VISMUT VA SURMA ASOSIDAGI TERMOELEKTR QATTIQ ERITMALARINING XUSUSIYATLARINI O'RGANISH.

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Annotatsiya: Maqolada past harorat oralig'i uchun eng yaxshi termoelektrik materiallar hisoblangan vismut va surma asosidagi qattiq eritmalarning xususiyatlari muhokama qilinadi. Termoelektrik materiallarda konversiya samaradorligini oshirish, birinchi navbatda, yarimo'tkazgich moddalarining qattiq eritmalarini hosil qilish orqali erishish mumkin bo'lgan samaradorlik koeffitsientining (Z) ortishi bilan bog'liq. Ushbu ishda vismut-tellurid asosidagi nikel qo‘shilgan qotishmadagi zaryad tashuvchilarning termoelektr quvvati, elektr o‘tkazuvchanligi va tarqalish mexanizmlari o‘rganildi. Natijalar shuni ko'rsatadiki, termoelektr quvvati bo'lingan valentlik zonasi mavjudligi sababli murakkab xatti-harakatlarni namoyon qiladi va Holl koeffitsienti materialning murakkab tarmoqli tuzilishini tasdiqlaydi. Shuningdek, termoelektr quvvati, elektr o'tkazuvchanligi va qotishmadagi zaryad tashuvchilarning harakatchanligi bilan bog'liq tenglamalar va hisoblar keltirilgan.

Kalit so'zlar: monokristal, issiqlik o'tkazuvchanlik, kengayish, harakatchanlik, termoelektr quvvati, degeneratsiya, effektiv massa, holatlarning zichligi.

ИССЛЕДОВАНИЕ СВОЙСТВ ТВЕРДЫХ РАСТВОРОВ ВИСМУТА И СУРЬМЫ ДЛЯ ТЕРМОЭЛЕКТРИЧЕСКИХ ПРИМЕНЕНИЙ.

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Аннотация: В статье рассматриваются свойства твердых растворов на основе висмута и сурьмы, которые считаются лучшими термоэлектрическими материалами для низкотемпературного диапазона. Повышение эффективности преобразования в термоэлектрических материалах в первую очередь связано с увеличением коэффициента полезного действия (z), что может быть достигнуто за счет образования твердых растворов полупроводниковых веществ. В статье исследованы термоэдс, электропроводность и механизмы рассеяния носителей заряда в сплаве на основе теллурида висмута с добавкой никеля. Результаты показывают, что термоЭДС имеет сложное поведение из-за наличия расщепленной валентной зоны, а коэффициент Холла подтверждает сложную зонную структуру материала. В статье также представлены уравнения и расчеты, связанные с термоэдс, электропроводностью и подвижностью носителей заряда в сплаве.

Ключевые слова: монокристалл, теплопроводность, расширение, подвижность, термоэдс, вырожденность, эффективная масса, плотность состояний.

EXPLORING THE PROPERTIES OF BISMUTH AND ANTIMONY SOLID SOLUTIONS FOR THERMOELECTRIC APPLICATIONS.

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Abstract: The article discusses the properties of solid solutions based on bismuth and antimony, which are considered the best thermoelectric materials for the low-temperature range. The increase in conversion efficiency in thermoelectric materials is primarily associated with an increase in the efficiency factor (z), which can be achieved by forming solid solutions of semiconductor substances. The article investigates the thermoelectric power, electrical conductivity, and scattering mechanisms of charge carriers in a bismuth telluride-based alloy with the addition of nickel. The results show that the thermoelectric power exhibits a complex behavior due to the presence of a split valence band, and the Hall coefficient confirms the complex band structure of the material. The article also presents equations and calculations related to the thermoelectric power, electrical conductivity, and mobility of charge carriers in the alloy.

Key words: single crystal, thermal conductivity, expansion, mobility, thermoelectric power, degenerate, effective mass, density of states.

Introduction:

This article aims to investigate the properties of solid solutions based on bismuth and antimony, with a particular focus on a Bi_2Te_3 + 0.04 wt% Ni alloy. The authors conducted an extensive study of the thermoelectric power, electrical conductivity, and magnetic field-dependent changes in the temperature range of 77 to 300 Kelvin [1-2]. Additionally, the Hall mobility of charge carriers and the Hall coefficient were calculated to further understand the material's characteristics.

The analysis revealed intriguing temperature-dependent behaviors of the thermoelectric power, suggesting the presence of a complex valence band in the Bi_2Te_3 + 0.04 wt% Ni alloy [3]. At low temperatures ($T < 180$ K), the electron gas's degenerate state correlated with a linear change in the thermopower, while higher temperatures exhibited a faster increase followed by saturation and subsequent decrease. These observations indicated the involvement of different subbands and highlighted the influence of carrier mobility and density of states near the Fermi level. Furthermore, the authors examined the Hall coefficient's temperature dependence, corroborating the presence of charge carriers of two sign types in the alloy's complex band structure.

The best thermoelectric materials for the low-temperature temperature range (200÷600 K) are solid solutions based on bismuth and antimony. It is therefore of tremendous scientific and practical relevance to conduct a thorough research of their properties. The improvement in thermoelectric material efficiency (Z) is principally responsible for the rise in conversion efficiency. The production of solid solutions of basic semiconductor substances and their compounds is one of the most common techniques for enhancing Z. In this instance, the extension of the forbidden zone, a change in the effective mass of current carriers, and a reduction in the thermal conductivity of the lattice all have an active impact on the scattering mechanism and the energy spectrum of electrons and phonons. In this way, on single crystals and coarse-grained polycrystals of solid solutions based on antimony and bismuth tellurides - Sb_2Te_3 - Bi_2Te_3 of p-type conductivity, Z values equal $(3 \div 3,4)\times 10^{-3} K^{-1}$ [4-7].

The decrease in resistivity is associated with a reduction in the polarity of the covalent bond, which increases the mobility of charge carriers. Conversely, the increase in the Seebeck coefficient is linked to an increase in the density of states near the Fermi level. Moreover, an increase in disordering also contributes to a decrease in the thermal conductivity of a material.

The mobility of charge carriers depends on the scattering of carriers due to temperature fluctuations of the periodic potential in the crystal lattice. Ionic crystals, in which atoms with positive and negative charges alternate, exhibit the most pronounced change in potential. Covalent bonding in a crystal enhances mobility because the interatomic bond is strongly expressed, leading to less pronounced temperature fluctuations of the crystal lattice potential.

Materials and Methods:

Thermal conductivity plays a crucial role in determining thermoelectric efficiency as it appears in the denominator of the efficiency expression. Therefore, it is essential to minimize the thermal conductivity without compromising electrical conductivity. The value of thermal conductivity depends directly on the frequency of thermal vibrations of the lattice. In the case of bismuth telluride, charge carriers scatter on acoustic phonons [8], which aligns with experimental observations and can be described by formula [9].

$$\alpha = \frac{2\pi^{\frac{2}{3}} k_0^2 m^{¿} T}{3^{\frac{5}{3}} e \hbar^2 p^{\frac{2}{3}}} \left(r + \frac{3}{2}\right) \quad (1)$$

where: k_0 – is the Boltzmann constant, m* - is the effective mass of the density of states, e – is the electron charge, ħ – is the Planck constant, p – is the concentration of charge carriers, r – is the scattering parameter and 3/2 for the acoustic scattering mechanism.

The total thermopower in this situation is defined as:

$$\alpha_{total} = \frac{\alpha_1 \sigma_1 + \alpha_2 \sigma_2}{\alpha_1 + \sigma_2} \quad (2)$$

Where thermopower

$$\alpha_1 = \frac{2\pi^{\frac{2}{3}} K_0^2 m^{¿} T}{3^{\frac{5}{3}} e \hbar^2 p^{\frac{2}{3}}} \left(r + \frac{3}{2}\right), \quad \alpha_2 = \frac{K_0}{e}\left[r + \frac{5}{2} + \ln \frac{2\left(2\pi m^{¿} K_0 T\right)^{\frac{3}{2}}}{\hbar^3 p}\right]$$

The electrical conductivity is a measure of a material's ability to conduct electricity. It quantifies the ease with which charge carriers can move through the material. The electrical conductivity can be calculated using the formula:

$$\sigma = \frac{I}{A \cdot L} \quad (3)$$

where I am the electrical current passing through the sample, A is the cross-sectional area, and L is the length of the sample.

The total thermoemf in this situation is defined as:

$$\alpha_{total} = \frac{\sum \alpha_p \sigma_p - \alpha_n \sigma_n}{\sum \left(\sigma_p + \sigma_n\right)} \quad (4)$$

where α_n, σ_n- respectively, thermoemf and electrical conductivity of electrons in the conduction band.

$$R = \frac{A}{peC_0} \frac{p_1 \mu_1^2 + p_2 \mu_2^2}{p_1 \mu_1 + p_2 \mu_2} \quad (5)$$

where A is the coefficient that determines the mechanism of hole scattering, p_1, μ_1, p_2, μ_2, respectively, the concentration and mobility of carriers in the sub bands.

We may suppose that the overall concentration of holes in the sub bands is $p = p_1 + p_2$ at low temperatures (T 100 K), and then

$$R = R_0 \frac{(1 + p_2/p_1)\left[1 + (p_2/p_1) b^2\right]}{\left[1 + (p_2/p_1) b\right]^2} \quad (6)$$

$R_0 = \frac{A}{p_2 eCo}, b = \frac{\mu_c}{\mu}$ The minor dependency of "b" on temperature may be accepted with a high enough degree of certainty.

Due to an increase in holes in the second subband and a reduction in the first, $R \approx R_0 (p_1/p_2)$ leads to an increase in R_H with rising temperature.

When the electrical conductivity σ_1-σ_2 values in the sub-zones are identical, the Hall coefficient reaches its maximum values, with

$$R_{max} = R_0 \frac{(1 + b^I)^2}{4 b^I} \quad (7)$$

The formula $R_H = \frac{A}{pec}$·states that after reaching its maximum value, the R_H value depends, like the other kinetic coefficients, mostly on the carriers of the second subzone. As their concentrations rise, the R_H value decreases. It should be noted that for semiconductor materials with complicated band structures, it is feasible to derive some band characteristics, such as $\frac{\mu_л}{\mu_m}, \frac{p_л}{p_m}, \Delta\varepsilon$, at temperatures where the maximum R_H is obtained by combining the values R_H and α_{total}.

The theory for a two-band model of the valence band's structure offers the following formula for the mobility of charge carriers [10]:

$$\mu = \frac{\mu_1 p_1 + \mu_2 p_2}{p} \quad (8)$$

where p_1, p_2 is the concentration and μ_1, μ_2 is the mobility of holes in the respective sub-zones.

As is well known, the mobility of charge carriers in the general case

$$\mu = \frac{\sqrt{\pi}}{\Gamma(r+3/2)} \frac{F_2+1/2(\mu^{¿})}{F_2+1/2(\mu^{¿})} \mu_0. \quad (9)$$

$$\mu_0 = \frac{2e}{3m^{¿}} \tau_0 (k_0 T)^2 \left(r+\frac{3}{2}\right) \frac{\Gamma(r+3/2)}{\Gamma(3/2)} \quad (10)$$

In the case when $\Gamma_{(s)} = \int_0^{\infty} x^{s-1} e^{-x} dx$ gammi function

Since it is known from (10), the mobility of current carriers depends on the temperature, the scattering mechanism, the effective mass of the density of states, and the degree of degeneracy of the electron gas, making it challenging to calculate it from measurements of the Hall effect, electrical conductivity, and thermopower.

The mobility, intensity (induction) of the magnetic field, and the degree of charge carrier degeneracy all affect how resistance changes in a magnetic field;

$$\rho_{(H)} = \rho_{(0)} \left[1 + \left(\frac{\mu H}{c} \right)^2 A \right] \quad (11)$$

$$A = \frac{(F_{3/2} \mu^{¿})^2}{F_{2+1}^4} \left[f_{r+1}(\mu^{¿}) f_{3r+1}(\mu^{¿}) - f^2_{2^r+\frac{1}{2}}(\mu^{¿}) \right] \quad (12)$$

$$f_{(H)} = f_{(0)}(0)[i+z+i].$$

in the case of the second sub band, for no degenerate semiconductors.

$$A = b_2 - a_2^r \quad (13)$$

$$a_r = \frac{3\sqrt{\pi}}{4} - \frac{F_{((2_{(r+3/2)}))}}{F^2(r+2)} \quad (14)$$

$$b = \frac{9}{16} \pi \frac{F_{(3^r+1)}}{F^3_{(r+2)}} \quad (15)$$

When the electronic spectrum of carriers degenerates either strongly or weakly (for the first sub band and in the region of both sub bands' activity),

Measurement of resistance in a magnetic field

$$\frac{\Delta\rho}{\rho} = \frac{\mu H^2}{c} \frac{\pi^2}{12} \frac{1}{\mu^{¿2}} \quad (16)$$

or the first subzone's area of influence,

$$\frac{\Delta\rho}{\rho}=\frac{\mu H^2}{c}B$$

for the predominant action of the second subzone.

Thus, it is clear from the formulas for $\frac{\Delta\rho}{\rho}$ that its variation is governed by the relationship between charge carriers' mobility and temperature. The development of $\frac{\Delta\rho}{\rho}$ - in the temperature range of 80-150 K is produced by two factors when the two-zone model of the valence band's structure is taken into consideration. First, there is an increase in mobility in the temperature range T150, followed by a drop in the first zone's carrier concentration and a corresponding drop in overall mobility.

The mobility of charge carriers in the second sub band is reduced in the temperature range T> 150 K due to an increase in the effective mass of the density of states and a reduction in mobility as a result of scattering by acoustic lattice vibrations. These changes result in a drop in the values of $\frac{\Delta\rho}{\rho}$.

Discussion of results

Up to values of T = 250–260 K, where saturation occurs and the thermopower then falls, a quicker increase in the thermopower values is seen than what is predicted by formula (1). We explain this thermopower behavior by assuming that the alloy under investigation has a complicated valence band that is typical of Bi_2Te_3. Bi_2Te_3 valence band is divided into two subbands with an energy gap of 0.02 eV between them [11]. The first sub band, the sub band of "light" holes, participates in conduction processes at low temperatures T 200 K. The state of charge carriers is degenerate at low temperatures because of high values of the concentration p, but as the temperature rises, some of the "light" holes move into the second sub band, the sub band of heavy holes, which has a higher effective mass of the

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The Bi_2Te_3 alloy with % Ni was prepared using a conventional solid-state reaction method. The raw materials, bismuth (Bi), tellurium (Te), and nickel (Ni), were mixed in appropriate proportions and subsequently subjected to a high-temperature sintering process. The resulting alloy was then characterized for its thermoelectric and galvanomagnetic properties.

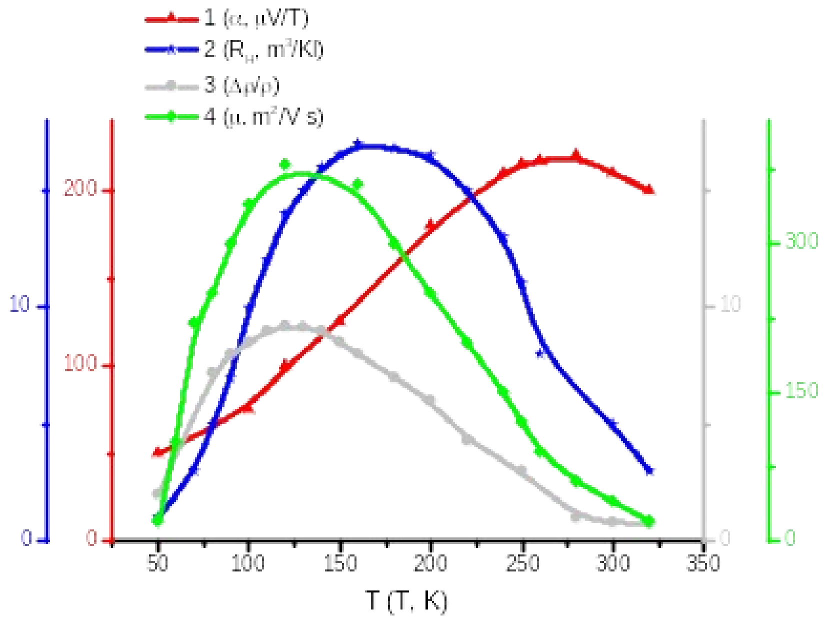

Fig 1. temperature dependence of the Seebeck and Hall coefficients for the Bi_2Te_3 + 0.04 wt% Ni alloy, along with the variations in charge carrier mobility and magnetic field resistance.

To identify the scattering mechanisms of charge carriers and establish a qualitative model of the band structure for the Bi_2Te_3+0.04 wt% Ni alloy, we conducted an investigation of thermoelectric power and electrical conductivity in the temperature range of 77 ÷ 300 K. Additionally, we observed their changes in a constant magnetic field within the same temperature range. We also calculated the Hall mobility of charge carriers and the Hall coefficient. The first line in the first figure illustrates the temperature dependence of the Seebeck coefficient (α). The linear change observed at T<180 K corresponds to the degenerate state of the electron gas [12]:

Furthermore, the exponential drop in the value of the thermopower, as evidenced by the approach of the research temperature to the region of intrinsic conductivity, is indicative of the non-standard structure of the valence band in the material under study. A temperature-dependent Hall coefficient was observed, as seen in the second row in the first figure, which follows the assumption of spherical bands and a consistent mechanism of hole scattering, similar to complex band structure substances like Be_2Te_2, Sb_2Te_3, and others that possess charge carriers of two types of sign. [12]

The mobility data, obtained from the simultaneous determination by the Hall effect and electrical conductivity, support the data on the change in $\frac{\Delta\rho}{\rho}$ that are provided. In fact, it is the third line of Figure 1 where the values of $(\frac{\Delta\rho}{\rho})$ change over the temperature range below T>150 K. The sole explanation given in the literature for this behavior $(\frac{\Delta\rho}{\rho})$ for Bi_2Te_3 and solid solutions based on it is a change in the scattering parameter r.

As can be seen from the fourth line of the graph, the effect of changing the resistance in the magnetic field can be used as a way to directly calculate the mobility without determining the factors mentioned above.

CONCLUSIONS:

Studies on thermoemf, electrical conductivity, and Hall coefficient revealed that the solid solution alloy of Bi_2Te_3 + 0.04 wt% Ni maintained the energy spectrum of charge carriers inherent to the p-type of bismuth sequin telluride.

At temperatures above 200 K, "heavy" holes are primarily responsible for the value of the thermoelectric parameters, while the subband of light holes participates in conduction processes in the temperature range of 80 to 150 K due to their lower effective mass of the density of states and higher carrier mobility.

In this study, we investigated the thermoelectric and galvanomagnetic properties of an alloy based on Bi_2Te_3 doped with 0.04 wt% Ni. The Seebeck coefficient (Z), electrical conductivity (σ), and thermal conductivity (κ) were evaluated in the temperature range of 77 ÷ 300 K. The calculated values of these parameters provide crucial insights into the alloy's thermoelectric performance. Further analysis and optimization of the doping percentage and fabrication conditions could potentially

The "light" and "heavy" holes' dispersion process relies mostly on the lattice's acoustic vibrations. The information on the change in resistance in a magnetic field and the findings of research on the determination of the scattering mechanism of charge carriers from thermoelectric characteristics are in good accord.

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