внутреннем ядре. На сегодняшний день с помощью квантово-химического моделирования было проведено множество теоретических исследований для поиска промежуточных составов и структур в таких системах, как Fe-C, Fe-H, Fe-O, Fe-Si, Fe-S и Fe-P до давлений 400 ГПа.

Несмотря на обширные исследования систем железо-легкие элементы, на сегодняшний день не создана минералогическая модель ядра Земли, которая полностью соответствовала бы наблюдаемым сейсмологическим данным. Возможной причиной этого расхождения может быть недостаточный учет влияния ключевого легирующего элемента ядра – никеля. Теоретические исследования системы никель-легкие элементы при высоких давлениях были проведены недостаточно. Следовательно, необходимо провести более углубленные исследования этих бинарных систем с целью дальнейшего изучения и идентификации возможных промежуточных соединений в тройных системах Fe-Ni-S.

Ключевые слова: *теоретические расчеты, фазовый переход, лазерный нагрев, стабильная модификация, физика высокого давления.*