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SELF-PROPAGATING HIGH TEMPERATURE SYNTHESIS OF SHAPE MEMORY TITANIUM-NICKEL ALLOYS

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Abstract. *Introduction* This research work is aimed at developing (establishing) an effective method for synthesizing nitinol alloy (Ni – Ti), a shape memory material using the self-propelled high-temperature synthesis (SHS) process. The synthesis was performed using condensed mixtures composed of titanium dioxide (TiO_2), nickel oxide (NiO), and magnesium (Mg), where magnesium served as a reducing agent. The mass fraction of magnesium was varied between 25% and 45% to determine its impact on combustion characteristics. The results showed that the highest combustion temperature reached 1845 °C, with a peak propagation velocity of 9.0 mm/s, demonstrating the system's strong exothermic nature. Thermogravimetric analysis revealed activation energies of 379.66 kJ/mol and 366.44 kJ/mol as calculated using the Kissinger and Ozawa methods, respectively. These values confirm the thermodynamic feasibility of the SHS reaction. X-ray diffraction (XRD) analysis identified the presence of multiple phases, including TiNi, MgO, and Mg_2TiO_4, indicating simultaneous reduction and intermetallic formation. Scanning electron microscopy (SEM) revealed a porous microstructure with pore sizes in the range of 50–200 nm, suggesting the suitability of the material for biomedical and sensor applications. Overall, the research confirms that SHS offers a promising pathway to synthesize porous NiTi alloys directly from metal oxides, reducing costs and avoiding complex vacuum-based melting techniques traditionally required in nitinol production.

Keywords: shape memory alloy, self-propagating high-temperature synthesis (SHS), nitinol (Ni-Ti), magnetothermal reduction, porous structure.

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1. Introduction

Shape Memory Alloys (SMAs) are functional materials with unique properties, and Ni-Ti alloys are among the most widely studied [1]. These materials undergo a martensitic thermoelastic transformation, during which changes in the relative positions of atoms in the crystal lattice occur through coordinated atomic movements. Displacements between neighboring atoms are small compared to interatomic distances. Such materials can 'remember' their original shape after being heated to high temperatures, and upon cooling to room temperature, they can be deformed and recover their original shape when reheated above 40°C. Unique properties such as exceptional flexibility and elasticity enable these materials to be widely used in medicine, aerospace engineering, robotics, space technology, and other fields [2]. The corrosion resistance, high mechanical strength, and biocompatibility of Ni-Ti alloys make them suitable for applications ranging from dental implants to cardiovascular devices [3,4].

In recent years, the fabrication of Ni-Ti alloys with a porous structure has become a significant focus of scientific research [5,6]. The unique properties of porous Ni-Ti alloys are attributed to their similarity to the natural bone structure. Such a structure supports cell metabolism and growth, a significant advantage for biomedical implants. Consequently, porous Ni-Ti alloys are used in orthopedics, trauma, and surgery. They are applied to produce artificial organs, bone fixators, and cardiovascular stents [7,8].

Various technologies based on powder metallurgy processes are used to synthesize porous Nitinol. Due to the high reactivity of nickel and titanium, melting processes are typically carried out under vacuum conditions. Among standard casting methods, vacuum induction, arc melting, electron beam melting, and plasma arc melting are widely used [9,10]. However, the need to operate in a vacuum environment and the high energy consumption of these methods significantly increase production costs. Today, one of the most efficient methods for obtaining Nitinol is Self-propagating High-temperature Synthesis (SHS) [11,12]. This method is attractive due to its relatively low cost, accessibility, and ability to produce highly porous materials. The SHS process typically involves homogenizing an equimolar mixture of titanium and nickel powders, compacting the mixture, and igniting the compact [13].

Many researchers have investigated the formation of Nitinol solid solutions by melting pure metals at high temperatures in synthesizing porous Ni-Ti alloys. However, the use of pure metals increases the overall cost of nitinol. Therefore, the main advantage of this study lies in the simultaneous synthesis of nitinol from metal oxides using the SHS method based on magnesiothermic reduction and in evaluating the efficiency of this synthesis approach.

2. Experimental Part

2.1. Materials

Magnesium powder (Sigma-Aldrich) was purchased as one of the initial components. Its active metal content was 99%. It was used as a reducing agent for

metal oxides. Nickel monoxide powder (GOST TU 6-09-4125-7580) was used to synthesize nickel. Titanium dioxide (GOST 9808-84) was used to synthesize titanium.

2.2. Preparation of samples from condensed mixtures based on TiO_2 + NiO + Mg

The initial components were weighed in various ratios and mixed using a ball mill to prepare a compacted mixture. The compacted mixture was then pressed using a press apparatus with a cylindrical mold to form cylindrical samples with a diameter of 20 mm and a height of 20 mm, applying a force of 100 kN.

2.3. *Study of the burning kinetics of TiO_2 + NiO + Mg - based condensed mixtures*

A cylindrical pressed sample (20×20 mm) is initiated by applying a 20 V voltage from a power source, using a spherical initiator. The burning process of the compacted mixture was recorded using a high-speed camera (Video camera Nikon 1SB-N5, 31 December 2012), and the burning rate was calculated. The burning temperature was measured using an infrared pyrometer (Kelvin PLC 2300, 02 February 2022). For each composition, the burning process was repeated three times.

2.4. Research Instruments

The morphology and elemental composition of the synthesized Ni-Ti alloy powder were determined using a Quanta 200i 3D scanning electron microscope (SEM) (FEI Company, Hillsboro, OR, USA). The phase composition of the synthesized products was analyzed using a Bruker D8 Advance diffractometer (Billerica, MA, USA) with CuKα radiation (40 kV, 40 mA). The thermal decomposition of the initial compacted mixture was studied using a BAXIT thermogravimetric analyzer (BXT-TGA-103) at various heating rates (°C/min).

3. Results and discussion

3.1. *Burning mechanism of a condensed mixture based on TiO_2 + NiO + Mg*

The cylindrical samples were ignited in an atmospheric environment using an open flame. The combustion cinegram of the self-propagating high-temperature synthesis process is shown in Figure 1.

Figure 1 – Burning cinegram of a condensed mixture based on TiO_2 + NiO + Mg

Figure 1 shows that the condensed mixture based on TiO_2 + NiO + Mg was completely combusted through the SHS method with a uniformly propagating

burning front. The synthesis process's burning temperature and velocity were measured and calculated. For the TiO_2 + NiO + Mg system, various ratios of the initial components were used, and the graph illustrating the correlation between the magnesium mass fraction and the burning temperature is presented in Figure 2.

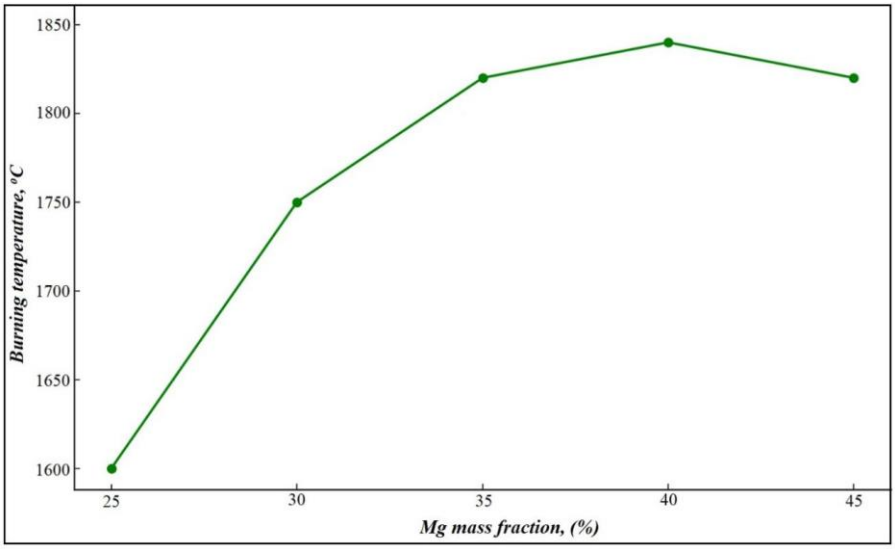

Figure 2 – Graph of the dependence of the burning temperature of a condensed mixture based on TiO_2 + NiO + Mg on the mass fraction of magnesium.

According to the combustion temperature graph, as the mass fraction of magnesium increases from 25% to 40%, the combustion temperature also rises, as there is a sufficient amount of reducing agent to drive the reaction in the system. However, when the amount of reducing agent exceeds 40%, the excess magnesium does not participate fully in the response, leading to a limited increase in temperature or a slight decrease. This may be due to the interaction of residual reactants' heat absorption capacity in exothermic reactions. In addition, the linear combustion velocity of the compacted mixture based on TiO_2 + NiO + Mg was calculated based on video recordings captured with a high-speed video camera. As the mass fraction of magnesium increased, the combustion velocity consistently rose, reaching a maximum value of 9.0 mm/s. However, at 45% Mg, the combustion velocity slightly decreased to 8.2 mm/s, indicating that excess Mg does not fully participate in the combustion, instead absorbing heat and slowing down the process.

3.2. Thermodynamics of the system TiO_2 + NiO + Mg

The TiO_2 + NiO + Mg-based system is an effective compacted composition for self-propagating high-temperature synthesis. This system is based on the

strong reducing properties of Mg and the formation of reaction products – NiTi intermetallic and MgO.

$$TiO_2 + NiO + 3Mg \rightarrow NiTi + 3MgO \quad (1)$$

The compacted mixture's activation energy (Ea) based on this reaction is crucial for calculating the combustion characteristics of the compacted mixture. The Kissinger and Ozawa methods are commonly used in Ea calculations, as they do not require knowledge of the reaction order or reaction models [14-15]. The following equation is proposed for calculating E_a according to the Kissinger method:

$$\frac{E_a}{R} = \frac{dln(\beta T_p^{-2})}{dT_p^{-1}} \quad (1)$$

where E_a is the activation energy; T_p is the highest temperature of thermal decomposition of the DTA curve; R is the universal gas constant; and β is the heating rate. These methods study the activation energy of high-energy density materials and compacted mixtures [16]. Therefore, in this research, calculating the Ea value through the Kissinger and Ozawa methods is essential for investigating the combustion mechanism of the TiO_2 + NiO + Mg-based compacted mixture.

The temperature-dependent mass loss behavior of the TiO_2 + NiO + Mg-based condensed composition at different heating rates is presented in Figure 3. Based on the onset temperatures of mass loss, the activation energy was calculated using various methods.

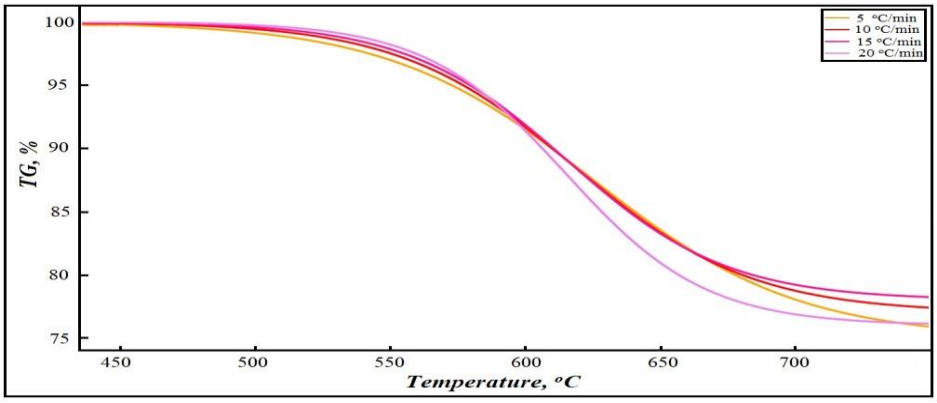

Figure 3 - Thermogravimetric analysis of TiO_2 + NiO + Mg-based compacted mixture

According to the results shown in Figure 3, mass loss occurred in the temperature range of 530 °C to 550 °C. This temperature range corresponds to the ignition of the condensed composition.

Figure 4 shows the dependency plots of $\ln(\beta/T_P^{-2})$ and T_P^{-1} for the activation energy calculation of the TiO_2 + NiO + Mg-based compacted mixture using the Kissinger (a) and Ozawa (b) methods. These relationships show nearly straight lines for each compacted mixture. The Ea values calculated using the Kissinger method were determined to be 379.66 kJ/mol for the compacted mix, while the Ea values computed using the Ozawa method were 366.44 kJ/mol. The Ea values calculated by the relatively different methods were very close.

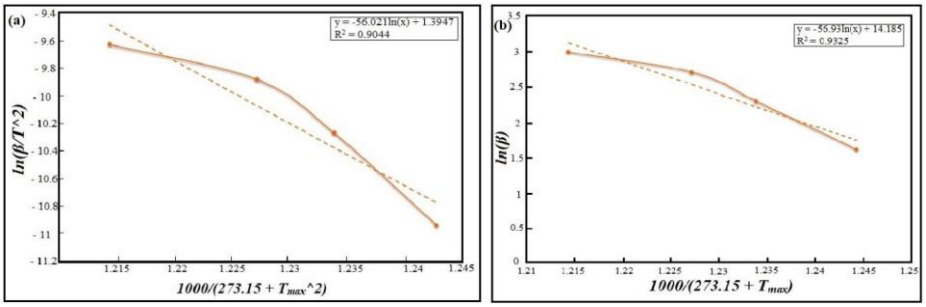

Figure 4 – Kissinger (a) and Ozawa (b) plots of an TiO_2 + NiO + Mg-based condensed mixture

The activation energies of the condensed mixture at different heating rates were calculated using the Kissinger (Ek) and Ozawa (Ea) methods. The calculated results are shown in Table 1.

Table 1 – Activation energy of a condensed mixture based on TiO_2 + NiO + Mg

Reactive Fuels	β (Heating Rate, °C/min)	T_p, °C	E_a/(kJ/mol) Kissinger's Method	R^2	E_a/(kJ/mol) Ozawa's Method	R^2
TiO_2 + NiO + Mg	5	530.5	365.15	0.93	366.44	0.93
	10	537.3				
	15	541.7				
	20	550.3				

The activation energy results calculated using the Kissinger and Ozawa methods showed relatively close values. However, these values indicate that the burning process of the TiO_2 + NiO + Mg system requires significant energy, but once ignited, the reaction proceeds steadily at high temperatures.

3.3. *Composition and morphology of synthesis products of the TiO_2 + NiO + Mg system*

When the TiO_2 + NiO + Mg system is synthesized using the SHS method, high-temperature exothermic reactions result in the formation of metallic nickel, titanium, and their intermetallic compounds (e.g., NiTi, Ni_3Ti) [17]. In this process, magnesium acts as a potent reducing agent, binding the oxygen in TiO_2 and NiO, making the reaction thermodynamically efficient. The obtained products' phase composition depends on the ratio of the starting components and

synthesis parameters. The phase composition of the synthesis products is shown in Figure 5.

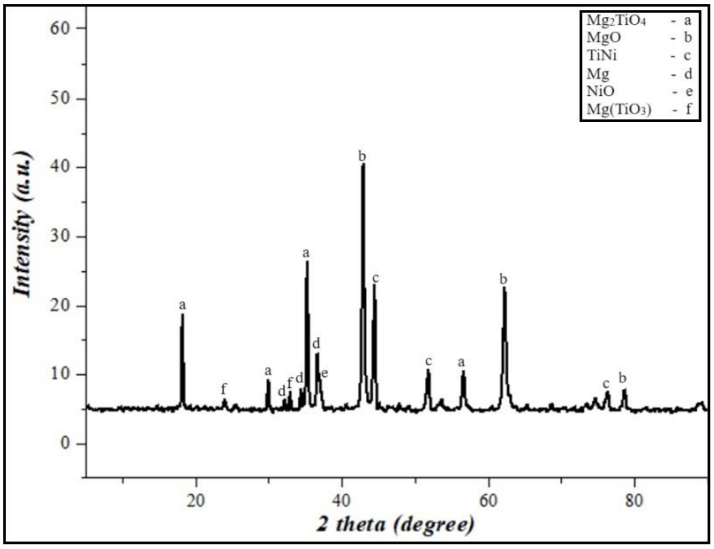

Figure 5 – Results of the phase composition of the burning products of a condensed mixture based on TiO_2 + NiO + Mg

According to the XRD analysis results, the products obtained via the SHS method exhibit a multiphase structure, where the main phases identified are MgO, TiNi, and Mg_2TiO_4. This indicates that simultaneous reduction, intermetallic compound formation, and complex titanate formation occur concurrently. It was determined that the synthesized products' structural complexity and phase composition directly depend on the initial component ratios and synthesis parameters (temperature, pressure, and time). Additionally, the morphology of the product synthesized by the SHS method is shown in Figure 6.

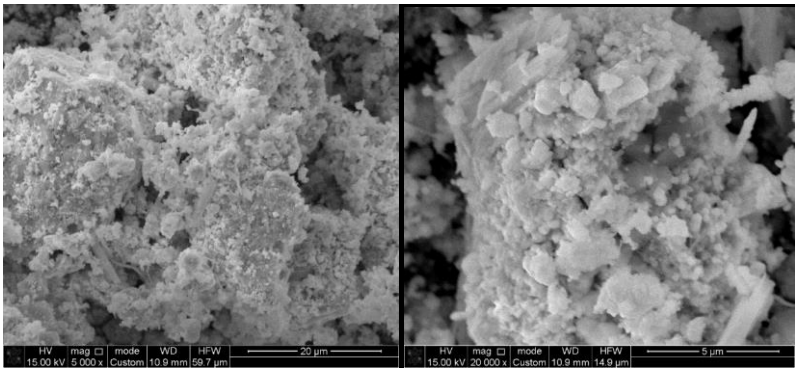

Figure 6 – SEM analysis results of the TiO2 + NiO + Mg system after the SHS process.

SEM analysis of the synthesized products of the TiO_2 + NiO + Mg system after the SHS process revealed a complex microstructure (Figure 5). Based on the conducted analyses, the morphology of the product was found to consist of a heterogeneous mixture of microcrystalline and nanostructured particles. The surface structure shows visible porosity, which may positively influence the catalytic activity of the material by forming favorable channels for gas diffusion. In the porous regions, the pore diameters range from approximately 50 to 200 nm, corresponding to a mesoporous structure. Overall, the obtained morphological and quantitative characteristics indicate not only the structural complexity of the material but also its functional potential. Such microstructures are of great interest for applications in high-temperature catalysis, sensor devices, energy storage systems, and shape memory alloys.

4. Conclusion

This study demonstrated the feasibility of efficiently synthesizing shape memory NiTi (nitinol) alloy via self-propagating high-temperature synthesis (SHS) based on the TiO_2 + NiO + Mg system. Magnesium acted as a reducing agent, creating favorable conditions for synthesizing intermetallic compounds from metal oxides. It was found that the combustion temperature and propagation rate depend on the ratio of the initial components: as the magnesium content increased, the intensity of the reaction also increased. The activation energy calculated using the Kissinger and Ozawa methods ranged from approximately 365 to 380 kJ/mol, indicating the energetic efficiency of the system. Phase composition analysis revealed that the synthesized product is multiphase (MgO, TiNi, Mg_2TiO_4), confirming that complex chemical processes occur during the synthesis. SEM microscopy showed a highly porous, microcrystalline structure, making the material promising for biomedical implants, high-temperature catalysts, and sensor systems as a shape memory alloy. Overall, the SHS method is a cost-effective, accessible, and environmentally friendly alternative technology for synthesizing complex materials such as nitinol from metal oxides.

ПІШІНДІ ЕСТЕ-САҚТАЙТЫН ТИТАН-НИКЕЛЬ ҚОРЫТПАЛАРЫНЫҢ ӨЗДІГІНЕН ТАРАЛАТЫН ЖОҒАРЫ ТЕМПЕРАТУРАЛЫҚ СИНТЕЗІ

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Түйіндеме: *Kipicne.* Бұл ғылыми-зерттеу жұмысы өздігінен таралатын жоғары температуралық синтез (ӨЖС) процесін пайдалана отырып, пішінді есте сақтайтын материал болып табылатын нитинол қорытпасын (Ni–Ti) синтездеудің тиімді әдісін әзірлеуге бағытталған. Синтез үшін титан диоксиді (TiO_2), никель оксиді (NiO) және магний (Mg) негізіндегі конденсирленген қоспалар пайдаланылды, мұнда магний тотықсыздандырғыш ретінде қолданылды. Магнийдің массалық үлесі 25%-дан 45%-ға дейін өзгертіліп, оның жану процесінің температурасы мен жылдамдығына әсері зерттелді. Нәтижесінде жану температурасы 1845 °C-қа дейін жетіп, жану жылдамдығы 9.0

мм/с мәніне ие болды, бұл қоспаның жоғары экзотермиялық реакция қабілетін көрсетті. Термогравиметриялық талдау нәтижесінде Киссинджер және Озава әдістері бойынша активтену энергиясы тиісінше 379.66 кДж/моль және 366.44 кДж/моль шамасында анықталды. Бұл көрсеткіштер жүйенің термодинамикалық тұрғыдан тиімді екенін растайды. Рентгендік фазалық талдау (РФТ) нәтижелері синтезделген өнімнің негізгі фазалары ретінде TiNi, MgO және Mg_2TiO_4 қосылыстарының түзілгенін көрсетті, бұл металл оксидтерінің бір мезгілде тотықсыздануы мен интерметалдық қосылыстардың түзілуі жүретінін дәлелдейді. Сканерлі электрондық микроскопия (СЭМ) нәтижелері материалдың 50–200 нм аралығындағы кеуектерге ие күрделі құрылымын анықтады, бұл оны биомедицина мен сенсорлық құрылғыларда қолдануға лайықты етеді. Жалпы алғанда, бұл зерттеу ӨЖС әдісі арқылы металл оксидтерінен тікелей кеуекті нитинол алу мүмкіндігін растайды және дәстүрлі вакуумдық балқыту әдістеріне балама ретінде өндіріс шығынын азайтатын технологиялық жол ұсынады.

Түйін сөздер: Пішінді жады қорытпасы, өздігінен таралатын жоғары температуралы синтез (SHS), нитинол (Ni-Ti), магнитотермиялық тотықсыздану, кеуекті құрылым.

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САМОРАСПРОСТРАНЯЮЩИЙСЯ ВЫСОКОТЕМПЕРАТУРНЫЙ СИНТЕЗ ТИТАНО-НИКЕЛЕВЫХ СПЛАВОВ С ПАМЯТЬЮ ФОРМЫ

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Резюме. *Введение.* Данная исследовательская работа направлена на разработку эффективного метода синтеза сплава нитинола (Ni – Ti), материала с памятью формы с использованием процесса самоходного высокотемпературного синтеза (СВС). Для синтеза использовались конденсированные смеси на основе диоксида титана (TiO_2), оксида никеля (NiO) и магния (Mg), где магний использовался в качестве восстановителя. Массовая доля магния была изменена с 25% до 45%, и было изучено его влияние на температуру и скорость процесса горения. В результате температура горения достигла 1845 °C, а скорость горения составила 9.0 мм/с, что свидетельствует о высокой способности смеси к экзотермической реакции. В результате термогравиметрического анализа энергия активации методами Киссинджера и Одзавы была определена в пределах 379.66 кДж/моль и 366.44 кДж/моль соответственно. Эти показатели подтверждают, что система термодинамически эффективна. Результаты рентгенофазного анализа (РФА) показали, что в качестве основных фаз синтезируемого продукта образуются соединения TiNi, MgO и Mg_2TiO_4, что доказывает, что происходит одновременное восстановление оксидов металлов и образование интерметаллических соединений. Результаты сканирующей электронной микроскопии (СЭМ) выявили сложную структуру материала с порами размером от 50 до 200 нм, что делает его подходящим для использования в биомедицине и сенсорных устройствах. В целом, это исследование подтверждает возможность получения непосредственно пористого нитинола из оксидов металлов методом СВС и предлагает технологический путь, который снижает производственные затраты в качестве альтернативы традиционным методам вакуумной плавки.

Ключевые слова: сплав с памятью формы, самораспространяющийся высокотемпературный синтез (СВС), нитинол (Ni-Ti), магнитотермическое восстановление, пористая структура.

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