X-RAY AND SEM ANALYSIS OF SILICON DIFFUSED WITH ZINC AND SULFUR IMPURITY ATOMS

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Abstract. In this work, Zn and S atoms were dopped into silicon by diffusion method, and the effect of Zn and S atoms on the crystal lattice of silicon was studied. Researches and measurements (XRD-6100 Shimadzu X-ray diffractometer, SEM-EVO MA 10 scanning electron microscope) were carried out on modern devices. Measurements were carried out at room temperature (T=300 °K). The results are the basis for our conclusion that ZnS binary compounds are formed on the surface of the Si sample.

Keywords: silicon, zinc, sulfur, binary compound, impurity, diffusion.

1. INTRODUCTION

Authors [1-6] formed islands of GaSb binary compounds on the surface of Si by the diffusion method and showed the forbidden field energy and lattice parameters of this material both theoretically and experimentally. It is known that the bandgap energy of GaSb binary compound semiconductor is smaller than the bandgap energy of silicon, the difference in lattice constants is ~12%. However, forming a ZnS binary compound semiconductor in silicon with a lattice constant equal to $a_{znS} = 5.41$ Å ($a_{si} = 5.43$ Å, the difference in lattice constants is ~0.37%), and the bandgap energy is higher than the bandgap energy of silicon ($E_{g,ZnS} = 3.54$ eV) is important both scientifically and practically. Due to the large bandgap energy, these materials are good candidates for the production of LEDs [7-11]. But obtaining this ZnS binary compound semiconductor single crystal is expensive, both technologically and in terms of raw materials. Therefore, the extraction technology can be solved by forming ZnS binary compounds in monocrystal Si, which has a rich reserve in the earth's crust, and obtaining new types of materials using the diffusion method.

It is known that the ZnS semiconductor is mainly formed in one of cubic sphalerite or hexagonal wurtzite structures [12-15].

2. MATERIALS AND METHODS

As an initial sample for the experiment, a monocrystalline silicon plate grown by the Chokhral method, dopped with phosphorus impurity atoms, with a resistivity of $\rho \sim 100 \ \Omega \cdot \text{cm}$ was selected (the amount of oxygen is equal to $N_0 \sim 10^{17} \text{ cm}^{-3}$). The monocrystalline silicon plate was cut in size $1 \times 4 \times 8 \text{ mm}^3$ and the surface of the samples was subjected to mechanical and chemical treatments. After that, Zn and S atoms were diffused into the samples in two stages.

After diffusion, the samples were repeatedly subjected to mechanical and chemical treatments. Elemental analysis and X-ray analysis of the samples were studied. All measurements were made at 300 °K, that is, at room temperature.

3. RESULTS AND DISCUSSION

3.1. Element analysis

Elemental analysis of samples was performed after two-step diffusion (Figure 1).

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Figure 1. Elemental composition of the surface of the Si sample after diffusing with Zn and S impurity atoms.

As can be seen from Fig. 1, Si, O, C, Zn, S elements were determined in the sample composition in 76.1, 17.7, 3.0, 2.0 and 1.2 mass fractions, respectively. From these results, we can conclude that silicon oxide (SiO₂) is formed on the surface of silicon, and ZnS binary compounds are also formed due to the closeness of Zn and S mass fractions.

3.2. X-ray analysis

In order to investigate the effect of Zn and S input atoms on the parameters of the crystal lattice of the silicon sample, X-ray analysis was carried out (Fig. 2).



Figure 2. X-ray analysis: a) silicon sample diffused with Zn and S impurity atoms; taken from COD (Crystallography Open Database), b) Si single crystal (No.: 96-901-1999); s) ZnS with

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sphalerite crystal structure (No.: 96-110-1051); d) Data of ZnS (No.: 96-110-1052) semiconductors with wurtzite crystal structure.

Figures 2-b and 2-c show that the crystal lattice parameters of ZnS semiconductors with silicon and sphalerite crystal structure are very close to each other. 20 peaks are identified in Fig. 2a, and it is known from the literature [16-20] that most of these peaks belong to Si, SiC, SiO2, ZnO, ZnS crystals. It is known that peak 5 in Fig. 2a belongs to the direction h=1, k=1, l=1 of Si and ZnS semiconductors with sphalerite crystal structure. A new peak was formed in the state adjacent to the 5th peak, in which the main peak 5 and the new peak formed were not clearly different from each other due to the closeness of the crystal lattice parameters of Si and ZnS semiconductors.

4. CONCLUSION

From what has been analysed and discussed above it can be inferred that the obtained experimental results showed that after two-step diffusion of Zn and S impurity atoms into the monocrystalline silicon sample, Zn and S do not form binary compound due to the fact that Zn and S are impurity atoms that form deep energy levels in silicon. Certain thermodynamic conditions are required for them to form a binary compound in the silicon crystal lattice. The obtained elemental analysis showed that Zn and S impurity atoms form a ZnS binary compound on the monocrystalline Si surface. This conclusion was confirmed by the X-ray analysis of the sample. The research results can be applied in real life situations and could be practically functioned in suitable cases.

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