Conference materials
UDC 538.9
DOI: https://doi.org/10.18721/JPM.153.103

Properties of solid solution $(Cd_{0.69}Zn_{0.31})_3As_2$

V. S. Zakhvalinskii [1] ✉, A. V. Borisenko [1], T. B. Nikulicheva [1], A. V. Kochura [2], Aung Zaw Htet [2], E. A. Pilyuk [1]

[1] Belgorod National Research University, Belgorod, Russia;
[2] Southwest State University, Kursk, Russia
✉ v_zaxval@mail.ru

Abstract: The modified Bridgeman method was used to obtain single crystals of $(Cd_{0,69}Zn_{0.31})_3As_2$. It has been established that the studied sample crystallizes in space group P42/nmc with lattice parameters a = 8.78 Å, b = 12.42 Å. We have investigated the electrical conductivity in the temperature range from 10 to 300 K and in a magnetic field of 1 T, and determined the temperature dependences of the concentration and mobility of charge carriers. We have established that hopping conduction with a variable length of the Mott-type hop takes place in the temperature range from 10 to 33 K, and determined its micro parameters.

Keywords: single crystals, solid solution, hopping conductivity

Citation: Zakhvalinskii V. S., Borisenko A. V., Nikulicheva T. B., Kochura A. V., Htet Aung Zaw, Pilyuk E. A. Properties of solid solution $(Cd_{0.69}Zn_{0,31})_3As_2$. St. Petersburg State Polytechnical University Journal. Physics and Mathematics. 15 (3.1) (2022) 22–26. DOI: https://doi.org/10.18721/JPM. 153.103

Материалы конференции
УДК 538.9
DOI: https://doi.org/10.18721/JPM.153.103

Свойства твердого раствора $(Cd_{0,69}Zn_{0,31})_3As_2$

В. С. Захвалинский [1] ✉, А. В. Борисенко [1], Т. Б. Никуличева [1], А. В. Кочура [2], А. З. Хтет [2], Е. А. Пилюк [1]

[1] Белгородский государственный национальный исследовательский университет, г. Белгород, Россия;
[2] Юго-Западный государственный университет, г. Курск, Россия
✉ v_zaxval@mail.ru

Аннотация. Модифицированный метод Бриджмена был использован для получения монокристаллов $(Cd_{0,69}Zn_{0,31})_3As_2$. Установлено, что исследуемый образец кристаллизуется в пространственной группе P42/nmc с параметрами решетки a = 8,78 Å, b = 12,42 Å. Была исследована электропроводность в диапазоне температур от 10 до 300 К и в магнитном поле 1 Тл, а также определены температурные зависимости концентрации и подвижности носителей заряда. Установлено, что в диапазоне температур от 10 до 33 К имеет место прыжковая проводимость с переменной длиной прыжка типа Мотта, и определены ее микропараметры.

Ключевые слова: монокристалл, твердый раствор, прыжковая проводимость

Ссылка при цитировании: Захвалинский В. С., Борисенко А. В., Никуличева Т. Б., Кочура А. В., Хтет А. З., Пилюк Е. А., Свойства твердого раствора $(Cd_{0,69}Zn_{0,31})_3As_2$ // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2022. Т. 15. № 3.1. С. 22–26. DOI: https://doi.org/10.18721/ JPM.153.103

Introduction

The narrow-gap semiconductor cadmium arsenide (Cd_3As_2) with an inverted structure of energy bands and the highest carrier mobility among semiconductors and semimetals (largely exceeding 10^4 $cm^2/(V·s)$ at room temperature) is distinguished by its chemical stability, low toxicity, and good manufacturability [1,2]. Cd_3As_2 is believed to manifest an inverted band structure due to the spin-orbital coupling (SOC) [3]. The 3D Dirac cones of Cd_3As_2 have been observed in angle-resolved photoemission spectroscopy (ARPES) [2,4,5]. A phase transition from a Dirac semimetal to a semiconductor with an increase in the Zn content was experimentally observed in single crystals of solid solutions $(Cd_{1-x}Zn_x)_3As_2$ at low temperatures [6]. In this study, we report single crystal $(Cd_{0.69}Zn_{0.31})_3As_2$ close to the composition of the concentration phase transition.

Materials and Methods

A modified Bridgman method was used to obtain $(Cd_{0.69}Zn_{0.31})_3As_2$ single crystals. Stoichiometric amounts of Cd_3As_2 and Zn_3As_2 binary compounds were placed in a graphitized and evacuated quartz ampoule. The CZA melt was slowly cooled from the melting temperature of 838 °C at a rate of 5 °C/h in the furnace temperature gradient.

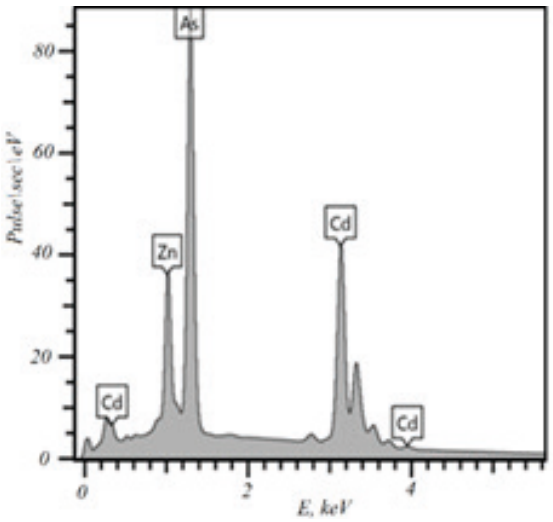

Fig. 1. EDX spectrum from the surface of $(Cd_{0.69}Zn_{0.31})_3As_2$ corresponding to the composition

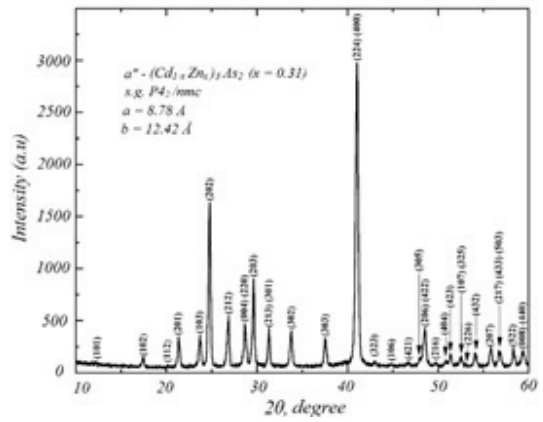

Fig. 2. Powder diffraction pattern of the $(Cd_{0.69}Zn_{0.31})_3As_2$ sample

The composition of the samples and their homogeneity were controlled by powder X-ray diffraction and energy dispersive X-ray spectroscopy (EDX). X-ray phase analysis (XPA) of the sample was performed using a GBC EMMA X-ray diffractometer (Cu Kα radiation, λ = 1.5401 Å) at room temperature. It has been established that the studied sample crystallizes in space group $P4_2/nmc$ with lattice parameters a = 8.78 Å, b = 12.42 Å [7]. To study the composition and distribution of elements on the surface, we used a JSM-6610LV (Jeol) scanning electron microscope (SEM) with an X-Max^N (Oxford Instruments) energy dispersive X-ray spectroscopy (EDX) attachment.

Fig. 1 shows the EDX spectrum from the surface of the $(Cd_{0.69}Zn_{0.31})_3As_2$ sample. Fig. 2 shows the powder diffraction pattern of the $(Cd_{0.69}Zn_{0.31})_3As_2$ sample.

Samples for the study of electrical conductivity by the six-probe method were parallelepipeds with the dimensions of 1.35×0.67×0.50 mm. The temperature dependence of electrical conductivity was studied in the temperature range from 10 to 300 K, and the Hall effect in a magnetic field of 1 T.

The results of the study of the temperature dependence of the resistivity of a solid solution single crystal $(Cd_{0.69}Zn_{0.31})_3As_2$ are shown in Fig. 3. The inset to Fig. 3 highlights the section corresponding to the variable range of the hopping conductivity according to Mott.

Results and discussions

As the temperature decreases from 320 K, the resistivity decreases from $2 \cdot 10^{-3}$ Ω·cm to a minimum of $5 \cdot 10^{-4}$ Ω·cm at 30 K, and then gradually increases. This behavior is typical of the Anderson transition [8]. The study of the Hall Effect in a magnetic field of 1 T made it possible to calculate the Hall coefficient R_H, the concentration and mobility of charge carriers. At a temperature of 10 K, the concentration of charge carriers was equal to $2.81 \cdot 10^{17}$ cm^{-3}, decreasing with increasing temperature to 30 K corresponding to the metal-insulator transition.

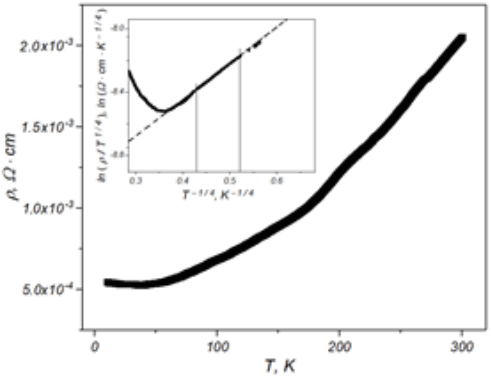

Fig. 3. Temperature dependence for resistivity of $(Cd_{0.69}Zn_{0.31})_3As_2$ solid solution single crystal. The temperature range of 10–33 K in the inset to Fig. 3 corresponds to the Mott variable range hopping conductivity

Above 30 K, an activation increase in the concentration of charge carriers was observed, which is typical for impurity semiconductors up to a value of $3.05 \cdot 10^{17}$ cm^{-3}. The mobility of charge carriers μ exhibits behavior characteristic of semiconductors, increasing with decreasing temperature. The value of mobility is maximum at the metal-dielectric transition point at a temperature of 30 K and is $4.51 \cdot 10^4$ cm^2·V^{-1}·s^{-1}. A further decrease in temperature leads to a decrease in mobility to $4.16 \cdot 10^4$ cm^2·V^{-1}·s^{-1} at a temperature of 10 K. The mechanisms of charge carrier scattering were evaluated.

At low temperatures, in the temperature range from 10 to 30 K, scattering by ionized impurity atoms and mobility $\mu \sim T^{3/2}$ prevail. In the temperature range from 30 to 300 K, scattering by thermal vibrations of the crystal lattice, $\mu \sim T^{-3/2}$, predominates (Fig. 4).

The inset to Fig. 3 shows a linear section of the temperature dependence of resistivity in the temperature range from 10 to 33 K, corresponding to the mechanism of hopping conduction by the states of the impurity band. Hopping conductivity is described by the universal equation (1) [8–10]:

$$\rho(T) = DT^m \exp\left[\left(T_0 / T\right)^p\right], \quad (1)$$

where D is a constant coefficient, T_0 is the characteristic temperature, and the parameters m and p depend on the mechanism of hopping conduction.

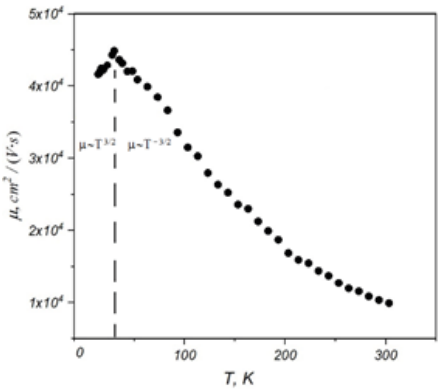

Fig. 4. Temperature dependence of mobility of $(Cd_{0.69}Zn_{0.31})_3As_2$ solid solution single crystal

We have determined the values of the parameters $m = 1/4$ and $p = 1/4$, which indicates the predominance of the mechanism of hopping conduction with a variable range hop according to Mott. When calculating the microparameters, the following obtained values of the coefficients were used: the characteristic temperature of the hopping conductivity $T_0 = 28.60$ K; hopping conduction onset temperature $T_V = 28.44$ K; coefficient $D = 8.488 \cdot 10^{-5}$ Ω·cm·K$^{-1/4.}$ For hopping conduction with a variable hop length, the following values of microparameters were obtained: Coulomb gap width in the density of localized states $\Delta = 0.43$ meV; acceptor zone width $W = 2.45$ meV; the value of the density of localized states outside the parabolic gap $g = 2.93 \cdot 10^{17}$ cm^{-3}·meV^{-1}; charge carrier localization radius $a = 307$ Å.

Conclusions

Single crystals of $(Cd_{0.69}Zn_{0.31})_3As_2$ solid solutions were obtained by the modified Bridgman method. Sample composition and element distribution was controlled using JSM -6610LV (Jeol) scanning electron microscope (SEM) with an X-Max^N (Oxford Instruments) energy dispersive X-ray spectroscopy (EDX) attachment.

It has been established that the studied sample crystallizes in space group $P4_2/nmc$ with lattice parameters $a = 8.78$ Å, $b = 12.42$ Å. We have investigated the electrical conductivity in the temperature range from 10 to 300 K and in a magnetic field of 1 T, and determined the temperature dependences of the concentration and mobility of charge carriers. It has been established that in the temperature range from 10 to 33 K, hopping conduction with a variable range of the Mott-type hop takes place, and its micro parameters have been determined: Coulomb gap width in the density of localized states $\Delta = 0.43$ meV, acceptor zone width $W = 2.45$ meV; charge carrier localization radius $a = 307$ Å. The obtained values do not contradict the literature data, which confirms the conclusion about the type of hopping conductivity.

REFERENCES

1. **Jeon S., Zhou B. B., Gyenis A., Feldman B. E., Kimchi I., Potter A. C., Gibson Q. D., Cava R. J., Vishwanath A., Yazdani A.,** Landau Quantization and Quasiparticle Interference in the Three-Dimensional Dirac Semimetal Cd_3As_2, Nature Materials. 13 (9) (2014) 851–856.

2. **Neupane M., Xu S.-Y., Sankar R., Alidoust N., Bian G., Liu C., Belopolski I., Chang T.-R., Jeng H.-T., Lin H., Bansil A., Chou F., Hasan M. Z.,** Observation of a three-dimensional topological Dirac semimetal phase in high-mobility Cd_3As_2, Nature Commun. 5 (2014) 3786.

3. **Aubin M. J., Caron L. G. & Jay-Gerin J. P.,** Band structure of cadmium arsenide at room temperature, Phys. Rev. B. 15 (1977) 3872–3878.

4. **Liu Z. K., et al,** A stable three-dimensional topological Dirac semimetal Cd_3As_2, Nat. Mater. 13 (2014) 677–681.

5. **Borisenko S., et al,** Experimental realization of a three-dimensional Dirac semimetal, Phys. Rev. Lett. 113 (2014) 027603.

6. **Hong Lu, Xiao Zhang, Yi Bian, Shuang Jia,** Topological Phase Transition in Single Crystals of $(Cd_{1-x}Zn_x)_3As_2$, Scientific Reports. 7 (2017) 3148.

7. **Arushanov E.K.,** Crystal growth and characterization of II3V2 compounds, Prog. Cryst. Growth Charact. 3 (1981) 211–255.

8. **Mott N. F.,** Metal–Insulator Transitions, London: Taylor and Francis, 1990.

9. **Mott N.F. and Davies Ye.A.,** Electron Processes in Non-Crystalline Materials / N.F. Mott. Oxford: Clarendon, 1979.

10. **Shklovskii B.I., Efros A.L.,** Electronic Propertie of Doped Semiconductors / B.I. Shklovskii. Berlin: Springer-Verlag, 1984.

11. **Amarnath R., Bhargavi K. S., Kubakaddi S. S.,** Thermoelectric transport properties in 3D Dirac semimetal Cd_3As_2. Journal of Physics Condensed Matter, 32 (22) (2020): 22570412.

12. **Armitage N.P., Mele E.J., Vishwanath A.,** Weyl and Dirac Semimetals in Three-Dimensional Solids, Rev. Mod. Phys. 90 (2018): 015001.

13. **Chorsi H. T., et al,** Widely Tunable Optical and Thermal Properties of Dirac Semimetal Cd_3As_2, Advanced Optical Materials. 8 (8) (2020) 120302 6.

14. **Crassee I., et al,** 3D Dirac semimetal Cd_3As_2: A review of material properties, Physical Review Materials. 2 (12) (2018) 120302 15.

THE AUTHORS

ZAKHVALINSKII Vasilii S.
v_zaxval@mail.ru
ORCID: 0000-0001-7055-8243

KOCHURA Alexey V.
akochura@mail.ru
ORCID: 0000-0002-7941-8404

BORISENKO Alexander V.
borisenko02.94@mail.ru
ORCID: 0000-0002-2539−3096

HTET Aung Zaw
zawh0898@gmail.com
ORCID: 0000-0003−3771−3082

NIKULICHEVA Tatyana B.
nikulicheva@bsu.edu.ru
ORCID: 0000-0001-6661−3959

PILYUK Evgeniy A.
pilyuk@yandex.ru
ORCID: 0000-0003−4979-5724

Received 14.05.2022. Approved after reviewing 15.07.2022. Accepted 16.07.2022.