East European Journal of Physics. **2.** 362-365 (2024)
DOI:10.26565/2312-4334-2024-2-44 ISSN 2312-4334

STUDY OF THE THERMOELECTRIC PROPERTIES OF CHROME SILICIDES

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Received April 2, 2024; revised May May 2, 2024; accepted May 11, 2024

The temperature dependences of the thermoelectromotive force of chromium mono and disilicides in the temperature range 200°C÷+600°C have been studied. For chromium disilicide, the dependence of the thermopower coefficient (α) on temperature (T) has three sections. Chromium monosilicide is characterized by a smooth increase in thermopower with increasing temperatures up to 200°C, and then its constancy. It was revealed that silicides rich in chromium atoms have lower thermopower values than silicides rich in silicon. The maximum thermo-EMF values of 110 μV/K and 190 μV/K were observed for chromium mono- and disilicides, respectively. It was revealed that for chromium silicides the dependence of the dimensionless parameter Q = Z·T on temperature is linear. The possibility of predicting the technology of synthesis of semiconductor material with optimal thermoelectric properties using the dependence of thermopower on conductivity and the parameter Q on temperature is shown.
Keywords: *Silicide; Thermal EMF; Hall Mobility; Doping; Saturation; Electrical Conductivity; Phase Diagram; Temperature Gradient*
PACS: 33.20.Ea, 33.20.Fb

INTRODUCTION

One of the pressing problems of microelectronics is the study of physical processes occurring in the surface and near-surface regions of silicon, diffusion-doped with impurities that create deep levels [1-6]. In the near-surface region of diffusion-doped silicon with chromium atoms, the formation of chromium silicides was revealed.

As is known [7-10], transition metal silicides are becoming the base material for new promising technological schemes of future generations due to their resistance to aggressive environments and high-temperature treatments. Therefore, a comprehensive study of the mechanism by which impurities enter the crystal volume and their interaction with both matrix atoms of the crystal and technological impurities is relevant.

From this point of view, the study of the formation of chromium silicides in the near-surface region of silicon during diffusion doping and the study of their thermal properties is of particular scientific importance in the context of the creation of new materials for micro- and nanoelectronics [11-15].

These materials will be used in thermal converters of spacecraft, in the petrochemical industry, in the energy sector and other industries.

In this regard, in this work, we studied the conductivity distribution profile of diffusion-doped silicon with chromium atoms and studied their temperature dependence of thermopower.

EXPERIMENTAL PART

To dope silicon with chromium, single-crystal p-type silicon ingots of the KDB-10 brand, grown by the Czochralski method, were used. Their initial parameters: resistivity 10 Ohm·cm, hole mobility 430 $cm^2/V·s$, hole concentration $1.5·10^{15}$ cm^{-3}. Chromium powder in an amount of 5 ÷ 6 mg was placed in the ampoule near the crystals. The ampoule with samples and diffusant was evacuated to a vacuum of ~10^{-3} mmHg. and soldered it.

The ampoules were placed in a horizontal diffusion oven and annealed at a temperature of 950-1020°C using laser irradiation for 30 minutes to 2 hours. Temperature fluctuations in the working furnace did not exceed ±5°C. After annealing, the samples were quenched by cooling at a rate of 100-150 K/s by dropping the ampoules into a vessel with water rotating at 33 rpm and kept to room temperature [16-19].

RESULTS AND DISCUSSION

The temperature dependences of the thermoelectromotive force of chromium silicides were studied in the temperature range -200°C ÷ +600°C, using a classical compensation scheme [20].

The dependence of the thermopower coefficient (α) on temperature for chromium monosilicides showed that α increases linearly with increasing temperature up to 200°C, and then remains constant (Fig. 1).

Cite as: A.T. Mamadalimov, M.Sh. Isaev, I.T. Bozarov, A.E. Rajabov, S.K. Vakhabova, East Eur. J. Phys. 2, 362 (2024), https://doi.org/10.26565/2312-4334-2024-2-44
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When studying this dependence for chromium disilicides, three sections were found in the curve: the first section is a section of linear growth of α as temperatures increase to 150°C, the second is a saturation section (temperature range +150°C ÷ +250°C) and the third is a section of a smooth decrease in α with increasing temperature (+250°C ÷ +600°C). The first section is explained by the effect of drag of charge carriers by phonons.

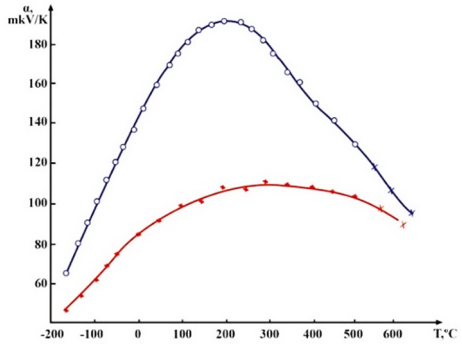

Figure 1. Temperature dependence of thermoEMF. 1 – $CrSi_2$; 2 – CrSi

The α(T) dependence for chromium monosilicides is explained by the fact that α increases up to +200°C due to the effect of hole entrainment by phonons, after 200°C α remains constant due to the disappearance of the effect of hole entrainment by phonons and due to an increase in the hole concentration and the acquisition of thermal kinetic energy.

The studied crystals are characterized by the fact that silicides rich in chromium have lower thermopower values than silicides rich in silicon. The maximum thermopower values of 1110 μV/K and 190 μV/K were observed for silicides CrSi and $CrSi_2$, respectively. Among the studied silicides, $CrSi_2$ has a linear dependence α(T) and can be used as a material for electronic thermometers and thermogenerators.

From the literature [21-24] it is known that the value of thermopower depends on the temperature difference and the type of material. When heating a metal silicide at high temperatures, the average energy of charge carriers and their concentration will be greater than in the region where the crystal temperature is lower. Consequently, the temperature gradient in such crystals leads to a gradient of the average energy of charge carriers and a gradient of their concentration, as a result of which thermopower arises.

The bell-shaped nature of the thermopower of chromium disilicide is explained by a change in the ratio of the concentration of charge carriers and their mobility in the temperature range of 150°C-250°C. In all other cases, a positive thermopower is observed, which indicates the formation of a negative space charge at the hot end of the crystal.

The measured temperature dependences of α, σ and χ are presented in Figs. 2 and 3.

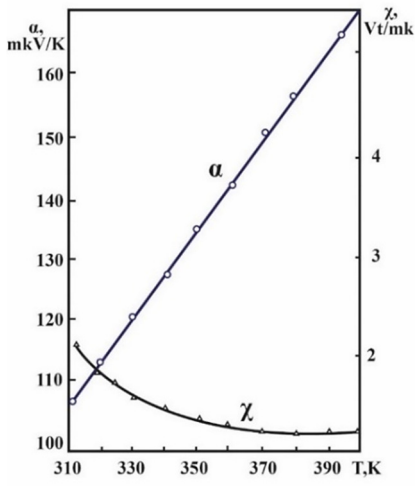

Figure 2. Temperature dependence of α and χ

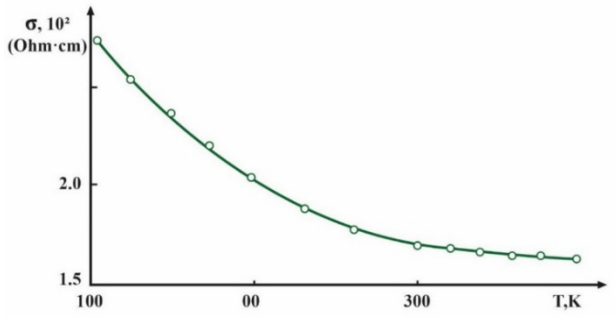

Figure 3. Temperature dependence of conductivity

To analyze the obtained thermoelectric properties of the samples, we will use generally accepted criteria.

The parameter Z, as well as the parameters α, ρ and χ, is a single-valued function of temperature, therefore it is practically more convenient to use the dimensionless parameter Q = Z·T, which is equal to 0.25, where T is the average temperature of the thermoelement branch. The relationship between electrical conductivity (σ) and thermoEMF (α) turned out to be a linearly decreasing function (Fig. 4).

The possibility of obtaining sufficiently high thermopower values in silicides was demonstrated by estimating the ratio of the radii of the silicon atom to the metal atom in the compound. The criterion for this ratio (k) is 0.59. It has been

established that at k <0.59 there is a conventional structure with embedded atoms. At k>0.59, a more complex structure appears that has semiconductor properties, the thermoelectric figure of merit of which can exceed by an order of magnitude the figure of merit of materials with a conventional structure. For chromium silicide k=0.94, which makes it possible to obtain high values of the thermoelectric figure of merit Z.

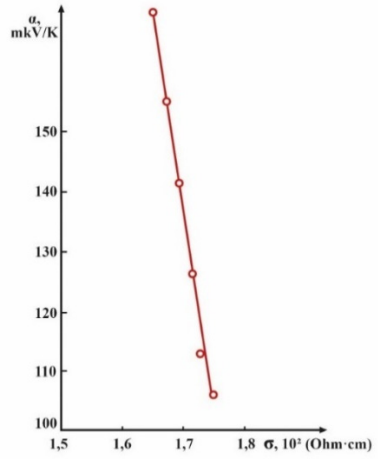

Figure 4. Dependence of thermopower on electrical conductivity

The convenience of the diffusion method for producing HCM of both electronic and hole type conductivity lies in the fact that it becomes possible to create the N and P branches of a thermogenerator from a material with identical electrical and thermoelectric properties.

Thus, the diffusion method for producing metal silicides opens up wide possibilities for varying parameters such as electrical conductivity, thermal conductivity and thermopower, and ultimately thermoelectric figure of merit, all of which contributes to the possibility of using chromium silicides as a promising material for thermoelectric converters in solar engineering.

CONCLUSION

1. Chromium mono- and disilicides were obtained by diffusion doping of silicon.
2. The electrical parameters of chromium disilicide were measured: charge carrier mobility 19 cm^2/V s, hole concentration $5.9 \cdot 10^{19}$ cm^{-3}, resistivity 1800 μOhm·cm, Hall constant $1.3 \cdot 10^{-2}$ cm^3/Kl.
3. Studies of the dependence α (T) for chromium disilicide revealed the formation of three sections: the first section is a section of linear growth of α as temperatures increase (-180℃ ÷ + 150℃), the second is a saturation section (-150℃ ÷ + 250℃) and the third is a section of smooth decrease α with increasing temperature. Chromium monosilicide is characterized by a smooth increase in thermopower with increasing temperature to 200℃, and then its constancy.
4. It was revealed that for chromium silicides the dependence of the dimensionless parameter Q = Z·T on temperature is linear. The possibility of predicting the technology of synthesis of semiconductor material with optimal thermoelectric properties using the dependence of thermopower on conductivity and the parameter Q on temperature is shown.

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ДОСЛІДЖЕННЯ ТЕРМОЕЛЕКТРИЧНИХ ВЛАСТИВОСТЕЙ СИЛІЦИДІВ ХРОМУ

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Досліджено температурні залежності термоелектрорушійної сили моно- та дисиліцидів хрому в інтервалі температур -200°C ÷ +600°C. Для дисиліциду хрому залежність коефіцієнта термоЕРС (α) від температури (T) має три ділянки. Для моносиліциду хрому характерне плавне зростання термоЕРС з підвищенням температури до 200°C, а потім її постійність. Виявлено, що силіциди, багаті атомами хрому, мають менші значення термоЕРС, ніж силіциди, багаті кремнієм. Максимальні значення термоЕРС 110 мкВ/К та 190 мкВ/К спостерігаються для моно- та дисиліцидів хрому відповідно. Виявлено, що для силіцидів хрому залежність безрозмірного параметра Q = Z·T від температури має лінійний характер. Показано можливість прогнозування технології синтезу напівпровідникового матеріалу з оптимальними термоелектричними властивостями на основі залежності термоЕРС від електропровідності та параметра Q від температури.

Ключові слова: *силіцид; термо-ЕРС; холлівська рухливість; легування; насичення; електропровідність; фазова діаграма; градієнт температури*