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Phase stability in nickel phosphides at high pressures

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We performed first-principles calculations on the crystal structure prediction and relative thermodynamic stability for Ni–P binary system at 100-400 GPa pressure range. Crystal structures of seven intermediate compositions, $Ni_{14}P$, $Ni_{12}P$, $Ni_{10}P$, Ni_8P, Ni_7P, Ni_5P, $Ni_3P, and Ni_2P$ stable against decomposition on the mixture of Ni and P are predicted in all investigated pressure range. First seven of them, present substitutional solid solutions of phosphorus in nickel face-centered cubic structure. Thus, up to 25 mol.% of P can be dissolved in crystal structure of Ni at low temperature and temperature can sufficiently increases this limit. For Ni_3P nickel phosphide, a new high-pressure phase with *Cmca* space group, which can be also considered as (Ni,P) solid solution within highly deformed *fcc* Ni structure, was found. This phase is stable in the range ... GPa. Ni_2P is found to be adopt allabogdanite structure at pressures above ... The *P-T* phase diagrams of Ni_2P and Ni_3P phosphides were calculated by the lattice dynamics method in the quasi-harmonic approximation.

1 Introduction

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

Fe end-members were intensively studied using both experimental and theoretical techniques. So far, most of the high-pressure investigations on iron phosphides have been restricted on Fe_4P,[?] Fe_3P,[?] Fe_2P[? ?] and FeP.[?] 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.[?] Theoretical modelling demonstrates that the stable phase of Fe_2P should be the *Pnma* with the lowest total energy at lower pressure, and the $P\bar{6}2m$ and *Pnma* phases would transform to the $P\bar{3}m$ phase with larger coordination number of iron at 125 GPa and 153 GPa, respectively.[?] Theoretical studies have shown that Fe_3P could decompose into Fe_2P and Fe_4P at pressures higher than 214 GPa [?], and Fe_3P and Fe would react with formation of Fe_4P at $\sim$100 GPa.[?] Fe_3P exhibits a structural phase transition from *I*4 to $P4/mnc$ at 64 GPa and 1600 K accompanied with an electronic state transition from high spin to low spin at around 20-40 GPa.[? ?] Upon compression, Fe_4P undergoes transition from ferromagnetic to nonmagnetic state at 80 GPa.[?] Britvin et al. reported two new structures of FeP (*Pnma*) and FeP_2 (*Pnnm*), found in the pyrometamorphic rocks.[? ?]

Alloying effect of Ni on physical properties and structure of Fe and it's alloys with light elements is also of geological interest, as according to geochemical assesment Earth's core could contain up to 10mol% of Ni (Уточнить и поставить ссылку на Чёрную Книжку (?)). Addition of nickel to iron phosphides affect the structure and phase stability. The example of Fe2P shows, that a small addition of Ni and Co stabilise the structure of alabogdanite against ... [? ? ?], and also slightly increases the bulk modulus of the allabogdanite phase.[?] А может здесь сослаться на нашу статью по алабогданиту (Bekker, Sagatov et al., 2020)? The incorporation of Ni in nonmagnetic Fe_4P results in reduction of the compressional and shear wave velocities enhancing their anisotropy.[?]

There are numerous phases were revealed in Ni–P system at ambient pressure. Among them are Ni_3P, Ni_8P_3, $Ni_{12}P_5$, Ni_2P, Ni_5P_4, NiP, NiP_2, and NiP_3. However, the data on this system at high-pressures, especially above 100 GPa, are limited. Donohue et al.[?] studied P-rich compositions ($NiP_{2.2-2.5}$) at 1.5-

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Table 1 Structural data for the predicted phases of Ni–P system Параметры ячейки лучше округлить до тысячных, четврётая цифра абсолютно не значима. Координаты атомов – до десятитысячных (именно так делает большинство авторов, например К. Пикард, лично я бы всё до тысячных округлял))

Phase	Pressure (GPa)	Space group	Lattice parameters (Å, degree)			Atomic coordinates			
						Atom	x	y	z
$Ni_{14}P$	400	$C2/m$ (#12)	a=6.8686Å	b=6.2097Å	c=5.0749Å	Ni1	0.00000	0.16860	0.00000
			α=90	β=119.559	γ=90	Ni2	0.09850	0.00000	0.39699
						Ni3	0.30065	0.00000	0.19837
						Ni4	0.70280	0.33474	0.80023
						Ni5	0.59887	0.16587	0.39807
						P1	0.00000	0.50000	0.00000
$Ni_{12}P$	400	$R\bar{3}$(#148)	a=7.4609Å	b=7.4609Å	c=5.0755Å	Ni1	0.53902	0.38422	0.00134
			α=90.00	β=90.00	γ=120	Ni2	-0.02851	0.40876	0.33153
						P1	0.00000	0.00000	0.00000
$Ni_{10}P$	300	$P\bar{1}$ (#2)	a=3.6654Å	b=4.7295Å	c=4.7339Å	Ni1	0.04502	0.41007	0.18032
			α=107.482	β=104.937	γ=97.456	Ni2	0.59015	0.31912	0.35915
						Ni3	0.13716	0.22851	0.54678
						Ni4	0.22672	0.04944	-0.09103
						Ni5	0.67759	0.13805	0.72806
						P1	0.50000	0.50000	0.00000
Ni_8P	200	$P\bar{1}$ (#2)	a=3.7669Å	b=3.7719Å	c=4.8694Å	Ni1	0.22148	0.11048	0.56082
			α=75.00	β=82.569	γ=80.481	Ni2	0.67093	0.33311	0.66740
						Ni3	0.44401	0.21845	0.11085
						Ni4	0.11116	0.55650	0.78047
						P1	0.00000	0.00000	0.00000
Ni_7P	100	$P\bar{1}$ (#2)	a=3.7553Å	b=3.7772Å	c=4.3925Å	Ni1	0.50201	0.00029	0.24766
			α=73.032	β=89.980	γ=79.849	Ni2	0.00000	0.00000	0.50000
						Ni3	0.75389	0.49840	0.12435
						Ni4	0.24895	0.50693	0.37130
						P1	0.00000	0.00000	0.00000
Ni_5P	200	$P6_3/mcm$ (#193)	a=3.7732Å	b=3.7732Å	c=7.0786Å	Ni1	0.33333	0.66667	0.00000
			α=90.00	β=90.00	γ=120	Ni2	0.67096	0.00000	0.25000
						P1	0.00000	0.00000	0.00000
Ni_3P	100	$Cmca$ (#64)	a=13.1666Å	b=4.4854Å	c=4.4851Å	Ni1	0.38137	0.00000	0.00000
			α=90.00	β=90.00	γ=90.00	Ni2	0.00000	0.18176	0.81801
						Ni3	0.25000	0.74729	0.25000
						P1	0.13651	0.00000	0.00000

6.5 GPa. Dera et. al.[?] synthesized a cubic NiP_2 phase at 6.5 GPa during heating at 1200°C and subsequent cooling to 900°C. Incongruent melting associated with formation of pyrite-type NiP_2 and amorphous Ni-P alloy was found at an intermediate pressure range, between 6.5 and 40 GPa. The phase transitions in Ni_2P were not observed in these experiments at pressures up to 50 GPa consistently with theoretical modelling.[?] Several reversible phase transitions were established in NiP at ambient temperature: (a) from *Pbca* to $Cmc2_1$ at 3.5 GPa, (b) to *Pnma*-phase at 8.5 GPa and again to $Cmc2_1$-phase, but with different crystal structure at 25 GPa.[? ?] Litasov et.al. studied the melting processes and subsolidus phase relations in the Ni-Ni_2P system at 6 GPa and 900-1600°C.[?] Хорошо бы в этой и других подобных ссылках отметить конкретный результат. А так получается просто констатация факта, что кто-то что-то исследовал. А что получено в результате? The stability of four intermediate compositions, Ni_3P, Ni_8P_3/Ni_5P_2, $Ni_{12}P_5$, and Ni_2P transjordanite was found. The $Ni_{12}P_5$ phase becomes unstable at 900°C and decomposes into Ni_5P_2 and Ni_2P.

The phase stability, elastic properties, hardness and related electronic structures of Ni–P crystal phases at ambient pressure and zero temperature were studied theoretically in Ref.[? ?]. According to calculations, at atmospheric pressure and zero temperature, Ni-P compounds can be ordered as the formation enthalpy increases as follows: $Ni_5P_4 < Ni_2P < Ni_{12}P_5 < NiP < Ni_8P_3 < Ni_3P < NiP_2 < NiP_3$. Как я понял, здесь считается энтальпия образования на атом, без учёта какой это атом. И какая информация получается в результате? что Ni_5P_4 стабильнее Ni_2P? Информативно ли это? Мне кажется что нет, но видимо я что-то не понимаю.

The equations of state and structural parameters of Ni_2P, NiP_2 (pyrite type) and Ni-doped Fe_2P (allabogdanite) at high pressures were determined with first-principles calculations.[?] There was not found barringerite-allabogdanite phase transition in Ni_2P at pressures up to 50 GPa. Bulk modulus of $(Fe_{1-x}Ni_x)_2P$ (allabogdanite) increases with Ni concentration. Increasing the concentration of Ni decreases the stability of structure and suppresses the total magnetic moment of the system.

In present research, we theoretically investigate Ni-P compounds in the pressure range from 100 to 400 GPa. A search for new crystalline structures is carried out. The relative stability of all predicted and well-known experimentally observed structures of the Ni–P system is investigated. The phase diagram of the Ni_2P system is calculated, where barringerite-allobogdanite structural phase transition occurs at pressures of 77-87 GPa depending on temperature. Similar calculations of the phase equilibrium between the new high-pressure Ni_3P phase and the schreibersite structure are also performed.

2 Computation Details

The structure predictions were performed using USPEX code based on evolutionary algorithms[?,?,?] and AIRSS based on a random sampling method.[?,?] Crystal structure prediction calculations were divided into two stages. At the first stage, the 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 calculations of the electronic structure were carried out within the DFT using the VASP 5.4 package.[?,?] The exchange-correlation interaction was taken into account in the generalized gradient approximation (GGA) in the form of the Perdew-Burke-Ernzerhof (PBE) functional[?] in a plane-wave basis set along with projector augmented-wave (PAW) pseudopotentials.[?] 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 $Ni_{10}P$, $Ni_{12}P$, and $Ni_{14}P$, 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 – $0.5Å^{-1}$. 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 $0.2Å^{-1}$.

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.[?]

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. 1. All found structures are dynamically stable,the corresponding phonon spectra presented in Supporting Information (SI).

The structures of Ni14P, Ni12P, Ni10P, Ni8P, Ni7P, Ni5P, and Ni3P are characterized by *fcc* packing, witi 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 sulphur adopt metallic properties[?] , this isomorphism became typical. Isomorphic replacement of iron on sulphur within *hcp* or *bcc* crystal structures can be given as exmaple[?] . Я здесь в обоих случаях на себя ссылаюсь, хорошо бы добавить и другие ссылки (например на Cote и Vocadlo), но сходу ничего предложить не могу. Typical for solid solutions, P atoms in found structures tend to

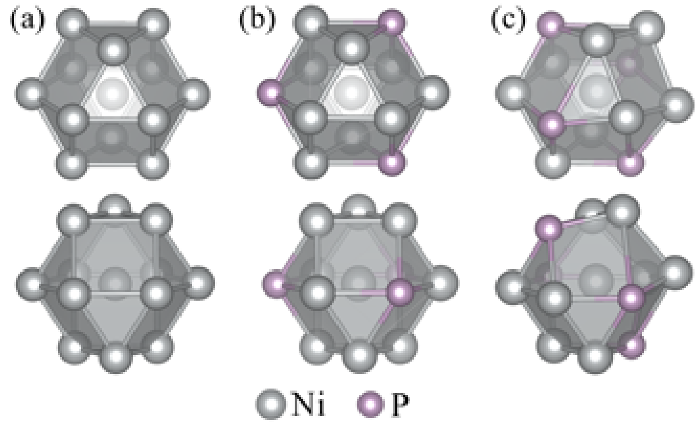

Fig. 1 Coordination cube-octahedron around Ni atoms in fcc-Ni (a), Ni_5P-$P6_3/mcm$ (b), and Ni_3P-*Cmca* (c) structures; upper row – view along three-fold axis, lower row – perpendicular to the three-fold axis Коллеги, я здесь запутался, получается что Ni_3P-*Cmca* – это тоже твёрдый раствор (Ni,P) просто сильно деформированный, т.е при давлении выше 70 ГПа просто стабилизируется твёрдый раствор, то же самое имеет место и в отношении других составов, кроме Ni2P. К рисунку с выпуклой оболочкой хорошо бы добавить ещё рисунок с фазовыми переходами, как мы это обычно делаем, их там практически нет, но всё равно, лучше для наглядности сделать, потому что мне было не просто разобраться. Структуру аллабогданита я бы тоже добавил, под буквой (d), а для имеющихся структур оставил только одну проекцию вдоль оси третьего порядка, слегка наклонённую. Ni8P3 – поду буквой (e)

be homogenically spread through the structure, without clustering or group formation.

The deformation of the ideal cubic *fcc* structure increases with increasing amount of phosphourus. The deformation of coordination cube-octahedron of ligand Ni and P atoms around central Ni atom can be traced by the changes of Ni-P and Ni-N bond lengths, shown in Supporting information Figure ??. Ni14P, Ni12P, Ni10P, Ni8P, Ni7P, Ni5P structures are characterised by almost ideal fcc packing, with both Ni-Ni and Ni-P bonds of the same length, equal to 2.7 Å at 100 GPa. The Ni-Ni bond in the pure *fcc* Ni is characterised by the same length. Ni3P structure is sufficiently deformed, as shown on Figure 1, 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 and it is sufficiently different from the described solid solutions, which indicate on the limit of (Ni,P) isomorphism. The calculations, which results will be presented below, show that experimentally synthesises at ambient pressure Ni8P3 structure is also stable up to 400 GPa. As well as Ni2P, the structure of this phase are also not related to the described solid solutions, Thus, around 15 mol.% of P can be dissolved in *fcc* structure of Ni, without heating. As temperature increases the limits of isomorphism, this value can be accepted as the lower boundary for (Ni,P) isomorphism at 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.

Spin-polarized calculations show the presence of a magnetic moment in structures with a relatively high nickel content from Ni_{14} to Ni_8P, as shown in Fig. 4. 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 $Ni_{14}P$, $Ni_{12}P$, $Ni_{10}P$, and Ni_8P 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.

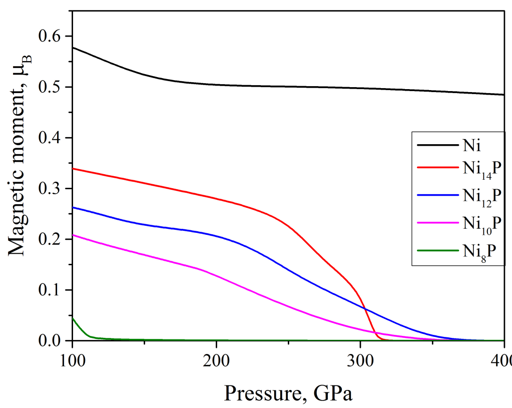

Fig. 2 Pressure dependence of magnatic moment (in Bohr magneton, μ_B) per Ni atom for predicted Ni–P crystal structures. The dependence of the magnetic moment on pressure for pure nickel is given for comparison.

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 ot the elemental solids Ni and P according to Eq. 1, in order to explore the thermodinamic stability of Ni–P:

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

where $H = U + PV$ is the entalpy of each compound, Z is a number of structure units in the unit cell 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.

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 Fig. 5. The stable phase lies on the convex hulls (the global stability lines). А почему в единственном числе? Here, we take into consideration the Ni_2P with allabogdanite structure and the new predicted Ni_3P structure. As will be shown below, these polymorphs are more thermodynamically favorable in the pressure range considered in the present paper.

All predicted $Ni_{14}P$, $Ni_{12}P$, $Ni_{10}P$, Ni_8P, and Ni_7P phases are stable through the entire range of considered pressures . The Ni_5P structure is metastable at a pressure of 100 GPa (ΔH=0.035 eV/atom), but it stabilizes at pressures of 200 GPa and higher. Ni_3P and Ni_2P become thermodynamically stable at pressures above 200 GPa. The structure of pyrite NiP_2 becomes metastable at pressures above 300 GPa.

~~The trend of phase stability for Ni–P compounds at zero pressure is Ni_5P_4 > Ni_2P > $Ni_{12}P_5$ > NiP > Ni_8P_3 > Ni_3P > NiP_2 > NiP_3.~~ Я уже приводил эту последовательность выше в Введении. Если лучше сослаться туда, можно это место переписать. As mentioned above, at atmospheric pressure Ni-P compounds can be ordered as the formation enthalpy increases as Ni_5P_4 < Ni_2P < $Ni_{12}P_5$ < NiP < Ni_8P_3 < Ni_3P < NiP_2 < NiP_3.[?, ?] Я бы избегал тут понятие тренд. Нигде кроме одной работы китайских исследователей я не видел. Опять же как считать стабильность в тренде? По идее нужно ссчитатть относительно соседей, т.к. именно эта разница энергий определяет стабильность, а здесь, как я понял, считается относительно Ni и P. With increasing pressure, this sequence changes. At a low phosphorus content, structures with an increase in their enthalpy of formation per atom are ordered as follows: Ni_3P < Ni_5P < Ni_7P < Ni_8P < $Ni_{10}P$ < $Ni_{12}P$ < $Ni_{14}P$. As mentioned above, structure Ni_5P is metastable at 100 GPa, and structure Ni_3P stabilizes at a pressure above 200 GPa. However, the value by which it is necessary to lower the enthalpies of these compounds to stabilize them is small and practically lies within the calculation error. At P=100 GPa, the most stable structure is NiP_2, whose enthalpy grows (with increasgin pressure?) with increasing pressure relative to the Ni_2P and Ni_8P_3, and it is metastable at a pressure of 400 GPa. At pressures of 200, 300, and 400 GPa, the most stable is the Ni_8P_3. Other intermediate compounds with known lattices stable at atmospheric pressure under the considered conditions become metastable

It has to be emphasized that the results presented in Fig.5 are obtained neglecting thermal effects. For their full consideration in the framework of the lattice dynamics method, it is necessary to calculate the vibrational spectra of all the structures considered. We performed phonon mode calculations for all considered Ni–P structures except the Ni_8P_3 lattice. For this structure, we encountered a technical difficulty related to the fact that the unit cell of this crystal contains 132 atoms on one side. On the other hand, due to its low symmetry, PHONOPY software generates 264 different unit cells with displaced atoms to calculate phonon modes. Our computer resources do not allow us to carry out such massive calculations, and we leave this question for further research in the future. However, using the experimental data of Oryshchyn et al.[?] , we can assume that the Ni_8P_3 phase is likely unstable at atmospheric pressure and 800°C. This structure is expected to be unstable at the higher pressures and sufficiently high temperatures.

3.2.0.1 PT phase diagrams of Ni_2P and Ni_3P

Structure prediction studies reveal the well-known allabogdanite structure of Ni_2P to be the most favorable phase in the range of 100-

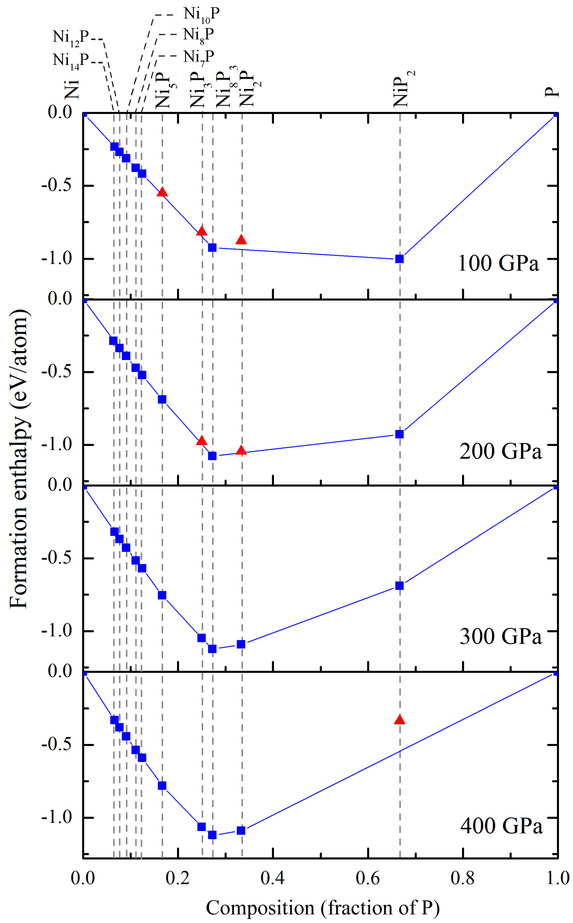

Fig. 3 Convex hulls of Ni–P system at various pressures and 0 K. Blue squares denote stable structures, red triangles - metastable structures.

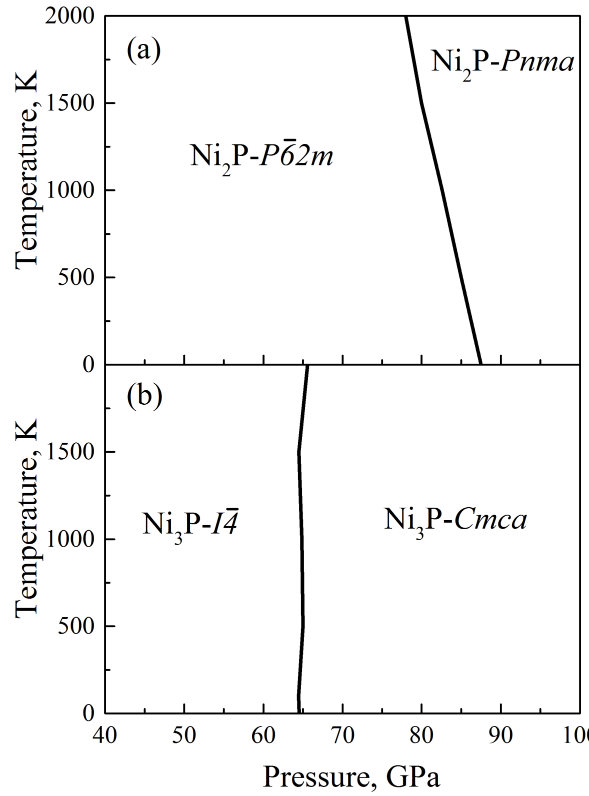

Fig. 4 P-T diagram of (a) Ni_2P and (b) Ni_3P. В обозначения протсранственных групп буквы пишутся италиком, а цифры – обычным шрифтом, а на рисунке – всё италиком Исправлено

400 GPa. On the other hand, it is well known that, at low pressures, the Ni_2P barringerite structure are more stable.[?] Experimental and theoretical studies conducted in the pressure range 0-50 GPa did not show the existence of a structural phase transition between these phases.[?,?] In the case of Ni_3P compounds, the schreibersite structure is the most stable in the low-pressure region,[?] while at the high-pressure we predicted the existence of the structure with *Cmca* symmetry. For both compositions, it is necessary to establish the PT stability fields of these polymorphs.

The results of calculations of phase diagrams in the $P-T$ plane, obtained by the lattice dynamics method in the QHA, are presented in Fig. 6. The structural phase transition barringerite-allabogdanite in the Ni_2P system occurs at a pressure of 88 GPa at low temperatures and 78 GPa at $T = 2000$ K. In the Ni_3P system, the pressure at which the phase transition occurs is practically independent of temperature and the structural transformation occurs at 62 GPa.

4 Conclusions

As a result of computer simulation, the existence of seven new crystalline modifications of nickel phosphide of various stoichiometries in the pressure range of 100-400 GPa was predicted.

Вот посмотрел я ещё раз на эти seven new crystalline modifications и подумал, а можно ли их рассматривать как новые фазы. Возьмём например твёрдый раствор (Fe,Mg)2SiO4. Во всё интервале составов это одна и та же структура, один и тот же минерал, одна и та же модификация. В нашем случае отличие только в том, что атомы по позициям распределены закономерно, а не беспорядочно, но это просто ограничении методики.Поэтому я бы тут так и писал шесть структуры соответствующей одной серии твёрдых растворов. ~~Six of these compounds turn to the fcc lattice of nickel if Ni atoms substitute phosphorus ones.~~ Six new structures are ordered substitutional solid solutions of phosphorus in the fcc lattice of Ni. For the phosphide of the Ni_3P composition, a new high-pressure phase of the *Cmca* space group is predicted. The transition from the low-pressure phase of Ni_3P-$I\bar{4}$ to the *Cmca* structure occurs at a pressure of 62 GPa, regardless of the external temperature. For Ni_2P, the allabogdanite lattice is a stable structure at high pressure. The phase transformation between these crystalline modifications occurs at a pressure of 88 GPa at low temperatures, and 78 GPa at $T = 2000$ K. New phases with a sufficiently high nickel content of $Ni_{14}P$, $Ni_{12}P$, $Ni_{10}P$, and Ni_8P can have a magnetic order. With increasing phosphorous content, the magnetic moment per nickel atom decreases.

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