



THE STATE OF ALLOYING ELEMENT ATOMS IN THE SILICON LATTICE

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Annotation

In this work, the arrangement of the elements in the crystal lattice of the semiconductor material silicon is analyzed.

Keywords: Electron, hole, silicon, doping, donor, acceptor, valence band, conduction band, solubility, valence.

Introduction

When atoms of alloying elements are dissolved in silicon, additional quantum levels are introduced, which are localized at the locations of the atoms associated with them. At a relatively low content of alloying elements in the silicon lattice, when foreign atoms are located at sufficiently large distances from each other, these additional levels do not split into zones. In heavily doped semiconductors, when the wave functions of the valence electrons of foreign atoms overlap, the levels of these electrons form a band that provides conduction if not all the levels in this band are occupied by electrons.

Methods

Let us consider what happens when atoms of alloying elements are dissolved in silicon, which have specific differences in the structure of the outer electron shells. It is known that silicon has four valence electrons and each atom in the crystal lattice is bound by covalent bonds with four neighboring atoms. Now, if silicon is doped with an element, for example, of group V of the periodic system, the atoms of which have five valence electrons, then when a germanium or silicon atom is replaced in the corresponding crystal lattice (Fig. 1, a), four electrons of the alloying element atom will go to the implementation of a chemical bond with four nearest neighbors, and the fifth electron can, under appropriate conditions, go into the conduction band. Therefore, alloying elements with a higher valence compared to silicon, which can give electrons to the conduction band, are called donor- type elements, or donors.



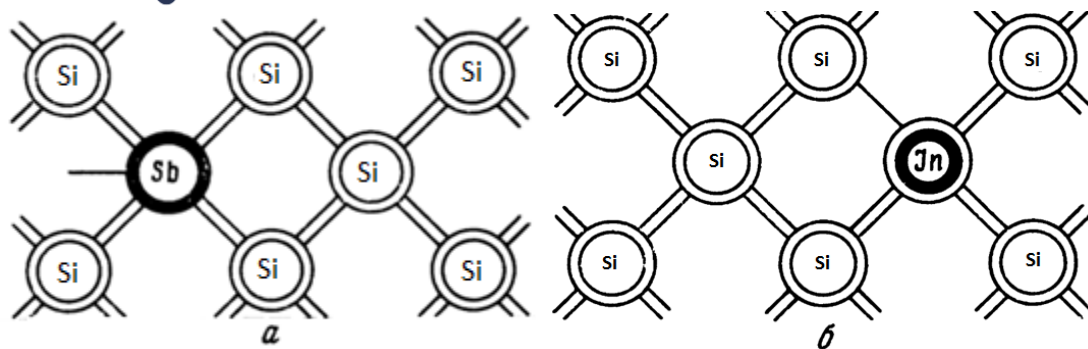


Fig. 1. Scheme of the formation of free electrons upon doping of silicon with elements of the donor type (a) and holes upon doping with elements of the acceptor type (b)

Results

When silicon is doped with elements with a lower valence, for example, elements of group III of the periodic system (Fig. 1, b), three valence electrons of the alloying element atom will go to the implementation of a chemical bond with three nearest neighbors, and the bond with the fourth neighbor turns out to be unsaturated. In this case, due to additional energy (for example, thermal motion), the electrons of other silicon atoms can occupy a free level associated with an atom of the alloying element, resulting in a hole in the valence band [1].

Alloy elements with a lower valence compared to silicon, which can accept electrons from the valence band, are called elements of the acceptor type, or acceptors.

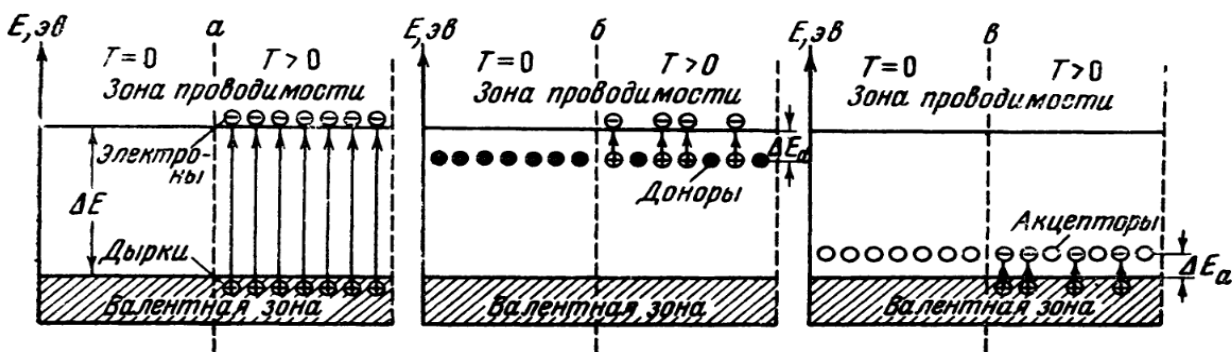


Fig. 2. Energy schemes of an undoped semiconductor (a), doped with donor (b) and acceptor (c) elements, illustrating the appearance of charge carriers with increasing temperature.

At low temperatures, the atoms of the alloying elements are non-ionized. The donor levels are located near the bottom of the conduction band at a distance corresponding to their ionization energy. The acceptor levels are located near the valence band. On fig. 2, b, c (see the left half of each figure) shows the schemes of the energy levels of the electron and hole semiconductors corresponding to the two considered cases.



Obviously, at a temperature of absolute zero, a doped semiconductor, like its own, must be an insulator. As the temperature rises, ionization of the atoms of the alloying elements will occur first. Shown in fig. 2 energy diagrams illustrate the appearance of charge carriers with increasing temperature in a semiconductor doped with elements of the donor and acceptor types. For comparison, a diagram of the appearance of electrons in an intrinsic semiconductor is also given. It follows from a qualitative comparison of these schemes that, in a fairly wide temperature range, the main role in the process of charge transfer will be played by carriers formed as a result of ionization of alloying element atoms.

It follows from the theory that the radius of a hydrogen atom placed in a dielectric medium and its ionization potential are determined by the following expressions:

$$r=0,53 \cdot 10^{-8} \epsilon \frac{m_0}{m^*} \quad (1) \quad \Delta E_d = \frac{13,53}{\epsilon^2} \cdot \frac{m^*}{m_0} \quad (2)$$

Simple calculations show that in silicon the ionization energy of the atoms of the alloying elements should not exceed 0.015-0.01 eV. This value is in good agreement with experimental data for most elements of group V of the periodic system. In table. Table 1 shows the values of the ionization energy and ionization of some alloying elements in silicon according to the data of [2, 3].

Table 1 Ionization energies of some alloying elements in silicon [4]:

alloying element	Group	Donor or acceptor	Energy level
Mn	VII	D	$E_c - 0.53$
Cu	II	D	$E_v + 0.24$
Zn	II	A	$E_v + 0.31$
Ni	VII	D	$E_c - 0.3$
Fe	VIII	D	$E_v + 0.4$

Note. E_c is the bottom of the conduction band; E_v is the top of the valence band.

Conclusion

It should be noted that when silicon is doped with some elements, several levels with different ionization energies are formed, and therefore, at some temperatures, the atoms of such elements can be donors, and at others, acceptors. An increase in concentration leads to a decrease in the ionization energy and ionization of the atoms of the alloying element. From Table. It follows from Table 1 that, at relatively low temperatures, the electrical properties of silicon doped with elements of the donor or acceptor type are determined mainly by the amount and state of the latter.



References

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