JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. 18 No 1, 01002(7pp) (2026)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том 18 № 1, 01002(7сс) (2026)

REGULAR ARTICLE

Formation of the (Ti, V)(C, N) Multicomponent Solid Solution by Mechanical Alloying of the $Ti_{PT\text{-}4}$–VN-C_{Gr} Powder Blend

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(Received 03 December 2025; revised manuscript received 15 February 2026; published online 25 February 2026)

Mechanically alloyed composite materials were obtained from the mixture of Titanium PT-4 grade (TiH_2–Ti mixture), VN and graphite powders. A detailed X-ray diffraction (XRD) study of the phase composition was provided for the test samples at every 2 hours processing in a planetary ball mill. The refinement of crystal structures of VN and TiH_2 phases present in the mixtures obtained has revealed that during the experiment (16 h of processing) the interaction between components of the charge occurs in two stages. Namely, the process of formation of vacancies in VN phase dominates at the first stage of synthesis (up to 5 h of treatment) with the subsequent penetration of released vanadium atoms into the tetrahedral voids of the TiH_2 structure. At the same stage, the interaction of TiH_2 titanium hydride with carbon atoms takes place, resulting in the formation of a ~ $TiV_{0.33}H_{0.66}C_{0.22}$ compound, which is gradually decomposing at further processing. At the second stage of mechanochemical synthesis (5-16 h of processing), titanium atoms formed as a result of the destroying of the α-Ti structure, are immersed in the VN crystal structure and the formation of a multicomponent (Ti, V)(C, N) solid solution takes place. XRD, SEM and EDS analysis have shown that the final product of mechanochemical synthesis contains the same amount of $V_{0.67}Ti_{0.33}N$ solid solution based on VN nitride and equiatomic (Ti, V)(C, N) solid solution, the formation of which during mechanical alloying is detected for the first time. Analysing the kinetics of interaction of the components of $Ti_{PT\text{-}4}$-VN-C_{Gr} charge, it was shown that the extreme shock loads and deformations that occur during mechanical alloying (MA) cause a high degree of structural instability of the phases and lead to close contact between the grains, activating the flow of diffusion processes. All this stimulates the process of a cold sintering and creates the conditions for further formation of the multicomponent solid solutions. However, considering the participation of nitrogen atoms in the diffusion processes, the formation of (Ti, V)(C, N) solid solution and its full densification is possible only at sintering of the MA mixture at high temperatures.

Keywords: Mechanical alloying, Carbide, Nitride, Crystal structure, Electron structure.

DOI: 10.21272/jnep.18(1).01002 PACS numbers: 81.05.Bx, 61.66.Dk, 61.05.cp

1. INTRODUCTION

Transition metal compounds such as TiC, TiN, VN and TiCN phases belong to the class of hard refractory metal materials due to their promising physical and chemical properties. Their high melting points, ultra-high hardness, corrosion resistance combined with good thermal conductivity, outstanding electrical and optical properties made these compounds implemented in many applications, especially in electrochemical devices, environmental remediation, gas sensing, photocatalysis, applied ceramics, and medicine [1-4]. In particular, TiC, TiN, VN and TiCN compounds have found their successful application as additives to improve the functional properties of ceramics [5-7] and also as components intended for applying biomedical coatings such as TiN, (TiCN) and (TiVN) [8-10].

According to the authors of [8-10] the (TiVN) and (TiCN) coatings obtained by PVD method are solid solutions of the NaCl type and have such advanced improved properties, such as wear resistance, hardness, corrosion resistance, and biocompatibilitym which make them considerable for due to considering the above materials are used for implant protection coatings with proper adhesion, uniformity, high purity, low cost, speed in processing, and ability to stimulate bone growth. Therefore, these multicomponents materials are highly relevant and promising.

In view of the above, a (TiVCN) solid solution that is a combination of (TiVN) and (TiCN) materials, may be a subject of increased of some interest. It is such a multicomponent solid solution (Ti, V)(C, N) of the NaCl-type that we have previously synthesized as a result of HPHT sintering (high pressure-high temperature sintering, 7.7 GPa, 2150 °C) of TiC-VN [11] and (TiH_2-Ti)-VN-C [12] mixtures, which have undergone preliminary mechanochemical processing in a high-energy planetary ball mill (rotation speed of 1400 rpm). It should be noted that, according to the results of a detailed study of the kinetics of the process of mechanical alloying of the TiC-VN [13] and (TiH_2-Ti)-VN-C mixtures [14], there was the formation of a $V_{0.67}Ti_{0.33}N$ solid solution based on the VN nitride, as well as solid solutions based on the TiC or TiH_2 and Ti phases.

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Cite this article as: N.M. Belyavina et al., *J. Nano- Electron. Phys.* 18 No 1, 01002 (2026) https://doi.org/10.21272/jnep.18(1).01002

It should be noted that previously [12, 14] as the initial charge (TiH_2-Ti)-VN-C intendent to obtain a (Ti, V)(C, N) solid solution we have used the industrial titanium powder of the PT-4 grade, which contains TiH_2 hydride. Thus, the authors of [15, 16] showed that the addition of TiH_2 hydride to the initial titanium charge leads to a densification of the microstructure, an increase in the plasticity of the manufactured material and allows obtaining a biocompatible material with a Young's modulus of 5.8-9.5 GPa, similar to the spongy tissue of human bone and with good mechanical compatibility between the bone and the metal titanium implant.

It should also be noted that we obtained a multicomponent (Ti, V)(C, N) solid solution only after HPHT sintering (high pressure-high temperature sintering) of the TiC-VN [11] and (TiH_2-Ti)-VN-C [12] mixtures previously mechanochemically activated for 8-10 h. However, the authors of [17] managed to partially synthesize a (Ti, Ta)(C, N) solid solution after a long (more than 48 h) mechanochemical processing of the Ti(C, N)-Ta charge.

Considering the above, the aim of this work was to study the kinetics of interactions of the phases of the Ti_{PT-4}-VN-C_{Gr} ((TiH_2-Ti)-VN-C_{Gr}) blends, subjected to long-term processing in a industrial BM6 pro planetary ball mill (rotation speed of 600 rpm). The components of the initial blend were industrial titanium powder PT-4 grade, containing its TiH_2 hydride as well as VN vanadium nitride and C_{Gr} graphite.

2. MATERIALS AND METHODS

The object of the study in this work was the Ti_{PT-4}–VN-C_{Gr} mixture, prepared from dispersed powders (diameters up to 50 μm) of industrial titanium (ПТ-4 grade, 98.0 wt. % purity), vanadium nitride (VN, 99.9 %) and graphite (C_{Gr}, 99.999 %). The composition of the charge was calculated with the aim of obtaining an equiatomic TiVCN solid solution in the future.

The mechanical alloying (MA) of the charge was carried out in planetary ball mill BM6 pro (POWTEQ, Китай) (marked as PM mill) according to the modes given in Table 1. Previously [14], a charge of similar composition was processed in a high energy planetary ball mill (Taras Shevchenko National University of Kyiv, Ukraine) (HEPM mill) (Table 1).

Table 1 – Mechanochemical processing modes

Modes	PM mill, this work	HEPM mill [14]
Material of vials and balls	ZrO_2	Steel
Number of balls, their diameter	16, ∅ 10 mm	20, ∅ 10 mm
Mass ratio between the balls and the powder	10:1	20:1
Rotational speed	600 rpm	1400 rpm
Cyclic mode: milling/cooling	8/2 min	20/10 min

The phase transformations that the components of the Ti_{PT-4}–VN-C_{Gr} blend udergo during MA processing were studied on the test samples selected after each 2 hour of treatment the initial mixture in a planetary mill. X-ray data were obtained on an automated diffractometer. DRON-4 diffractometer (Burevestnik factory, USSR) with CuKα radiation operating in a discrete mode with the following scanning parameters: observation range 2θ = (20–100)°, step scan of 0.05° and counting time per step at 3 s. The original software package, including full complex of standard Rietveld procedures, has been used for analysis and interpretation of the X-ray diffraction patterns obtained, namely, determination of both peak positions and integral intensities of the Bragg reflections by means of full profile analysis; qualitative phase analysis using the least square method for lattice parameters refinement; refining crystal structures of the phases (including atomic position filling) and calculation of the parameters of their real structure (coherent block sizes and microdeformation values). The full methodology is described in [18] and is available at x-ray.knu.ua.

The microstructure of the compacted samples was examined via scanning electron microscopy (SEM) using a ZEISS EVO 50 XVP instrument (Carl Zeiss Microscopy GmbH, Germany). Imaging was performed in material contrast mode using a Compact Zeiss BackScattered Detector (CZ BSD) to collect backscattered electrons. Elemental and phase composition were determined by means of energy-dispersive X-ray spectroscopy (EDS) using an Ultim Max 100 detector (Oxford Instruments, UK).

3. RESULTS AND DISCUSSION

3.1 XRD Analysis

The results of X-ray diffraction studies show that the initial Ti_{PT-4}–VN-C_{Gr} blend contains VN vanadium nitride, C_{Gr} graphite and titanium powder of the PT-4 grade, which is a mixture of TiH_2 titanium hydride and α-Ti in a ratio of 3:2 (Fig. 1). With an increase in the MA treatment duration, the phase composition of the mixture gradually changes, namely, the reflections of the CGr graphite, TiH_2 titanium hydride and α-Ti disappear but after 8 h of exposure, new reflections appear on the diffraction patterns of test samples, the intensity of which gradually increases (in Fig. 1, these reflections are marked as red stars). It should also be noted that the presence of ZrO_2 oxide, which is the material of the reaction zone of the planetary mill, was recorded in the test samples that underwent long-term MA treatment.

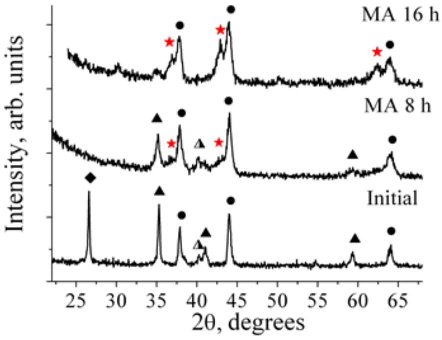


Fig. 1 – Fragments of diffraction patterns of the Ti_{PT-4}–VN-C blend: initial and after processing in a planetary mill. Reflection of VN are marked as ●, of TiH_2 as ▲, of α-Ti as △, of C_{Gr} as ◆ and (Ti, V)(C, N) as ★

The calculations show that the main phase components of the test samples are VN and TiH_2, which undergo certain structural changes during mechanochemical processing. First of all, this concerns variations in the crystal lattice parameters of these phases (Fig. 2).

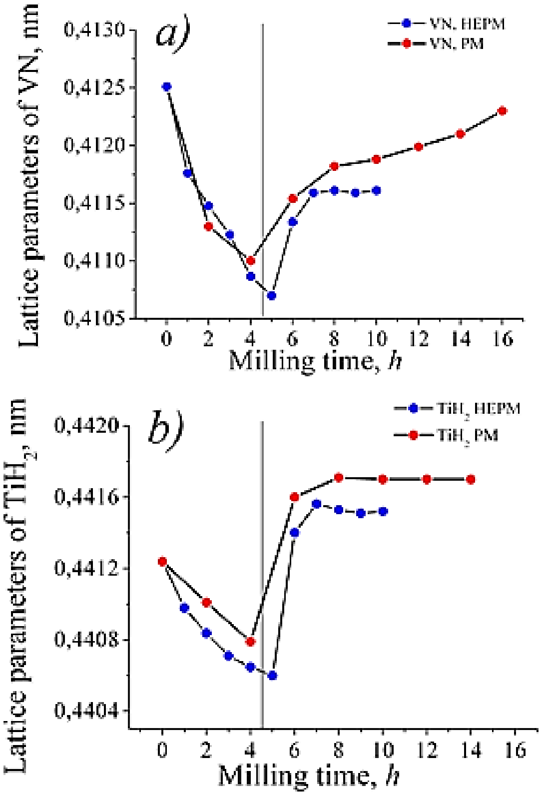
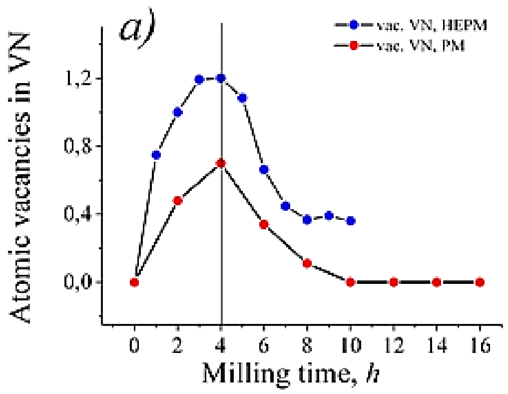


Fig. 2 – Dependences of lattice parameters of VN nitride (a) and TiH_2 hydride (b) present in the $Ti_{PT\text{-}4}$–VN-C blend after their processing in a planetary mill. Data obtained in this work are marked as red circle (PM mill) and data obtained earlier [14] are marked as blue circle (HEPM mill)

In addition, it was found that at the beginning of the process of mechanical alloying of the $Ti_{PT\text{-}4}$–VN-C_{Gr} blend (up to 4 h) the crystal structure of VN vanadium nitride gradually accumulates vacancies in the position occupied by vanadium atoms (Table 2). However, after 4 h of treatment, these vacancies are gradually filled by titanium atoms. The nature of the change in the total number of available atomic vacancies in the VN lattice is presented on Fig. 3a.



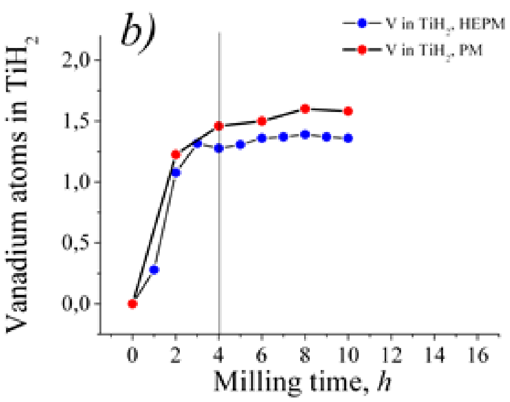


Fig. 3 – Dependences of atomic vacancies in VN nitride (a) and additional vanadium atoms in TiH_2 hydride present in the $Ti_{PT\text{-}4}$–VN-C_{Gr} blend after their processing in a planetary mill. Data obtained in this work are marked as red circle (PM mill) and data obtained earlier [14] are marked as blue circle (HEPM mill)

The crystal structure of the TiH_2 hydride undergoes more complex transformations. Thus, if at the beginning of the MA synthesis this phase still retains a cubic structure of the CaF_2 type, then after 2 hours of treatment it is internally deformed and can be described within the framework of the rhombohedral model. In this case external deformation of the structure is practically absent, due to which the lattice parameters of TiH_2 can be given in cubic syngony (Fig. 2b). That is why in the work the lattice parameters of TiH_2 will be given in the cubic aspect.

According to the calculations carried out within the framework of the model proposed by us in [14] (Table 1), at the beginning of the MA treatment process, half of the tetrahedral pores of the TiH_2 hydride gradually lose hydrogen atoms and are filled with carbon atoms, while the other half of the tetrahedral pores, displacing hydrogen atoms, are partially filled with vanadium atoms, due to which these pores are somewhat deformed. The nature of the accumulation of vanadium and carbon atoms in the TiH_2 structure is illustrated in Fig. 3b and Fig. 4.

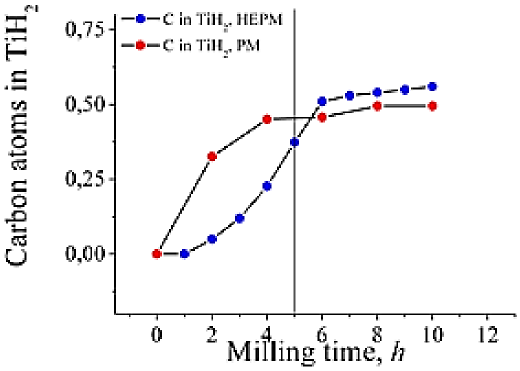


Fig. 4 – Dependences of additional carbon atoms in TiH_2 hydride present in the $Ti_{PT\text{-}4}$–VN-C_{Gr} blend after their processing in a planetary ball mill. Data obtained in this work are marked as red circle (PM mill) and data obtained earlier [14] are marked as blue circle (HEPM mill)

Table 2 – Crystal data for VN nitride and TiH_2 hydride present in the Ti_{PT-4}–VN-C_{Gr} blend after its processing in a planetary mill (4 hour of treatment)

Atom	Site	Site occ.	*x*	*y*	*z*
VN nitride (NaCl-type structure)					
V1)	*4a*	0.827(4)	0	0	0
N	*4b*	1.000	0.5	0.5	0.5
Space group			*F-43m* (no.216)		
Lattice parameters, *a* nm			0.41122(8)		
Total isotropic *B* factor, nm^2			$B = 3.04(3) \cdot 10^{-2}$		
Phase			$V_{0.83}N$		
Reliability factor			$R_B = 0.02$		
Atom	Site	Site occ.	*x*	*y*	z
TiH_2 hydride (rhombohedrically distorted CaF_2-type structure)					
Ti	*3a*	1.00(1)	0	0	0
V	*3a*	0.36(1)	0	0	0.328(2)
H(1)	*3a*	0.64(1)	0	0	0.328(2)
H(2)	*3a*	0.89(1)	0	0	0.666(2)
C	*3a*	0.11(2)	0	0	0.666(2)
Space group			*R3m* (no. 160)		
Lattice parameters, *a, c,* nm			*a* = 0,3135(2); *c* = 0,7681(3);		
Total isotropic *B* factor, nm^2			$B = 2.61(3) \cdot 10^{-2}$		
Calculated phase content, at. %			$TiV_{0.36}H_{1.51}C_{0.11}$		
Reliability factor1)			$R_B = 0.04$		

Taking into account the results of XRD calculations, the process of vacancy formation in the VN structure and the process of accumulation of additional vanadium and carbon atoms in the TiH_2 structure gradually stabilize after 4 hours of MA (Figs. 3, 4). After that, according to the phase analysis study, the TiH_2 and α-Ti phases gradually disappear, and instead a new phase is formed, the diffraction reflections of which are well indexed in the cubic lattice with $a = 0.4220$ nm (in Fig. 1 this phase is marked as ★).

3.2 SEM and EDS Analysis

In order to determine the elemental composition of the phases present in the Ti_{PT-4}–VN-C_{Gr} mixture processed in a planetary ball mill for 16 h, electron microscopy study has performed.

SEM image of the powder obtained shows a mixture of a large number of small grains (size of 1-2 μm) with the inclusion of individual large grains (up to 25 μm) (Fig. 5). According to the XRD studies, the coherent scattering blocks size is ~ 20 nm.

The EDS analysis data, obtained from different areas of the MA Ti_{PT-4}–VN-C_{Gr} mixture, showed the presence of the grains of two different compositions, namely, vanadium-enriched grains (Grain 1 in Fig. 5) and grains with a parity content of titanium and vanadium (Grain 2 in Fig. 5). In addition, there are a small number of fine grains with a high titanium content (apparently, residues of solid solutions based on TiH_2 and α-Ti phases). It should also be noted that the uncertainty of EDS data for carbon and nitrogen is significantly lower than for metals, since the efficiency of the EDS detector in registering quanta with an energy below 1 KeV is limited.

In general, summarizing the XRD and EDS analysis data, it can be stated that as a result of MA processing of the Ti_{PT-4}–VN-C_{Gr} mixture in a planetary ball mill, two solid solutions were formed, namely, ~ $V_{0.66}Ti_{0.33}N$ with $a = 0.41230(6)$ nm and $Ti_{0.25}V_{0.25}C_{0.25}N_{0.25}$ (or TiVCN) with $a = 0.4220(1)$ nm.

The spectra (Fig. 4, 5) calculated illustrate the change in DOS of TiC and VN phases, which occurs when those phases accumulate maximal number of structural defects in the form of vacancies (after 3-6 h of MA), and during the subsequent formation of mutual

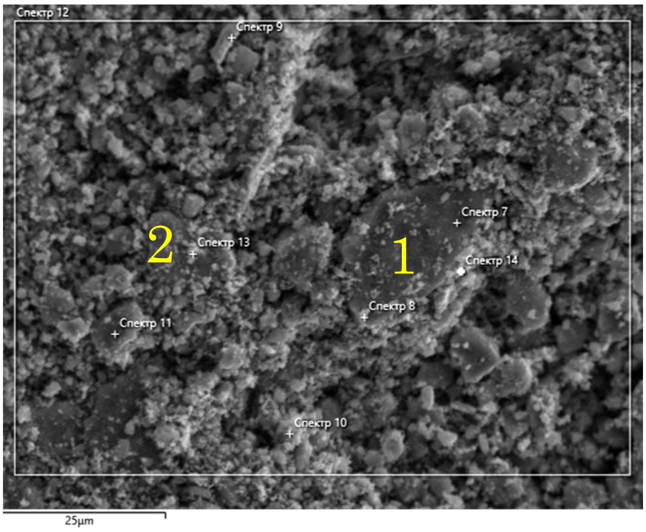
The formation of a similar additional asymmetric peak, which in the highest occupied state exists slightly above the Fermi level, was shown by the authors of Ref. [12] when studying the electronic structure of $ScMeN_2$ polynitrides (Me-V, Nb, Ta) in the initial state and in the presence of defects in the form of vacancies and atoms C, O, F embedded in the lattice. According to the authors of [12], such a local maximum of the DOS near the Fermi level often correlates to a first approximation with the degree of structural instability, since the formation of a vacancy corresponds to the separation between the binding and anti-binding states of the compound.

4. DISCUSSION

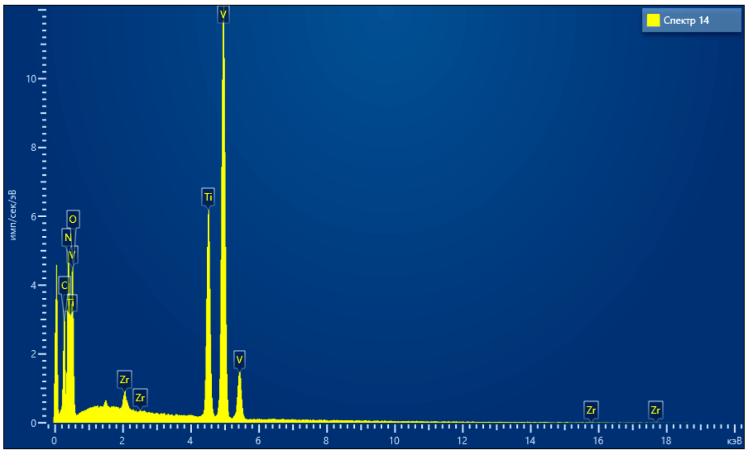
Since the results of XRD studies of the test samples, obtained after a certain time of mechanochemical processing of the charge, provide information about the kinetics of the interaction of the phases present, it was of interest to compare the data of this work on MA treatment of the Ti_{PT-4}–VN-C mixture with the data of our previous work [14] on MA treatment of a similar composition mixture. However, these experiments were carried out, first, in different ball mills (conventionally designated as PM and HEPM), second, under different processing modes (Table 1), and in addition, graphite (C_{Gr}) was used as the carbon component of the charge in this work, while graphite (C_{Gr}) or/and carbon nanotubes (CNT) were used in the previous work [14] (the graphs in Fig. 2-4 show the averaged data [14] for three Ti_{PT-4}–VN-C_{Gr}, Ti_{PT-4}–VN-CNT and

$Ti_{PT\text{-}4}$–VN-(C_{Gr}+CNT)) mixtures). It is clearly seen that the kinetic curves presented in Fig. 2-4 are practically identical and show that the mechanochemical synthesis occurs in two stages, each of which is dominated by different interaction mechanisms.

At the first stage of mechanochemical synthesis (up to 5 h of processing), as a result of the applied shock load, part of the vanadium atoms leaves the crystal structure of VN nitride with the formation of individual vanadium clusters in the reaction zone of the mill. This process is accompanied by the accumulation of vacancies in VN (Fig. 3a) while most of the vanadium clusters formed (probably in the form of ions) are embedded in the tetrahedral voids of the rhombohedrically distorted TiH_2 structure which are released during its dehydrogenation (Fig. 3b). At the same stage, the process of filling the released voids of the TiH_2 structure with carbon atoms begins (Fig. 4).



Grain 1	
Element	Weight, %
C	13.04
N	24.16
O	21.65
Ti	12.53
V	27.64
Zr	0.98
Total	100.00



Grain 2	
Element	Weight, %
C	12.37
N	10.90
O	16.24
Ti	29.39
V	28.85
Zr	2.25
Total	100.00

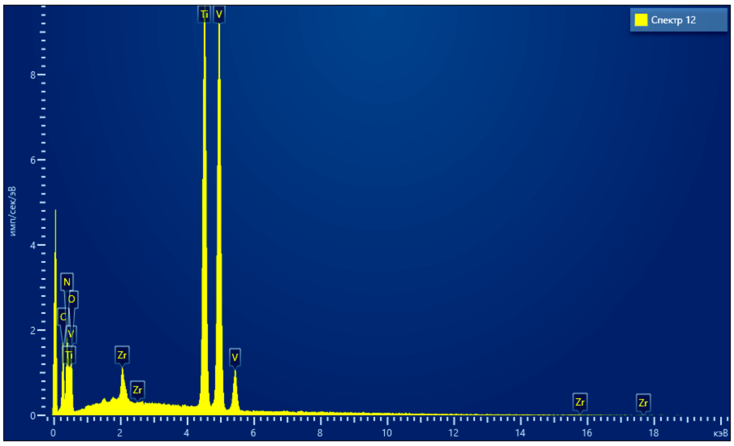


Fig. 5 – SEM image and EDS spectra for $Ti_{PT\text{-}4}$–VN-C powder after 16 h processing in planetary ball mill

At the end of the first stage of MA, the TiH_2 dehydration and transformation of becomes more balanced (the number of embedded vanadium atoms does not change (Fig. 3b)), and therefore, *at the second stage* of synthesis (after 5 h of MA), in our opinion, the process of immersion of titanium clusters formed during partial decomposition of α-Ti into the crystal lattice of VN prevails, which leads to a significant decrease of vacancies fraction in it (Fig. 3a) and to the lattice parameter increasing (Fig. 2a).

In the course of the experiments, it was shown that the interaction of TiH_2 with VN and carbon leads to the formation of a compound with the composition ~ $TiV_{0.33}H_{0.66}C_{0.22}$ [14] after 5 h of MA processing, which subsequently begins to decompose (Fig. 1). In turn, VN nitride accumulates a certain fraction of titanium atoms with the formation of $V_{0.67}Ti_{0.33}N$ solid solution These data fully correspond: firstly, to the data of the authors of [19], who synthesized a $V_{0.75}Ti_{0.25}N_{0.87}$ solid solution by a mechanochemical method in a nitrogen environment from pure metals (titanium and vanadium); and secondly, to our data [20] present results of MA synthesis of a $V_{0.75}Ti_{0.25}N_{1.6}$ solid solution from VN and TiN nitrides (however, in this synthesis, the solid solution was significantly oversaturated with nitrogen).

In this work, the MA of the $Ti_{PT\text{-}4}$–VN-C charge was prolonged to 16 hour, which led to the formation of a multicomponent equiatomic (Ti,V)(C,N) solid solution, the composition of which was determined by the EDS method. Previously, using the MA $Ti_{PT\text{-}4}$–VN-C mixture [14], a similar solid solution in the form of single-phase compact sample was synthesized by us under high pressures and temperatures sintering (HPHT method, 7.7 GPa, 2150 °C) [12].

Hence, it is obvious that extreme loads and deformations that occur during the MA cause a high degree of structural instability of the phases [21] and lead to close contact between grains, activating the flow of diffusion processes. All this stimulates the process of cold sintering and creates conditions for further solid solutions formation. However, given the participation of nitrogen in the diffusion processes, to complete the process of formation of (Ti, V)(C, N) solid solution and achieve its full densification, in our opinion, is possible only during the sintering of the MA-treated mixture at high temperatures.

5. CONCLUSIONS

A detailed XRD study of the test samples selected after every 2 hours of mechanochemical processing in a planetary ball mill of the $Ti_{PT\text{-}4}$–VN-C_{Gr} mixture was carried out. In this case initial mixture contains VN vanadium nitride, C_{Gr} graphite, and also industrial titanium of the PT-4 grade (a mixture of TiH_2 and α-Ti).

The nature of interaction between the phases existing in the MA treated $Ti_{PT\text{-}4}$–VN- C_{Gr} mixture was determined based on the results of the refinement of the crystal structure of the VN nitride and TiH_2 hydride present in selected test sample.

It is shown that 16-hour mechanochemical processing of the $Ti_{PT\text{-}4}$–VN-C_{Gr} mixture leads to the formation of $V_{0.67}Ti_{0.33}N$ solid solution based on VN nitride and to the formation of a (Ti, V)(C, N) solid solution, which is a product of the reactive interaction of the charge components.

The final products of mechanochemical synthesis obtained in the work will be subjected to sintering by the reactive hot pressing method (RHP method) to determine the stability of the solid solution formed, as well as to study the properties of the manufactured compacts and the prospects for their use for applying protective biomedical coatings.

ACKNOWLEDGEMENTS

This work was financially supported by the Ministry of Education and Science of Ukraine (project No. 24BF051-01, registration number 0124U001075)

REFERENCES

1. B. Mazumder, A.L. Hector, *J. Mater. Chem.* **19** No 27, 4673 (2009).
2. *Transition Metal Carbides and Nitrides* (Ed. by L. Toth) (Elsevier: 2014).
3. S.A. Rasaki, B. Zhang, K. Anbalgam, T. Thomas, M. Yang, *Prog. Solid State Chem.* **50**, 1 (2018).
4. M. Mhadhbi, M. Driss, *J. Brill. Eng.* **2**, 1 (2021).
5. K.V. Slipchenko, I.A. Petrusha, V.Z. Turkevich, D.A. Stratiichuk, V.M. Slipchenko, N.M. Bilyavina, J.E. Stahl, *Metallofiz. Nov. Tekhnol.* **41** No 12, 1599 (2019).
6. K. Slipchenko, V. Bushlya, D. Stratiichuk, I. Petrusha, A. Can, V. Turkevich, F. Lenrick, *J. Eur. Ceram. Soc.* **42** No 11, 4513 (2022).
7. A. Aramian, Z. Sadeghian, M. Narimani, N. Razavi, F. Berto, *Int. J. Refract. Met. Hard Mater.* **115**, 106320 (2023).
8. A.P. Serro, C. Completo, R. Colaço, F. Dos Santos, C.L. Da Silva, J.M.S. Cabral, B. Saramago, *Surf. Coat. Technol.* **203**, No 24, 3701 (2009).
9. M. Madej, K. Piotrowska, *Coatings* **14**, No. 6, 775 (2024).
10. J. Bautista-Ruiz, A. Elhadad, W. Aperador, *Mater. Chem. Phys.* **326**, 129856 (2024).
11. N.M. Belyavina, V.V. Kuryliuk, A.M. Kuryliuk, D.A. Stratiichuk, S.P. Starik, O.I. Nakonechna, *Mater. Adv.* **6**, 7443 (2025).
12. N.M. Belyavina, V.V. Kuryliuk, A.M. Kuryliuk, D.A. Stratiichuk, S.P. Starik, *Next Mater.* **10**, 101366 (2026).
13. N.M. Bilyavina, V.V. Kuryliuk, V.V. Dibrov, A.M. Kuryliuk, *Metallofiz. Nov. Tekhnol.* **47** No 1, 25 (2025).
14. N.M. Bilyavina, A.M. Kuryliuk, P.P. Kogutyuk, R.V. Ostapenko, *Metallofiz. Nov. Tekhnol.* **47** No 5, 555 (2025).
15. H.T. Wang, M. Lefler, Z.Z. Fang, T. Lei, S.M. Fang, J.M. Zhang, Q. Zhao, *Key Eng. Mater.* **436**, 157 (2010).
16. F. Kuang, Y. Pan, J. Sun, Y. Liu, C. Lei, X. Lu, *J. Mater. Process. Technol.* **329**, 118459 (2024).
17. M. Naidoo, J. Raethel, I. Sigalas, M. Herrmann, *Int. J. Refract. Met. Hard Mater.* **35**, 178 (2012).
18. M. Dashevskyi, O. Boshko, O. Nakonechna, N. Belyavina, *Metallofiz. Nov. Tekhnol.* **39** No 4, 541 (2017).
19. M.A. Roldán, M.D. Alcalá, C. Real, *Ceram. Int.* **38**, No 1, 687 (2012).
20. O. Nakonechna, N. Belyavina, A. Kuryliuk, P. Kogutyuk, D. Stratiichuk, V. Turkevich, *Mater. Proc.* **14** No 1, 16 (2023).
21. N.M. Belyavina, A.M. Kuryliuk, V.V. Zavodyannyi, M.P. Semenko, *J. Nano- Electron. Phys.* **17** No 1, 01001 (2025).

Формування багатокомпонентного твердого розчину (Ti, V)(C, N) шляхом механохімічного синтезу порошкової суміші $Ti_{PT\text{-}4}$–VN-C_{Gr}

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Проведено докладне рентгенівське дослідження фазового складу тестових проб, відібраних через кожні 2 години механохімічної обробки у планетарному млині суміші $Ti_{ПТ\text{-}4}$-VN-C за участю нітриду ванадію VN, графіту C, а також порошу промислового титану марки ПТ-4, який являє собою суміш гідриду титану TiH_2 та α-Ti в співвідношенні 3:2. В результаті уточнення кристалічних структур основних фазових складових VN та TiH_2, наявних в оброблених сумішах, показано, що за час проведення експерименту (16 год обробки) взаємодія між компонентами шихти проходить в два етапи. А саме, на першому етапі синтезу (до 5 год обробки) домінує процес формування вакансій в нітриді VN з подальшим зануренням атомів ванадію, які при цьому вивільнися, до тетраедричних пор структури TiH_2. На цьому ж етапі відбувається взаємодія гідриду титану TiH_2 з вуглецем, яка в сукупності із взаємодією з ванадієм призводить до утворення сполуки складу ~ $TiV_{0.33}H_{0.66}C_{0.22}$, яка при подальшої обробці починає поступове розпадатися. На другому етапі механохімічного синтезу (5-16 год обробки) відбувається занурення до структури нітриду VN атомів титану, які утворюються в результаті руйнування структури Ti, а також формування мультікомпонентного твердого розчину (Ti, V)(C, N). Із застосуванням методів XRD, SEM та EDS аналізів показано, що фінальний продукт механохімічного синтезу містить однакову кількість твердого розчину $V_{0.67}Ti_{0.33}N_{0.93}$ на базі нітриду VN та еквіатомного твердого розчину (Ti, V)(C, N), формування якого в процесі механохімічного обробки зафіксовано вперше. При аналізі кінетики взаємодії компонентів шихти $Ti_{ПТ\text{-}4}$-VN-C показано, що екстремальні ударні навантаження та деформації, які виникають в процесі МХ синтезу, викликають високий ступінь структурної нестабільності фаз та призводять до тісного контакту між зернами, активуючи протікання дифузійних процесів. Все це в сукупності стимулює процес холодного спікання та створює передмови для подальшого формування твердих розчинів. Проте зважаючи на участь в дифузійних процесах атомів азоту, завершити процес формування твердого розчину (Ti, V)(C, N) та досягнути його повне ущільнення можливе лише під час спікання МХ обробленої суміші при високих температурах.

Ключові слова: Механохімічний синтез, Карбід, Нітрид, Кристалічна структура, Електронна структура.