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The Research of Temperature Dependences of Electrical Conductivity and Thermopower of WS_2 and WSe_2 with Partial Replacement of W on Nb

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The temperature dependences of electrical conductivity and thermopower of tungsten disulfide and tungsten diselenide have been investigated in this paper. These materials have the low value of electrical conductivity. The main idea of this paper is the increase of electrical conductivity for obtaining high thermoelectric efficiency. Niobium have served as an acceptor impurity. It has been revealed that the replacements of metal atoms have increased of electrical conductivity of $W_{0.85}Nb_{0.15}Se_2$ *by 4 order of magnitude. While the thermopower has decreased with increasing of impurity concentration. The thermoelectric power factor has been calculated for materials. The figure of merit ZT of the best composition* $W_{0.95}Nb_{0.05}Se_2$ *has been estimated and has had a value of 0.02 at room temperature.*

Keywords: thermopower, tungsten disulfide, tungsten diselenide, power factor.
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Introduction

The thermoelectricity is based on the Seebeck effect. The Seebeck effect is the direct conversion of temperature difference to electric voltage. The efficiency of thermoelectric material is characterized by figure of merit $ZT = S^2 \cdot \sigma \cdot T/k$, where S is thermopower, σ is electrical conductivity, k is thermal conductivity, T is temperature. Consequently, high-performance thermoelectric materials have to possess high value of electrical conductivity, thermopower and low value of thermal conductivity. In this paper tungsten disulfide (WS_2) and tungsten diselenide(WSe_2) have been investigated. These materials belong to the layered transition metal dichalcogenides. The properties of WS_2 and WSe_2 have been researched at high temperature [1–6]. It has been found that these materials has a high value of thermopower and low value of electrical conductivity and thermal conductivity. The aim of this paper is to research the influence of partial replacement tungsten atom on niobium atom in WS_2 and WSe_2. The Nb has one less electron in electron shell, as a consequence the uncompensated charge arises. As a result, p-type carriers are created. Nb acts as acceptor impurity. In this article temperature dependence of electrical conductivity and thermopower of $W_{1-x}Nb_xS_2$ and $W_{1-x}Nb_xSe_2$ (where $x = 0$, 0.05, 0.10 and 0.15) are presented.

1. Sample preparation and measurement procedure

A series of the samples $W_{1-x}Nb_xSe_2$ and $W_{1-x}Nb_xS_2$ ($x = 0$, 0.05, 0.10 и 0.15) have been synthesized by high-ampoule method. The powders obtained have been pressed. The sample researched have been cut to the size 2x2x8 mm^3. The temperature dependences of electrical conductivity have been researched by four-contact technique from 4.2 to 300 K in helium atmosphere. The temperature dependences of thermopower have been investigated by two-gradient technique from 80 to 300 K in helium atmosphere.

2. Temperature dependences of electrical conductivity

The measurement results of electrical conductivity and thermopower are presented in the Fig. 1. The WS_2 and WSe_2 have the exponential increase of electrical conductivity with increase of temperature. Such behavior is typical for semiconductors. The $W_{1-x}Nb_xSe_2$ samples have a linear decrease of electrical conductivity with increase of temperature. Such behavior is typical for metals. The $W_{1-x}Nb_xS_2$ have a linear increase of electrical conductivity with increase of temperature. It should be noted that addition of Nb atoms increases the electrical conductivity. Thus we have succeed in increasing of electrical conductivity by 4 orders of magnitude.

3. The temperature dependences of thermopower

The WS_2 and WSe_2 are the semiconductors. The electron transport of these materials occurs within the hopping conductivity with a variable hopping length according to the formula [7, 8]:

$$\sigma(T) = \sigma_0 exp[-(T_0/T)^{1/4}]. \tag{1}$$

With such conductivity model thermopower is described by the formula [9]:

$$S(T) = \frac{\xi_1}{e}[-(T_0/T)^{1/4}], \tag{2}$$

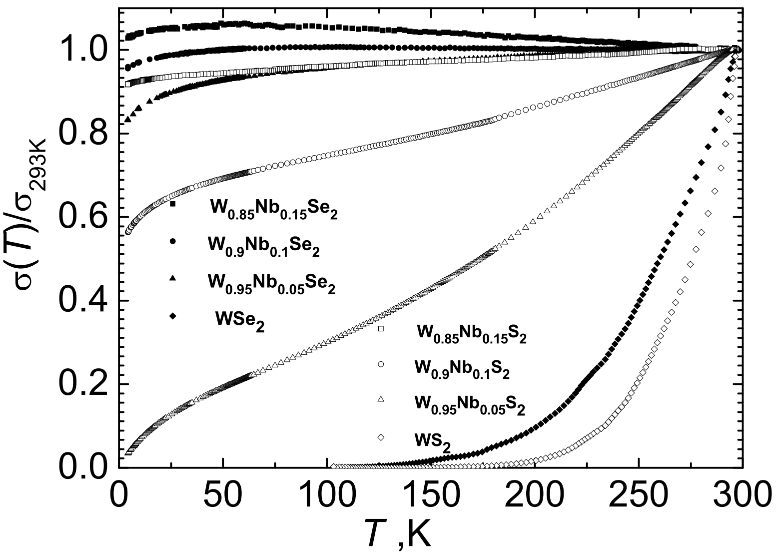

Fig. 1. The temperature dependences of electrical conductivity of $W_{1-x}Nb_xS_2$ and $W_{1-x}Nb_xSe_2$

where T_0 is parameter, $\xi_1 = 1/4$. The temperature dependence of electrical conductivity and thermopower of WS_2 and WSe_2 within the hopping model are presented in the Fig. 2. With decrease of thermopower the electrical conductivity increases.

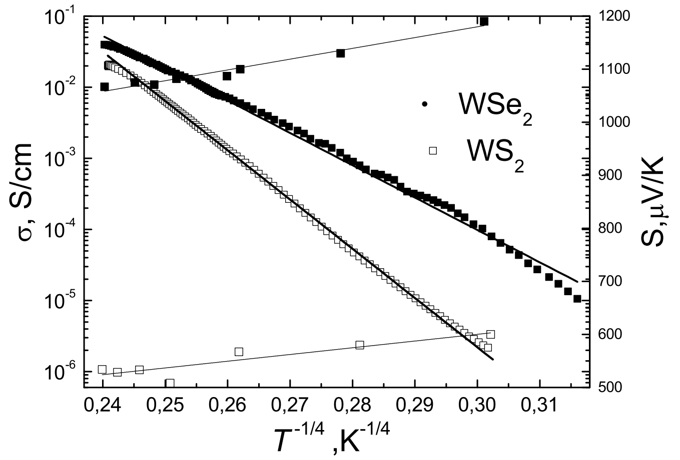

Fig. 2. The temperature dependences of electrical conductivity σ and thermopower S of WS_2 and WSe_2

The temperature dependences of thermopower of $W_{1-x}Nb_xSe_2$ and $W_{1-x}Nb_xS_2$ are presented on the Fig. 3.

In the $W_{1-x}Nb_xSe_2$ samples the linear increase of temperature dependence of thermopower are observed. With Nb addition material have a metallic behavior. It can be seen on temperature dependence of termopower. The metals are characterized by linear temperature dependence of

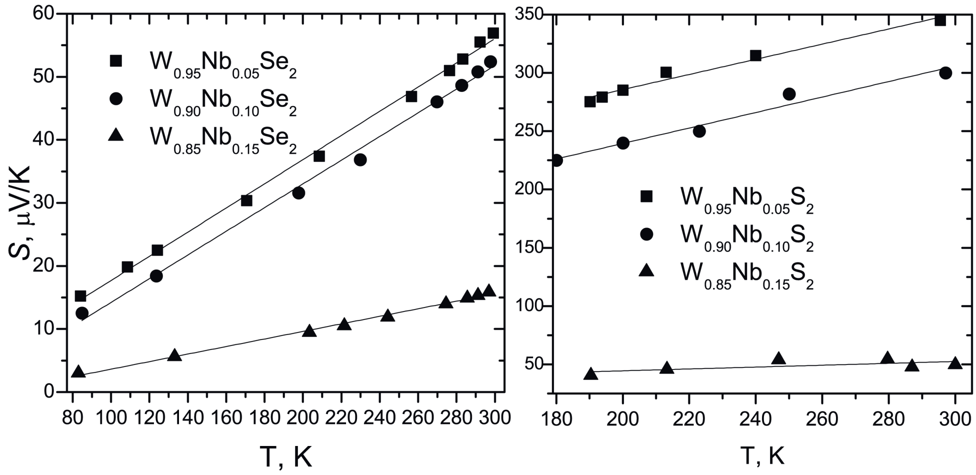

Fig. 3. The temperature dependences of thermopower of $W_{1-x}Nb_xSe_2$ and $W_{1-x}Nb_xS_2$ samples

the thermopower according to the formula[10]:

$$S(T) = -\frac{\pi^2}{6}\frac{k_B}{e}\frac{k_B T}{E_F}, \tag{3}$$

where k_B is Boltzmann constant, e is electron charge, E_F is Fermi energy.

With addition of Nb thermopower of the samples decreases. Respectively, the more concentration of Nb the less thermopower is observed. The$W_{1-x}Nb_xS_2$ samples had a loose structure. Perhaps this fact affected on the measurement. As a result, the temperature range is small in comparison with$W_{1-x}Nb_xSe_2$ samples. In these samples the increase of electrical conductivity is accompanied by increase of thermopower.

Such behavior of thermopower and electrical conductivity can be explained by the presence of n- and p-type carriers in the materials. The n- and p-type carriers make different contributions at various temperatures. Just as in the case of WSe_2, with addition of Nb the thermopower of $W_{1-x}Nb_xS_2$ samples decreases.

4. Power factor

In this paper the power factor has been calculated in order to estimate the replacement of W on Nb according to the formula $P = S^2 \cdot \sigma$. The results of power factor calculation are presented on the Fig. 4.

According the data obtained, the best value of power factor has $W_{0.95}Nb_{0.05}Se_2$ samples. The maximum value of power factor is 72 μW/m·K^2 at room temperature. The power factor cannot fully characterize the thermoelectric efficiency of materials. Because the thermal conductivity is not taken into account. Using literature data ($k = 1$ W/m·K) the figure of merit ZT of $W_{0.95}Nb_{0.05}Se_2$ has been estimated. This value is 0.02 at room temperature.

5. Conclusion

In this paper the temperature dependences of electrical conductivity and thermopower of $W_{1-x}Nb_xSe_2$ and $W_{1-x}Nb_xS_2$ samples have been investigated. It has been found that the

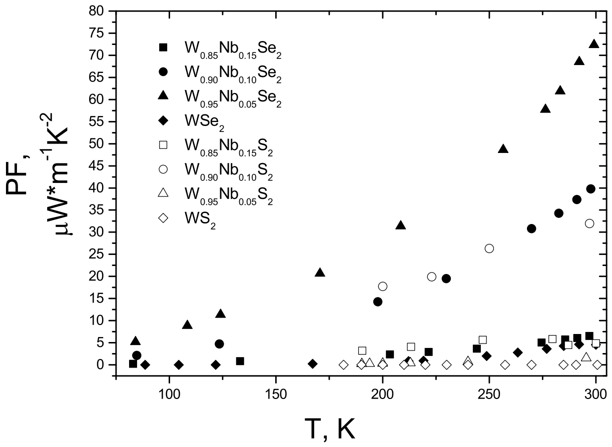

Fig. 4. The temperature dependences of power factor of $W_{1-x}Nb_xSe_2$ and $W_{1-x}Nb_xS_2$ samples

increase of Nb concentration has led to change from semiconductors to metallic behavior. The figure of merit *ZT* has been estimated for the $W_{0.95}Nb_{0.05}Se_2$ sample and has had a value 0.02 at room temperature. This value is to small in order to compete with modern thermoelectric materials. The modern thermoelectric materials have a value of figure of merit *ZT* about 1 and above. Probably, $W_{1-x}Nb_xSe_2$ and $W_{1-x}Nb_xS_2$ will have a higher thermoelectric efficiency at high temperature.

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Исследование температурных зависимостей электропроводности и термоЭДС WS_2 и WSe_2 с частичным замещением W на Nb

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В данной работе исследованы температурные зависимости электропроводности и термоЭДС дисульфида вольфрама и диселенида вольфрама. Так как данные материалы имеют низкую электропроводность, то основной целью данной работы было увеличение этого параметра, необходимого для высокой термоэлектрической эффективности. В качестве акцепторной примеси выступал ниобий. Было выявлено, что такое замещение увеличивает электропроводность материала на четыре порядка в образцах состава $W_{0.85}Nb_{0.15}Se_2$*. При этом термоЭДС уменьшается в зависимости от концентрации примеси. Измеренные параметры использовались для оценки термоэлектрического фактора мощности. Для наилучшего состава* $W_{0.95}Nb_{0.05}Se_2$ *был оценен фактор добротности, который составил 0.02 при комнатной температуре.*

Ключевые слова: термоЭДС, дисульфид вольфрама, диселенид вольфрама, фактор мощности.