UDC 621.315.592; 538.91

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INCLUDING OF ADMIXTURE BORON ATOMS IN THE ELECTRIC NONACTIVE STATE TO SILICON SINGLE-CRYSTAL

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According of to experimental data by means of mathematical modeling was evaluated the proportion of those nonactive boron atoms, which are part of a single crystal silicon in an electrically inactive state at various stages of his growing by the of Czochralskij method.
Keywords: silicon, single crystal, boron, nonactive, electrically inactive impurity

Introduction. The single-crystals of silicon for providing of p-type for conductivity alloy by an acceptor impurity, mostly - by boron. However part of atoms of boron in a crystal can enter in the complement of various microflaws and complexes [1]. Such atoms do not form covalently connections with the atoms of silicon and can not form a hole, id est. there are electric nonactive.

The size of concentration and state of alloying admixture determine one of major factors of quality of silicon single-crystals - its specific electric resistance. A control by the concentration of all admixtures in the given limits is an actual task at the production of silicon single-crystals for microelectronics and sun energy.

State of question. The concentration of admixture in a single-crystal which is grown from fusion depends on the effective coefficient of distribution of this admixture between the liquid and hard phases k [2]:

$$k = \frac{N_{тв}}{N_p} \cdot \frac{\gamma_p}{\gamma_{тв}} , \tag{1}$$

where $N_{тв}$, N_p are a concentration of admixture atoms accordingly in hard and liquid phases, at/sm^3; γ_p, $\gamma_{тв}$ are a density of these phases, тт/m^3.

Effective coefficient for distribution of most admixtures in silicon less than one (for boron $0.8 \le k \le 1.0$) [3] as a result of their partial pushing away from front of crystallization in fusion. Therefore in the process of drawing out of single-crystal in fusion by Czochralskij method there is a gradual accumulation of boron admixture in fusion, thus its concentration in the grown single-crystal increases gradually. Distribution of admixture in fusion and single-crystal for the tend of crystallization it is possible to characterize analytical expressions which are based on V. Pfann works [4]:

$$N_p(g) = N_0(1-g)^{k-1}, \tag{2}$$

$$N_{тв}(g) = \frac{\gamma_{тв}}{\gamma_p} \cdot k \cdot N_0 \cdot (1-g)^{k-1}, \tag{3}$$

where N_0 is an initial concentration of admixture atoms n a liquid phase (to beginning of crystallization), at/sm^3; g is part of initial mass of fusion, which passed to the hard phase in the moment of crystallization of portion crystal with the concentration of admixture of $N_{тв}(g)$, at/sm^3

In work [2] it was shown by a mathematical analysis, that a function $N_{тв}(g)$ from equation (3) is ambiguous, and the physical admissions used for its conclusion executed not on all stages of process of grow after Czochralskij method. In this work a new model was worked out for dependence $N_{тв}(g)$, which is based on equation of balance of atoms of not volatile admixture of boron during all process of drawing out from fusion of single-crystal by Czochralskij method. With use of this model the effective coefficient of distribution k is determined on experimental dependence $N_{тв}(g)$:

$$k(g)=\frac{(1-g)\cdot N_{тв}(g)}{\frac{\gamma_{тв}}{\gamma_{ж}}\cdot N_0-\int_0^g N_{тв}(g)\,dg} \quad . \tag{4}$$

On the same principle there were the worked out models of $N_{тв}(g)$ and $k(g)$ for the carbon and oxygen admixtures [5]. In Czochralskij method speed of crystallization V on the finishing stage of growing is diminished on technological reasons. From the kinetic theory of crystallization from fusion follows, that with diminishing V the effective coefficient of distribution for any admixture k must also diminish. In this work it was shown that in an experiment the coefficients of admixtures for carbon k_C and oxygen k_O diminish with diminishing V of single-crystal of silicon, alloying by far stronger than it is forecast by the kinetic theory of crystallization. At the same time the size of effective coefficient of distribution for boron k with diminishing of speed of single-crystal growing from fusion instead of diminishing grows. At fact of considerable difference of experimental dependences k(g) admixtures in silicon from speed of height from theoretical in work [6] admission was done, that during growing by Czochralskij method the processes of complexaction change in the single-crystal silicon as a result of change correlation of concentrations for all admixtures.

Problem formulation. Task of this research is estimation on experimental data in the single-crystals silicon part of atoms of alloying admixture of boron, which are electric nonactive as a result of included in composition of complexes and microflaws.

Basic part of researches. Seven single-crystals silicon of brand KGB 0.5-1.7/10 with diameter a 135 mm and a crystallography orientation {100} are investigated. Crystals were grown by Czochralskij method at industrial conditions in setting as "Redmet-30" from identical raw material. A concentration electric active atoms of alloying admixture of boron was calculated on the size of specific electric resistance, that measured by four-prove method [7,8]. The experimental results of concentration electric active atoms of boron $N_{тв}(g)$ generalized on seven single-crystals are offered to fig. 1, and calculated for to data $N_{тв}(g)$ dependence of effective coefficient of distribution electric active atoms of boron $k(a)$ - on fig. 2. Accepting that the looked increase of size $k(a)$ on the late stages of growing is related to diminishing of part electric nonactive atoms of boron in single-crystals. For determination of effective coefficient distribution for all atoms of boron k (electric active and nonactive) will consider their distribution between liquid and hard phases at the beginning of single-crystal growing.

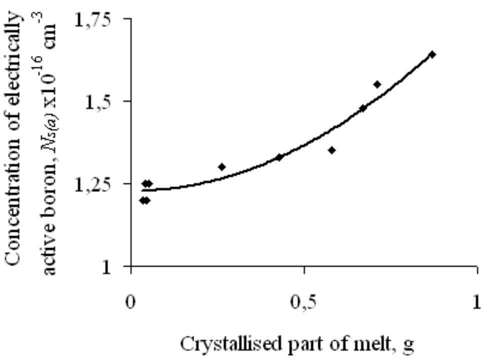

Figure 1 is distribution electric active atoms of boron in single-crystals silicon

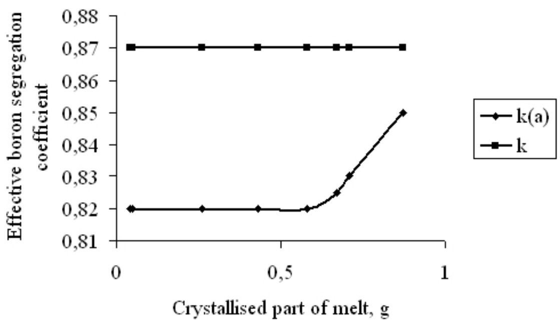

Figure 2 is the effective coefficient of distribution of the boron: $k(a)$ - electric active atoms; k - general

As industrial conditions measure the concentration of admixtures in fusion N_p is impossible, we determine its on data of measuring $N_{тв}(g)$ on a formula (1)

$$N_p(g) = \frac{N_{тв(a)}(g)}{k_{(a)}} \cdot \frac{\gamma_p}{\gamma_{тв}}. \qquad (5)$$

On the graphic fig. 1 and fig. 2 by approximations determine $N_{тв}(0.01)$ and k(0,01), id est. in the overhead crossing of single-crystal, when $g = 0.01$.

From formula (5) find the concentration of boron atoms in fusion $N_p(0.01)$. The complete concentration of boron in initial fusion N_0 we determine on its concentration in raw material:

$$N_0 = N_{сир} \cdot \frac{\gamma_p}{\gamma_{тв}} = 1{,}45 \cdot 10^{16} \cdot \frac{2{,}53}{2{,}33} = 1{,}574 \cdot 10^{16} \text{ sm}^{-3}.$$

Farther from formula (2) find the value of effective coefficient of distribution for all atoms of boron k (together electric active and nonactive).

Where:

$$k = 1 + \frac{\log \frac{N_p(0{,}01)}{N_0}}{\log 0{,}99}. \qquad (6)$$

After the substitution of data g = 0,01; $N_{ТВ}(0{,}01) = 1{,}19 \cdot 10^{16}$ sm^{-3}; k(0,01) = 0,82; $\gamma_p = 2{,}53$ t/m^3 and $\gamma_{тв} = 2.33$ t/m^3 we find: $k = 0.87$. Now from formula (1) it is possible to find dependence of concentration electric nonactive atoms of boron $N_{тв(н)}$ in a single-crystal on the different stages of its growing:

$$k(g) = \frac{N_{тв(a)}(g) + N_{тв(н)}(g)}{N_p(g)} \cdot \frac{\gamma_p}{\gamma_{тв}}, \qquad (7)$$

where $N_{тв(н)}(g)=\frac{\gamma_{тв}}{\gamma_p}\cdot k(g)\cdot N_0\cdot(1-g)^{k-1}-N_{тв(а)}(g)$.

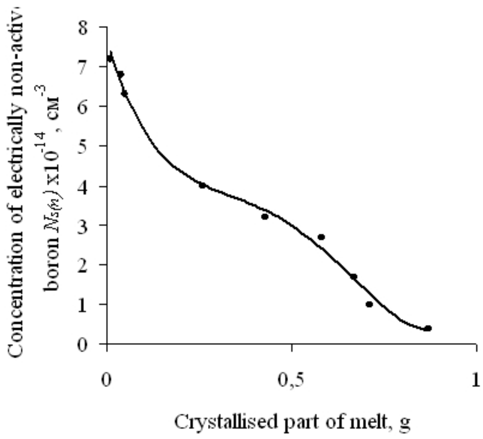

Figure 3 is concentration electric of nonactive atoms to boron in the single-crystals of silicon

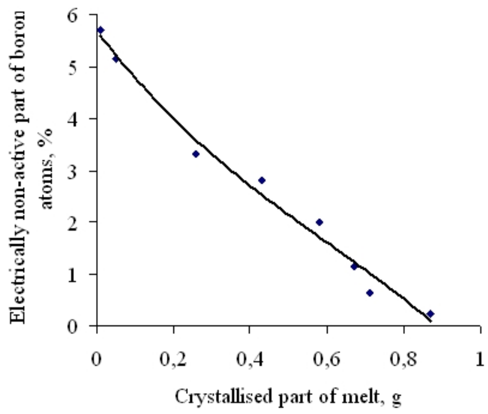

Figure 4 is relative concentration electric of atoms of boron in the single-crystals of silicon

We accept, that $k(g)$ = const, as it was accepted in work [4], id est. $k(g)$ = 0.87 (fig. 2). Using experimental data $N_{тв}(g)$ from fig. 1, expect dependence $N_{тв}$ fig. 3) and $N_{тв}(g)/N_{тв}$ (fig. 4). From data of fig. 4 it is evidently that during growing of single-crystal part electric nonactive atoms of boron in its diminishes substantially.

Conclusions. From estimations, got from experimental data by a mathematical modeling, follows, that part of alloying admixture boron, which is in the single-crystal silicon in electric nonactive state, diminishes during the process of crystallization. The most credible reason of such phenomenon it is possible to consider diminishing of formation of complexes boron-oxygen as a result of the gradual diminishing of concentration of admixture of oxygen in the single-crystal of silicon from overheard to its underbody during growing on Czochralskij method.

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