MATHEMATICAL MODEL OF OXYGEN OUTDIFFUSION①

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ABSTRACT

A new mathematical model of oxygen outdiffusion was proposed. Experimental results demonstrated that theoretical calculation based on this model meets these results perfectly.

Key words: CZSi outdiffusion intrinsic gettering

1 INTRODUCTION

The first step in intrinsic gettering is oxygen outdiffusion. When width of denuded-zone is calculated, exactly known vertical distribution of oxygen after oxygen outdiffusion is required. Ruiz and Pollack[1] once put forward an error function:

$$C = C_F + (C_0 - C_F)\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \qquad (1)$$

where C_F is solid solubility of oxygen in silicon; C_0 is initial interstitial oxygen concentration; D is diffusion coefficient of oxygen in silicon; t is diffusion time. A mathematical model is proposed in the form of series. Experiment shows that this model describes vertical distribution of oxygen after outdiffusion more exactly than the error function.

2 MATHEMATICAL MODEL

During the outdiffusion, the thickness of silicon wafer is much larger than vertical depth of diffusion. Thus diffusion can be expressed as a one-dimension equation:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \qquad (2)$$

where C is shorthand of $C(x, t)$.

There is a boundary condition when outdiffusion carries out in protective atmosphere:

when $t > 0,\ C(0, t) = C(l, t) = 0$

where l is thickness of silicon wafer;

and an initial condition:

$$C(x, 0) = C_0$$

where C_0 is initial interstitial oxygen concentration of sillicon wafer.

The solution of series in equation (2) which satisfies boundary and initial condition is:

$$C(x, t) = \frac{4}{\pi}C_0\sum_{k=1}^{\infty}\frac{1}{2k-1}\exp\left[-\frac{(2k-1)^2}{l^2}Dt\right] \times \sin\left(\frac{2k-1}{l}\pi x\right) \qquad (3)$$

where t is outdiffusion time; k is integer larger than or equal to zero; D is diffusion coefficient of oxygen in silicon under outdiffusion temperature T. The relation between D and T can be defined as:

$$D = 0.17\exp\left(\frac{A}{KT}\right) \qquad (4)$$

where K is Boltzmann constant, $A = 2.54$ eV.

According to equations (3) and (4), it is assumed that initial interstitial oxygen concentration in silicon is $10\times10^{-4}\%\sim30\times10^{-4}\%$, outdiffusion temperature and time are 1 050~1 200 ℃ and 1 ~ 5 h respectively. The calculated results are drawn in Fig. 1.

3 EXPERIMENTAL

3.1 *Experiment Theory*

All wafers used are N type, thus there is a resistivity equation:

$$\rho = 1/(\mu_n q N_D) \qquad (5)$$

where μ_n is electron mobility; q is electron charge; N_D is donor concentration.

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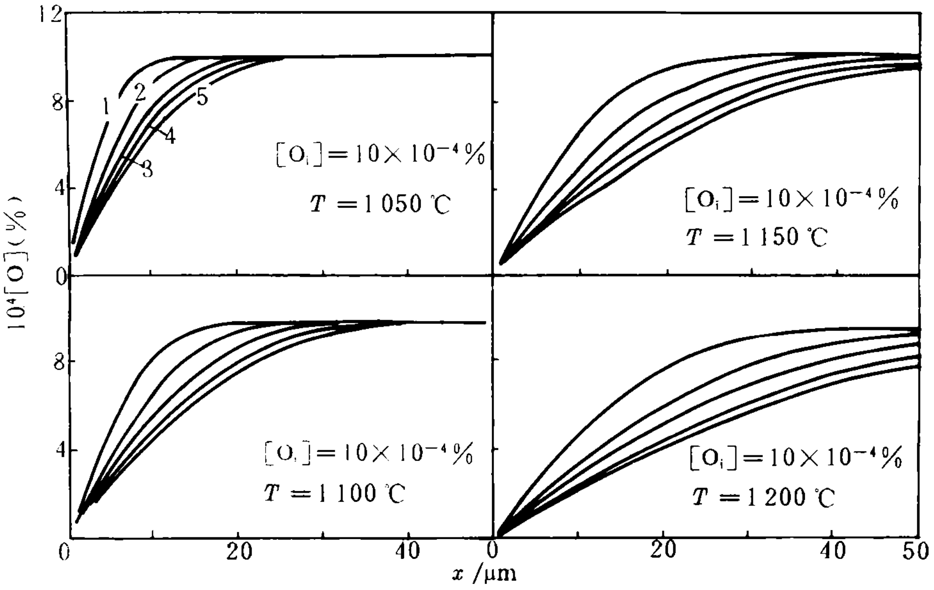

Fig. 1 Calculated vertical distribution of oxygen after outdiffusion (1)

1—1 h; 2—2 h; 3—3 h; 4—4 h; 5—5 h

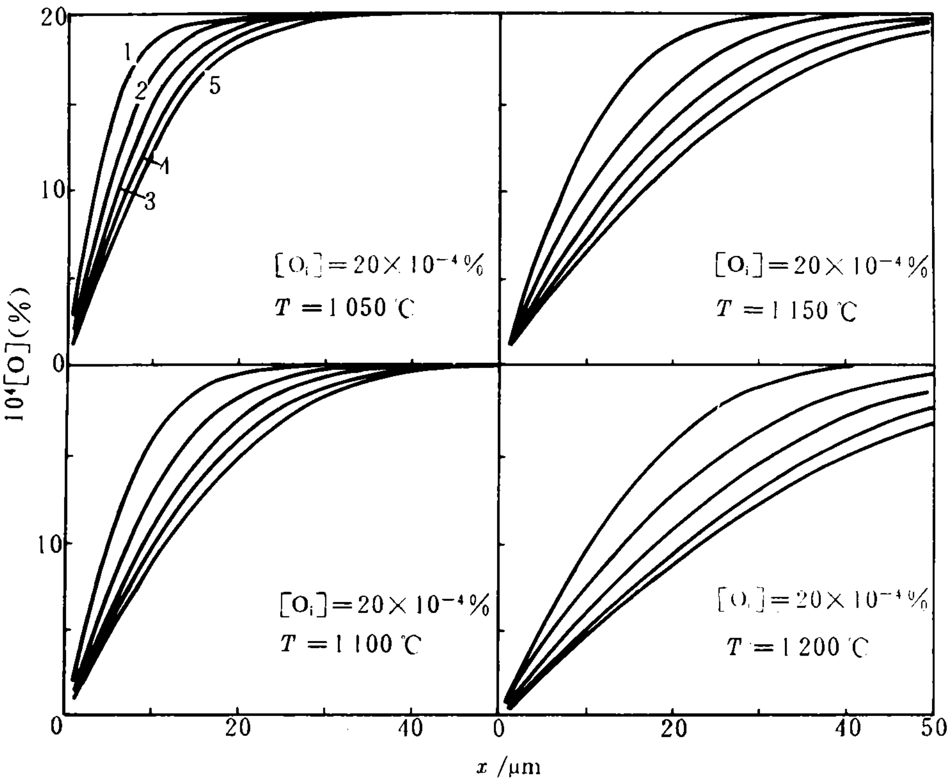

Fig. 1 Calculated vertical distribution of oxygen after outdiffusion (2)

1—1 h; 2—2 h; 3—3 h; 4—4 h; 5—5 h

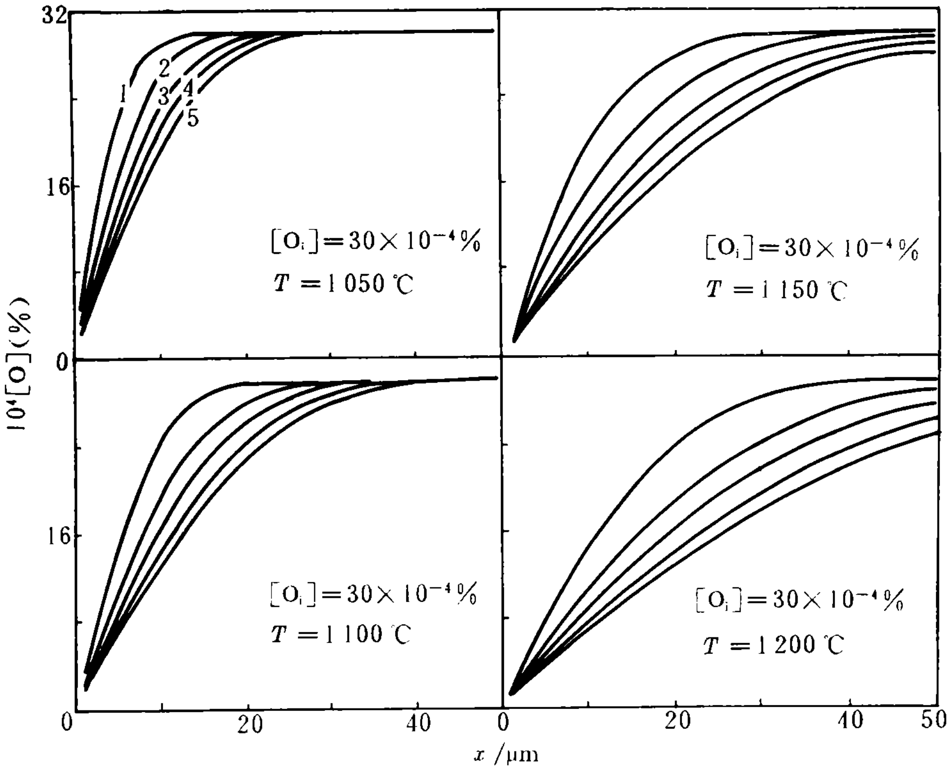

Fig. 1 Calculated vertical distribution of oxygen after outdiffusion (3)

1—1 h; 2—2 h; 3—3 h; 4—4 h; 5—5 h

Spreading resistance probe can be used when testing the concentration of carrier in micro-region. The relation between spreading resistance R_S and resistivity ρ is:

$$R_S = \rho/(4a) \tag{6}$$

where a is effective radius of spreading resistance probe. Its value is a constant for a fixed apparatus. Combining equations (5) and (6), we have:

$$N_D = 1/(4a\mu_n q R_S) = K_0/R_S \tag{7}$$

where $K_0 = 1/(4a\mu_n q)$ is a constant.

In the range 300—500 ℃, oxygen becomes a thermal donor. Its saturated concentration N_{DT} has a bearing on initial interstitial oxygen concentration $[O_i]_0$ as follows:

$$N_{DT} = K_m[O_i]_0^3 \tag{8}$$

where K_m is a constant.

Suppose the donor concentration in wafers is N_{D0} before thermal donor changes. Thus the total donor concentration after changing is:

$$N_D = N_{D0} + N_{DT} \tag{9}$$

substituting equation (9) into (7), we have:

$$N_{D0} + N_{DT} = K_0/R_S$$

combining with (8), we have:

$$[O_i]_0^3 = \frac{K_0}{K_m}\left(\frac{1}{R_S} - \frac{N_{D0}}{K_0}\right) \tag{10}$$

When oxygen distributes unevenly, equation (10) is:

$$[O_i]_0^3(x) = \frac{K_0}{K_m}\left(\frac{1}{R_S} - \frac{N_{D0}}{K_0}\right) \tag{11}$$

Uneven distribution of oxygen is formed by outdiffusion. Before diffusion, oxygen distributes evenly, and its concentration is C_0. After diffusion, if x is large enough (i. e. it reaches the stage in curve of oxygen distribution), it still exists:

$$[O_i](x) = C_0$$

Suppose R_{S1} is spreading resistance in stage tested by spreading resistance probe, and R_{S2} represents that in surface. A group of equations can be drawn from equation (11):

$$\frac{K_0}{K_m}\left(\frac{1}{R_{S2}} - \frac{N_{D0}}{K_0}\right) = 0$$

$$\frac{K_0}{K_m}\left(\frac{1}{R_{S1}} - \frac{N_{D0}}{K_0}\right) = C_0^3$$

Therefore

$$N_{D0} = K_0/R_{S2}$$

and

$$\frac{K_0}{K_m} = \frac{C_0^3}{1/R_{S1} - 1/R_{S2}}$$

substituting them into equation (11), we have:

$$[O_i]^3(x) = C_0^3(1/R_S - 1/R_{S2}) / (1/R_{S1} - 1/R_{S2}) \qquad (12)$$

In equation (12), C_0 can be determined by infrared spectrum, all of R_S, R_{S1} and R_{S2} can be decided by spreading resistance probe. Thus $[O_i](x)$ curve can be obtained from tested $R_S(x)$ curve. Conversely, the later can also get from the former.

3.2 *Experimental Methods and Results*

Wafers used are provided by Semiconductor Plant of Zhejiang University, Second Shanghai Smeltery Plant and Luoyang Monocrystalline Silicon Plant. The related parameters are listed in Table 1.

After cleaning wafers, outdiffusion was carried out on NW32 at 1 150 ℃ for 2 h, and on NW34, LC14 and LC44 at 1 200 ℃ for 2h. Then all the wafers have been done thermal donor conversion at 456 ℃ for 100h, in order to form thermal donor and reach their saturated concentration. Heat treatment was performed under argon shield. After heat treatment, the lapped angle of wafer is shown in Fig. 2. Then, ASR-210C$_2$ spreading resistance probe was employed to determine spreading resistance point by point at the pace of 5 um (converse to 0.5 μm in vertical direction). The distribution of tested spreading resistance in vertical direction was described in Fig. 3. It can be learned from Fig. 3. resistance of low-carbon (LC14, LC44) and trace-nitrogen wafers presents a curve distribution. This is the formation of thermal donor, i. e. interstitial oxygen concentration shows a curve distribution. Obviously, they are results of oxygen outdiffusion within several microns on surface, data are irregular. It may cause by abrasive piling on one side of wafers on laping machine.

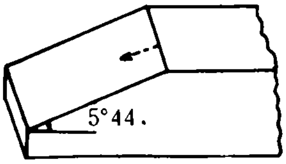

Fig. 2 Tested spreading resistance wafer

3.3 *Calculated Curve Compared With Experimental Curve*

The experimental data were showed in Fig. 4 (XXX). The curves calculated according to equations (3) and (12) and based on experimental condition was shown in Fig. 4 (—). It demonstrates that calculated curve meets experimental one very well except for several micron on surface. It also shows that data of spreading resistance tested on trace-nitrogen silicon wafer are dispersed compared with these on low-carbon silicon. This may be resulted from nitrogen pair-silicon-oxygen complexes showing electrical activity and its scattering carriers. Both the curve calculated from equation (1) and experimental curve are shown in Fig. 5. They do not meet very well than series equation (3).

Table 1 Parameters of wafers

N_D	$\rho/\Omega\cdot$cm	$[O_i]_0/10^{-4}\%$	$[C_S]$ $\times 10^{16}/\text{cm}^{-3}$	$[N_p]$ $\times 10^{15}/\text{cm}^{-3}$	type	Crystal direction	Diameter /cm	Thickness /mm
NW32	7.15	11.472	below tested limit	3.46	N	[111]	4.4	4.687
NW34	7.15	11.472	below tested limit	3.46	N	[111]	4.4	4.687
LC14	4.59	12.432	2.97	0	N	[111]	8.2	2.170
LC44	5.25	15.188	2.10	0	N	[111]	8.2	1.880

Note: Coverse $[O_i]$, $[C_S]$, $[N_p]$ according to $[O_i] = 4.90\,\alpha_{1106} \times 10^{-4}\%$, $[C_s] = 1.1 \times 10^{17}\alpha_{607}$ (cm^{-3}), $[N_p] = 1.83 \times 10^{17}\alpha_{963}$ (cm^{-3})

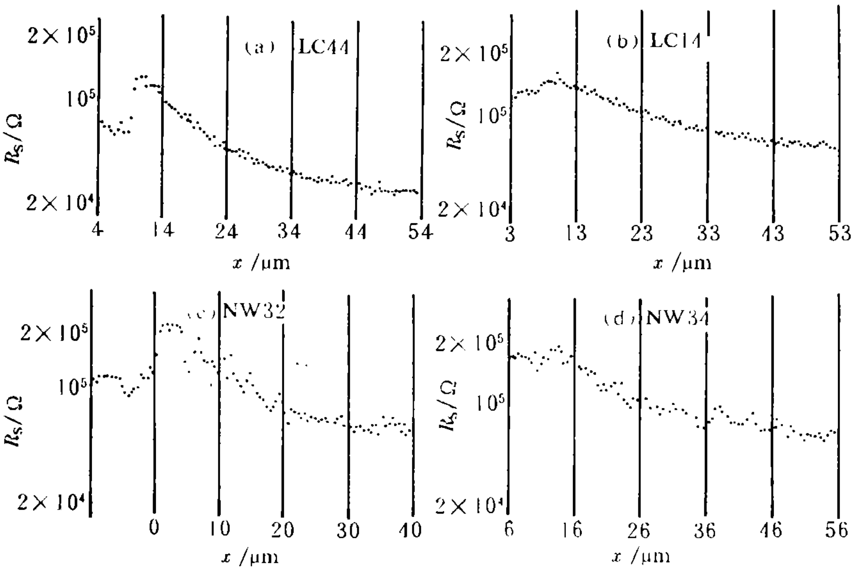

Fig. 3 After oxygen outdiffusion in low-carbon(a, b) and trace-nitrogen(c, d) CZSi wafer, distribution of vertical spreading resistance through heat donor conversion(456 ℃, 100h)

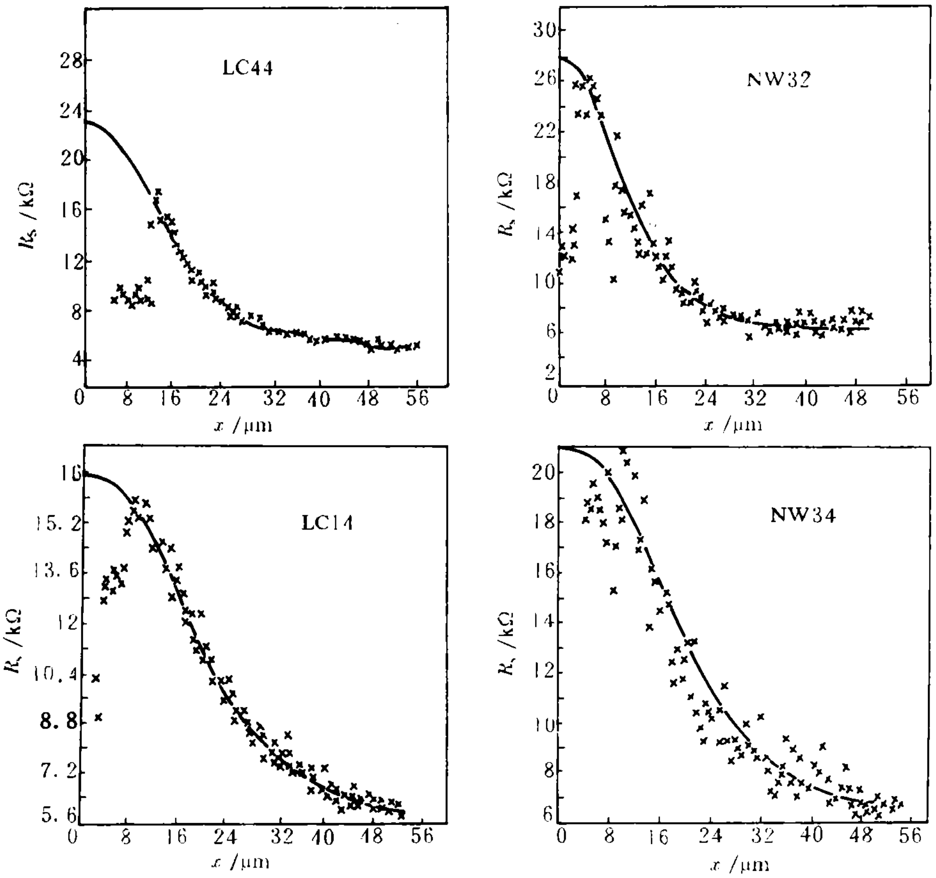

Fig. 4 Comparison of calculated curve(—)based on series equation (3) with experimental curve(XXX)

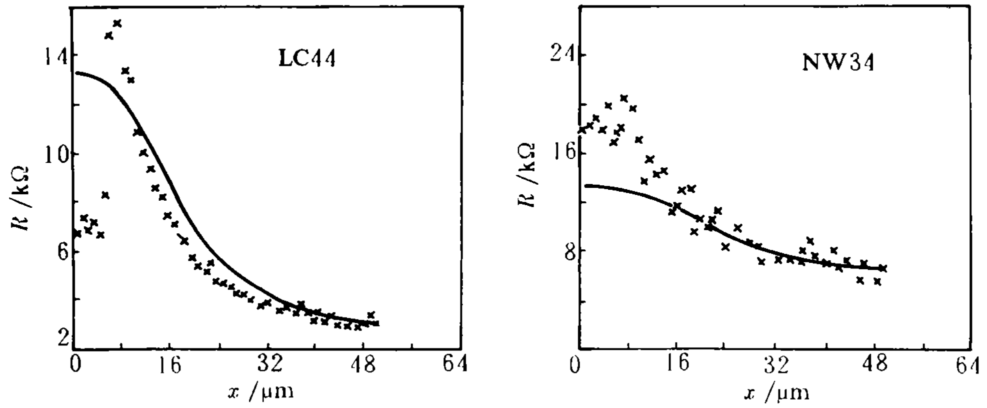

Fig. 5 **Comparison of calculated curve(—)according to error equation with experimental curve(XXX)**

4 RESULTS

Vertical distribution of oxygen after outdiffusion can be described in form of series equation (3).

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(*From page 70*)

obvious. When a superpartial moves towards the GB under an applied stress, the increase of GB energy is obscure, especially for the boron-doped Ni-rich GB.

4 CONCLUSIONS

(1) The segregation of boron lowers the energy barrier needed to be overcome to the absorption and emission of dislocations at the GB, which eases the release of stress concentration caused by the pile-up of dislocations at the GB and reduces the tendency of intergranular fracture.

(2) The effect of boron to lower the energy barrier is more pronounced in Ni-rich GBs than in Al-rich GBs. The Σ3(111) GB behaviors the lowest energy barrier to the dislocation motion. The (111)SISF superdislocation dissociation is more unfavorable, from an energy viewpoint, to the dislocation motion in the GB region than the (111)APB and (010)APB dissociations.

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