9.1 Introduction

Silicon is by far the most important material in the electronics industry. Especially the Czochralski-grown silicon crystals are suited for low-power devices, particularly for the LSI (large scale integration) and VLSI (very large scale integration) devices which are needed in logic and control electronics [1, 2]. Oxygen is the main impurity present in this material and its presence may directly or indirectly affect the electronic properties of devices. On the other hand, a controlled annealing treatment of silicon wafers known as a 'gettering process' may purify the silicon by the segregation or coprecipitation at dislocations of metallic and oxygen impurity atoms.

In the present chapter, the author has discussed the content of oxygen and vacancies in a Czochralski grown silicon in sections 9.2 and 9.3. Taking into consideration of oxygen and vacancies in the bulk the author has used a model of oxygen-vacancy - silicon clusters in the bulk to develop the thermodynamical part of the study. The model will be described in section 9.4. The large volume difference between the silicon and silicon-dioxide precipitates creates a lot of strain in the system considered. The author has calculated the strain energy as a function of temperature for various values of the number of vacancies in the
cluster in section 9.5. The results of the thermodynamic considerations are presented in section 9.6 using a systematic mathematical approach to the silicon-oxygen-vacancy complexes.

9.2 Oxygen Content in CZ Silicon

Liquid silicon reacts with the silica of the crucible as follows

\[
\text{Si} + \text{SiO}_2 \rightleftharpoons 2 (\text{SiO})
\]  

(9.1)

Until today it is not clear in which manner the oxygen is incorporated into the silicon melt [2] as dissolved [SiO]_Si or as dissolved [O]_Si. However, it is well-known that after transport through melt, the oxygen evaporates easily and rapidly at the melt surface in the form of silicon-monoxide, even at high inert gas pressure. To avoid the sublimation of SiO near the crystallisation front, i.e. at the crystal surface or in the gas above the melt, a constant stream of argon is led over the melt in order to carry away the gaseous SiO. In this way the SiO partial pressure above the melt is kept low and the evaporation of SiO is not restrained.

Substantial efforts have been and are being directed at the related problem of achieving a uniform oxygen distribution in CZ crystals. In a typical single-crucible
arrangement, the rate of oxygen incorporation is related to the rate of silica crucible dissolution and the net rate of oxygen flux into the melt. The net rate of flux into the melt is related to the algebraic sum of the rates resulting from silica crucible dissolution, due to evaporation of SiO at the melt-ambient interface and that incorporated into the growing crystal through [3, 4]

$$\frac{dQ}{dt} = \alpha_1 A_1 - \alpha_2 q A_2 - k q R A_3, \quad (9.2)$$

where $k$ is the effective oxygen segregation coefficient, $R$ is the crystal growth rate, $q$ is the oxygen concentration in the bulk of melt, $A_1$, $A_2$, and $A_3$ are crucible-melt, melt-ambient, and crystal-melt interface areas and $\alpha_1$ and $\alpha_2$ are dissolution rate of crucible and diffusion limited oxygen evaporation coefficient respectively. Eq. 9.2 is solved for the axial variation in oxygen concentration for the case of varying rates of crucible dissolution and evaporation coefficients.

According to measurements of Chaney and Varker [5] the silica is dissolved by the silicon melt at the rate of 1.5 mg SiO$_2$/hcm$^2$ ($= 6.9$ $\mu$m/h) and according to Nozaki and coworkers [6, 7], who investigated the binary phase system Si - O near the Si side, the equilibrium distribution coefficient of oxygen in silicon is 1.4. Fig. 9.1 shows
FIG. 9-1. AXIAL OXYGEN DISTRIBUTIONS IN CZ Si SINGLE CRYSTALS GROWN WITH DIFFERENT PULLING PARAMETERS. CURVES 1 AND 2 REPRESENT TYPICAL AXIAL DISTRIBUTIONS CURVES 3 TO 11 ARE FROM CRYSTALS GROWN WITH IMPROVED PROCESSES WHICH ALLOW TO GROW CRYSTALS HAVING MORE UNIFORM AXIAL OXYGEN CONCENTRATION BOTH ON HIGH AND LOW LEVELS.
\( \text{\(\bigcirc\)} = \text{ATOMS, LOCATED AT THE SURFACE OF THE UNIT CELL} \)

\( \text{\(\bigcirc\bigcirc\)} = \text{ATOMS, LOCATED AT THE INNER OF THE UNIT CELL} \)

\( a = \text{LATTICE CONSTANT} \)

\text{FIG. 9.2 SCHEMATIC VIEW OF THE DIAMOND LATTICE.}
very different axial oxygen distributions in Czochralski grown silicon single crystals, as pulled under the same conditions of pressure and argon flow. Their pulling processes differed with respect to the crystal and crucible rotation, the geometry and temperature distribution of the melt, and the direction of the argon flow above the melt. The radial variation of oxygen concentration cannot be described by a satisfactory model. The requirement of radial homogeneity suggests that the crystal rotation rate should dominate the fluid flow. In addition, a uniform boundary layer can normally be achieved only if the crucible diameter is appreciably larger than the crystal diameter by more than a factor 2 or 3. The axial gradient in oxygen can be controlled by varying the atmosphere above the melt, change or by varying the fluid flow. Lin and Pearce [8] report good radial and axial oxygen uniformity with the double crucible method.

9.3 Vacancies in CZ Silicon

Silicon crystallizes in the diamond lattice type of which the elementary cell is shown schematically in fig. 9.2. If one assembles a model of this crystal lattice with 'hard spheres', large interstices will be seen between the atoms. In these space spheres with the same radius as the lattice atoms can be placed without shifting the neighbouring atoms.
The geometrical conditions in the diamond lattice naturally favour the incorporation of interstitial atoms, whereas in the face centered cubic lattice interstitial incorporation may be difficult. On the other hand, it is plausible that in the fcc lattice vacancies, as a state of disorder, are more probable than in the diamond lattice.

These probably are the main reasons why the silicon lattice has far fewer vacancies than the well-known typical metal lattices in thermal equilibrium. However, the question of just how many vacancies and/or interstitials are present in Si in thermal equilibrium is still a hotly disputed item. Masters et al [9] give the vacancy concentration, $X_v$, in silicon as

$$X_v \approx 1000 \times \exp \left(- \frac{3.66 \text{ eV}}{kT} \right)$$

with $k = \text{Boltzmann constant} = 8.617 \times 10^{-5} \text{ eV/K}$. This expression results in a vacancy concentration of only $1.3 \times 10^{-8}$ at the melting point ($1693^\circ\text{K}$) of silicon, whereas according to Schulze [10] a typical metal lattice would have a vacancy concentration of $\approx 1 \times 10^{-3}$.

In contrast, the concentration of silicon self-interstitials amounts to $4.0 \times 10^{-7}$ at the same temperature, according to Seegar et al [11]. For the equilibrium concentration of $X_i$ of silicon self-interstitials these
authors give the following expression

\[ X_j = f_1 \exp \left( \frac{S_j^F}{k} \right) \exp \left( -\frac{H_j^F}{kT} \right) \]  

(9.4)

where \( f_1 = 1 \), \( S_j^F = 1.00 \) k \( \text{eV} \) at 570 K, \( H_j^F = 2.59 \) eV at 570 K, \( = 5.02 \) k \( \text{eV} \) at 1320 K, \( = 6.11 \) k \( \text{eV} \) at 1658 K.

Both kinds of point defects are supposed to have a high diffusivity. The diffusion coefficient of vacancies is given by [9]

\[ D_V \approx 10 \text{ cm}^2/\text{sec.} \times \exp (-1.47 \text{ eV/kT}) \]  

(9.5)

whereas according to Seeger et al [11], the diffusion coefficient \( D_I \) of self-interstitials is given by

\[ D_I = f_2 \exp \left( \frac{S_I^M}{k} \right) \exp \left( -\frac{H_I^M}{kT} \right) \]  

(9.6)

where \( f_2 = 4.2 \times 10^{-3} \text{ cm}^2/\text{sec} \)

\[ S_I^M = 1.00 \) k \( \text{eV} \) at 570 K, \( = 5.69 \) k \( \text{eV} \) at 1320 K, \( = 6.96 \) k \( \text{eV} \) at 1658 K.

The concentration and diffusion coefficients given in table 9.1 have been calculated using eqs. 9.3 and 9.6. The vacancy type precipitates in silicon is reported by Yasuami et al [12] who used diffuse X-ray scattering. According to Seeger et al [11], the self-diffusion in
Table 9.1
Concentration $X_V$ and diffusion coefficients $D_V$ of vacancies in silicon (according to refs. [9], [11]).

<table>
<thead>
<tr>
<th>Temp (K)</th>
<th>$X_V$</th>
<th>$D_V$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1693</td>
<td>$1.3 \times 10^{-8}$</td>
<td>$4.2 \times 10^{-4}$</td>
</tr>
<tr>
<td>1500</td>
<td>$5.0 \times 10^{-10}$</td>
<td>$1.2 \times 10^{-4}$</td>
</tr>
<tr>
<td>1300</td>
<td>$6.5 \times 10^{-12}$</td>
<td>$2.0 \times 10^{-5}$</td>
</tr>
<tr>
<td>1100</td>
<td>$1.7 \times 10^{-14}$</td>
<td>$1.8 \times 10^{-6}$</td>
</tr>
</tbody>
</table>
silicon is controlled by self-interstitials above 1200°K: below this temperature the diffusion of mono-vacancies predominates.

9.4 **Precipitation Model**

When the silicon wafers are annealed at any temperature in the range 400°C to 1175°C, it is expected to cause interstitial oxygen to come out of supersaturated solution in the silicon lattice according to the general formula

\[
\text{Si}(s) + x \text{I}_0 + p \text{V}_{\text{Si}} \rightleftharpoons \text{SiO}_x(s_j) + \text{strain} \quad (9.7)
\]

where \( V_{\text{Si}} \) is the silicon vacancy, \( \text{I}_0 \) is the oxygen interstitial and \( j \) refers to the type of silica phase. This is a variant of the very familiar reaction

\[
\text{Si}(s) + 0.2(0) \rightleftharpoons \text{SiO}_2(s) \quad (9.8)
\]

so obviously, one has to consider the addition reactions

\[
0.2(0) \rightleftharpoons 2.0(0) \rightleftharpoons 2 \text{I}_0 \quad (9.9)
\]

in order to develop the thermodynamic driving force for the precipitation process and this part is dealt in detail in section 9.6. The molecular volume of \( \text{SiO}_2 \) (cristobalite) is \( 4.54 \times 10^{-23} \text{ cm}^3 \) whereas the atomic volume of silicon is only \( 2 \times 10^{-23} \text{ cm}^3 \). Because of the molar volume of \( \text{SiO}_2 \) is about 2.2 times the molar volume for silicon, the formation of \( \text{SiO}_x \) from interstitial oxygen species requires the
presence of free volume in order to minimize the strain to acceptable limits. As indicated in eq. (9.7), an influx of vacancies to the forming or growing precipitate will reduce the stored strain energy and enhance the precipitation formation. Besides the available vacancies in the system, an additional source of free volume is given via the reaction involving substitutional silicon, $S_{Si}$,

$$S_{Si} \leftrightarrow I_{Si} + V_{Si}.$$  \hspace{1cm} (9.10)

One can expect eqs. (9.7) to (9.10) to occur simultaneously as oxide precipitates form and grow in size.

Recently Tiller et al [13] showed that the different precipitate morphologies could be understood by considering that the total free energy available to derive the precipitation process, $\Delta G_{\text{tot}}$, is partitioned into five sub-processes namely [14],

i) $\Delta G_{\text{o}}$, the driving force needed to transport the interstitial oxygen species to the precipitate surface

ii) $\Delta G_{\text{S}}$, the strain energy

iii) $\Delta G_{\text{f}}$, the excess free energy associated with the interfacial energy

iv) $\Delta G_{\text{V}}$, the free energy consumed in the creation of free volume and

v) $\Delta G_{\text{K}}$, the free energy needed to activate the molecular attachment process at the $\text{SiO}_{2}/\text{Si}$ interface.

This classification is represented in fig. 9.3.
\[ \text{SiO}_2 \quad \text{SILICON} \]

\[ n_{I_0}^{(0)} \quad n_{I_0}^{(\infty)} \]

\[ \Delta G_S \quad \Delta G_0 \quad \Delta G_\gamma \quad \Delta G_I \quad \Delta G_K \quad \Delta G_\infty \]

\text{FIG. 9.3}
9.5 Strain Energy

The electron microscopy data of Ponce et al [15] has shown that the different SiO₂ precipitate morphologies occur in different temperature ranges and these morphologies reveal that strain fields play an important role in this precipitation process [13, 14]. This is not surprising in view of the large difference in specific volumes between SiO₂ and Si and one can expect the need for free volume to dominate this internal SiO₂ precipitation process just as it does the external oxidation process [16].

Taking into consideration of eq. (9.7) for the precipitation of SiO₂, each SiO₂ molecule precipitating consumes p vacancies and 2 interstitial oxygen atoms for the given strain. The reaction can be written as

\[ \Delta X_{Si} + 2 \Delta X_{O} + p \Delta X_{V} \rightleftharpoons \Delta X_{p} \]  

(9.11)

where \( \Delta X_{i} \) is the change in the i species (i = Si, O, V and precipitate (SiO₂)). That is, for the given strained state, \( X_{p} \) silicon atoms, \( 2X_{p} \) interstitial oxygen atoms and \( p X_{p} \) vacancies are consumed in the formation of \( X \) silicon dioxide molecules (where \( X_{p} \) is the molefraction of SiO₂ molecules in the bulk). If \( p = 1.3 \), then a condition of zero strain is produced.

The strain in the sample, which is defined as the ratio of change in volume to the original volume, is calculated as
follows. As discussed before, to precipitate $X_p$ silicon dioxide molecules, $X_p$ silicon atoms, $2X_0$ interstitial oxygen atoms and $p X_p$ vacancies have to be consumed. Since the oxygen atoms are in the interstitial state, it is neglected to evaluate the strain. After the formation of $X_p$, the mole fraction of SiO$_2$, the bulk silicon, the change in the volume $\Delta V$

$$\Delta V = (1 - X_p) \frac{\alpha_{Si}}{1 - p X_p} - X_p(1 + p) \frac{\alpha_{Si}}{1 - X_p} - p \frac{\alpha_{SiO2}}{1 - X_p} - X_p \frac{\alpha_{Si}}{1 - X_p}$$

(9.12)

where $\frac{\alpha_{Si}}{1 - X_p}$ and $\frac{\alpha_{SiO2}}{1 - X_p}$ are the specific volumes of silicon and silicon dioxide. Therefore the strain

$$\frac{\text{change in the volume}}{\text{original volume}} = \frac{X_p \frac{\alpha_{SiO2}}{1 - X_p} - X_p(1 + p) \frac{\alpha_{Si}}{1 - X_p}}{\frac{\alpha_{Si}}{1 - X_p}} = X_p \frac{\alpha_{SiO2}}{\alpha_{Si}} - X_p (1 + p) = X_p (1.266 - p).$$

(9.13)

As an example of the relation (9.13) derived above, a silicon wafer containing oxygen of $2 \times 10^{18}/cm^3$ is considered. Using the Craven's solubility data [17]

$$\log n_0^{eq} = 21.506 - \frac{5200}{T},$$

(9.14)

and assuming the excess oxygen in the wafer gets precipitated, the mole fraction of SiO$_2$ in the same is calculated as
\[ X_p = \frac{n_0 - n_0^{\text{eq}}}{n_{\text{Si}}} \] (9.15)

where \( n_{\text{Si}} \) is the number of silicon atoms in one mole = 4.995 x 10^{22}/cm^3. Numerical values of the average strain of eq. (9.13) is presented in fig. 9.4 for various values of \( p \), the number of vacancies in the silicon-oxygen-vacancy complexes.

For a dilute solution of spherical precipitates, the strain energy per SiO_2 molecule is given by [14]

\[ \frac{\Delta G}{\Delta P} = 2 \alpha \mu_{\text{Si}} \frac{N}{n_{\text{SiO}_2}} \left( \frac{(1.3 - p) - n_{\text{Si}}}{n_{\text{SiO}_2}} \right)^2 \left( \frac{\tilde{\kappa}_{\text{SiO}_2}}{3\kappa_{\text{SiO}_2} + 4\mu_{\text{Si}}} + \Omega_{\text{SiO}_2} \right), \] (9.16)

where \( \tilde{\mu}_{\text{Si}} \) is the shear modulus of silicon, \( \tilde{\kappa}_{\text{SiO}_2} \) is the effective bulk modulus of SiO_2, \( \Omega_{\text{Si}} \) is the atomic volume of silicon and \( \Omega_{\text{SiO}_2} \) is the strained molecular volume of SiO_2, ie.,

\[ \Omega_{\text{SiO}_2} = (1 + p) \Omega_{\text{Si}} \] (9.17)

which yields

\[ \frac{\Delta G}{\Delta P} = \frac{(1.3 - p)^2}{1 + p} \Omega_{\text{Si}} \left( \frac{\tilde{\mu}_{\text{Si}} \tilde{\kappa}_{\text{SiO}_2}}{2\tilde{\mu}_{\text{Si}} + 1.5 \kappa_{\text{SiO}_2}} \right) = \tilde{\beta} \left( \frac{(1.3 - p)^2}{1 + p} \right), \] (9.18)

where

\[ \tilde{\beta} = \left( \frac{\tilde{\mu}_{\text{Si}} \tilde{\kappa}_{\text{SiO}_2}}{2\tilde{\mu}_{\text{Si}} + 1.5 \kappa_{\text{SiO}_2}} \right) \Omega_{\text{Si}} \] (9.19)
FIG. 9-4. MODULUS OF AVERAGE STRAIN AS A FUNCTION OF TEMPERATURE FOR VARIOUS VALUES OF $p$. 
FIG. 9-5. STRAIN ENERGY AS A FUNCTION OF THE NUMBER OF VACANCIES IN THE COMPLEX.
FIG. 9-6. STRAIN ENERGY AS A FUNCTION OF ASPECT RATIO.
The numerical results of the eq. (9.18) is shown in fig. 9.5 which shows the strain energy as a function of $p$, the number of vacancies in the complex. As already mentioned, when $p = 1.3$, the strain energy of the SiO$_2$ molecules is zero. The strain energy dependence of precipitate shape is a well-studied phenomenon and depends upon whether the precipitate is coherent or incoherent with the matrix and whether the two phases are elastically isotropic or anisotropic. Considering, for illustrative purposes, the simplest case of an incoherent precipitate and isotropic phases, fig. 9.6 shows the stored strain energy of an ellipsoidally shaped precipitate with semi axis $(R, R, \gamma)$ as a function of aspect ratio for the given value of $p$. From the figure, it is observed that the strain energy is maximum when the precipitate is sphere ($\frac{\gamma}{R} = 1$) and strain energy is minimum for a disc and intermediate for a rod.

9.6 Equilibrium Thermodynamics

If no free volume is provided to the SiO$_2$/Si interface, the volume strain, $\varepsilon_0$, will be so large that the strain energy $\Delta G_0$ will be larger than the total driving force, $\Delta G_\infty$ and precipitation cannot thermodynamically occur until incredibly low temperatures are reached. At the other extreme, an infinite supply of free volume allows an unstrained precipitate to form and the precipitation process can thermodynamically-
cally occur at any temperature of interest. For the realistic state inbetween, one must consider the thermodynamic process for forming a strained precipitate constrained to \( \varepsilon < \varepsilon_0 \) and must consider the mechanisms that provide the free volume to reduce the volume strain by an amount \( \varepsilon_0 - \varepsilon \).

From standard thermodynamics, one obtains the quasi-equilibrium interstitial oxygen concentration in the silicon, subject to the presence of precipitates constrained to have a volume strain of \( \varepsilon \) as follows.

\[
\text{Si(s)} + O_2(g) \rightleftharpoons \text{SiO}_2(s) + \varepsilon; \quad K_1 \exp \left( \frac{\Delta G_1}{RT} \right) \approx P_{O_2}^{-1}
\]

\[(9.20)\]

\[
O_2(g) \rightleftharpoons 2 O(g); \quad K_2 \approx P_{O_2}^{-1} P_O^2
\]

\[(9.21)\]

and

\[
O(g) \rightarrow I_0(s); \quad K_3 \approx C_0(s) P_O^{-1}
\]

\[(9.22)\]

so that

\[
C_0(s) \approx K_3 P_O \approx \exp \left\{ \left[ -\frac{\Delta G_1}{2} + \Delta G_0 \right] - \left( \Delta G_3 + \frac{\Delta G_2}{2} \right) \right\} / RT
\]

\[(9.23)\]

In eq. (9.23), \( K_3 \) has the role of a Henry's law constant and \( \Delta G_j \) are reaction free energies for equations (9.1), (9.2) and (9.3). Thus, the greater is the stored strain energy, \( \Delta G_0 \), the larger will be \( C_0 \) in the silicon.
The free energy of a system of one mole of total silicon with interstitial oxygen, vacancy and interstitial silicon defects and silicon dioxide precipitate particles and constrained to a state of volume strain $\varepsilon$ is given by

$$G = N \left[ \mu_{Si} + X_0 \mu_0 + X_V \mu_V + X_I \mu_I + X_p(\mu_p - \mu_{Si}) \right] + \Delta G_0.$$  

(9.24)

In eq. (9.24), $X_0$, $X_V$, $X_I$ and $X_p$ are the mole fractions of interstitial oxygen, vacancy, interstitial silicon and SiO$_2$ species respectively and $\mu_j$ is the chemical potential of $j$ ($j = O$, $V$, $I$ and $p$). At equilibrium, the free energy of the system, eq. 9.24, should be minimum with respect to $X_0$. In order to get the relations between the change in quantities of $X_O$, $X_V$ and $X_p$, eq. (9.11) is again used. As already discussed it is assumed in this model that the formation of each SiO$_2$ molecule consumes $p$ vacancies to produce the volume strain $\varepsilon$ and that the interstitial silicon formation reaction is independent of the precipitation reaction. Thus

$$\mu_I = 0$$  

(9.25)

$$\frac{\delta X_p}{\delta X_0} = -\frac{1}{2}$$  

(9.26)

and

$$\frac{\delta X_p}{\delta X_V} = -\frac{1}{p}$$  

(9.27)

which requires that

$$\frac{\delta X_V}{\delta X_0} = \frac{p}{2}.$$  

(9.28)
Neglecting the effect of strain on \( \mu_0, \mu_V \) and \( \mu_I \), eq. (9.24) with eq. (9.18) becomes

\[
G = N \left[ \mu_{Si} + X_0 \mu_0 + X_V \mu_V + X_p \mu_p - \mu_{Si} + \beta \frac{(1 - 3 - p)^2}{1 + p} \right].
\]

(9.29)

At any temperature, for a given \( p \), the system will seek a minimum free energy with respect to \( X_q \), i.e.,

\[
\frac{\partial G}{\partial X_q} \bigg|_p = 0.
\]

(9.30)

Since \( \mu_0 \) and \( \mu_V \), the chemical potential of interstitial oxygen and vacancy, are of the form

\[
\mu_j = H_j - TS_j + kT \ln X_j, \quad (j = 0, V)
\]

(9.31)

when \( H_j \) and \( S_j \) are the ethalphy and entropy of formation of \( j \).

From eq. (9.31) \( \frac{\partial \mu_j}{\partial X_j} = kT/X_j \), \( (j = 0, V) \)

(9.32)

so that eq. (9.30) becomes, using eqs. (9.26) - (9.28)

\[
\mu_0 + kT + \frac{p}{2} (\mu_V + kT) = \frac{1}{2} (\mu_p - \mu_{Si}) + \beta \frac{(1 - 3 - p)^2}{1 + p}.
\]

(9.33)

Fig. 9.7 shows numerically the value of \( \mu_0 + \frac{p}{2} \mu_V \) as a function of \( T \) for various values of \( p \). Thus as expected, one finds that \( X_0 \) and \( X_V \) are related for a given \( p \). Craven's experimental data [17] on the variation of \( X_0 \) allows one to evaluate both \( \Delta X_p \) and \( \Delta X_V \) and thus \( \mu_V (p) \) provided the values of \( H_V \) and \( S_V \) are known.
FIG. 9.7. NUMERICAL VALUES OF $\mu_0 + \frac{p}{2} \mu_V$ AS A FUNCTION OF TEMPERATURE FOR VARIOUS VALUES OF p.
9.7 Conclusion

Oxygen is invariably present in Czochralski grown silicon crystals at concentration levels in the vicinity of $10^{18}$ cm$^{-3}$. It originates primarily from the interaction of molten silicon with the SiO$_2$ crucible like all impurities in silicon, oxygen is not uniformly distributed. It is a highly undesirable impurity in a number of device applications.

In this chapter, the author has made an attempt to study the incorporation of oxygen in Czochralski grown silicon crystals. Taking into consideration of oxygen-vacancy-silicon complexes, a systematic mathematical approach has been made to give the qualitative treatment to the precipitation of oxides in CZ silicon crystals. Since the volume difference between the specific volumes of silicon and silicon dioxide is very large, the strain energy is evaluated due to the formation of silicon dioxide precipitates. Equilibrium thermodynamic studies have been made to the system chosen and it is shown that the equilibrium concentration of oxygen in the CZ silicon can be calculated.
References

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