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REGULAR ARTICLE

Microstructure and Morphological Properties of Granulated Mg_3Sb_2 Thermoelectric Material

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This article presents the results of studying the microstructure and morphological properties of a rod-shaped granular Mg_3Sb_2 nanosemiconductor thermoelectric material prepared by resistance annealing. This method is based on placing a mixture of Mg_3Sb_2 particles prepared using 70 % ethyl alcohol on a tubular heat-resistant substrate, for example, a ceramic substrate, and heating the particles using a resistance annealing. The Mg_3Sb_2 semiconductor thermoelectric material obtained by resistance annealing consists of a granular particle assembly and interparticle boundary regions formed between them, forming a structure characteristic of polycrystalline. The particle assembly core consists of Mg_3Sb_2, and its surface regions are composed of oxidized nanocomposite coatings such as $Mg_4Sb_2O_9$, $Mg(Sb_2O_5)_2$, MgO_2, SbO_3. According to the analysis, the amount of oxygen atoms is distributed from the core of the Mg_3Sb_2 compound to the surface, forming an oxidized nanocomposite coating on the surface areas.

Keywords: Granulated Mg_3Sb_2 nanosemiconductor, Thermoelectric material, Microstructure, Morphology, $Mg_4Sb_2O_9$, $Mg(Sb_2O_5)_2$, MgO_2, SbO_3 compounds, Oxidized nanocomposite coating, Heat-resistant ceramic substrate, Thermal bonding, Interparticle boundary regions, Polycrystalline structure.

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1. INTRODUCTION

In the world energy sector, the development of new types of energy sources that do not emit harmful substances into the environment, are one of the most pressing problems today. In this area, the direct conversion of thermal energy into electrical energy using semiconductor thermoelectric materials or thermoelectric devices occupies a leading position. The efficiency of a thermoelectric material is $ZT = \alpha^2\sigma T/\lambda$, and its main parameters are high electrical conductivity (σ) and the Seebeck coefficient (α), while low electrical resistance (ρ) and thermal conductivity (λ) are required [1, 2]. Among semiconductor materials, the low thermal conductivity of Mg_3Sb_2 materials has increased interest in them. In particular, the main thermoelectric characteristics of Mg_3Sb_2 depend on the structure, temperature, and Mg atoms of the material (for example, [1, 2] and references therein). It was observed that with increasing temperature, the formation of electron-hole pairs in its band gap increases σ and α, while, conversely, the decrease in phonon mobility in the crystal lattice decreases λ, which in turn increases ZT. Theoretical and practical studies have shown that such a result can be achieved by controlling the structure of the material and the effect of an additional Mg atom on it, as well as the method of obtaining Mg_3Sb_2. In particular, in [1, 2], we studied the dependence of the electrical and thermoelectric parameters of granulated Mg_3Sb_2 on the properties of granulated Mg_3Sb_2 particles.

The electrical and thermoelectric properties of granulated Mg_3Sb_2 particles depend mainly on the structure of the interparticle boundary regions and the physical processes occurring in the boundary region. With increasing temperature, the ionization of localized traps in the interparticle boundary regions and the trapping of charge carriers in them leads to a decrease in electrical conductivity. Also, the Seebeck coefficient (α) increases with the formation of temperature differences due to the potential difference and phonon absorption. In this case, thermoelectric effects appear due to the formation of electron-hole pairs in the interparticle boundary regions with energy levels E_{in}. As a result, the total λ increases simultaneously with the thermal conductivity of the two connected interparticle boundary regions. The convergence of the electrical conductivity and the potential difference leads to a relatively stable change in λ. These processes are related to the morphological properties of the granulated

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Mg_3Sb_2 particles, which are shown to lead to a change in the ZT index from ~0.021 to ~1.3 at $T = 300 – 700$ K. In addition, it is recognized that the thermoelectric characteristics of granulated Mg_3Sb_2 can be improved by controlling the morphological properties of the particles. However, the microstructure and morphological properties of the granulated Mg_3Sb_2 particles, as well as the mechanisms for the formation of interparticle boundary regions, have not been fully resolved.

2. RESEARCH METHODS

Granulated Mg_3Sb_2 particles prepared by powder technology were selected for the study [1, 2]. The samples were prepared by preparing a mixture of granular Mg_3Sb_2 particles using ethyl alcohol, placing the mixture on a heat-resistant, for example, tubular ceramic substrate, and heating the particles with a resistance [1-5]. As a result, the aggregate of granular Mg_3Sb_2 particles inside the ceramic substrate takes on the shape of a rod. [6] The structural model and charge transfer processes of granular nano-semiconductor particles placed on a tubular ceramic substrate were studied. According to the authors, interparticle boundary regions are formed between the granular nano-semiconductor particles, and the charge transfer processes are explained precisely by the morphological characteristics of the interparticle boundary regions.

Fig. 1 shows a simplified diagram of the method of heating and bonding granulated Mg_3Sb_2 particles with a resistance device. A mixture of Mg_3Sb_2 particles placed on a tubular heat-resistant ceramic substrate is pressed under pressure P through rod-shaped MA and MB ohmic contacts. Then, the Mg_3Sb_2 particles are thermally treated by applying heat Q through a resistance device. Thermal treatment is carried out in the processes of increasing and decreasing the temperature $T = 300 – 700$ K.

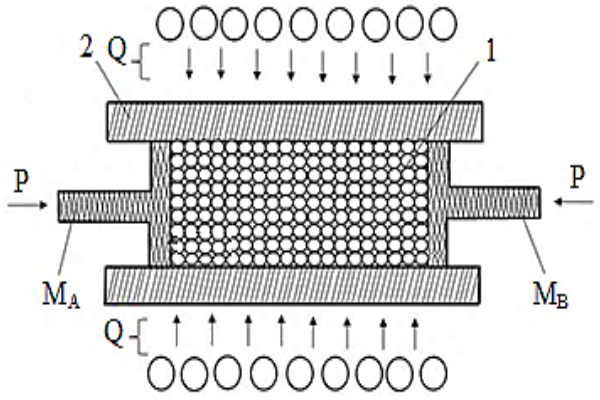

Fig. 1 – Simplified diagram of the method of heating granulated particles with a resistance device. Here, 1 – Mg_3Sb_2 particles, 2 – heat-resistant dielectric body, MA and MB ohmic contacts and thermocouples

Studies have shown that the method of heating with a resistance medium has been found to allow the formation of rod-shaped polycrystalline structures. The microstructure and morphology of the rod-shaped polycrystalline structure were studied on a JEOL JXA-8800R electron microscope. It should be noted that the voltage applied to the accelerator is 0.1÷30 kV, which can magnify microphotographs of structures up to 1 nm by 25 to 650,000 times and allows determining the chemical composition with an error of up to 10^{-3}%.

3. MICROSTRUCTURE AND MORPHOLOGICAL CHARACTERISTICS OF GRANULATED MG_3SB_2

Fig. 2 shows a micrograph of a polycrystalline structure. The sample was isolated by breaking a tubular heat-resistant ceramic substrate. Fig. 2 shows that the resistance annealing method produces a polycrystalline structure consisting of rod-shaped particles and interparticle boundaries. The chemical composition of a sample of granulated Mg_3Sb_2 particles was studied in several different areas of the sample (Fig. 2b). Fig. 3 shows the X-ray diffraction characteristic of the granular Mg_3Sb_2 semiconductor sample.

It should be noted that the studies were carried out point and point. According to X-ray spectral characteristics, the sample consists of magnesium, antimony, oxygen, silicon and other types of elements. Their number or chemical composition varies in the region of interparticles and interparticles. In particular, it is noted that the number of oxygen atoms increases from the center of the particle junction to the outside.

In addition, silicon and carbon atoms were also observed in some areas of the surface in addition to oxygen atoms (Fig. 3a-3f). It is known that ceramic materials consist of silicon or alumina compounds [1-5], which contain various forms of compounds consisting of Si, C, O and other elements. Heating was carried out in the process of simultaneous temperature increase from 300 K to $T = 800$ K. The temperature increase time was 30 minutes, and the maximum temperature was kept for 20 minutes. It was then cooled at the same rate. The heating stage was completed 6 and 7 times. In addition, at each stage, sample particles with metal contacts MA and MB on both sides were printed (Fig. 1). In this case, the pressure force P was controlled by controlling the resistance R of the particles by the metal contacts MA and MB. In our case, $R = 1$ kOhm. Such processes make it possible to create strong joints not only between particles, but also with the surface of the ceramic tube. Thus, extraneous atoms (Figs. 3a-3f), such as silicon or carbon, occurring in some surface regions may refer to heat-resistant ceramic bases.

As you know, today electronic programs have been developed that allow you to determine using chemical equations any types of compounds and their atomic structure, or, conversely, chemical equations of any types of compounds and the atomic structure of the compound using them [7, 8]. In this work, the chemical equation of the formation of granular Mg_3Sb_2 semiconductor particles and their atomic structure were studied. Let's look at the results of the study.

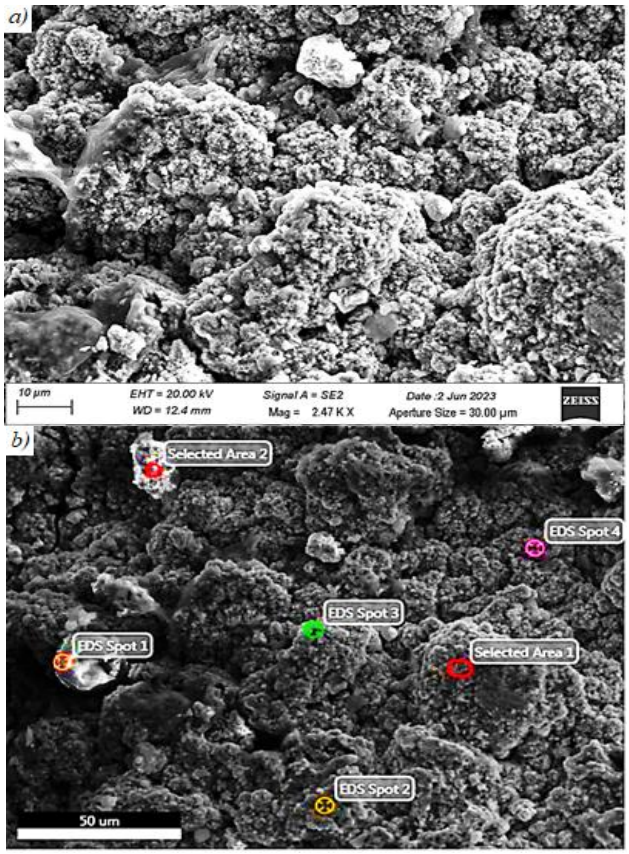

Fig. 2 – Micrograph of granular Mg_3Sb_2 particles

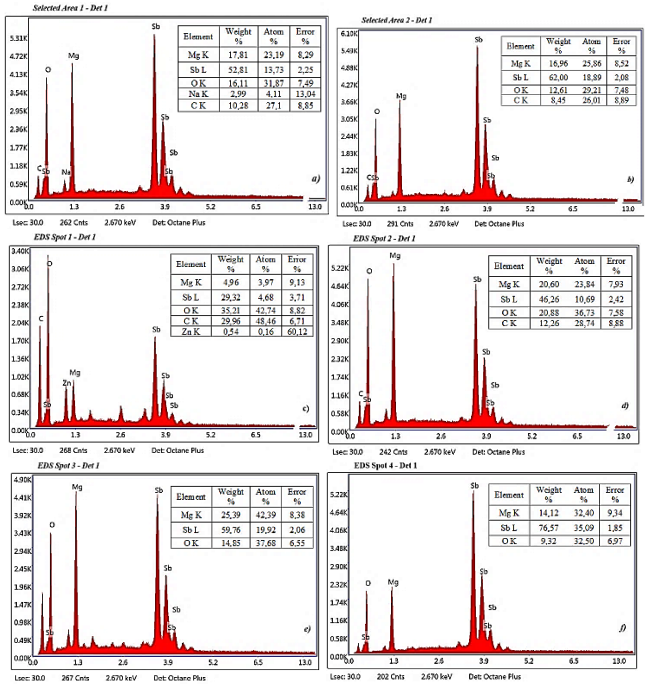

Fig. 3 – X-ray spectral characteristics of granular Mg3Sb2 particles

For the studies, we use the X-ray spectral characteristics given in Fig. 3, as well as the composition and number of elements defined in the tables. The composition of the particles can be described as the amount of each element and the formula of the compound by converting the mass of the substance into a commodity using the mass of the weight and atoms of the elements [9]:

$$\text{Weight \%}\frac{1\ mol}{\text{Atom weight,g}} = mol \qquad (1)$$

(1) divide the ratio of each commodity, determined based on the expression, by the smallest value:

$$\frac{mol}{\text{mol}_{smallest}} = x \qquad (2)$$

By formula (2) we can determine the corresponding values for each element. Thus, using expression (1), we calculate the weight of the element shown in Fig. 3a and the amount of mass of the element using atomic masses.

For magnesium; $Mg_{71,84}\frac{1}{Mg_{24,305}} = Mg_{0,733}\ mol$

For antimony; $Sb_{52,81}\frac{1}{Sb_{121,76}} = Sb_{0,434}\ mol$

For oxygen; $O_{16,11}\frac{1}{O_{15,999}} = O_{1,01}\ mol$

For sodium; $Na_{2,99}\frac{1}{Na_{22,99}} = Na_{0,13}\ mol$

For carbon; $C_{10,28}\frac{1}{C_{2,011}} = C_{5,112}\ mol$

It can be seen from the calculation that the sodium element content is the smallest. (1) based on the expression, divide the proportion of each element by the lowest value of the sodium content:

For magnesium; $\frac{Mg_{0,733}}{Na_{0,13}} = 5{,}6$

For antimony; $\frac{Sb_{0,434}}{Na_{0,13}} = 3{,}3$

For oxygen; $\frac{O_{1,01}}{Na_{0,13}} = 7{,}7$

For sodium; $\frac{Na_{0,13}}{Na_{0,13}} = 1$

For carbon; $\frac{C_{5,112}}{Na_{0,13}} = 39{,}3$

To convert the residuals to an integer, multiply them by 2. So, Mg – 11; Sat – 7 units; O – 15 units; Na – 2; C – 79 pcs. Since some of the oxygen, as well as sodium and carbon atoms, belong to ceramic bases, we do not take them into account. Thus, according to the research method [9], using the results of calculations, it is possible to determine the particle structure formula using a chemical reaction calculator. We carry out the reaction using a chemical collider.

$$11Mg + 7Sb + 9O = 3(Mg_3Sb_2) + Mg_4Sb_2O_9$$

Table 1 shows the yield results and the formula of the partial structure or defined compound using it.

Table 1

Element	(Weight %)	Atomic mass, g	Core of particles	Oxide layer
Mg	17.81	24.305	3	4
Sb	52.81	121.76	2	2
O	16.11	15.999		9
Na	2.99	22.99		
C	10.28	2.011		
Fractional structure formula			Mg_3Sb_2	$Mg_4Sb_2O_9$

So, the core of the particle compound consists of the Mg_3Sb_2 structure of the $Mg_4Sb_2O_9$ and its surface regions. Now we define the structure of these connections using an electronic application [7, 8].

Fig. 4a shows the cryptographic structure of the Mg_3Sb_2 compound. Mg_3Sb_2 crystallizes in the trigonal $P\bar{3}m1$ space group. There are two inequivalent Mg^{2+} sites. In the first Mg^{2+} site, Mg^{2+} is bonded to six equivalent Sb^{3-} atoms to form $MgSb_6$ octahedra that share corners with twelve equivalent $MgSb_4$ tetrahedra, edges with six equivalent $MgSb_6$ octahedra, and edges with six equivalent $MgSb_4$ tetrahedra. All Mg-Sb bond lengths are 3.11 Å. In the second Mg^{2+} site, Mg^{2+} is bonded to four equivalent Sb^{3-} atoms to form $MgSb_4$ tetrahedra that share corners with six equivalent $MgSb_6$ octahedra, corners with six equivalent $MgSb_4$ tetrahedra, edges with three equivalent $MgSb_6$ octahedra, and edges with three equivalent $MgSb_4$ tetrahedra. The corner-sharing octahedral tilt angles range from 11-58°. There are three shorter (2.82 Å) and one longer (2.94 Å) Mg-Sb bond length. Sb^{3-} is bonded to seven Mg^{2+} atoms to form a mixture of distorted corner and edge-sharing $SbMg_7$ pentagonal bipyramids. This structure has 5 atoms, a density of 4.01 g cm^{-3}, and the oxidation state can be Mg^{2+}, Sb^{3-}.

Fig. 4b shows the cryptographic structure of the $Mg_4Sb_2O_9$ compound. This material is an ordered representation of a disordered structure. $Mg_4Sb_2O_9$ is Ilmenitelike structured and crystallizes in the triclinic $P\bar{1}$ space group. There are four inequivalent Mg^{2+} sites. In the first Mg^{2+} site, Mg^{2+} is bonded in a 6-coordinate geometry to six O^{2-} atoms. There are a spread of Mg-O bond distances ranging from 1.98-2.42 Å. In the second Mg^{2+} site, Mg^{2+} is bonded to six O^{2-} atoms to form distorted MgO_6 octahedra that share corners with six MgO_6 octahedra, edges with three SbO_6 octahedra, and a faceface with one MgO_6 octahedra. The corner-sharing octahedral tilt angles range from 44-64°. There are a spread of Mg-O bond distances ranging from 2.00-2.22 Å. In the third Mg^{2+} site, Mg^{2+} is bonded to six O^{2-} atoms to form MgO_6 octahedra that share corners with two equivalent MgO_6 octahedra, corners with seven SbO_6 octahedra, edges with three MgO_6 octahedra, and a faceface with one MgO_6 octahedra. The corner-sharing octahedral tilt angles range from 43-64°. There are a spread of Mg-O bond distances ranging from 2.03-2.18 Å. In the fourth Mg^{2+} site, Mg^{2+} is bonded to six O^{2-} atoms to form distorted MgO_6 octahedra that share corners with four equivalent MgO_6 octahedra, corners with five SbO_6 octahedra, edges with two equivalent MgO_6 octahedra, and a faceface with one SbO_6 octahedra. The corner-sharing octahedral tilt angles range from 44-63°. There are a spread of Mg-O bond distances ranging from 2.02-2.19 Å. There are two inequivalent Sb^{5+} sites. In the first Sb^{5+} site, Sb^{5+} is bonded to six O^{2-} atoms to form SbO_6 octahedra that share corners with four MgO_6 octahedra, an edgeedge with one MgO_6 octahedra, and edges with two equivalent SbO_6 octahedra. The corner-sharing octahedral tilt angles range from 46-63°. There are a spread of Sb-O bond distances ranging from 1.90-2.10 Å. In the second Sb^{5+} site, Sb^{5+} is bonded to six O^{2-} atoms to form SbO_6 octahedra that share corners with eight MgO_6 octahedra, an edgeedge with one SbO_6 octahedra, edges with two equivalent MgO_6 octahedra, and a faceface with one MgO_6 octahedra. The corner-sharing octahedral tilt angles range from 43-60°. There are a spread of Sb-O bond distances ranging from 1.95-2.12 Å. There are nine inequivalent O^{2-} sites. In the first O^{2-} site, O^{2-} is bonded to three Mg^{2+} and one Sb^{5+} atom to form a mixture of distorted corner and edge-sharing OMg_3Sb trigonal pyramids. In the second O^{2-} site, O^{2-} is bonded in a distorted see-saw-like geometry to three Mg^{2+} and one Sb^{5+} atom. In the third O^{2-} site, O^{2-} is bonded to three Mg^{2+} and one Sb^{5+} atom to form distorted OMg_3Sb trigonal pyramids that share corners with six OMg_3Sb trigonal pyramids and edges with two OMg_2Sb_2 trigonal pyramids. In the fourth O^{2-} site, O^{2-} is bonded in a 4-coordinate geometry to two equivalent Mg^{2+} and two equivalent Sb^{5+} atoms. In the fifth O^{2-} site, O^{2-} is bonded to three Mg^{2+} and one Sb^{5+} atom to form distorted OMg_3Sb trigonal pyramids that share corners with six OMg_3Sb trigonal pyramids and edges with two OMg_2Sb_2 trigonal pyramids. In the sixth O^{2-} site, O^{2-} is bonded in a distorted see-saw-like geometry to three Mg^{2+} and one Sb^{5+} atom. In the seventh O^{2-} site, O^{2-} is bonded to two Mg^{2+} and two equivalent Sb^{5+} atoms to form distorted OMg_2Sb_2 trigonal pyramids that share corners with five OMg_3Sb trigonal pyramids and edges with two OMg_2Sb_2 trigonal pyramids. In the eighth O^{2-} site, O^{2-} is bonded to two Mg^{2+} and two equivalent Sb^{5+} atoms to form a mixture of distorted corner and edge-sharing OMg_2Sb_2 trigonal pyramids. In the ninth O^{2-} site, O^{2-} is bonded in a distorted see-saw-like geometry to three Mg^{2+} and one Sb^{5+} atom. This oxidized compound has 9 atoms, a density of 3.00 g cm^{-3}, and an oxidation state of Mg^{2+}, O-.

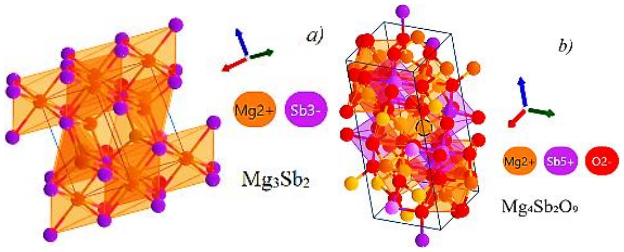

Fig. 4 – Critical Mg_3Sb_2 structure and term $Mg_4Sb_2O_9$. The crystal structure of the compounds is based on programs

Let's take a look at the other results shown in Fig. 3. Table 2 is given for the results shown in Fig. 3b. According to the results of calculations, the structure consists of 3 atoms of Mg, 2 Sb and O and C. And here we do not take into account oxygen and carbon atoms, since they belong to ceramic bases. Thus, according to the research method [9], using the results of calculations, it is possible to determine the particle structure formula using a chemical reaction calculator. We carry out the reaction using a chemical collider.

$$3Mg + 2Sb = Mg_3Sb_2$$

Thus, the structure consists of a compound related to the Mg_3Sb_2 and ceramic base material. It can be assumed that the crystal structure of Mg_3Sb_2 compound corresponds to the results of Fig. 5a.

Table 2

Element	(Weight %)	Atomic mass, g	Core of particles	Oxide layer
Mg	16.96	24.305	3	
Sb	62.00	121.76	2	
O	12.61	15.999		7
C	8.45	2.011		17
Fractional structure formula			Mg_3Sb_2	Cermic bottom

For the results shown in Fig. 3c in Table 3, the extraction results and the formula of the partial structure or defined compound using it are given. According to the results of calculations, the structure consists of 4 atoms Mg, 6 Sb and O and C. Since part of the oxygen and carbon atoms belong to ceramic bases, we do not take them into account. Thus, according to the research method [9], using the results of calculations, it is possible to determine the particle structure formula using a chemical reaction calculator. We carry out the reaction using a chemical collider.

$$4Mg + 6Sb + 10O = Mg_3Sb_2 + Mg(Sb_2O_5)_2$$

Thus, the structure consists of a compound related to Mg_3Sb_2, $Mg(Sb_2O_5)_2$ and a ceramic base material. The crystal structure of Mg_3Sb_2 compound corresponds to the results of Fig. 3a. The crystal lattice structure of the compound $Mg(Sb_2O_5)_2$ can be described as follows (Fig. 6).

Table 3

Element	(Weight %)	Atomic mass, g	Core of particles	Oxide layer
Mg	4.96	24.305	3	1
Sb	29.32	121.76	2	4
O	35.21	15.999		10
C	29.96	2.011		
Zn	0.54	65.38		
Fractional structure formula			Mg_3Sb_2	$Mg(Sb_2O_5)_2$

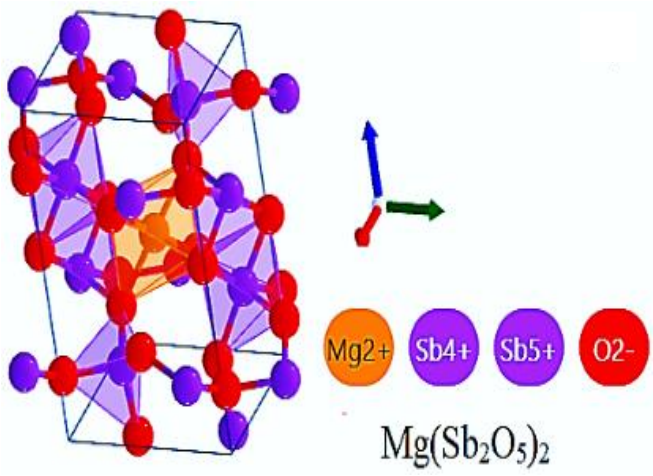

Fig. 6 – Critical structure of $Mg(Sb_2O_5)_2$ compound

Fig. 6 shows the cryptographic structure of the $Mg(Sb_2O_5)_2$ compound. $Mg(Sb_2O_5)_2$ crystallizes in the triclinic P1 space group. Mg is bonded to six O atoms to form MgO_6 octahedra, that share corners with four equivalent SbO_4 tetrahedra and edges with four equivalent SbO_6 octahedra. There are a spread of Mg-O bond distances ranging from 2.05-2.14 Å. Sb is bonded to six O atoms to form SbO_6 octahedra that share corners with four equivalent SbO4 tetrahedra, an edgeedge with one SbO6 octahedra, and edges with two equivalent MgO6 octahedra. There are a spread of Sb-O bond distances ranging from 1.99-2.07 Å. Sb is bonded to four O atoms to form SbO_4 tetrahedra that share corners with two equivalent MgO_6 octahedra and corners with four equivalent SbO_6 octahedra. The corner-sharing octahedral tilt angles range from 42-61°. There are a spread of Sb-O bond distances ranging from 1.95-2.05 Å. There are five inequivalent O sites. In the first O site, O is bonded in a bent 150° degrees geometry to one Sb (in SbO_6 octahedra) and one Sb (in SbO_4 tetrahedra) atom. In the second O site, O is bonded in a distorted trigonal planar geometry to one Mg (in MgO_6 octahedra), one Sb (in SbO_6 octahedra) and one Sb (in SbO_4 tetrahedra) atom. In the third O site, O is bonded in a distorted bent 150° degrees geometry to one Sb (in SbO_6 octahedra) and one Sb (in SbO_4 tetrahedra) atom. In the fourth O site, O is bonded in a distorted trigonal non-coplanar geometry to one Mg (in MgO_6 octahedra) and two equivalent Sb (in SbO_6 octahedra) atoms. In the fifth O site, O is bonded in a distorted trigonal planar geometry to one Mg (in MgO_6 octahedra), one Sb (in SbO_6 octahedra) and one Sb (in SbO_4 tetrahedra) atom. This oxidized compound has 15 atoms, a density of 5.07 g cm^{-3}, and oxidation states Sb^{4+}, Mg^{2+}, Sb^{5+}, O^{2-}.

Table 4 shows the harvest results for the results shown in the 3d figure. According to the results of calculations, the structure consists of 4 Mg atoms, 2 Sb and O and C. Since part of the oxygen and carbon atoms belong to ceramic bases, we do not take them into account. We carry out the reaction using a chemical collider.

$$4Mg + Sb + 2O = Mg_3Sb_2 + MgO_2$$

Table 4

Element	(Weight %)	Atomic mass, g	Core of particles	Oxide layer
Mg	20.6	24.305	3	1
Sb	46.26	121.76	2	
O	20.88	15.999		2
C	12.26	2.011		
Fractional structure formula			Mg_3Sb_2	MgO_2

Let's examine the crystal structure of MgO_2 (Fig. 7). MgO_2 has a Marcasite-like structure and crystallizes in the trigonal $R\bar{3}m$ space group. In this structure: Mg^{2+} is bonded to six equivalent O^{1-} atoms to form edge-sharing MgO_6 octahedra. All Mg–O bond lengths are 2.11 Å. O^{1-} is bonded in a 4-coordinate geometry to three equivalent Mg^{2+} and one O^{1-} atom. The O–O bond length is 1.49 Å. This oxidized com-pound has 9 atoms, a density of 3.00 g cm^{-3}, and the oxidation states of Mg^{2+} and O^{-}.

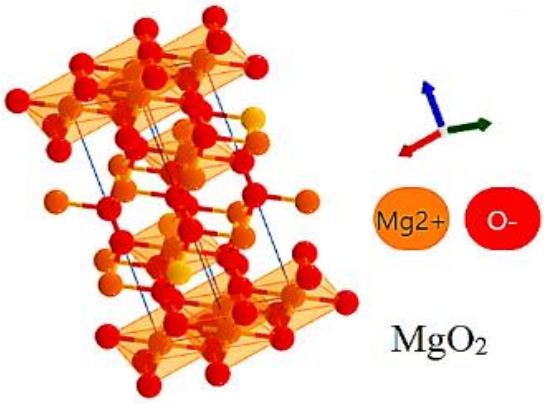

Fig. 7 – Critical structure of the MgO_2 connection. The crystal structure of the compounds is based on programs

For the results shown in Fig. 3e in Table 5, the extraction results and the formula of the partial structure or defined compound using it are given. The results of the calculation showed that the structure formula, as in Table 5, consists of Mg_3Sb_2, MgO_2, and the crystal lattice structure of the Mg_3Sb_2 compound corresponds to the results of Fig. 3a, and the crystal lattice structure of the MgO_2 compound corresponds to the results of Fig. 7.

Table 5

Element	(Weight %)	Atomic mass, g	Core of particles	Oxide layer
Mg	25.39	24.305	3	1
Sb	59.79	121.76	2	
O	14.85	15.999		2
Fractional structure formula			Mg_3Sb_2	MgO_2

For the results shown in Fig. 3f in Table 6, the extraction results and the formula of the partial structure or a specific compound using it are given. According to the results of calculations, the structure consists of 3 Mg atoms, 3 Sb and 3 O atoms. We carry out the reaction using a chemical collider.

$$3Mg + 3Sb + 3O = Mg_3Sb_2 + SbO_3$$

The structure consists of Mg_3Sb_2 and SbO_3 compounds. Again, the crystal structure of Mg_3Sb_2 compound corresponds to the results of Fig. 3a. The crystal lattice structure of SbO_3 compound can be described as follows (Fig. 8).

Table 6

Element	(Weight %)	Atomic mass, g	Core of particles	Oxide layer
Mg	14.12	24.305	3	
Sb	76.57	121.76	2	1
O	9.32	15.999		3
Fractional structure formula			Mg_3Sb_2	SbO_3

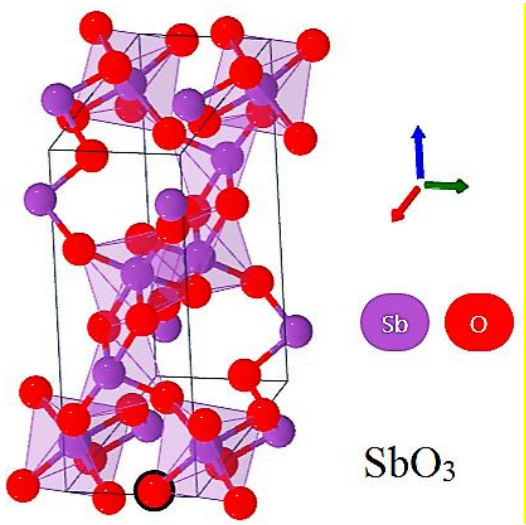

Fig. 8 – Critical structure of the SbO_3 connection

SbO_3 crystallizes in the monoclinic $P2_1/c$ space group. Sb is bonded to six O atoms to form a mixture of corner and edge-sharing SbO_6 octahedra. The corner-sharing octahedral tilt angles are 47°. There are a spread of Sb-O bond distances ranging from 1.96-2.05 Å. There are three inequivalent O sites. In the first O site, O is bonded in a water-like geometry to two equivalent Sb atoms. In the second O site, O is bonded in a bent 120 degrees' geometry to two equivalent Sb atoms. In the third O site, O is bonded in a water-like geometry to two equivalent Sb atoms. This oxidized compound has 34 atoms, a density of 4.02 g cm^{-3}, and an unknown oxidation state.

4. CONCLUSIONS

Thus, a method was developed for the manufacture of

granular Mg_3Sb_2 nano-semiconductor materials in the form of stereotypes by heating and attaching nanoparticles by means of resistance. It is made of 70% ethyl alcohol Mg_3Sb_2 is based on the heat resistance of a mixture of particles, for example, on a ceramic substrate, heating and fixing the particles with resistance means. The heating temperature of the Mg_3Sb_2 particles was 300÷700 K. Obtained by heating and fixing powdered particles using resistance, the granular Mg_3Sb_2 in the form of sterein forms a polycrystalline structure consisting of a compound of granular particles and interparticle boundaries. Granulated particles consist of Mg_3Sb_2 compounds, their surface areas consist of oxidized nanocomposite coatings, such as $Mg_4Sb_2O_9$, $Mg(Sb_2O_5)_2$, MgO_2, SbO_3.

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Мікроструктура та морфологічні властивості гранульованого термоелектричного матеріалу Mg_3Sb_2

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У цій статті представлено результати дослідження мікроструктури та морфологічних властивостей стрижнеподібного гранульованого нанонапівпровідникового термоелектричного матеріалу Mg_3Sb_2, отриманого методом відпалу з використанням електричного опору. Суть методу полягає в нанесенні суміші частинок Mg_3Sb_2, підготовлених у 70 % етиловому спирті, на трубчасту термостійку підкладку (наприклад, керамічну), з подальшим нагріванням через електричний опір. Отриманий матеріал має полікристалічну структуру, що складається з гранульованого скупчення частинок Mg_3Sb_2 і міжчастинкових межових областей. Ядро частинок складається з чистого Mg_3Sb_2, тоді як поверхневі області вкриті окисненими нанокомпозитними плівками, такими як: $Mg_4Sb_2O_9$, $Mg(Sb_2O_5)_2$, MgO_2, SbO_3. Згідно з проведеним аналізом, атомарний кисень розподіляється від ядра до поверхні частинок, формуючи нанокомпозитне окисне покриття. Це свідчить про активне поверхневе окислення внаслідок термічного впливу. Таким чином, представлений метод резистивного відпалу дозволяє отримати гранульовану полікристалічну термоелектричну структуру із сформованими окисними прошарками, що може впливати на електричні та теплові властивості матеріалу.

Ключові слова: Гранульований нанонапівпровідник Mg_3Sb_2, Термоелектричний матеріал, Мікроструктура, Морфологія, $Mg_4Sb_2O_9$, $Mg(Sb_2O_5)_2$, MgO_2, SbO_3, Окиснене нанокомпозитне покриття, Термостійка керамічна підкладка, Термічне спікання, Міжчастинкові межі, Полікристалічна структура.