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ON HOW TO CALCULATE THE BAND GAP OF SULFUR AND ZINC-DOPED SILICON

Abstract. The value of the band gap (E_g) is a core parameter of a semiconductor material. An exact knowledge of the band gap in such materials makes it possible to manipulate key performance characteristics of semiconductor devices developed on the basis of such materials [1]. Therefore, comprehensive knowledge of E_g in a semiconductor material is one of the main issues of semiconductor physics and technology [2].

Keywords: semiconductor, new materials, value of the band gap, electronics, photoenergetics.

Experimental technique

The process of diffusion of impurity atoms of sulfur and zinc in silicon was carried out as follows. Initially, *n* – type conductivity phosphor-doped silicon samples with resistivity of ρ =100 Ω cm (size $1 \times 5 \times \times 10\,mm^3$) were prepared as reference samples. These samples were divided into 2 groups and thereafter a two-stage process of diffusion of impurity atoms of sulfur and zinc in silicon was carried out from gaseous phase installation. At the first stage of diffusion, impurity atoms of sulfur were doped in silicon from gaseous phase in a vacuumed ($P \approx 10^{-6}$ mm. Hg)

quartz ampoules at temperature of T = 1250 °C for t = 10 hours. Reference samples in the second group, i.e., not doped with impurity atoms of sulfur and zinc were put into in a separate quartz ampoule and subjected to annealing under similar thermal and technological conditions. At the second stage, silicon samples from both groups were placed in quartz ampoules and diffused with impurity atoms of zinc. Diffusion of zinc atoms was carried out in separate quartz ampoules under the same conditions at a temperature of T = 1200 °C for t = 5 minutes.

After diffusion, the surfaces of silicon samples were cleaned by mechanical and chemical treatment. Diffusion of impurity atoms of sulfur and zinc in silicon allowed us to receive structures with a ρ –n junction. After the diffusion process has been accomplished, 100 μm-thick samples were polished (i.e., surface layers) by mechanical grinding from five sides (with the exception of one side). (Figure 1 a, b).

a) b)

Figure 1. Structure of ρ –n junction, formed on the basis of n – type conductivity phosphor-doped silicon samples with resistivity of ρ = 100% cm *a) samples of the 1st group, b) samples of the 2nd group*

In the process of grinding, in order to determine the depth of diffusion of impurity atoms in silicon samples, the type of conductivity of ρ – n junctions on the surface of the samples were assessed using a two-probe technique (thermal probe). The depth of of zinc and sulfur impurity atoms in silicon was calculated using theoretical formulas taking into account the diffusion mechanism of sulfur and zinc impurity atoms in silicon. The calculated depth of impurity atoms in silicon samples and the actual depth determined after the diffusion process were in good concordance only with negligent difference of ~5% [3–5].

At various temperatures, the authors measured the current-voltage characteristics (CVC) of the samples where ρ – n junction were formed. Their spectral sensitivity was also measured at room temperature by using IKS-12 spectrophotometer in the visible light range.

Measurement technique

For measuring the current-voltage characteristics (CVC), a device was used that was designed as per (Fig. 2). Current-voltage characteristics of *Si* < *P*, *Zn* > and *Si* < *P*, *S*, *Zn* > samples with ρ – n junction were measured at two temperatures: T_1 = 30 °C and T_2 = 80 °C.

The current-voltage characteristics of the samples were measured using a DC source with a voltage of U = 5V and U = 12V, a multi-stage potentiometer with a resistance of 10 kOhm, while current measurements were carried out using a Rigol DM3068-type device, voltage measurements were carried out with a Mastech MS8040 device, a thermostat connected to a constant voltage source, digital temperature meter type Espada TPM10 with scale division of Δt = 0.1 °C. In order to prevent significant overheating of ρ – n structures, the measurements were carried out by applying short-term impulse voltages. The results of the current-voltage characteristics of samples with a ρ – n junction are shown in (Fig. 3).

The authors in [1] based on I–V characteristics of ρ – n structures suggested the final formula for determining the band gap (E_g) of a semiconductor material with a ρ – n junction:

$$E_g = \frac{T_1 T_2}{T_2 - T_1}\left[\left(\frac{\varphi_{c1}}{T_1} - \frac{\varphi_{c2}}{T_2}\right) - 3k\ln\frac{T_2}{T_1}\right] \qquad (1)$$

where: T_1 and T_2 are experimental temperatures; $\varphi_{c1} = U^c_{cut1}$ and $\varphi_{c2} = U^c_{cut2}$; is the Boltzmann constant; E_g is the band gap energy of a semiconductor material.

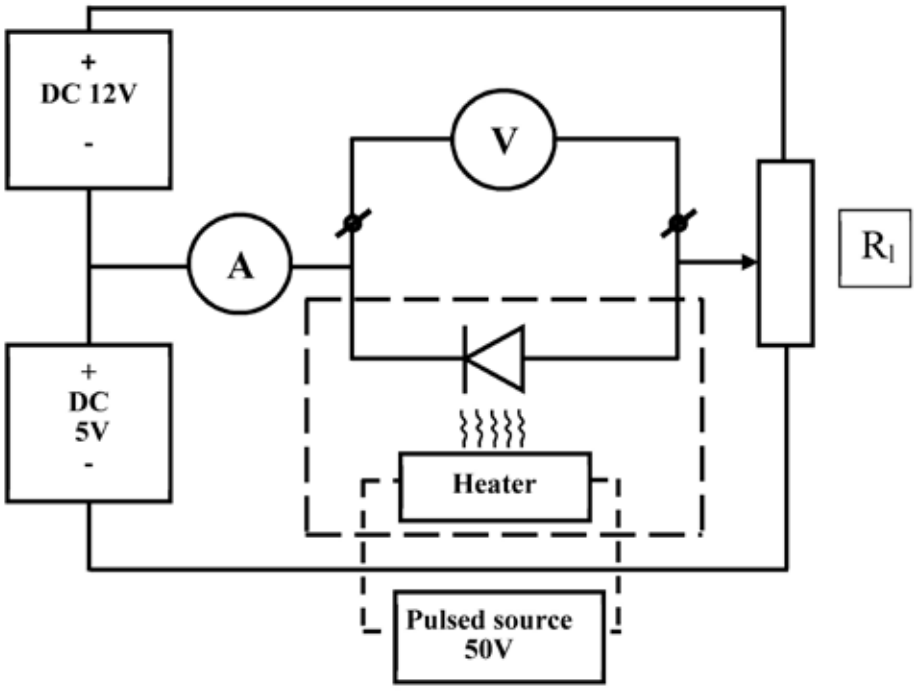
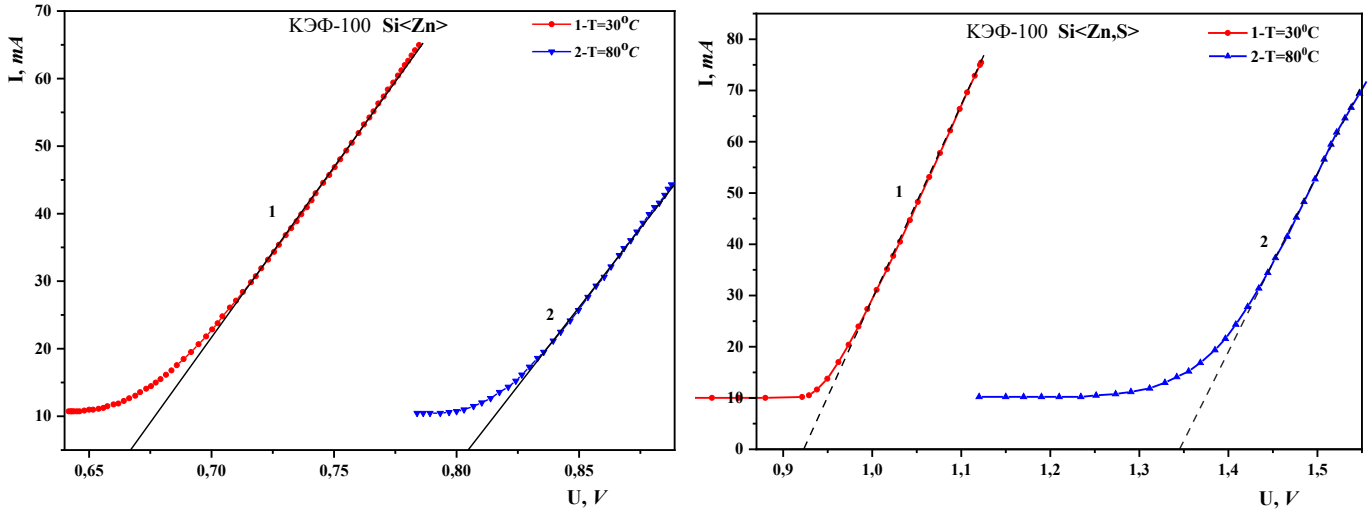


Figure 2. The device for measurement of current-voltage characteristics of the samples

Afterwards, straight lines were drawn from the linear parts of the current-voltage characteristics of the samples at temperatures T_1 = 30 °C and T_2 = 80 °C, and from the points of their intersection with the voltage axis, the values U_{cut1}^{C} and U_{cut2}^{C} were determined. As a result of measurement of I–V characteristics of the samples and by applying formula 1, the value of the energy of the band gap, was determined [6].



a) b)

Figure 3. Current-voltage characteristics (CVC) of silicon samples containing impurity atoms of zinc and sulfur, measured at temperatures: T = 30 °C and 2– T = 80 C: a) Zn-doped silicon (initial sample of n-type conductivity phosphor-doped silicon with resistivity of $\rho = 100\,\Omega$ cm); b) *Zn* and *S* doped silicon (initial sample of *n* – type conductivity phosphor-doped silicon with resistivity of $\rho = 100\,\Omega$ cm)

As a result of measurements and the data presented in (Fig. 3) and further by applying formula 1, the band gap energies were determined: $Eg_{Si_{Zn}} \approx 1.14\,eV$ – for silicon samples containing zinc

atoms and $Eg_{Si_{Zn}} \approx 1.38 eV$ – for silicon samples containing binary compounds of impurity atoms of sulfur and zinc.

It is well known that the fundamental value of the band gap of a single crystalline silicon equals $Eg \approx 1.12\ eV$, whereas the value of the band gap of a pure single-crystalline zinc-sulfide semiconductor compound is $Eg \approx 3.72\ eV$. The value of the band gap energy of the formed ZnS binary compound in silicon, determined experimentally, looks likely to be $Eg_{Si<Zn>S} = 1.38\ eV$, which is also confirmed by theoretical calculations $\left(Eg_{Si} < Eg_{Si<ZnS>} > Eg_{ZnS}\right)$ using formula 1.

Based on the analysis of the experiments, the authors suggest that new sulfide-zinc binary compounds type $(ZnS)_x(Si_2)_{1-x}$ must be formed in the bulk of single-crystalline silicon. In the course of investigation at room temperature of spectral sensitivity of the obtained silicon samples with impurity atoms of zinc as well as of silicon samples sequentially doped with impurity atoms of sulfur and zinc, it was determined that in silicon samples containing impurity atoms of sulfur and zinc one might evidence the increase in the sensitivity and expansion of the spectral range towards visible diapason [7–9].

As can be seen from (Fig. 4), the maximum photocurrent density of silicon samples containing sulfur and zinc atoms (second curve) is almost 3 times higher than the maximum photocurrent density of silicon samples containing only zinc atoms (first curve). In addition, the expansion of the range of absorption of light rays from $\Delta E_1 = 0.4\ eV$ to $\Delta E_2 = 0.93$ eV is well evidenced.

The experimental results suggest that by embedding sulfur and zinc atoms into the lattice of single-crystal silicon, one might form binary neutral compounds of $Zn - S^{++}$ type. It has been established that these binary compounds formed in the volume of silicon lead to a change in the fundamental parameters of silicon, which makes it possible to obtain a material with absolutely novel electrophysical parameters.

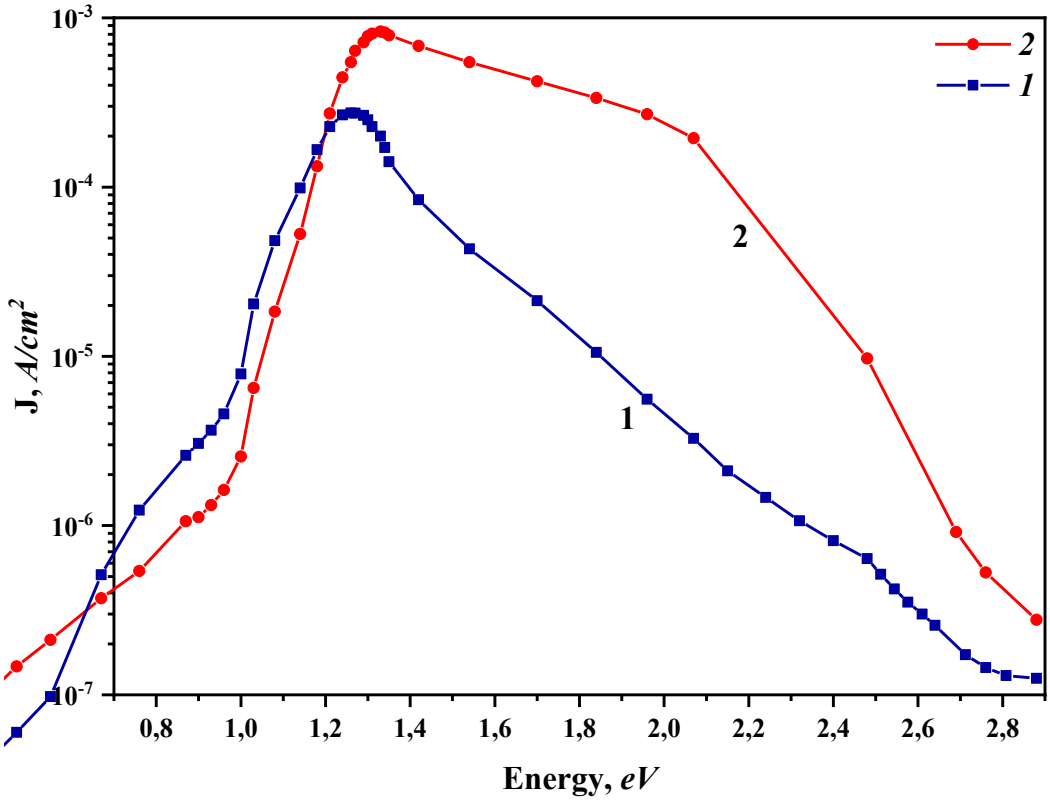


Figure 4. Spectral characteristics of samples: 1 – *Si* < *P, Zn* > ; 2 – *Si* < *P, S, Zn* >, *T* = 300 *K*, *U* = 10 *V*

The parameters of such a material fundamentally differ from the fundamental parameters of silicon. As a result of X-ray diffraction studies, it was established that the formed binary compounds of sulfur and zinc do not affect the crystal structure of the initial silicon [10–12].

Conclusion

Thus, the authors report that a technology has been developed that would allow obtaining new materials with impurity atoms of sulfur and zinc in silicon, which leads to the formation of binary compounds from sulfur and zinc atoms, thus changing the fundamental parameters of the source material. It is shown that the obtained silicon samples containing binary compounds of impurity atoms of sulfur and zinc could help to design cheap devices for their implementation in electronics, optoelectronics, and photoenergetics.

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