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Тел.: +7 (7172) 709-500, (ішкі 31-410).
E-mail: vest_phys@enu.kz

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Тел: +7 (7172)709-500 (ішкі 31-410). Сайт: http://bulphysast.enu.kz

Editorial address: **2, Satpayev str., of. 402**
L.N. Gumilyov Eurasian National University, Astana, Kazakhstan, 010008
Tel.: **+7 (7172) 709-500, (ext. 31-410),**
E-mail: **vest_phys@enu.kz**

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Адрес редакции: **010008, Казахстан, г. Астана, ул. Сатпаева, 2**
Евразийский национальный университет имени Л.Н. Гумилева, каб. 402
Тел.: **+7(7172) 709-500, (вн. 31-410),**
E-mail: **vest_phys@enu.kz**

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Comparative study of dose for different fluence of neutron

K. Zhumadilov[1], A. Amangeldina*[1], V. Stepanenko[2], M. Hoshi[3]

[1]Department of Nuclear Physics, New Materials and Technologies, L.N. Gumilyov Eurasian National University, Astana, Kazakhstan
[2]A. Tsyb Medical Radiological Research Center – Branch of the National Medical Research Radiological Center of the Ministry of Health of the Russian Federation, Koroleva Str., 4., Obninsk, Kaluga Region 2490036, Russian Federation
[3]Hiroshima University, Hiroshima, Japan

*(E-mail: [1]zhumadilov_ksh@enu.kz, *[1]alimka.02@mail.ru, [2]valerifs@yahoo.com, [3]mhoshi-hiroshima-u.ac.jp)*

Abstract. *The comparative study aims to investigate the dose received by materials exposed to different fluence of neutron radiation. The research is significant in the field of nuclear energy and radiation protection as neutron radiation is one of the most common types of radiation produced by nuclear reactions. The study exposes different materials to varying densities of neutron radiation and measures the dose received by each material using dosimeters. The results showed that the dose received by the materials increased with increasing fluence of neutron radiation. Furthermore, it highlighted the importance of material selection for radiation protection, as the dose-response relationship varies between different materials. The study concludes that a better understanding of the dose-response relationship for different materials can help in the development of more effective radiation shielding materials and improve radiation safety in various applications.*

Keywords: *fluence of neutron, radiation, dosimetry, Gray, Kazakhstan*

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1. Introduction

Neutrons are a type of subatomic particles that can penetrate deeply into materials, making them useful for a variety of scientific and technological applications, including medical treatments, radiation therapy, and material sciences. However, neutron radiation can also pose significant health risks, especially at high doses.

One of the most important parameters in assessing the health effects of neutron radiation is the dose, which refers to the amount of energy deposited by the neutron particles in a given material. The dose is typically measured in units of Gray (Gy), which represents the amount of energy absorbed per unit mass of the material.

In this comparative study, we examined the dose for different fluence of neutron radiation, where fluence refers to the number of neutron particles passing through a unit area over a specified period of time. Specifically, we compared the dose for low fluence neutron radiation (less than 10^{10} neutrons per square centimeter per second) with that for high fluence neutron radiation (greater than 10^{10} neutrons per square centimeter per second).

Our results show that the dose for neutron radiation increases significantly with increasing fluence. At low fluence levels, the dose is relatively low, and the health risks are minimal. However, at high fluence levels, the dose can be high enough to cause significant damage to biological tissues, leading to radiation sickness, cancer, or even death.

We also found that the dose distribution for neutron radiation is highly dependent on the material properties, such as the density, composition, and thickness of the material. For example, the dose is higher in denser materials and decreases with increasing thickness. Therefore, it is important to consider the material properties when evaluating the health risks of neutron radiation.

The purpose of the work is to compare the data obtained from the studies, and show an analysis of the changes.

2. Methods

Neutron activation of manganese dioxide powder was conducted at the IVG.1 M research reactor (Kazakhstan). The IVG.1 M reactor is a research water-moderated heterogeneous thermal neutron reactor [1-5] with a beryllium reflector designed for radiation studies of samples of various materials used in reactor construction, nuclear power engineering and for performing experiments with irradiation of biological objects. Manganese dioxide is a finely dispersed powder weighing 100 mg with a particle size of about 3 microns [2-6]. Special construction for exposure of laboratory animals to sprayed powder $^{56}MnO_2$ has been developed. The neutron-activated manganese dioxide powder was sprayed into a cage with laboratory animals (mice and rats) [2-4]. To exclude the possibility of $^{56}MnO_2$ powder particles to enter the working room, the cage with experimental animals (mice and rats) was placed in an external box [2].

There were several experiments carried out. Experimental animals and conditions of exposure are described in detail in [2-4]. Briefly, experiments were performed with 11-week-old male Wistar rats and with 10-week-old CD-1, C57BL, and BALB/C mice. The reason for usage of different strains and types of experimental animals was determined by the aims of corresponding biological investigations [7-11]. Experimental animals were exposed to 100 mg portion of sprayed radioactive manganese dioxide powder with various initial activities of ^{56}Mn – in the range from 8.0 × 10^7 Bq to 8.0 × 10^8 Bq – as it was planned in biological experiments [12-14]. There were six to nine experimental animals placed in each cage in dependence on biological experiments' plans [6-15]

Tables 1 and 2 present the pooled information regarding values of internal irradiation among organs of mice from different strains after exposure to the sprayed neutron-activated ^{56}Mn dioxide powder with various levels of activity. As it follows from the Table 1, the doses of internal irradiation in organs and tissues resulting from exposure to sprayed 2.74 × 10^8 Bq activity of ^{56}Mn dioxide powder are not statistically different in different strains of mice. A similar picture takes place under irradiation to 8 × 10^8 Bq activity (Table 2). This means that the distribution of the radioactive powder in the body of mice of different strains but of the same age was practically the same in the case of exposure to the same activity of $^{56}MnO_2$ powder.

Table1. Doses of internal irradiation and corresponding standard deviations (D±SD), Gy, in organs resulted from exposure to 2,74 x 10^8 Bq activity of sprayed neutron activated $^{56}MnO_2$ powder among different strains of 10 week old mice.

Dose (D±SD), Gy, in investigated organs

Activity of ^{56}Mn, Bq and strains		2.74 x 10^8 C57bl	2.74 x 10^8 C57bl	2.74 x 10^8 BALB/C
Lungs	D	0.096	0.14	0.11
	SD	0.013	0.02	0.03
Small intestine	D	0.91	1.1	0.86
	SD	0.15	0.2	0.21
Large intestine	D	4.2	4.5	3.8
	SD	0.5	0.5	0.6
Stomach	D	0.98	1.2	0.91
	SD	0.16	0.2	0.22
Whole body	D	0.38	0.33	0.41
	SD	0.07	0.07	0.09
Skin	D	0.29	0.34	0.21
	SD	0.05	0.06	0.07
Esophagus	D	0.087	0.079	0.093
	SD	0.013	0.013	0.016
Trachea	D	0.039	0.047	0.05
	SD	0.003	0.008	0.01

Eyes	D	0.14	0.13	0.16
	SD	0.05	0.02	0.03
Liver	D	0.0066	0.0086	0.0076
	SD	0.0011	0.0014	0.0012
Heart	D	0.056	0.007	0.061
	SD	0.011	0.01	0.014
Spleen	D	0.0025	0.0028	0.0032
	SD	0.0007	0.0006	0.0008
Kidney	D	0.0028	0.0021	0.0026
		0.0005	0.0006	0.0004

Table 2. Doses of internal irradiation and corresponding standard deviations (D±SD), Gy, in organs resulted from exposure to 8 x 10^8 Bq activity of sprayed neutron activated $^{56}MnO_2$ powder among different strains of 10-week-old mice

Dose (D±SD), Gy, in investigated organs

Activity of ^{56}Mn, Bq and strains		8,0 x 10^8 C57bl	8,0 x 10^8 C57bl	8,0 x 10^8 BALB/C
Lungs	D	0.25	0.34	0.38
	SD	0.05	0.07	0.07
Small intestine	D	2.3	2.8	2.4
	SD	0.2	0.4	0.4
Large intestine	D	10.1	11	9.5
	SD	1.4	2.1	2.1
Stomach	D	2.4	2.2	3.2
	SD	0.5	0.3	0.5
Whole body	D	0.97	1.1	1.2
	SD	0.22	0.2	0.3
Skin	D	0.96	0.91	0.99
	SD	0.21	0.16	0.23
Esophagus	D	0.29	0.17	0.21
	SD	0.05	0.024	0.04
Trachea	D	0.14	0.16	0.13
	SD	0.06	0.04	0.03
Eyes	D	0.39	0.32	0.34
	SD	0.08	0.07	0.07
Liver	D	0.023	0.022	0.024
	SD	0.002	0.004	0.005

Heart	D	0.12	0.18	0.15
	SD	0.02	0.04	0.04
Spleen	D	0.006	0.008	0.007
	SD	0.001	0.002	0.002
Kidney	D	0.007	0.006	0.007
		0.002	0.002	0.002

3. Results and Discussion

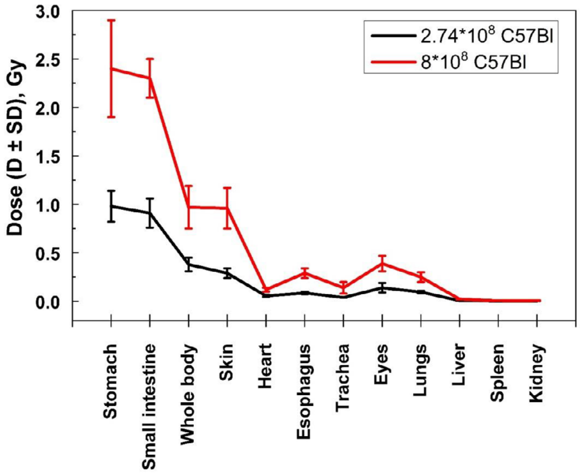

*Fig. 1. Dose comparison for 2.74*10^8 C57BI and 8*10^8 C57BI (from table 1 [15])*

Figure 1 compares the two doses for different neutron fluences and shows a significant difference in dose magnitude for the stomach, small intestine, whole body, and skin. The doses for the liver, spleen, and kidney are almost identical (as confirmed by statistical analysis using a t-test).

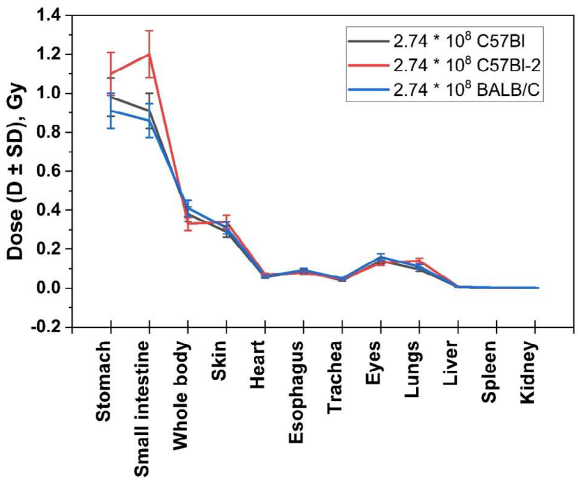

*Fig. 2. Dose comparison for 2.74*10^8 C57BI for different type of irradiated (from table 1 [15])*

Figure 2 compares three types of rats for fluence of neutrons $2.74*10^8$. The doses for different fluencies of neutrons show significant differences in the amount of doses for the stomach, small intestine, whole body, and skin. However, the doses for the liver, spleen, and kidney are almost the same, as confirmed by statistical analysis using a t-test.

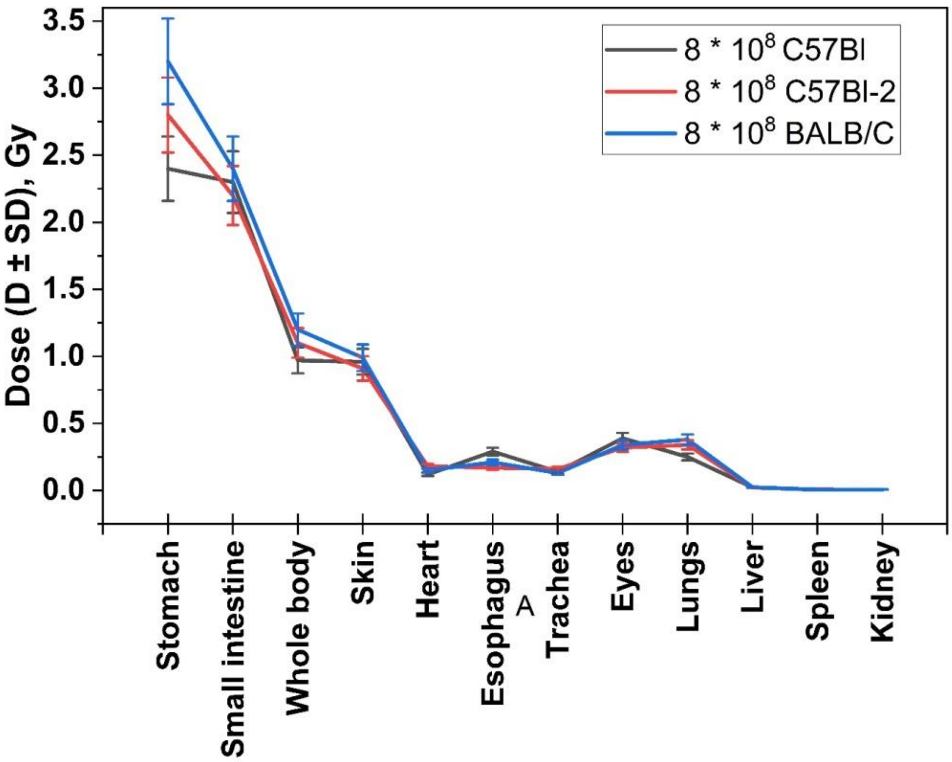

Fig. 3. Dose comparison for $8*10^8$ C57BI for different type of irradiated rats (from table 1 [15])

Figure 3 compares of three types of rats for fluence of neutrons $8*10^8$. The doses for different fluencies of neutrons show significant differences in the amount of doses for the stomach, small intestine, whole body, and skin. However, for the liver, spleen, and kidney, the doses are almost the same (statistically confirmed by t-test) [16].

Unpaired t test results (stomach, small intestine, skin)

P value and statistical significance:

The two-tailed P value equals 0.1629

By conventional criteria, this difference is considered to be not statistically significant.

Confidence interval:

The mean of 2.74 minus 8 equals -0.24033

95% confidence interval of this difference: From -0.63115 to 0.15048

Intermediate values used in calculations:

t = 1.7074

df = 4

standard error of difference = 0.141
Unpaired t test results (heart, esophagus, trachea, eyes, lungs)
P value and statistical significance:
The two-tailed P value equals 0.0905
By conventional criteria, this difference is considered to be not quite statistically significant.
Confidence interval:
The mean of 2.74 minus 8 equals -0.027015
95% confidence interval of this difference: From -0.059562 to 0.005532
Intermediate values used in calculations:
t = 1.9627
df = 7
standard error of difference = 0.014
Unpaired t test results (liver, spleen, kidney)
P value and statistical significance:
The two-tailed P value equals 0.4979
By conventional criteria, this difference is considered to be not statistically significant.
Confidence interval:
The mean of 2.74 minus 8 equals -0.0020800
95% confidence interval of this difference: From -0.0106884 to 0.0065284
Intermediate values used in calculations:
t = 0.7690
df = 3
standard error of difference = 0.003

4. Conclusions

In conclusion, a comparative study of dose for different fluence of neutron is a crucial area of research that requires interdisciplinary collaboration and careful execution. The findings of such studies can provide valuable insights into the dose-response relationship for different neutron fluence rates and can help in developing effective radiation protection measures to safeguard human health and the environment.

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Author Contributions

Alima Amangeldina – results calculation, writing the text and critically revising its content, approval of the final version of the article for publication;

Kassym Zhumadilov – writing the text and critically revising its content, approval of the final version of the article for publication, agreement to be responsible for all aspects of the work, proper examination and resolution of issues related to the reliability of the data.

Valeriy Stepanenko – approval of the final version of the article for publication, agreement to be responsible for all aspects of the work, proper examination and resolution of issues related to the reliability of the data.

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Жумадилов Қасым[1], Амангельдина Алима[1*], Валерий Степаненко[2], Масахару Хоши[3]

[1]Қазақстан, Астана қаласы, Л.Н. Гумилев атындағы Еуразия ұлттық университеті, ядролық физика, жаңа материалдар және технологиялар кафедрасы

[2]А. Цыба Медициналық Радиологиялық Зерттеу Орталығы-ресей Федерациясы Денсаулық Сақтау Министрлігінің Ұлттық Медициналық Зерттеу Радиологиялық Орталығының Филиалы, Королева Көшесі., 4., Обнинск Қ., Ресей Федерациясы

[3]Хиросима университеті, Хиросима, Жапония

Нейтронның әр түрлі флюенциясының дозасын салыстырмалы зерттеу

Абстракт. Салыстырмалы зерттеудің мақсаты әртүрлі қарқындылықтағы нейтрондық сәулеленуге ұшыраған материалдардан алынған дозаны зерттеу болып табылады. Зерттеулер атом энергетикасы мен радиациядан қорғауда маңызды, өйткені Нейтрондық сәулелену ядролық реакциялар нәтижесінде пайда болатын сәулеленудің ең көп таралған түрлерінің бірі болып табылады. Бұл зерттеуде әртүрлі материалдар әртүрлі қарқындылықтағы нейтрондық сәулеленуге ұшырады және әрбір материал алған доза дозиметрлермен өлшенді. Нәтижелер материалдардан алынған дозаның нейтрондық сәулеленудің жоғарылауымен жоғарылағанын көрсетті. Сонымен қатар, зерттеу доза-әсер қатынасы әртүрлі материалдарда өзгеретінін көрсетті, бұл радиациялық қорғаныс үшін материалды таңдаудың маңыздылығын көрсетеді. Зерттеу әртүрлі материалдар үшін доза-әсер қатынасын жақсырақ түсіну радиациядан қорғау үшін тиімдірек материалдарды әзірлеуге және әртүрлі қолданбаларда радиациялық қауіпсіздікті арттыруға көмектесуі мүмкін деген қорытындыға келді.

Түйін сөздер: нейтрондар ағыны, радиация, дозиметрия, Грей, Қазақстан.

Жумадилов Касым[1], Амангельдина Алима[1]*, Валерий Степаненко[2], Масахару Хоши[3]
[1]*Кафедра ядерной физики, новых материалов и технологий,*
Евразийский национальный университет им. Л.Н. Гумилева, Астана, Казахстан
[2]*Медицинский радиологический научный центр им. А.Цыба – филиал Национального медицинского исследовательского радиологического центра Министерства здравоохранения Российской Федерации, ул. Королева, д.4., Обнинск, Калужская область, Российская Федерация*
[3]*Университет Хиросима, Хиросима, Япония*

Сравнительное исследование доз для разных флюенсов нейтронов

Абстракт. Сравнительное исследование направлено на изучение дозы, получаемой материалами, подвергшимися воздействию нейтронного излучения различной плотности. Исследования имеют важное значение в области ядерной энергетики и радиационной защиты, поскольку нейтронное излучение является одним из наиболее распространенных видов излучений, образующихся в результате ядерных реакций. В этом исследовании различные материалы подвергаются разной плотности нейтронного излучения, а доза, полученная каждым материалом, измерялась с помощью дозиметров. Результаты показали, что доза, получаемая материалами, увеличивается с увеличением флюенса нейтронного излучения. Кроме того, исследование показало, что взаимосвязь «доза-реакция» различна для разных материалов, что подчеркивает важность выбора материала для радиационной защиты. В исследовании делается вывод, что лучшее понимание зависимости «доза-реакция» для различных материалов может помочь в разработке более эффективных материалов радиационной защиты и улучшить радиационную безопасность в различных приложениях.

Ключевые слова: поток нейтронов, излучение, дозиметрия, Грей, Казахстан.

Сведения об авторах:

Амангельдина А.Қ. – Л.Н. Гумилев атындағы Еуразия ұлттық университеті, «Ядролық физика, жаңа материалдар және технологиялар» кафедрасының 1 курс магистранты, 010008, Астана қ., Қажымұқан к-сі, 13.

Жумадилов Қ.Ш. – PhD, профессор, «Ядролық физика, жаңа материалдар және технологиялар» кафедрасының меңгерушісі, Л.Н. Гумилев атындағы Еуразия ұлттық университеті, 010008, Астана қ., Қажымұқан к-сі, 13.

Степаненко В.Ф. – биология ғылымдарының докторы, профессор, Ресей Денсаулық сақтау министрлігінің "нмиц радиология" ФМБУ филиалы А. Ф. Цыба атындағы мрнц медициналық-экологиялық дозиметрия және радиациялық қауіпсіздік зертханасының меңгерушісі, Королева Көшесі., 4., Обнинск Қ., Ресей Федерациясы

Масахару Хоши – Хиросима университетінің құрметті профессоры, Хиросима, Жапон.

Амангельдина А.К. – магистрант, Евразийский национальный университет им. Л. Н. Гумилева, 010008, г. Астана, ул. Кажымукана, 13.

Жумадилов К.Ш. – PhD, профессор, Евразийский национальный университет имени Л.Н. Гумилева, 010008, г. Астана, ул. Кажымукана, 13.

Степаненко В.Ф. – доктор биологических наук, профессор, заведующий лабораторией медико-экологической дозиметрии и радиационной безопасности МРНЦ имени А.Ф. Цыба – филиала ФГБУ «НМИЦ радиологии» Минздрава России, ул. Королева, д.4., Обнинск, Калужская область Российская Федерация.

Масахару Хоши – почетный профессор Университета Хиросимы, Хиросима, Япония.

Information about authors:

Amangeldina A.K. – 1st year master's student the Department of Nuclear Physics, New Materials and Technologies, L. N. Gumilyov Eurasian National University, 010008, Kazhymukan Str., 13, Astana

Zhumadilov K.Sh. – PhD, Professor, Head of the Department of Nuclear Physics, New Materials and Technologies, L.N. Gumilyov Eurasian National University,", 010008, Kazhymukan Str., 13, Astana

Stepanenko V.F. – Doctor of Biological Sciences, Professor, Head of the Laboratory of Medical-Ecological Dosimetry and Radiation Safety of the MRRC named after A.F. Tsyba - a branch of the Federal State Budgetary Institution "National Medical Research Center of Radiology" of the Russian Ministry of Health, Koroleva Str., 4., Obninsk, Kaluga Region 2490036, Russian Federation

Masaharu Hoshi – Emeritus professor at Hiroshima University.

Л.Н. Гумилев атындағы Еуразия ұлттық университетінің ХАБАРШЫСЫ.
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Mechanical properties of nickel nitrides under high pressures

N. Sagatov*[1,2], D. Sagatova[1,3]

[1]*Sobolev Institute of Geology and Mineralogy SB RAS, Novosibirsk, Russian Federation*
[2]*Novosibirsk State University, Novosibirsk, Russian Federation*
[3]*Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russian Federation*

*(E-mail: *sagatinho23@gmail.com)*

Abstract. *Transition metal nitrides are durable ceramic materials with a range of impressive characteristics, such as a high melting point, exceptional resistance to oxidation, wear, and corrosion, as well as chemical stability and strong electrical conductivity. These exceptional properties are mainly due to the distinctive electronic and geometric structures of transition metal nitrides. The Fe-N system, a common example of transition metal nitrides, has been thoroughly studied to investigate its compounds not only as functional materials but also as a possible component of the Earth's interior layers. Unlike iron nitrides, nickel nitrides have been less studied, although they, like iron nitrides, are of interest not only from the point of view of materials science, but also from the point of view of Earth sciences. In present study, the mechanical properties of previously known nickel nitrides,* Ni_6N*-*$R\bar{3}$*,* Ni_3N*-*$P6_322$*,* Ni_3N*-Cmcm, and Ni7*N_3*-Pbca, were calculated from first principles using density functional theory in the pressure range of 0-400 GPa. Considered nickel nitrides are mechanically stable in the entire considered pressure ranges. It was shown that all phases are ductile and have low Vickers hardness values which are below the minimal criteria of hard materials,* $H_V > 20$ *GPa. In addition, the fracture toughness was estimated.*

Keywords: *high pressures, nitrides, hardness, elastic moduli, density functional theory.*

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1. Introduction

Transition-metal nitrides exhibit a variety of electronic, mechanical, and chemical characteristics that make them well-suited for various technological uses, including hard wear-resistant coatings, diffusion barriers in microelectronics, protective and decorative coatings, and energy storage applications. Transition-metal nitrides have low compressibility and high hardness because of their exceptionally strong and short bonteleds, which differ significantly from those found in pure metals. Consequently, extensive research efforts have been dedicated to discovering novel transition-metal nitrides characterized by exceptional hardness and superior fracture resistance, with the expectation that they may be utilized in cutting tools and as durable coatings. To date, a significant amount of research is focused on investigating transition-metal nitrides under high pressure conditions. The reason for this is that elevated pressure allows for the exploration of different structural configurations of known nitrides and the creation of unique compounds that are not possible to produce under standard atmospheric conditions. Among the transition metal nitrides, iron and nickel nitrides are not only useful for practical purposes but also hold significance in the field of Earth sciences. The inner core (329-364 GPa) is believed to be solid and composed mainly of iron, ~5% nickel and a small proportion of light elements [1-3]. Nitrogen is considered one of the possible light elements in the inner core. Therefore, iron and nickel nitrides and their elastic properties are of interest for studying the structure and composition of the Earth's inner core.

A considerable amount of research, spanning both theoretical and experimental approaches, has focused on iron nitrides [4-10], whereas there is a limited number of studies dedicated to nickel nitrides. In the nickel-nitrogen system, Ni3N is the only stable intermediate compound that has been identified at atmospheric pressure. The ambient-pressure structure of Ni_3N was shown to remain it stability at least up to 20 GPa [11]. Subsequently, through the application of a laser-heated diamond anvil cell method, nickel pernitride, NiN_2, featuring a marcasite-type structure, was successfully produced at a pressure of 40 GPa [12]. Recently, four new stable phases, Ni_6N-R$\bar{3}$, Ni_3N-Cmcm, Ni_7N_3-Pbca, and NiN_2-Pa$\bar{3}$, were obtained, based on crystal structure prediction calculations [13]. It was shown that ambient-pressure phase Ni_3N-P$6_3$22 is stable up to 96 GPa and above this pressure decompose to Ni_7N_3 + Ni. New predicted nitride Ni_6N-R$\bar{3}$, is stable in the pressure range of 98-114 GPa. Ni_7N_3-Pbca becomes stable relative to neighboring nitrides (Ni_3N + NiN_2) above 93 GPa and stable at least up to 400 GPa. Previously known nickel pernitride with marcasite structure, NiN_2-Pnnm, was shown to be stable above 14 GPa, and at 96 GPa phase transition to new modification with pyrite structure, NiN_2-Pa$\bar{3}$, occurs. Furthermore, it was demonstrated that at pressures exceeding 331 GPa, a new phase of Ni3N with a Cmcm structure becomes stabilized and maintains its stability up to at least 400 GPa. While the elastic and mechanical properties of NiN_2 have been studied, the mechanical properties of the other nickel nitrides remain to be evaluated. This highlights the importance of assessing the mechanical properties of the remaining nickel nitrides. In this study, we present the results of the calculations on mechanical properties of Ni_6N-R$\bar{3}$, Ni_3N-P$6_3$22, Ni3N-Cmcm, and Ni_7N_3-Pbca at pressure range up to 400 GPa.

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2. Methodology

All computations were carried out using the density functional theory (DFT) method implemented in the VASP software package [14, 15]. Exchange-correlation effects were accounted for using the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof functional [16]. The electron–ion interaction was modeled using the projector-augmented-wave (PAW) method, with the valence electron configurations of Ni being $3d^8 4s^2$ and N being $2s^2 2p^3$. The calculation settings were as follows: cutoff energy of plane wave basis set – 600 eV, density of Monkhorst-Pack [18] k-point grid – 0.2 A^{-1}, electronic smearing – according to the Methfessel-Paxton scheme [19] with a parameter σ equal to 0.1 eV. The self-consistent field tolerance was set to 10^{-8} eV.

In order to assess characteristics like hardness and fracture toughness, we derived the static elastic stiffness tensor components (C_{ij}) from the stress (σ) – strain (ε) relationship, expressed as $\sigma_i = C_{ij}\varepsilon_j$. Utilizing the determined C_{ij} values, we computed the bulk (B) and shear (G) moduli using the Voigt-Reuss-Hill method [20, 21]. For hexagonal and trigonal phases, bulk and shear moduli were calculated by next formula:

$$\begin{cases} B_V = \frac{1}{9}(2C_{11} + C_{33}) + \frac{2}{9}(2C_{13} + C_{12}) \\ B_R = \frac{A}{M} \\ G_V = \frac{1}{30}(M + 12C_{44} + 12C_{66}) \\ G_R = \frac{5(AC_{44}C_{66})}{4B_V C_{44}C_{66} + A(C_{44} + C_{66})} \\ A = (C_{11} + C_{12})C_{33} - 2C_{13}^2 \\ M = C_{11} + C_{12} + 2C_{33} - 4C_{13} \\ B = \frac{B_V + B_R}{2} \\ G = \frac{G_V + G_R}{2} \end{cases} \quad (1)$$

For orthorhombic phases, to calculate bulk and shear moduli next formulas were used:

$$\begin{cases} B_V = \frac{1}{9}[C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})] \\ B_R = \Delta\begin{bmatrix} C_{11}(C_{22} + C_{33} - 2C_{23}) + C_{22}(C_{33} - 2C_{13}) - 2C_{33}C_{12} + C_{12}(2C_{23} - C_{12}) \\ + C_{13}(2C_{12} - C_{13}) + C_{23}(2C_{13} - C_{23}) \end{bmatrix}^{-1} \\ G_V = \frac{1}{15}[C_{11} + C_{22} + C_{33} + 3(C_{44} + C_{55} + C_{66}) - (C_{12} + C_{13} + C_{23})] \\ G_R = 15\left\{\frac{4\begin{bmatrix} C_{11}(C_{22} + C_{33} + C_{23}) + C_{22}(C_{33} + C_{13}) + C_{33}C_{12} - \\ C_{12}(C_{23} + C_{12}) - C_{13}(C_{12} + C_{13}) - C_{23}(C_{13} + C_{23}) \end{bmatrix}}{\Delta} + 3\left(\frac{1}{C_{44}} + \frac{1}{C_{55}} + \frac{1}{C_{66}}\right)\right\}^{-1} \\ \Delta = C_{13}(C_{12}C_{23} - C_{22}C_{13}) + C_{23}(C_{12}C_{13} - C_{23}C_{11}) + C_{33}(C_{11}C_{22} - C_{12}^2) \\ B = \frac{B_V + B_R}{2} \\ G = \frac{G_V + G_R}{2} \end{cases} \quad (2)$$

Using obtained bulk and shear moduli Young's modulus (E) and Poisson's ratio (ν) could be calculated as follows:

$$E = \frac{9BG}{3B + G}$$
$$\nu = \frac{3B - 2G}{2(3B + G)} \quad (3)$$

In order to analyze the Vickers hardness of the nitrides under study, we utilized the empirical models proposed by Chen [22] and Tian [23]:

$$H_V^{Chen} = 2 \cdot (k^2 \cdot G)^{0.585} - 3$$
$$H_V^{Tian} = 0.92 \cdot k^{1.137} \cdot G^{0.708} \quad (4)$$

where k = G/B.

In our study, H_V was estimated as average value obtained from equations (4):

$$H_V = \frac{H_V^{Chen} + H_V^{Tian}}{2} \quad (5)$$

To estimate the fracture toughness the following empirical formula was used [24]:

$$K_{IC} = V_0^{1/6} \cdot G \cdot \left(\frac{B}{G}\right)^{1/2} \quad (6)$$

where V_0 is the volume per atom (in m^3/atom) and K_{IC} is fracture toughness (in MPa $m^{1/2}$).

3. Results and discussion

To investigate the mechanical properties of previously known nickel nitrides the elastic constants C_{ij} of Ni_6N-R$\bar{3}$, Ni_3N-P$6_3$22, Ni_3N-Cmcm, and Ni_7N_3-Pbca were calculated in the pressure ranges of 100-120 GPa, 0-100 GPa, 300-400 GPa, and 100-400 GPa, respectively. The pressure ranges were chosen to cover the stability field of each phase as reported at ref [13]. The results of the elastic constants calculations are summarized in the Table 1. Due to the symmetry of the considered nitrides, Ni_6N-R$\bar{3}$ and Ni_3N-P$6_3$22 have five independent elastic constants, C_{11}, C_{33}, C_{44}, C_{12}, and C_{13}, and Ni_3N-Cmcm, and Ni_7N_3-Pbca have nine independent elastic constants, C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13}, and C_{23}.

The elastic constants C_{ij} can be used to assess the mechanical stability of the phases, as the criteria for the mechanical stability of hexagonal (trigonal) and orthorhombic crystals are typically defined by the following conditions:

for Ni_6N-R$\bar{3}$, Ni_3N-P$6_3$22

$$\begin{cases} C_{44} > 0 \\ C_{11} > |C_{12}| \\ (C_{11} + 2C_{12})C_{33} - 2C_{13}^2 > 0 \end{cases},$$

for Ni_3N-Cmcm, and Ni_7N_3-Pbca

$$\begin{cases} C_{ii} > 0 \;\; (i = 1-6) \\ [C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})] > 0 \\ (C_{11} + C_{22} - 2C_{12}) > 0 \\ (C_{11} + C_{33} - 2C_{13}) > 0 \\ (C_{22} + C_{33} - 2C_{23}) > 0 \end{cases}.$$

As indicated in Table 1, the calculated C_{ij} of all considered nickel nitrides satisfy above criteria, which indicate that they are mechanically stable in the considered pressure ranges. This result is in accordance with the previous results of the formation enthalpy calculations [13].

Table 1. Elastic constants (C_{ij} in GPa) of nickel nitrides at various pressures (in GPa).

Phase	Pressure	C_{11}	C_{12}	C_{13}	C_{22}	C_{23}	C_{33}	C_{44}	C_{55}	C_{66}
Ni_6N-R$\bar{3}$	100	879	524	480			852	159		177
	110	930	559	512			901	167		186
	120	981	592	545			948	175		192
Ni_3N-P$6_3$22	0	286	152	155			278	89		67
	25	445	260	267			419	122		93
	50	582	354	363			549	150		114
	75	708	445	457			669	175		131
	100	825	532	547			782	196		146
Ni_3N-Cmcm	300	1677	1244	1175	1706	1188	1739	187	433	475
	350	1873	1409	1319	1906	1334	1972	235	484	533
	400	2069	1567	1461	2106	1477	2203	277	536	591

Ni_7N_3-Pbca	100	824	540	533	801	608	800	136	60	85
	150	1052	703	697	1060	779	1055	175	86	110
	200	1270	863	856	1297	945	1294	210	112	139
	300	1684	1175	1163	1739	1266	1741	266	160	197
	400	2078	1478	1463	2154	1579	2160	317	210	252

At the next step, the bulk modulus, shear modulus, Poisson's ratio and Young's modulus were calculated based on obtained C_{ij} using equations (1-3). The elastic moduli (bulk modulus, shear modulus, Young's modulus, and Poisson's ratio) are numerical quantities which identify the mechanical behavior of a material when some stress is applied. These are listed in Table 2. From the obtained results it could be seen that bulk moduli of all nickel nitrides are increased with increasing pressure and lies almost at the same line (Figure 1).This means that considered nickel nitrides have almost the same incompressibility. Calculated shear and Young's moduli also increases with pressure increase (Figure 1). The relation of shear and Young's moduli of nitrides are almost identical. The shear and Young's moduli of Ni_3N-$P6_322$ are on average 8% lower than those of Ni_6N-$R\bar{3}$, and 35% higher than those of Ni_7N_3-Pbca. The shear and Young's moduli of Ni_3N-Cmcm are on average 25% higher than those of Ni_7N_3-Pbca. The Poisson's ratios of the considered nitrides are slightly dependent to pressure. A more obvious dependence of Poisson's ratio on pressure is shown by Ni_3N-$P6_322$. In the considered pressure range of 0-100 GPa its Poisson's ratio increases on 15 %. The change in the Poisson ratios with pressure of the remaining nitrides does not exceed ~1%. As a result, we see that the Ni7N3-Pbca has the highest Poisson's ratio among known nickel nitrides, ~0.424. This high value is identical to the Poisson's ratio of gold (~0.42) and close to the maximum possible Poisson's ratio of 0.5, which characterizes the elastic properties, for instance, of rubber.

It should be noted that among iron nitrides there is an isostructural analog of Ni_7N_3-Pbca, Fe_7N_3-Pbca [10]. The Ni_7N_3-Pbca has on 11% higher values of bulk, shear, and Young's moduli than that of Fe_7N_3-Pbca [10], while Poisson's ratios of Ni_7N_3-Pbca and Fe_7N_3-Pbca are almost identical (~0.424).

In addition, the percentage of elastic anisotropy for bulk modulus A_B and shear modulus A_G in polycrystalline materials were estimated (Table 2). A value of 0% represents elastic isotropy and a value of 100% is the largest possible anisotropy. Ni_6N-$R\bar{3}$ is almost isotropic crystal because the values A_B and A_G are not exceeded 1%. All other phases show weak anisotropy of shear modulus.

Table 2. Calculated bulk modulus (B in GPa), shear modulus (G in GPa), Poisson's ratio (ν), Young's modulus (E in GPa), the B/G ratio, Vickers hardness (H_V in GPa), fracture toughness (K_{IC} in MPa×$m^{1/2}$) and anisotropy of bulk and shear moduli (A_B and A_G in %) of nickel nitrides at various pressures (in GPa).

Phase	Pressure	B	G	ν	E	B/G	H_V	K_{IC}	A_B	A_G
Ni_6N-R$\bar{3}$	100	619	173	0.372	475	3.57	7.26	7.68	0.079	0.361
	110	658	182	0.373	500	3.62	7.41	8.09	0.081	0.351
	120	696	189	0.375	521	3.68	7.47	8.47	0.078	0.303
Ni_3N-$P6_322$	0	197	74	0.333	197	2.67	5.61	2.50	0.005	1.207
	25	322	100	0.359	273	3.21	5.49	3.67	0.027	1.438
	50	430	123	0.370	337	3.50	5.70	4.64	0.026	1.473
	75	533	142	0.377	392	3.75	5.80	5.51	0.023	1.635
	100	631	159	0.384	439	3.98	5.81	6.28	0.018	1.729
Ni_3N-Cmcm	300	1371	301	0.398	840	4.56	7.93	13.72	0.009	6.462
	350	1542	343	0.396	958	4.49	8.95	15.46	0.008	5.753
	400	1710	385	0.395	1073	4.45	9.88	17.14	0.010	5.478
Ni_7N_3-Pbca	100	643	100	0.426	286	6.40	1.64	7.32	0.046	5.459
	150	835	134	0.424	382	6.22	2.42	9.55	0.088	4.296
	200	1020	166	0.423	473	6.13	3.07	11.64	0.101	3.348
	300	1373	224	0.423	636	6.14	4.02	15.44	0.113	2.184
	400	1713	277	0.423	787	6.19	4.78	18.97	0.115	1.449

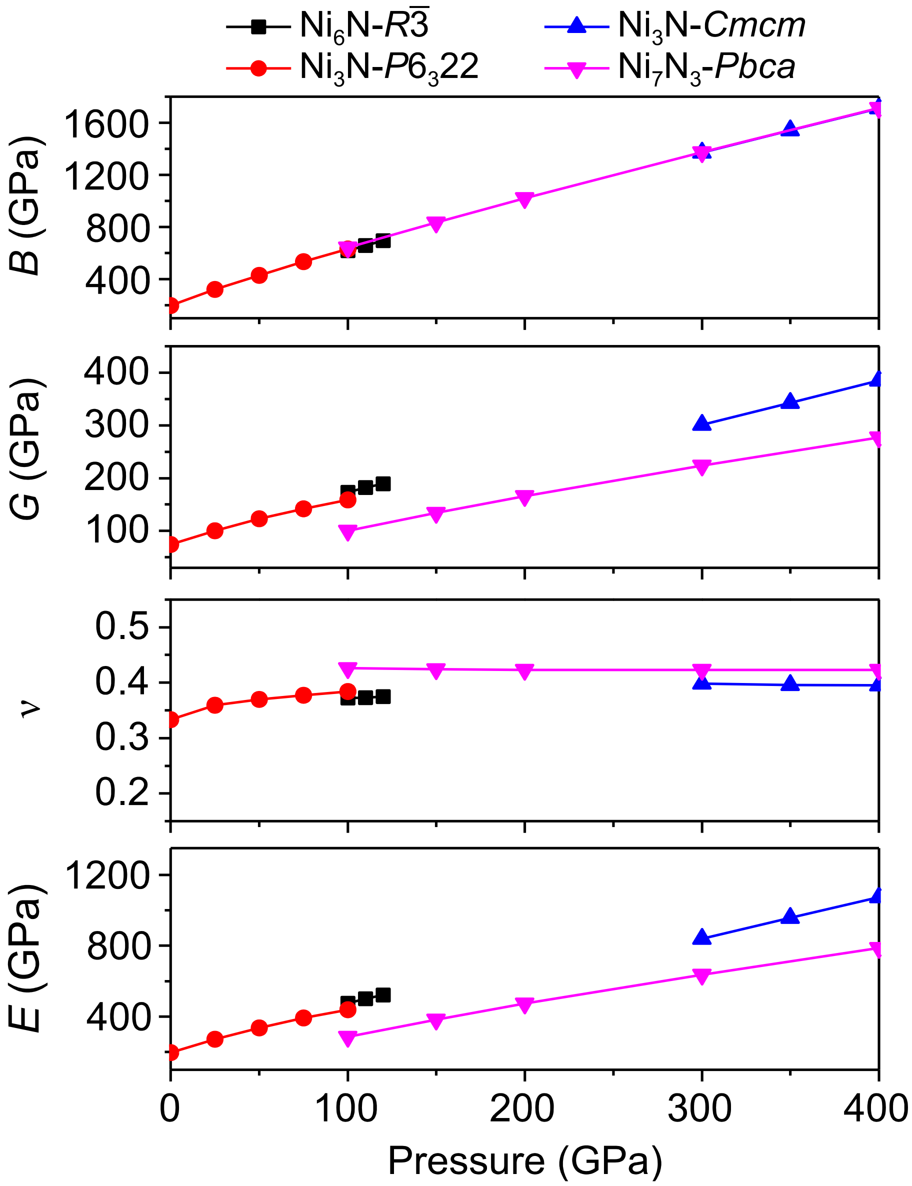

Figure 1. Calculated bulk modulus (B), shear modulus (G), Poisson's ratio (ν), and Young's modulus (E) of nickel nitrides as a function of pressure.

Poisson's ratio is a useful indicator for determining the nature of a material, its compressibility, and bonding characteristics. Additionally, the B/G ratio serves as a reliable criterion for assessing the ductility or brittleness of materials. There are specific threshold values for both Poisson's ratio (0.26) and the B/G ratio (1.75) that can be used to distinguish between ductile and brittle materials. If a material's Poisson's ratio and B/G ratio exceed these thresholds, it is considered ductile, and vice versa. Our analysis of nickel nitrides reveals that their Poisson's ratios and B/G ratios (as shown in Figure 2 and Table 2) consistently surpass these threshold values across various pressures, indicating that these phases exhibit ductile behavior.

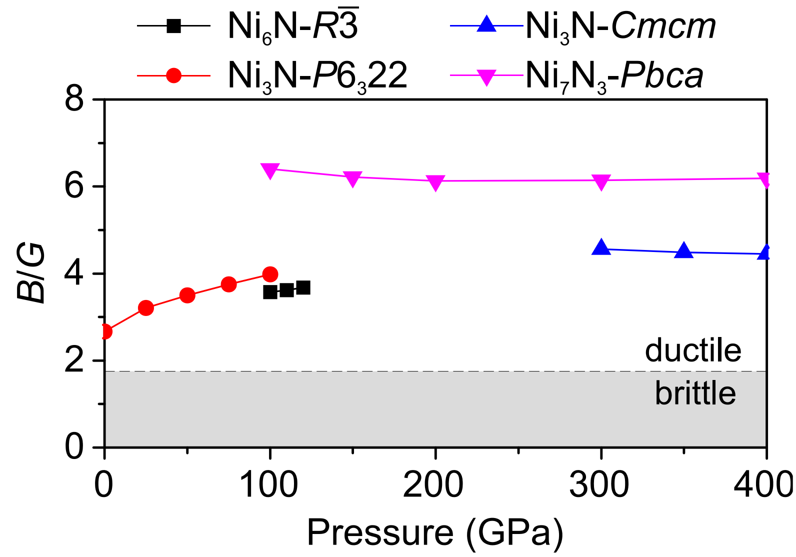

Figure 2. Calculated B/G ratio of nickel nitrides as a function of pressure

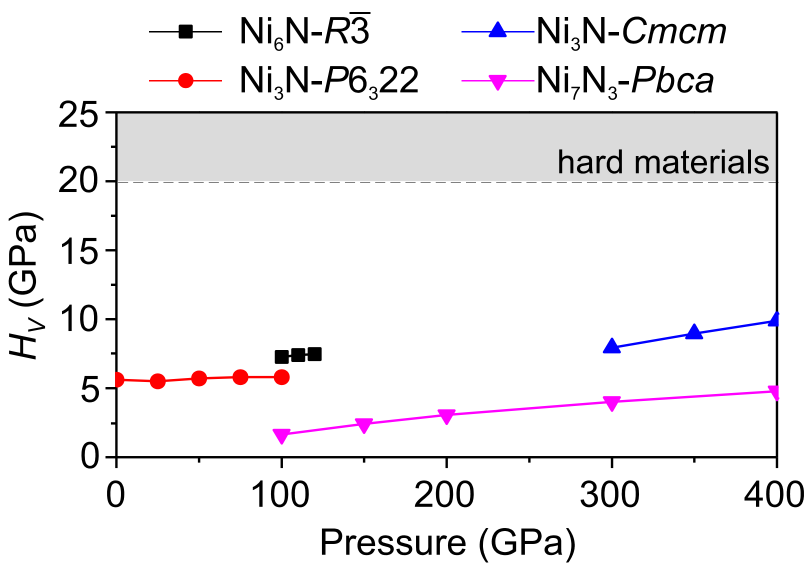

Figure 3. Calculated value of hardness (HV) of nickel nitrides as a function of pressure

The relationship between the hardness of a material and its bulk modulus and shear modulus is significant, as hardness is a measure of a crystal's ability to withstand plastic deformation under various types of stress. This suggests that Ni_3N-Cmcm is expected to exhibit the highest hardness compared to other nitrides based on calculations of elastic moduli. The Vickers hardness (H_V) of nickel nitrides was evaluated using empirical models (equations 4-5). Ni_3N-Cmcm indeed showed the highest Vickers hardness value. However, the calculated Vickers hardness values for Ni_3N-Cmcm (8-10 GPa) and other nickel nitrides fall below the minimum threshold for hard materials, which is $H_V > 20$ GPa (Figure 3, Table 2).

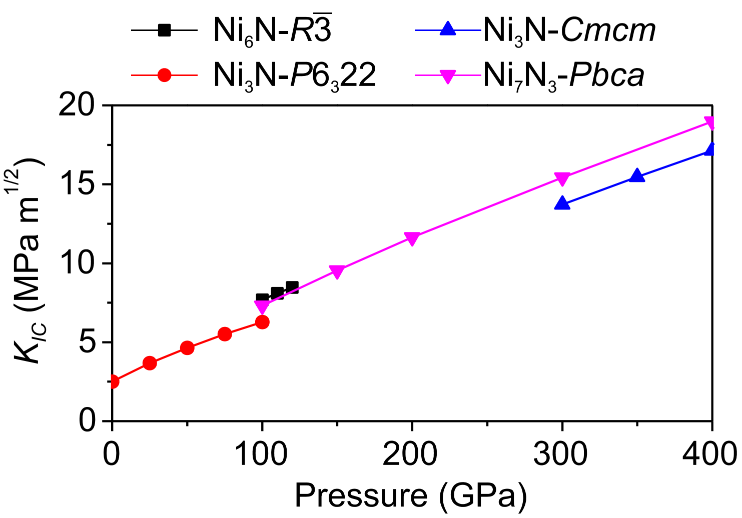

Figure 4. Calculated fracture toughness of nickel nitrides as a function of pressure

The capacity of a substance to withstand the spread of cracks and fractures when exposed to external forces is known as fracture toughness (K_{IC}). The calculated K_{IC} of the considered phases increase with increasing pressure (Figure 4, Table 2). The nitride Ni_3N-P$6_3$22 has the lowest K_{IC} value of 2.5-6.3 MPa $m^{1/2}$ among considered phases. For comparison, K_{IC} of ceramic materials, such aluminum oxide and silicon carbide, is equal to 3-5 MPa $m^{1/2}$. This result indicates that Ni_3N-P$6_3$22 is more prone to cracks than other nickel nitrides. All other phases have K_{IC} values as those of metals. For comparison, K_{IC} of pure aluminum is equal to 14-28 MPa $m^{1/2}$.

4. Conclusion

Based on the ab initio calculation within the density functional theory elastic constants C_{ij} were obtained and then the elastic moduli and mechanical properties, such as brittleness/ductility, hardness and fracture toughness, of Ni_6N-R$\bar{3}$, Ni_3N-P$6_3$22, Ni_3N-Cmcm, and Ni_7N_3-Pbca were estimated. Among considered nitrides, the highest bulk, shear, and Young's moduli belong to Ni_3N-Cmcm, while Ni_7N_3-Pbca has the highest Poisson's ratio (~0.424). Considered nickel nitrides are isotropic with respect to bulk modulus and slightly anisotropic with respect to the shear modulus. It was shown that all phases are ductile and have low Vickers hardness values which are below the minimal criteria of hard materials, $H_V > 20$ GPa. In addition, the fracture toughness was estimated.

Conflicts of interest

There are no conflicts to declare.

Authorship contribution statement

N. Sagatov: Investigation, Methodology, Analysis, Writing – original draft.
D. Sagatova: Investigation, Methodology, Analysis, Writing – original draft.

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Н. Сағатов[1,2], Д. Сағатова[1,3]
[1]В.С. Соболев ат. геология және минералогия институты СТ РҒА, Новосибирск, Ресей Федерациясы
[2]Новосибирск мемлекеттік университеті, Новосибирск, Ресей Федерациясы.
3А.В.Николаев ат. бейорганикалық химия институты СТ РҒА, Новосибирск, Ресей Федерациясы

Жоғары қысымдағы никель нитридтерінің механикалық қасиеттері

Аннотация. Өтпелі металл нитридтері жоғары балқу температуралары, тотығуға, тозуға және коррозияға ерекше төзімділік, сондай-ақ химиялық тұрақтылық және жоғары электр өткізгіштік сияқты бірқатар әсерлі сипаттамалары бар берік керамикалық материалдар болып табылады. Бұл ерекше қасиеттер негізінен өтпелі металл нитридтерінің ерекше электронды және геометриялық құрылымына байланысты. Fe-N жүйесі, өтпелі металдар нитридтерінің кең таралған мысалы, оның қосылыстарын тек функционалды материалдар ретінде ғана емес, сонымен қатар Жердің ішкі қабықтарының ықтимал құрамдас бөлігі ретінде зерттеу үшін кеңінен зерттелді. Темір нитридтерінен айырмашылығы, никель нитридтері аз зерттелген, бірақ олар темір нитридтері сияқты материалтану тұрғысынан ғана емес, сонымен қатар Жер туралы ғылымдар тұрғысынан да қызығушылық тудырады. Бұл жұмыста алғашқы принциптерден тығыздық функционалдық теориясын қолдана отырып, бұрын белгілі никель нитридтерінің Ni_6N-R$\bar{3}$, Ni_3N-P$6_3$22, Ni_3N-Cmcm және Ni_7N_3-Pbca механикалық қасиеттері әртүрлі қысымдарда есептелді. Қарастырылған никель нитридтері барлық қарастырылған қысым диапазонында механикалық тұрақты. Көрсетілгендей, барлық фазалар иілімді болып табылады және қатты материалдардың $H_V > 20$ ГПа ең төменгі критерийінен төмен болатын Викерс қаттылығының төмен мәндері бар. Сондай-ақ сызатқа беріктігі бағаланды.

Түйін сөздер: жоғары қысымдар, нитридтер, қаттылық, серпімділік модульдері, тығыздық функционалдық теориясы

Н.Сагатов[1,2], Д.Сагатова[1,3]
[1]Институт геологии и минералогии им В.С. Соболева СО РАН, Новосибирск, Российская Федерация
[2]Новосибирский государственный университет, Новосибирск, Российская Федерация
[3]Институт неорганической химии им. А.В.Николаева СО РАН, Новосибирск, Российская Федерация

Механические свойства нитридов никеля при высоких давлениях

Аннотация. Нитриды переходных металлов – это прочные керамические материалы с рядом впечатляющих характеристик, таких, как высокая температура плавления, исключительная стойкость к окислению, износу и коррозии, а также химическая стабильность и высокая электропроводность. Эти исключительные свойства обусловлены главным образом отличительной электронной и геометрической структурой нитридов переходных металлов. Система Fe-N, распространенный пример нитридов переходных металлов, была тщательно исследована с целью изучения ее соединений не только в качестве функциональных материалов, но и как возможного компонента внутренних оболочек Земли. В отличие от нитридов железа, нитриды никеля изучены меньше, хотя они, как и нитриды железа, представляют интерес не только с точки зрения материаловедения, но и с точки зрения наук о Земле. В данной работе из первых принципов с использованием теории функционала плотности были рассчитаны механические свойства ранее известных нитридов никеля Ni_6N-$R\bar{3}$, Ni_3N-$P6_322$, Ni_3N-Cmcm и Ni_7N_3-Pbca при различных давлениях. Рассмотренные нитриды никеля являются механически стабильными во всем рассмотренном диапазоне давлений. Показано, что все фазы пластичны и имеют низкие значения твердости по Виккерсу, которые лежат ниже минимального критерия для твердых материалов $H_V > 20$ ГПа. Также была оценена трещиностойкость.

Ключевые слова: высокие давления, нитриды, твердость, модули упругости, теория функционала плотности.

Сведения об авторах:

Сағатов Н. – корреспонденция авторы, физика-математика ғылымдарының кандидаты, В.С. Соболев атындағы Геология және Минералогия институтінің ғылыми қызметкері, академик Коптюг даңғылы, 3, Новосибирск, Ресей Федерациясы.

Сағатова Д. – геология-минералогия ғылымдарының кандидаты, В.С. Соболев атындағы Геология және Минералогия институтінің ғылыми қызметкері, академик Коптюг даңғылы, 3, Новосибирск, Ресей Федерациясы.

Сагатов Н. – автор для корреспонденции, кандидат физико-математических наук, научный сотрудник Института геологии и минералогии им В.С. Соболева СО РАН, проспект академика Коптюга, 3, Новосибирск, Российская Федерация.

Сагатова Д. – кандидат геолого-минералогических наук, научный сотрудник Института геологии и минералогии им В.С. Соболева СО РАН, проспект академика Коптюга, 3, Новосибирск, Российская Федерация.

Information about authors:

Sagatov N. – corresponding author, candidate of physical and mathematical sciences, researcher of the Sobolev Institute of geology and mineralogy SB RAS, prospect akademika Koptyuga, 3, Novosibirsk, Russian Federation.

Sagatova D. – candidate of geological and mineralogical sciences, researcher of the Sobolev Institute of geology and mineralogy SB RAS, prospect akademika Koptyuga, 3, Novosibirsk, Russian Federation.

Бас редакторы: К.Ш. Жумадилов
Компьютерде беттеген: Д. Нурушева

Авторларға арналған нұсқаулықтар,
жарияланым этикасы журнал сайтында берілген: http://bulphysast.enu.kz

Л.Н. Гумилев атындағы Еуразия ұлттық университетінің Хабаршысы.
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Редакция мекен-жайы: 010008, Қазақстан Республикасы Астана қ., Сәтбаев көшесі, 2.
Л.Н. Гумилев атындағы Еуразия ұлттық университеті Тел.: +7(71-72) 70-95-00 (ішкі 31-410)
Л.Н. Гумилев атындағы Еуразия ұлттық университетінің баспасында басылды.