Table 1 Structural data for the found phases of Ni-P system at P=100~GPa. The pressures at which the structures were predicted are indicated in the corresponding column

Phase	Pressure (GPa)	Space group				Atomic coordinates			
			Lattice parameters (Å, degree)			Atom	х	у	Z
Ni ₁₄ P	400	C2/m~(#12)	$a=7.538 \\ \alpha=90$	b = 6.816 $\beta = 120$	$c{=}5.567$ $\gamma{=}90$	Ni1 Ni2 Ni3	$0.000 \\ 0.099 \\ 0.301$	$0.169 \\ 0.000 \\ 0.000$	$0.000 \\ 0.397 \\ 0.198$
						Ni4 Ni5 P1	0.703 0.599 0.000	$0.335 \\ 0.166 \\ 0.500$	$0.800 \\ 0.398 \\ 0.000$
$\mathrm{Ni}_{12}\mathrm{P}$	400	$R\bar{3}(\#148)$	$a=8.032 \\ \alpha=90$	b = 8.032 $\beta = 90$	$c{=}5.261 \\ \gamma{=}120$	Ni1 Ni2 P1	$0.539 \\ -0.029 \\ 0.000$	$0.384 \\ 0.409 \\ 0.000$	$0.001 \\ 0.332 \\ 0.000$
Ni ₁₀ P	300	PĪ (#2)	a=3.932 $\alpha=107.5$	b = 5.074 $\beta = 105.0$	$c{=}5.079$ $\gamma{=}97.4$	Ni1 Ni2 Ni3 Ni4 Ni5 P1	0.0450 0.5902 0.1372 0.2267 0.6776 0.5000	0.4101 0.3191 0.2285 0.0494 0.1381 0.5000	0.1803 0.3592 0.5468 -0.0910 0.7281 0.0000
Ni ₈ P	200	PĪ (#2)	$a=3.927 \\ \alpha=75.0$	b = 3.932 $\beta = 82.6$	$c{=}5.076 \ \gamma{=}80.5$	Ni1 Ni2 Ni3 Ni4 P1	$\begin{array}{c} 0.22148 \\ 0.67093 \\ 0.44401 \\ 0.11116 \\ 0.00000 \end{array}$	$\begin{array}{c} 0.11048 \\ 0.33311 \\ 0.21845 \\ 0.55650 \\ 0.00000 \end{array}$	$\begin{array}{c} 0.56082 \\ 0.66740 \\ 0.11085 \\ 0.78047 \\ 0.00000 \end{array}$
Ni ₇ P	100	PĪ (#2)	$a=3.755 \ \alpha=73.0$	b = 3.777 $\beta = 90.0$	$c{=}4.393$ $\gamma{=}79.9$	Ni1 Ni2 Ni3 Ni4 P1	0.5020 0.0000 0.7539 0.2490 0.0000	0.0003 0.0000 0.4984 0.5069 0.0000	0.2477 0.5000 0.1244 0.3713 0.0000
Ni ₅ P	200	P6 ₃ /mcm (#193)	$a=3.934 \\ \alpha=90$	b = 3.934 $\beta = 90$	$c{=}7.372 \\ \gamma{=}120$	Ni1 Ni2 P1	0.3333 0.6710 0.0000	0.6667 0.0000 0.0000	0.0000 0.2500 0.0000
Ni ₃ P	100	Cmca (#64)	$a{=}13.1666 \ \alpha{=}90$	b = 4.4854 $\beta = 90$	$c{=}4.4851 \ \gamma{=}90$	Ni1 Ni2 Ni3 P1	0.3814 0.0000 0.2500 0.1365	0.0000 0.1818 0.7473 0.0000	0.0000 0.8180 0.2500 0.0000
Ni ₂ P	100	Pnma (#64)	a=4.271 $\alpha=90$	$b=3.307 \ \beta=90$	$c{=}6.247 \ \gamma{=}90$	Ni1 Ni2 P1	0.4537 0.8260 0.8021	$0.2500 \\ 0.2500 \\ 0.2500$	0.7890 0.0589 0.3870

 $\textbf{b}, \textbf{b}, \textbf{b}, \textbf{m}, \textbf{m}, \textbf{u}, \textbf{m}, \textbf{v}, \textbf{u}, \textbf{x}, \boldsymbol{\phi}, \textbf{y}, \textbf{r}, \textbf{c}, \textbf{p}, \textbf{n}, \textbf{o}, \textbf{m}, \textbf{m}, \textbf{x}, \textbf{x}, \textbf{u}, \textbf{u}, \textbf{x}, \textbf{s}, \boldsymbol{\delta}, \textbf{a}, \textbf{x}, \textbf{f}, \textbf{o}, \textbf{s}, \textbf{s}, \textbf{h}, \textbf{s}, \textbf{h}, \textbf{s}, \textbf{h}, \textbf{h}, \textbf{s}, \textbf{h}, \textbf{h}$

1 Introduction

Phosphides play a significant role in the mineralogy of iron meteorites as the components of the ternary Fe-Ni-P system. Although being rare, accessory minerals with composition $(Fe,Ni)_xP$, they give important information about phosphorus geochemistry on the early stages of the universe formation. ^{1–10} The occurrence of these minerals in meteoritic samples is believed to originate either from the equilibrium condensation of protoplanetary materials taking place in the solar nebulae or from crystallization processes in the cores of parent bodies.

Iron-rich end-members of Fe-P system were intensively studied using both experimental and theoretical techniques. So far, most of the high-pressure investigations on iron phosphides have been restricted on Fe₄P, ¹¹ Fe₃P, ¹² Fe₂P ^{13,14}, and FeP. ¹⁵ Several structural and magnetic phase transitions have been revealed as the result. Dera et al. observed that on heating at 8 GPa phase of Fe₂P transforms to a high-pressure modification, which could be quenched to ambient conditions. ¹³ Theoretical modelling demonstrates that the stable phase of Fe₂P should be the *Pnma* with the lowest total energy in the low pressure region, and the $P\bar{6}2m$ and Pnma phases would transform to the $P\bar{5}m$ Journal Name, [vol.], [vol.] distation number of iron at 125 GPa and 153 GPa, respectively. ¹⁴ Theoretical studies have shown that Fe₂P could decompose into Fe₂P and Fe₄P at pressures

allabogdanite against barringerite ^{3,4,19}, and also slightly increases the bulk modulus of the allabogdanite phase. ¹⁹ A может здесь сослаться на нашу статью по алабогданиту (Bekker, Sagatov et al., 2020)? The incorporation of Ni in nonmagnetic Fe₄P results in reduction of the compressional and shear wave velocities enhancing their anisotropy. ¹¹

There are numerous phases were revealed in Ni-P system at ambient pressure. Among them are Ni₃P, Ni₈P₃, Ni₁₂P₅, Ni₂P, Ni₅P₄, NiP, NiP₂, and NiP₃. However, the data on this system at high-pressures, especially above 100 GPa, are limited. Donohue et al. ²⁰ studied P-rich compositions (NiP_{2,2-2,5}) at 1.5- $6.5~\mathrm{GPa}$. Dera et. al. 21 synthesized a cubic NiP₂ phase at 6.5GPa during heating at 1200°C and subsequent cooling to 900°C. Incongruent melting associated with formation of pyrite-type NiP₂ and amorphous Ni-P alloy was found at an intermediate pressure range, between 6.5 and 40 GPa. The phase transitions in Ni₂P were not observed in these experiments at pressures up to 50 GPa consistently with theoretical predictions. 19 Several reversible phase transitions were established in NiP at ambient temperature: (a) from Pbca to Cmc2₁ at 3.5 GPa, (b) to Pnma-phase at 8.5 GPa and to another Cmc2₁-phase, but with different crystal structure at 25 GPa. 22,23 Litasov et.al. studied the melting processes and subsolidus phase relations in the Ni-Ni₂P system at 6 GPa and 900-1600°C. At 6 GPa and 900-1600°C the Ni-Ni₂P system has four stable phosphides: Ni₃P

the magn

search for stable structures of intermediate compositions was performed using the USPEX package. At the second stage, the predictions were performed for the fixed compositions represented on the convex hull constructed at the first stage using USPEX and AIRSS. The crystal structure prediction calculations were performed at 100, 200, 300, and 400 GPa for 1-4 formula units. The size of the first generation in the calculations with USPEX was equal to 60 structures. 60% of the structures with the lowest enthalpy were selected after the optimization and then used for the production of the next generation (30% - by heredity, 20% - by atomic mutation, 15% by lattice permutation, and 35% - randomly). Using AIRSS 1500-2000 structures were randomly generated and optimized, and those with the lowest enthalpy were selected. The calculations of the electronic structure were carried out within the DFT using the VASP 5.4 package. ^{32,33} The exchange-correlation interaction was taken into account in the generalized gradient approximation (GGA) in the form of the Perdew-Burke-Ernzerhof (PBE) functional³⁴ in a plane-wave basis set along with projector augmented-wave (PAW) pseudopotentials. 35 For all studied structures, calculations were performed, taking into account the spin polarization. It was found that in all cases, except for the new predicted phases Ni₁₀P, Ni₁₂P, and Ni₁₄P, the magnetic moment is equal to zero. The computation parameters were as follows: energy cut-off - 450 eV; the density of the grid of Monkhorst-Pack k-point mesh -0.5\AA^{-1} . The most promising predicted structures were then optimized with higher accuracy at various pressures. In these calculations, the cut-off energy was 700 eV and the density of k-points was 0.2Å^{-1} . Tyt, как уже было отмечено, нужно добавить про оптимизацию структур, взятых из литературных источников.

To take into account the temperature effect and predict the phase diagrams, we used the method of lattice dynamics within the quasi-harmonic approximation (QHA). For this task, the phonon frequencies were calculated with the PHONOPY code. ³⁶ Coordination polyhedrons for predicted structures were visualized with VESTA software?

3 Results and Discussion

3.1 The analysis of HP crystal structures

Structural data of the new phases predicted with USPEX and AIRSS codes are summarized in Table 1 and shown in Fig. ??. All found structures are dynamically stable, the corresponding phonon spectra presented in Supporting Information (SI) in Fig. S1. New structures were predicted at different pressures. Table 1 shows the unit cell parameters after the optimization of the volume of unit cells corresponding to an external pressure of 100 GPa.

The structures of $Ni_{14}P$, $Ni_{12}P$, $Ni_{10}P$, $Ni_{8}P$, $Ni_{7}P$, $Ni_{5}P$, and $Ni_{3}P$ are characterized by fcc packing, with Ni atoms partially substituted by P atoms. The pure Ni also present in the fcc form up to 400 GPa. Thus, the found structures can be considered as (Ni,P) solid solutions. This type of isomorphism between d-metal and light element is unusual at ambient pressures. At extreme pressures of the Earth's core, when elements which are

typical non-metals like sulfur adopt metallic properties ³⁷, this isomorphism became widespread. Isomorphic replacement of iron on S, Si and C within *hcp* or *bcc* crystal structures can be given as an example ^{38?}. Добавил ссылку, но bibtex ее не видит. Как и некоторые другие выше. Phosphorus atoms in found structures tend to be homogeniously spread through the structure, without clustering or group formation.

Ni₁₄P, Ni₁₂P, Ni₁₀P, Ni₈P, Ni₇P, Ni₅P structures are characterised by almost ideal fcc packing, with both Ni-Ni and Ni-P bonds are of the same length, equal to 2.7 Å at 100 GPa. The Ni-Ni bond in the pure Ni is characterised by the same length. Ni₃P structure is sufficiently deformed, as shown on Figure ??, the Ni-P bond is equal to 2.25 Å while length of Ni-Ni bonds vary in the range 2.25-2.35Å. The found Ni₂P-Pnma structure is the analogue of allabogdanite mineral with composition Fe₂P. Allabogdanite is of cottunite-type, does not having close-packing of atoms, in contrast to fcc structure which is 3layered close-packing. The calculations, which results will be presented below, show that experimentally synthesised at ambient pressure Ni₈P₃ structure is also stable up to 400 GPa. As well as Ni₂P, the structure of this phase are not of closed packing type. Thus, at nearly 25 mol.% of P content in (Ni,P) alloy, the change of the structural type takes place. This value can be accepted as the estimation for the phosphorus solubility in Ni structure at high pressures and low temperatures. As temperature increases the limits of isomorphism, this value can be sufficiently higher for the conditions of the cores of the Earth or planets. The fact, that similar isomorphism was not found in Fe-P systems, likely shows that solubility of P in (Fe,Ni) alloy will be higher than in the pure Fe.

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Spin-polarized calculations show the presence of a magnetic moment in structures with a relatively high nickel content from Ni₁₄ to Ni₈P, as shown in Fig. 2. In all other cases, the magnetic order is absent. The magnetic moment per nickel atom decreases with an increase in the specific phosphorus content in the system. With increasing pressure, the magnetic moment and magnetic ordering completely disappear at a pressure of 315, 360, 350, and 115 GPa for the Ni₁₄P, Ni₁₂P, Ni₁₀P, and Ni₈P lattices, respectively. Unlike the considered phosphides, the magnitude of the magnetic moment in pure nickel weakly depends on external pressure. With an increase in pressure from 100 to 200 GPa, the magnetic moment per nickel atom decreases from 0.58 μ_B to 0.5 μ_B and then remains practically unchanged.

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3.2 Thermodynamic of Ni–P compounds

Both sets of the predicted and experimentally observed Ni-P binary compounds were used to evaluate the formation enthalpy ΔH with respect to the elemental solids Ni and P according to Eq. 1, in order to explore the thermodynamic stability of Ni-P:

$$\Delta H(\mathrm{Ni}_n\mathrm{P}_m) = \frac{H(\mathrm{Ni}_n\mathrm{P}_m) - nH(\mathrm{Ni}) - mH(\mathrm{P})}{Z(n+m)}, \tag{1}$$

where H = U + PV is the enthalpy of each compound, Z is a number of formula units in the unit cell of the structure and ΔH is the enthalpy of formation per formula unit. Herein, U, P, and V are internal energy, pressure and volume, correspondingly. Detailed information about the element solids can be found in SI. Ссылка на рисунок.

The relative stabilities of the considered compositions at the selected pressures of 100, 200, 300, and 400 GPa, with ΔH evaluated per atom, are shown in the form of the so-called convex hull Fig. ??, useful for assesing of the phases thermodynamic stability. Points corresponding to the phases with enthalpy lower than the enthalpy of mechanical mixture of the neighbouring compounds forms the convex hull on such a plot. All points above the convex hull corresponds to the unstable phases, decomposing on the mixture of neighbouring compounds. In addition to the predicted and described above Ni₁₄P, Ni₁₂P, Ni₁₀P, Ni₈P, Ni₇P, Ni₅P, Ni₃P, and Ni₂P structures, we have also considered Ni₈P₃, Ni₁2P₄, Ni₅P₂, NiP₂, and NiP₃ structures, synthesised experimentally at ambient pressure.

Predicted solid solutions Ni₁₄P - Ni₇P are stable within all pressure range from 100 to 400 GPa, while solid solution enriched with phosphorus are stabilised with pressure. Ni₅P became stable from 200 GPa and above, while Ni₃P from 300 GPa and above. Allabogdanite-Ni₂P is also stabilised against decomposition at 200 GPa. Experimental phase Ni₈P₃ is stable at the entire pressure range, while NiP2 destabilised above 300 GPa. Experimental phases Ni₁2P₅, Ni₅P₂, and NiP₃ are thermodynamically unstable at the considered pressure range.

It has to be emphasized, that the results presented in Fig.?? are obtained neglecting thermal effects. In order to account for the effect of temperature on Gibbs energy, we use method of lattice dynamic. Within this method, it is necessary to calculate the vibrational spectra of all the structures considered. We performed phonon mode calculations for all predicted structures, described above. Experimentally synthesised Ni₈P₃ was not considered in this context, due to the large size of the unit cell, containing 132 atoms. Speculatively we assume thermodynamic instability of such a low symmetric structure in the filed of high temperatures, due to effect of entropy.

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Due to natural ocurence of schreibersite-Ni₃P, allabogdanite-Ni₂P, and transjordanite-Ni₂P phases and their findings in metoritic rocks, we determined PT phase diagrams for these compounds, presented in Fig. ??. The diagrams shows, that transition from barringerite to allabogdanite structure in the Ni₂P system occurs in the pressure range 77-88 GPa at temperatures 0-2000 K. The transition from schreibersite to the found Cmcm structure occurs at 62 GPa and pressure of phase transition is almost independent from temperature.

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