Precision Interplanar Spacing Measurements of Boron-Doped Silicon

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Abstract
A study of the lattice parameters of boron-doped silicon (10¹⁴-10¹⁹ cm⁻³) grown in ⟨111⟩ and ⟨001⟩ directions by the Czochralski technique has been undertaken. Interplanar spacings (d) were measured by the pseudo-Kossel technique to a precision of 0.001%; different procedures to obtain d and the errors are discussed. The crystallographic planes are found to contract preferentially and the usual study of parameter variation must be made as a function of d. The diffused B particularly contracts the ⟨333⟩ plane, which is more pronounced in high concentrations. An orientation dependence of the diffusion during growth was observed.

Introduction
The silicon crystal-lattice distortion, resulting from impurity diffusion, has been widely studied owing to interest in solid-state devices. Pearson & Bardeen (1949) studying the electrical properties of undoped and boron-doped silicon verified that the presence of substitutional B in the silicon lattice as acceptor impurity produces a lattice contraction. Horn (1955) arrived at the same conclusion, employing density measurements in addition to lattice parameters, electrical and chemical analyses. The B diffusion (5 × 10²⁰ cm⁻³) in silicon wafers reduces the lattice parameter because of the different values of the ionic radii of Si atoms (1.7 Å) and substitutional B atoms (0.98 Å) (Queisser, 1961; Carruthers, Hoffman & Ashner, 1963); this reduction introduces a uniform deformation and for adequately large values it favours the formation of dislocations, regularly distributed in the slip planes. Cohen (1967) considered that discrepancies found in the contraction coefficient of the silicon lattice are due to the non-consideration of deformation produced by diffusion process and the defect complexes formed; the generation of excess vacancies would be one of the factors contributing to make the diffusion a function of the temperature (Jain & Van Overstraeten, 1973).

Fukuhara & Takano (1977), employing X-ray techniques, confirmed some of the results of Queisser (1961) verifying the proportionality between the elastic deformation and the B concentration; after a critical value of deformation, defects like dislocations appear in order to relax that deformation and proportionality is no longer valid.

The B diffusion process is certainly related to the so-called microdefects in Si. Despite intensive efforts, basic questions about point defects in Si are still unanswered or hotly disputed, with the consequence that all the important diffusion mechanisms of impurities are still not known with certainty (Föll, Gösselle & Kolbesen, 1981). Besides that, some crystallographic aspects of the B diffusion process are not well known.

In previous papers describing the silicon crystal-lattice distortion resulting from boron diffusion, a uniform lattice contraction was assumed since it is usually expressed in terms of a variation Δa of the cubic cell parameter a. This paper presents an accurate study of the crystalline parameter variation of boron-doped silicon single crystals grown by the Czochralski method and doped by diffusion during growth. The orientation dependence of diffusion of B in silicon slices has been pointed out (Allen & Anand, 1971, among others) but a possible relation among the crystal growth direction, diffusion process and alteration of crystallographic parameters has not been established. This paper also presents a correlation between growth direction (⟨100⟩ and ⟨111⟩) and interplanar spacing of the silicon doped lattice during growth.

The back-reflection pseudo-Kossel technique was employed to determine lattice parameters with a precision of 0.002% (Berg & Hall, 1974). This technique has the advantage of allowing the separate determination of interplanar spacings from planes of the same family, providing a technique for investigating anisotropy (Newman & Shrier, 1970).

Several methods of measuring interplanar spacings with precision, using the back-reflection X-ray divergent-beam technique, have been suggested (for a
difficulty with this technique is that the pseudo-Kossel lines are complicated fourth-degree equations and the assumption that they are conics would lead to significant error (Newman, 1970). The incomplete formation of the curves, due to some sub-structure in the specimen, constitutes another limitation for several methods.

In order to overcome these difficulties Schneider & Weik (1967) have suggested geometrical methods, utilizing double exposures, which are conveniently applicable to the study of anisotropic distortions in single crystals. A discussion of the geometrical limitation of this method was presented by Newman & Shrier (1970) who suggested another method utilizing the coordinates of general points of the lines rather than their special geometrical properties. A double exposure of the film is also employed by Newman & Shrier but the corresponding points are established by utilizing discontinuities produced by fine shadows of a wire grid on the pseudo-Kossel curve; from the measurements of the shadow displacements due to film translation the direction cosines of a particular diffracted beam can be determined.

Aristov, Shekhtman & Shmytko (1974) employed an analogous method utilizing a screen of copper wires (\(\phi \sim 1 \text{ mm}\)) in the form of a radial net to create sharp breaks on the diffraction lines; interplanar spacing measurements have shown that the method guarantees an error \(\Delta d/d\) of less than 0.0005. Employing basically the same experimental procedure, another approach to this technique was given by Aristov & Shmytko (1978); they considered that the precision of lattice-parameter measurements can be increased if the calculation of the Bragg angle is obtained by combining the approach based on the direction cosines of three arbitrary diffracted rays on the same diffraction surface and that employed in the Debye–Scherrer method; this procedure allows high accuracy \(\Delta d/d = 3 \times 10^{-5}\), but it is comparatively more labour consuming.

Aristov, Shekhtman & Shmytko (1974) have proposed that the precision in the determination of the crystallographic parameters by their method can be improved if necessary by increasing the number of exposures, the number of breaks on the lines, the \(\Delta z\) displacement of the cassette, as well as by a special mathematical treatment. The accuracy constraints of this technique are associated with the comparatively high error in determining each of the coordinates of the gap points (Aristov & Shmytko, 1978).

This paper employs the method suggested by Newman & Shrier (1970) and Aristov, Shekhtman & Shmytko (1974) improving some experimental procedures, such as employing a screen of very thin tungsten wires to create the breaks on the diffraction lines (Koishi & Gilles, 1979). A brief discussion of the procedures employed to determine the interplanar spacings and of the errors involved is also presented.

**Experimental**

Silicon single crystals were grown by the Czochralski method and doped by a diffusion process during the growth. The doping was carried out with acceptor-type impurity (boron) at concentrations in the solid up to \(10^{19} \text{ cm}^{-3}\). The silicon wafers were 4 cm in diameter, nominally 200 \(\mu\)m thick with the surface crystallographic plane perpendicular to the growth direction \((<111>\) and \(<001>)\). In order to remove the surface stress introduced by the cutting process, the wafers were polished by the usual chemical–mechanical process. The silicon wafers of normal semiconductor-grade specifications belong to batches usually utilized in microcircuit devices in the Microelectronic Laboratory of the Politechnic School, S. Paulo University.

The concentrations of electrically active dopants were determined with the four-point probe technique; this measurement also allows the verification of the resistive homogeneity of the samples within 0.5%. Thickness homogeneity was verified with a precision of 0.1 \(\mu\)m by a capacitive process. The radius of curvature was determined from a light interferometer and in some samples also by a transmission topographic camera (Lang type). The profile analysis of the Bragg reflection in an X-ray double diffractometer was employed to ensure the crystalline homogeneity (Brito Filho, 1981; Pimentel & Brito Filho, 1983).

In order to characterize the general perfection of the wafers, the X-ray transmission topographies of samples 1, 3 and 5 (Table 1) were obtained (Pimentel, 1982). They show a monotonous grey feature without the typical images of line dislocations and surface imperfections due to growth, cutting and polishing processes. The topography from the 444 reflection of sample 5 shows the swirl defect. The X-ray topographic sections show interference fringes of high uniformity for boron concentrations \(C_B \leq 10^{18} \text{ cm}^{-3}\) with some internal distortion for \(C_B \geq 10^{18} \text{ cm}^{-3}\); the dynamical image of the microdefects could be seen in some topographic sections.

The samples with boron concentration higher than \(10^{18} \text{ cm}^{-3}\), despite their thinness, were completely (100%) absorbent to infrared radiation, making impossible any infrared absorption spectroscopic analysis. For the samples with lower B concentration this analysis was performed in a differential form, employing a standard floating-zone silicon crystal from the General Diode Corp. (200 \(\Omega\) cm resistivity) with low carbon and oxygen concentration; the differential curves obtained did not show oxygen or carbon absorption lines. When the growth conditions, the electrical performance and the general crystallographic characteristics are considered, it is
Table 1. General characteristics of boron-doped silicon samples, mean interplanar spacings for \{hkl\} planes and the corresponding standard deviation of the mean value (68% confidence level)

<table>
<thead>
<tr>
<th>Sample</th>
<th>Growth direction</th>
<th>Resistivity (Ω cm)</th>
<th>Concentration (cm⁻³)</th>
<th>Mean interplanar spacing (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>⟨100⟩</td>
<td>19</td>
<td>7·0 × 10¹⁴</td>
<td>0·82854</td>
</tr>
<tr>
<td></td>
<td></td>
<td>7·0 × 10¹⁴</td>
<td>8·5829</td>
<td>0·91894</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0·9 × 12</td>
<td>1·5 × 10¹⁴</td>
<td>0·00016</td>
</tr>
<tr>
<td>2</td>
<td>⟨111⟩</td>
<td>9</td>
<td>7·0 × 10¹⁴</td>
<td>0·82743</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1·5 × 10¹⁴</td>
<td>8·5862</td>
<td>0·91757</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0·015</td>
<td>0·82750</td>
<td>0·00009</td>
</tr>
<tr>
<td>3</td>
<td>⟨100⟩</td>
<td>0·9 × 12</td>
<td>1·6 × 10¹⁴</td>
<td>0·00009</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1·6 × 10¹⁴</td>
<td>8·5840</td>
<td>0·91883</td>
</tr>
<tr>
<td>4</td>
<td>⟨111⟩</td>
<td>0·0108</td>
<td>7·0 × 10¹⁴</td>
<td>0·000038</td>
</tr>
<tr>
<td></td>
<td></td>
<td>7·0 × 10¹⁴</td>
<td>8·5859</td>
<td>0·91722</td>
</tr>
<tr>
<td>5</td>
<td>⟨100⟩</td>
<td>0·0108</td>
<td>9·6 × 10¹⁴</td>
<td>0·00038</td>
</tr>
<tr>
<td></td>
<td></td>
<td>9·6 × 10¹⁴</td>
<td>8·5808</td>
<td>0·91751</td>
</tr>
<tr>
<td>6</td>
<td>⟨111⟩</td>
<td>0·0058</td>
<td>2·0 × 10¹⁵</td>
<td>0·000011</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2·0 × 10¹⁵</td>
<td>8·5866</td>
<td>0·91640</td>
</tr>
</tbody>
</table>

The characteristics of the silicon samples (growth orientation, electrical resistivity and boron concentration) are shown in Table 1, together with the experimental results.

The pseudo-Kossel back-reflection patterns were obtained with a Rigaku Microflex apparatus employing Cu Kα radiation (40 kV, 65 μA) with a focal spot of 60 μm: a screen of tungsten wires (Ω ~ 0·2 mm) in the form of a quadratic net of 20 × 25 cm between the crystal and the film produced the 'shadows' on the patterns. The focus-screen distance was 55 and 75 mm, respectively, in the first and second exposures. It is necessary to avoid the contribution of the crystal edge to the patterns since the polishing process may change the edge thickness, with consequent variation of the sample curvature. On the other hand, only for sample-focus distances > 3·0 mm is it possible to obtain the pseudo-Kossel lines corresponding to {533} and {444} of crystals with growth directions respectively ⟨111⟩ and ⟨001⟩. These facts have limited the sample-focus distance to 3·0–3·5 mm. The samples were mounted vertically in a goniometer and set parallel to the film cassette. Sakura and Kodak films with one emulsion removed were used.

Several factors contribute to the precision of the measurements and careful calculations or estimates were made for each source of error. The temperature of the sample during exposure can be taken to be within ±0·2 K and the determined interplanar spacing values correspond to 294 K. For the silicon, a temperature change of 0·1 K near 298 K and 2θ₀ = 157° (Hubbard, Swanson & Mauer, 1975) alters this d₃₂₅ interplanar value by ~4 × 10⁻⁵%. A variation of ±2 K changes both extreme measured interplanar spacings by about 0·001% or, in other terms, changes d₀₀₄ and d₄₄₄ respectively by ±5 × 10⁻⁶ Å and ±5 × 10⁻⁷ Å. Hence, changes in temperature several times the controlled tolerance would not affect the calculated interplanar spacings. The error due to sample curvature (Berg & Hall, 1974) is less than 10⁻⁶ Å since the curvature radius is larger than 200 m, except for sample 2 (curvature radius ~ 8 m), for which the estimated error is less than 3 × 10⁻⁵ Å. The calculated precision in the displacement z of the cassette and the estimated buckling of the film in the cassette show that both may introduce an error in dₙₙₙ of less than 0·05%. The shrinkage of the photographic material was calculated and the error introduced by the development process in dₙₙₙ is about 0·001%. Measurements on the film were made with an Enraf-Nonius microdensitometer fitted with a 3 x telescope; this coordinate measuring constitutes the main source of error and is due to the absolute uncertainty in the reading (±0·005 mm), the observer, the line width and the edges of breaks, despite their sharpness. In order to minimize this error, for each particular (hk1) plane the coordinates (x, y) were measured from seven to twelve pairs of discontinuities on the hk1 diffraction lines.

Considerations of the pseudo-Kossel method

The pseudo-Kossel lines were indexed by comparison with a theoretical pattern obtained by a computer program (Koishi & Gilles, 1979) that takes into account the experimental conditions and gives reflection conics on the crystal surface. Table 2 shows the plane family {hkl} and reflections hkl appearing in the pseudo-Kossel patterns in the particular experimental conditions for samples with ⟨111⟩ and ⟨001⟩ growth directions.

A computer program has calculated the direction cosines of the diffracted rays defined for each pair of coordinates (x, y) and the displacement z of the film.
Table 2. hkl reflections appearing in pseudo-Kossel patterns for samples with ⟨111⟩ and ⟨001⟩ growth directions parallel to the incident beam

<table>
<thead>
<tr>
<th>(hkl) plane</th>
<th>⟨111⟩</th>
<th>⟨001⟩</th>
</tr>
</thead>
<tbody>
<tr>
<td>(444)</td>
<td>(444)</td>
<td>(335)</td>
</tr>
<tr>
<td>(533)</td>
<td>(335)</td>
<td>(335)</td>
</tr>
<tr>
<td>(620)</td>
<td>(315)</td>
<td>(015)</td>
</tr>
<tr>
<td>(531)</td>
<td>(315)</td>
<td>(135)</td>
</tr>
<tr>
<td>(440)</td>
<td>(315)</td>
<td>(035)</td>
</tr>
<tr>
<td>(511)</td>
<td>(315)</td>
<td>(135)</td>
</tr>
<tr>
<td>(333)</td>
<td>(315)</td>
<td>(135)</td>
</tr>
<tr>
<td>(242)</td>
<td>(315)</td>
<td>(135)</td>
</tr>
<tr>
<td>(004)</td>
<td>(315)</td>
<td>(135)</td>
</tr>
</tbody>
</table>

providing N directions (N = 7 to 12 in this paper); the direction cosines of the normal to an (hkl) plane was obtained from the system of equations (Newman & Shrier, 1970):

\[
s_i, m = \sin \theta_i \quad (i = 1, 2, ..., N)\]

where \(s_i\) represents the direction cosine of the diffracted ray (DCD), the components of \(m\) represent the direction cosines of a solution for the unit vector normal to an (hkl) plane (DCN) and \(\theta\) the Bragg angle.

By procedure I, one solution for DCN was obtained from each triplet of DCD; the N DCD values were combined three at a time, leading to \(N'\) solutions or \(N'\) values for DCN. Consequently, \(N'\) values for \(\sin \theta\) were determined and employing the Bragg law and the \(\lambda\) value, \(N'\) values for \(d(hkl)\) were obtained (Koishi & Gilles, 1979). In this paper selected data reducing the \(N'\) values to \(n < N'\) were employed in order to avoid the introduction of rough errors in the mean value \(\bar{d}_{(hkl)}\). This can particularly occur when the triplet of DCD corresponds to consecutive discontinuities on a diffraction line near to the centre of the film; in this case, the distances between the discontinuities are very small leading to high values for the relative errors. The mean interplanar spacing of an (hkl) plane \([\bar{d}_{(hkl)}]\) was given by the arithmetic average for the \(n\) values; \(\sigma_i\) is the standard deviation of the distribution.

For an {hkl} plane family,

\[
\bar{d} = \frac{\sum_{i=1}^{r} \omega_i d_i}{\sum_{i=1}^{r} \omega_i}, \quad \sigma_i = \frac{n_i d_i}{\sum_{i=1}^{r} n_i \sigma_i^2}
\]

where \(r\) corresponds to the number of (hkl) planes of a same {hkl} family, and \(\omega_i = n_i/\sigma_i^2\). The standard deviation of this global mean value is given by

\[
\sigma_{\bar{d}}^2 = \frac{1}{n-r+1} \sum_{i=1}^{n-r} \frac{(\bar{d} - \bar{d}_i)^2}{\sigma_i^2}
\]

Employing algebraic artifices and definitions of mean values and deviation, it is possible to simplify and rewrite this last expression:

\[
\sigma_{\bar{d}}^2 = \frac{n-r+1}{n-1} \sum_{i=1}^{n-r} \frac{1}{\sigma_i^2}
\]

Procedure II followed the approach suggested by Newman & Shrier (1970); (1) was rewritten in a more suitable form:

\[
s_{zi} = a s_{xi} + b s_{yi} + c,
\]

where

\[
a = -\frac{n_x}{n_z}, \quad b = -\frac{n_y}{n_z} \quad \text{and} \quad c = \frac{\sin \theta_i}{n_z}
\]

and \(i = 1, ..., N\). In this paper, in order to determine the parameters \(a, b, c\) of the system of \(N\) equations, the REGRE/IBM program was used employing multiple linear regression (Ostle, 1954). The mean interplanar spacing of an (hkl) plane is given by

\[
\bar{d}_i = \frac{\lambda (1 + a^2 + h^2)^{1/2}}{2 |c|}
\]

For an {hkl} plane family, the average interplanar spacing \(\bar{d}\) is given by the arithmetic average of the \(r\) values of \(d_i:\)

\[
\bar{d} = \frac{\sum_{i=1}^{r} d_i}{r} \quad (r = 3 \text{ to } 8)
\]

and the corresponding standard deviation by
Table 3. Values of mean interplanar spacing ($\overline{d}$), standard deviation ($\sigma_d$), standard deviation of the mean value ($\sigma_\overline{d}$) and degrees of freedom (n) for \{hkl\} planes obtained from procedures I and II (sample 5)

<table>
<thead>
<tr>
<th>{hkl}</th>
<th>Procedure</th>
<th>$\overline{d}$</th>
<th>$\sigma_d$</th>
<th>$\sigma_\overline{d}$</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>{531}</td>
<td>I</td>
<td>0.91758</td>
<td>0.00397</td>
<td>0.00018</td>
<td>487</td>
</tr>
<tr>
<td></td>
<td>II</td>
<td>0.91751</td>
<td>0.00065</td>
<td>0.00023</td>
<td>8</td>
</tr>
<tr>
<td>{620}</td>
<td>I</td>
<td>0.85803</td>
<td>0.00135</td>
<td>0.00010</td>
<td>198</td>
</tr>
<tr>
<td></td>
<td>II</td>
<td>0.85808</td>
<td>0.00064</td>
<td>0.00038</td>
<td>4</td>
</tr>
<tr>
<td>{335}</td>
<td>I</td>
<td>0.82800</td>
<td>0.00162</td>
<td>0.00012</td>
<td>182</td>
</tr>
<tr>
<td></td>
<td>II</td>
<td>0.82810</td>
<td>0.00017</td>
<td>0.00011</td>
<td>4</td>
</tr>
</tbody>
</table>

The values of $\overline{d}$, $\sigma_d$ (and the corresponding standard deviation of the mean value, $\sigma_\overline{d}$) obtained from procedures I (expressions 2, 3) and II (expressions 4, 5) are shown in Table 3 for some planes \{hkl\}.

The relative discrepancy between the $\overline{d}$ values obtained from procedures I and II is in general less than 0.01% and is always within the standard deviation of the mean value. The largest difference between these procedures occurs in the $\sigma_\overline{d}$ values since procedure I leads to a set of $d_{(hkl)}$ values much more dispersive than procedure II, despite the mean value being practically the same, as well as their standard error (perhaps a little under-estimated in procedure I).

Expressions (1) can be thought of as equations of a plane where $\sin \theta_i$ is the origin–plane distance and the components of $s_i$ are coordinates of a point belonging to that plane. Procedure I determines a plane for each triplet of points and therefore the corresponding $d_{(hkl)}$ value; this means that not all these $d_{(hkl)}$ values are independent. In this procedure, sets of very close and very distant points were given equal weighting. This implies a not very well defined average and an over-estimated dispersion among the $d_{(hkl)}$ values: therefore it is impossible to employ the $\sigma_\overline{d}$ values in order to estimate the dispersion among the $\overline{r}$ values of $d_{(hkl)}$ planes which would give an idea about the anisotropic alterations in planes belonging to the same family. Procedure II adjusts the best plane containing the N points and the distances between the points are taken as weight. It was considered that this last procedure leads to a best determination of $\overline{d}$ values with an improved precision ($\sigma_\overline{d}$ low) and it was utilized in this paper.

**Results and discussion**

A typical back-reflection pseudo-Kossel pattern is shown in Fig. 1. The pseudo-Kossel lines of all the patterns did not show displacements, breaks or preferential enlargement, which are related to several types of local defect in atomic planes (Vasil’ev & Ivanov, 1970); in particular, the anisotropic pseudo-Kossel line broadening is mainly due to the presence of dislocations (Barabash & Ryaboshapka, 1976). A quantitative measurement of the width of the pseudo-Kossel line was performed in a microdensitometer (Joyce Loebel, type 3 CS) for samples 1, 5 and 6 and for another \langle 111 \rangle Si sample ($\rho \sim 200 \Omega$ cm) from Hooboken. Samples 1 and 5 did not show significant alterations in the 400 line width. On the other hand, a broadening of about 80% was observed in the 333 line width from sample Hooboken to sample 6 but it occurs isotropically, without preferential enlargement. A quantitative analysis of the line-width broadening has not been performed yet.

Table 1 shows the values of mean interplanar spacings and the corresponding standard error for the most significant planes. It is worth while to note that although it is possible to obtain in the pseudo-Kossel patterns the \{hkl\} reflections presented in Table 2 some of them are not adequate for precise measurements: low-order reflections are characterized by large errors; reflection lines 444 cover a very small area and are not always completely available on the film.

The usual procedure to study the lattice-parameter variation in a cubic system investigates the cell parameter $a$. The precision determination of this $a$ parameter by the X-ray divergent-beam method was carried out by adopting the sequence of steps given by Ellis, Nanni, Shrier, Weissmann, Padawer & Hosokawa (1964). The lattice parameters $\overline{a}$ were computed using the relation $\overline{a} = \overline{d(r^2 + k^2 + l^2)}^{1/2}$. The $d$-spacing errors, and therefore the error in $\overline{a}$, diminishes with increasing $\overline{r}$; this behaviour is common to all diffraction methods in which the highest precision of measurements is obtained from lines with the largest diffraction angles (Ellis, Nanni, Shrier, Weissmann, Padawer & Hosokawa, 1964). As proposed by these authors, a value of the Nelson–Riley function was determined for each $\overline{a}$ of an

Fig. 1. A typical back-reflection pseudo-Kossel pattern of B-doped Si (part of the pattern). The sharp lines do not show displacements, breaks or preferential enlargements.
The lattice parameter $a_0$ was obtained by extrapolation of the Nelson–Riley plot of the weighted $(1/\sigma^2)a'$ values. For samples with high $B$ concentration the analysis of this graph has shown a dispersion from that linear function, higher than the experimental error. Besides that, it was observed that the more dispersive $d$ values presented high $\sigma_d$ values, meaning that they did not contribute practically to the $a_0$ value extrapolated. If the physical significance of $\sigma_d$ is taken into account and related to the residual strain distribution in the crystal (Ellis, Nanni, Shrier, Weissmann, Padawer & Hosokawa, 1964), it can be seen that the planes $\{hkl\}$ most affected by the boron diffusion process are those that contribute least in obtaining the estimate of the lattice-parameter alteration. Of course, that procedure would have been valid if the $B$ diffusion process should affect equivalently all the planes, which means an isotropic contraction. Therefore it was considered that in the present study the relationship between the $B$ concentration and the contraction of specific interplanar spacings should be investigated.

Fig. 2 shows graphs of mean interplanar spacings of several planes $\{hkl\}$ related to boron concentration values; the plotted values are identified according to the growth directions of the samples. The interplanar spacings for high-purity perfect silicon measured by the same X-ray method (Aristov & Shmytko, 1978) are also shown on the graphs in order to compare the lattice interplanar spacings of undoped and B-doped silicon single crystals.

Fig. 2. Variation of mean interplanar spacings $d$ of $\{hkl\}$ planes with the boron concentration $C$ of silicon samples grown in $\{111\}$ ($\{1\}$) and $\{001\}$ ($\{2\}$) directions ($\{3\}$ values from Aristov & Shmytko, 1978).

The diverse behaviour of the distinct planes, suffering preferential contractions or little affected by the doping, is evident. The actual occurrence of this particular behaviour did not allow the usual analysis of the lattice contraction coefficient to be carried out as a function of doping concentration, taking into account just an average of the cell parameter $a_0$. This is particularly serious if the boron concentration is $10^{18}$-$10^{19}$ cm$^{-3}$.

As a general tendency, a decrease of the $d$ values with the increase of $B$ concentration can be seen, and in a more pronounced form for $10^{18}$-$10^{19}$ cm$^{-3}$, meaning that in general the interplanar spacings tend to contract. Nevertheless, the $\{hkl\}$ planes have suffered different contractions, the $\{333\}$ apparently being most affected and the $\{620\}$ planes the least.

An interesting aspect is the systematic behaviour of samples depending on the growth direction. It can be noted that interplanar spacings of $\{533\}$ and $\{531\}$ planes from $\{111\}$ are smaller than those for the $\{001\}$ samples; in a not well-defined form, the reverse seems to occur for the $\{620\}$ planes. This indicates an orientation dependence of the diffusion of boron in silicon during growth, analogous to the observation in silicon slices where boron depositions were carried out (Allen & Anand, 1971; Allen, 1973). For both growth directions, each particular reflection shows similar dependence of the interplanar spacing with $B$ concentration.

The causes of that contraction should not be immediately attributed to the presence of substitutional boron in the silicon lattice. The two major non-intentionally doped impurities in silicon crystals, oxygen and carbon, may also contribute to alter the lattice parameters. The oxygen is incorporated into the silicon lattice as a solid solution occupying interstitial sites, causing a lattice expansion; on the other hand, the carbon occupies substitutional sites, contracting the Si lattice, but it may also be located interstitially (for concentration $\sim 10^{18}$ cm$^{-3}$), expanding the lattice (Liaw, 1979). It is possible that these impurities may contribute to some non-uniform behaviour of the $d$ parameter as a function of the $B$ concentration. Nevertheless, based on the previous considerations on the presence of $C$ and $O$, it is possible to propose that the marked contraction in the $\{333\}$ plane for concentrations $\sim 10^{18}$-$10^{19}$ cm$^{-3}$ is due to the presence of the doping. This could be better understood if it were to be established that the substitutional boron was located preferentially on the $\{111\}$ planes. However, to obtain such information would necessitate undertaking a considerably more detailed and precise investigation of the lattice contraction than reported in the present paper. The possibility of a preferential distribution of microdefects particularly in heavily doped silicon samples is not discarded (Brito Filho, 1981; Pimentel & Brito Filho, 1983).
Conclusions

It is concluded that the boron doping process in silicon during the Czochralski growth introduces preferential alterations in the Si lattice; the usual study of parameter variation must be done as a function of interplanar spacings of the lattice since the diffusion process affects differently the crystallographic planes. The presence of boron in the Si lattice produces a concentration-dependent contraction of the lattice, at least for concentrations up to $10^{18}$ cm$^{-3}$. This reinforces the hypothesis of the presence of substitutional B in the Si lattice. For identical crystallographic planes the interplanar spacings of samples grown in different orientations suffer distinct alterations with the B concentration. Hence, it is concluded that there is an orientation dependence of the diffusion of B in Si during the Czochralski growth.

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