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# Mathematic modeling the oxygen distribution mechanism in Si ingots during growing processes

**A.P. Oksanich, S.E. Pritchin, A.V. Vasheruk**
*Institute of Economics and Advanced Technologies, 24/37 , Proletarska street, 36900, Kremenchuk, Ukraine*
*Phone/fax.: +380 (5366) 31124, E-mail oksanich@cat-ua.com*

**Abstract.** The article provides specified mathematic modeling of oxygen distribution mechanism in Si ingots. Experimentally such model parameters as quartz melting speed for different melting zones, initial oxygen concentration in melt, influence of crucible rotation speed on melting rate. The work outlines the results of computer modeling. The results of theoretical and experimental investigations carried make possible to predict oxygen concentration in Si ingot and define the technology parameters for growing ingots of stated concentration.

**Keywords:** Si ingots, oxygen, crucible, mathematic modeling.

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## 1. Introduction

In microelectronics and instrument-making the most common growing method of Si single-crystal ingots is that of Czochralski one though during the process silicon is saturated with hydrogen from quartz crucible. Hydrogen is the main dopant in silicon [1], determining the thermodonor behavior, the support of charge life thermal stability, microdefects formation.

The Si ingot diameter and length being increased, the hydrogen dopant influence on their electro-physical properties extends [2].

Obtaining Si ingots with stated oxygen distribution along the ingot is subject to carrying out technological process with programmed variations of technological parameters. In this case, mathematic modeling of oxygen distribution along the ingot is necessary to determine these parameters.

Existing mathematic models [3] that describe oxygen inflow in the melt and its distribution in the ingot need further specification as they cannot be used for obtaining accurate modeling results to practise oxygen concentration prediction and choose technological parameters in the process of the ingot growth with the diameter more than 150 mm. Consequently, the problem of oxygen distribution during the growth of Si ingots with the above mentioned diameter is the issue of the day.

## 2. Problem definition and solution suggested.

During melting different dopant, otherwise stated, may occur in silicon. The most important of them is oxygen with concentration dependent on process conditions and the ingot diameter [4]. The main source of oxygen in the melt during ingot growth is quartz crucible in which melted burden is loaded. Then the ingot is grown from the melt with oxygen in it. The crystallization process is carried out at high temperatures; crucible melts slowly and under convection current oxygen of the crucible transfers to melt.

The problem of oxygen inflow from the crucible in the melt and its influence on dopant distribution in growing crystal has been widely discussed. Formulas obtained are sophisticated and require digital integration. Thus, for example in work [5], the equilibrium obtained for determining the oxygen concentration in the melt does not take into account the cylindrical form of the crucible.

In this case, we can use equilibrium describing the dopant distribution along the ingot [6]:

$$\begin{aligned} C = k_0 C_0 [1 - \frac{\pi R^2 v_p}{v_s (k_0 - 1) C_0} - \frac{2 V_p v_p}{R v_s (k_0 - 2) C_0}] \times \\ \times (1-g)^{k_0 - 1} + \frac{2 V_0 v_p k_0}{R v_s (k_0 - 2)} (1-g) + \frac{\pi R^2 v_p k_0}{v_s (k_0 - 1)}, \end{aligned} \tag{1}$$

where $k_0$ is the equilibrium distribution ratio equal to 0.25; $C_0$ – initial oxygen concentration in the melt; $p$ – melted silicon density equal to 2.53 g/cm$^3$; $R$ – crucible radius; $v_p$ – speed of the oxygen inflow in the melt with 1 cm$^2$ contact surface of crucible and melt; $V_p$ – melt amount; $V_0$ – initial melt amount; $v_s$ – growth speed; $g$ –part of the melt crystallized calculated as

$$g = \frac{W}{W_0}, \tag{2}$$

where $W$ – ingot oblong mass; $W_0$ – melt and ingot total mass.

Programming technological process parameters is achieved by bringing a variable parameter to the ingot length and radius, and equilibrium (1) should be expressed through the ingot length $L$ and radius $R_s$.

After simple equilibrium transformation (1), we have:

$$C = [k_0 C_0 - \frac{\pi R^2 v_p k_0}{v_s(k_0-1)} - \frac{2V_p v_p k}{R v_s(k_0-2)}] \times \\ \times (1-g)^{k_0-1} + \frac{2V_0 v_p k_0}{R v_s(k_0-2)}(1-g) + \frac{\pi R^2 v_p k_0}{v_s(k_0-1)}, \tag{3}$$

The oxygen concentration in ingot is defined as

$$C_s = C \times V_s, \tag{4}$$

where $V_s$ is the amount of grown ingot part equal to

$$V_s = \pi R_s{}^2 L, \tag{5}$$

where $R_s$ – ingot radius, $L$ – ingot length.

Then, using (3) and (5) in (4) and defining $k_0 C_0$ as $A$ we have:

$$C = \left[ [A - \frac{\pi R^2 v_p k_0}{v_s(k_0-1)} - \frac{2V_p v_p k}{R v_s(k_0-2)}] \times (1-g)^{k_0-1} + \right. \\ \left. + \frac{2V_0 v_p k_0}{R v_s(k_0-2)}(1-g) + \frac{\pi R^2 v_p k_0}{v_s(k_0-1)} \right] \left(\pi R_s^2 L\right), \tag{6}$$

concentration distribution along the ingot is determined by equilibrium:

$$C_l = \int_0^L C_s dL. \tag{7}$$

Then, integrating (6) we have:

$$\int_0^L A\pi R_s^2 L dl = \frac{A\pi R_s^2 L^2}{2}; \tag{8}$$

$$\int_0^L \frac{\pi R^2 v_p k_0 \pi R_s^2 L}{v_s(k_0-1)} dL = \frac{\pi^2 R^2 v_p k_0 L^2}{2v_s(k_0-1)}; \tag{9}$$

$$\int_0^L \frac{2\pi R_s{}^2 L k_0 \pi R_s^2 L}{R v_s(k_0-2)} dL = \frac{2\pi^2 R_s^4 L^3 k_0}{3R v_s(k_0-2)}; \tag{10}$$

$$\int_0^L \frac{\pi R^2 v_p k_0 \pi R_s^2 L}{v_s(k_0-1)} dL = \frac{\pi^2 R^2 v_p k_0 R_s L^2}{2v_s(k_0-1)}. \tag{11}$$

Putting equilibrium (8) as A1, equilibrium (9) as A2, equilibrium (10) as A3, equilibrium (11) as A4 and introducing A5 = $\pi R_s{}^2 L$, we get as a result:

$$C_l = ((A_1 - A_2 - A_3)(1-g)^{k-1} + A_4(1-g)) \times A_5. \tag{12}$$

It is necessary to determine speed transfer of the dopant in the melt as well as initial oxygen concentration at the beginning of the cylindrical ingot part growth for calculating equilibrium (12).

Oxygen inflow speed from quartz crucible in melt is determined by speed of the crucible melting dependant on the interaction character between melt and crucible. Heater temperature and crucible rotation ratio are main technological parameters affecting this process. As it is shown in [6] this problem has not been sent analytically.

Authors used measuring method for determining crucible melting speed. It conveys weighing of crucible parts with definite dimensions after finishing of ingot growth process. We used crucible of natural quartz glass made by GE Quartz Europe GmbH with diameter 350 mm, during ingots growth, diameter being 155 mm. the growth was effected with utmost usage of the melt in the crucible.

In the growing process by means of automated control growth system [7] archiving data of ingot diameter, length, rotation ratio, lifting speed, rotation frequency of ingot and crucible and data discrete filing, equal to 120 sec. We define 4 contact zones crucible-melt (See figure 1).

First zone mostly takes no part in oxygen saturation of the melt, consequently its examining poses no practical interest.

Second zone is characterized by well defined flute of breadth up to 2 mm. This zone is developed due to the fact that at the process beginning flute is melted at higher temperature and the melt, after complete flute melting, has a higher temperature up to 1480°C. It determines the oxygen concentration at the initial stage of growth process.

Third and fourth zones determine oxygen concentration in melt during basic part ingot growth and, consequently, oxygen concentration in ingot.

After ingot withdrawal rectangular wafers were cut of the quartz, with size 10 × 100 mm, which were weighted with accuracy to 0.001 g.

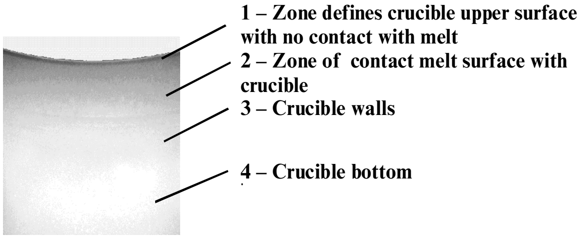

**Fig. 1.** Contact zones of melt and the crucible.

During the ingot growth process for lower melt level compensation that takes place due to silicon transformations from liquid phase (melt) to solid (ingot) crucible lifting is made with ratio determined by means of equilibrium [8]:

$$v_t = v_s\left(1 + \frac{1}{\dfrac{D_t^2}{D_s^2} \times \dfrac{\rho_s}{\rho_m} - 1}\right), \tag{13}$$

where $D_s$ – ingot diameter, $D_t$ – crucible diameter.

Thus, the time of measured wafer in the melt is defined as:

$$t_p = \frac{H}{v_t}, \tag{14}$$

where $H$ – melt level from flute beginning at crucible to lower wafer, $v_t$ – crucible lifting speed.

The crucible melting speed is calculated as:

$$v_p = \frac{M_0 - M_p}{S_p \cdot t_p}, \tag{15}$$

where $M_0$ – wafer sample mass cut from the crucible not used in the growth process = 10.98 g; $M_p$ – wafer sample mass; $S_p$ – wafer measured dimensions = 500 mm$^2$.

Experiments were carried out for the fixed crucible rotation ratio 5, 10, and 15 r/min. At every rotation ratio three processes took place and measured results of crucible melting speed were approximated.

The results of the experiments are shown in Fig. 2.

Experiments proved that crucible melting speed varies in different zones. Crucible melting speed for these zones for crucible of natural quartz glass made by GE Quartz Europe GmbH with the diameter 330 mm is 7.5 mg/(cm$^2$·h) – for the second zone; 3.2 mg/(cm$^2$·h) – for the third zone, and 4.3 mg/(cm$^2$·h) – for the fourth one.

The initial oxygen concentration in the melt $C_0$ is defined by the degree of crucible melt in the process of flute melting at high temperatures. It is possible to evaluate the initial oxygen concentration in the melt by means of the oxygen concentration varying in the upper part of the ingot. We carried out a research of the oxygen concentration in the upper part of 128 ingots grown in identical conditions to define the initial oxygen concentration. The results of verifications are given in Fig. 3.

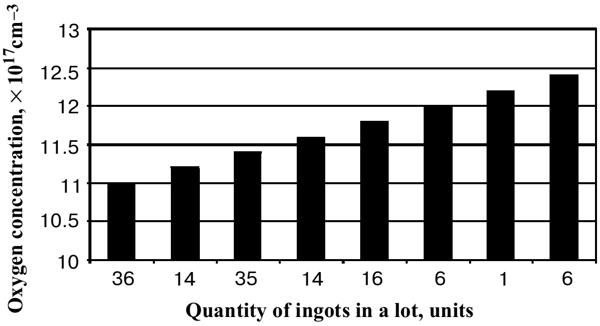

**Fig. 3.** Initial oxygen concentration in Si melt.

The initial oxygen concentration in melt was defined as average meaning of the concentration in ingots with equilibrium:

$$C_0 = \frac{1}{n}\sum_{1}^{n} N_0, \tag{16}$$

where $n$ – quantity of samples measured, $N_0$ – oxygen concentration in samples.

On the basis of these experiments, we established the meaning of the initial oxygen concentration in the melt equal to 1.14·10$^{18}$ cm$^{-3}$.

Applying LabView and using the equilibrium obtained by the authors (12) as well as the results of experimental data concerning establishing quartz crucible melting speed and the initial oxygen concentration in melt, we made computer modeling the oxygen concentration in melt. For this purpose, a virtual instrument was worked out. The results of modeling are given in Fig. 4.

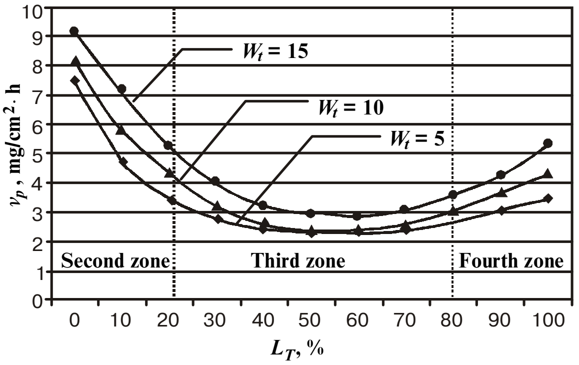

**Fig. 2.** Dependence of quartz crucible melting speed on crucible rotation ratio: $v_p$ – quartz crucible melting speed, mg/(cm$^2$·h); $W_t$ - crucible rotation ratio, r/min; $L_T$ – ratio melt height in crucible to crucible height, %.

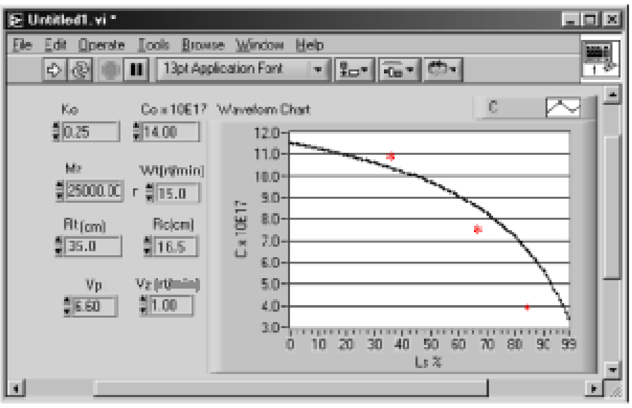
Ko 0.25
Co x 10E17 14.00
Mz 25000.00
Wt[r/min] 15.0
Rt(cm) 35.0
Rc(cm) 16.5
Vp 6.60
Vz [r/min] 1.00

**Fig. 4.** Oxygen concentration in silicon.

Comparison of the modeling results with those experimental data of oxygen concentration in Si ingots along their length presented quite accurate coincidence of theoretical and experimental data.

## 3. Conclusions

The given model makes it possible to describe approximately the character of oxygen concentration verifications in the melt and correct technological process parameters on the basis of data obtained.

Model parameters were determined, namely:

- Natural quartz crucible melting speed with diameter 350 mm, that makes 7.5 mg/(cm$^2$·h) – for the second zone; 3.2 mg/(cm$^2$·h) – for the third zone, and 4.3 mg/(cm$^2$·h) – for the fourth one;
- Initial oxygen concentration in melt that makes $1.14 \cdot 10^{18}$ cm$^{-1}$.

The experiment to find the dependence between quartz crucible melting speed and crucible rotation ratio has been carried out. This dependence possesses a non-linear character.

The results of theoretical and experimental data make it possible to predict the oxygen concentration in Si ingot and determine technologic process parameters for obtaining ingots with a given oxygen concentration.

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