Microdefect formation in heavily-doped silicon crystals

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Introduction

• Large diameter crystals with increasingly higher doping levels are required to support the expanding market of discrete devices.
• The increase in dopant concentration affects significantly the crystal quality, changing dramatically the paradigms established for lightly-doped crystals and commonly accepted in the technical community.
• This talk describes the impact of a high concentration of donor atoms on the properties of 200mm diameter Czochralski-grown silicon crystals, and specifically on the formation of voids (COPs).

Point Defects

Vacancies

Microdefects

Voids
(v-clusters, D Defects or COPs)

COP formation in heavily-doped silicon crystals
COP formation in heavily-doped silicon crystals

• 200mm diameter, <100> oriented CZ silicon crystals
• Donor type dopants: phosphorus, arsenic, antimony.
• The resistivity axial profile was measured by 4-point probe.
• Resistivity range covered:
  – 12 - 50mΩ•cm for antimony,
  – 2.1 - 6.5mΩ•cm for arsenic
  – 1.1 - 4.3mΩ•cm for phosphorus.
• Grown-in microdefects were revealed by copper decoration (900°C for 20min), preferential etching and inspection under collimated light.
• Wafers were sampled at selected locations based on the resistivity profile.
• For each position, sister wafers were taken. All wafers were identified with a unique laser mark and processed through the wafering line as a single lot, to assure the same processing conditions, in particular the same surface finish (polishing and cleaning).
Experimental - 2

• Group 1: surface defects were counted by means of Tencor SP1, adopting a threshold of 0.12 microns (latex sphere equivalent). The measurement was done in oblique mode, in order to separate surface particles from voids. After the first measurement, the wafers were submitted to repeated cleaning cycles and remeasured, to check the impact of a prolonged cleaning on the enlargement of the void size and therefore on their detectability.

• Group 2: the defects identified by laser inspection (SP1 events) were evaluated by Atomic Force Microscope using AFM Dimension5000 in tapping mode at higher resolution to examine their morphology and confirm their nature as voids. This was additionally checked by examining selected wafers after Secco etch to reveal the formation of Flow Pattern Defects (FPD).
Results – COPs Vs Resistivity

Void counts in dependence of the resistivity for P-doped wafers (empty circles), As-doped wafers (full circles) and Sb-doped wafers (patterned circles). The lines are just an aid to the eye.
Results – COPs & repeated cleaning

Void counts after repeated cleaning cycles as a function of the wafer resistivity. The numbers 1, 3, 5, 7 indicate the number of cleaning cycles applied.

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AFM image of a single void in arsenic-doped wafer (6.7 mΩ·cm) in the centre of the wafer. The SP1 size is 0.155 µm.

AFM image of a double void in arsenic-doped wafer (4.5 mΩ·cm) near the edge of the wafer. The SP1 size is 0.148 µm.

In the case of antimony, six defects were analysed and all were single voids. For phosphorus, one defect out of 4 was a double-void (25%). In the case of arsenic, 8 defects out of 13 were double voids (60%).
Results – Flow Pattern Defects

Images of flow pattern defects observed under optical microscope on the surface of wafers after Secco etch. **Left**: phosphorus-doped, **Center**: arsenic-doped, **Right**: antimony-doped sample. The images show the defects upside down. The scale marker corresponds to 20 microns.

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Results – SP1 maps - As

COP formation in heavily-doped silicon crystals
Results – SP1 maps - P

COP formation in heavily-doped silicon crystals
Results – SP1 maps - Sb

COP formation in heavily-doped silicon crystals

12\text{m}\Omega\cdot\text{cm} 

17\text{m}\Omega\cdot\text{cm} 

30\text{m}\Omega\cdot\text{cm}
Results - Copper decoration test

Microdefect pattern of copper-decorated As-doped samples with a resistivity decreasing from left to right.
Discussion

Impurities can affect the value of the critical V/G ratio between the pull speed V and the axial thermal gradient G that separates the vacancy-rich and the interstitial-rich growth regime.

The increase in vacancy concentration with increasing donor doping can be explained by the formation of dopant-vacancy complexes (VMₘ), such as SbV or AsV, which act as trapped vacancies and preserve them from annihilation with interstitials, making them available for void formation. The sharp reduction of void formation at even higher donor concentration (here observed only for As and P) can be explained assuming that, above a certain concentration, the trapping of interstitials by interstitial-donor atoms (I + Mₛ ↔ Mᵢ) starts dominating over the trapping of vacancies (V + Mᵢ ↔ Mₛ).

In any case, a concentration-based mechanism is consistent with the observed radial uniformity of the defects.

V.V. Voronkov and R. Falster, Microelectronic Engineering 56, 165 (2001)
Voronkov’s model

- The concentration ratio $[\text{VM}_s] / [\text{M}_i]$ depends on the doping concentration $[\text{M}_s]$ - when $[\text{M}_s]$ becomes larger than the intrinsic electron concentration $n_i$. It occurs if the charge states of the two defects $\text{VM}_s$ and $\text{M}_i$ are different.
- The $\text{VM}_s$ defect is most likely of the same charge $+1$ as $\text{M}_s$ since $V$ is considered to be a neutral defect in intrinsic $\text{Si}$. The $\text{M}_i$ defect may have an opposite charge state $-1$. Then the equilibrium ratio for the two defects depends on the electron concentration $n$ as $n^2$:
  - $[\text{VM}_s]/[\text{M}_i] = R_{vi} (n_i/n)^2 \quad (1)$
  - where $R_{vi}$ is the ratio for the intrinsic $\text{Si}$.
  - Therefore, at larger doping level – when $n$ becomes well above the intrinsic value of $n_i$ – the ratio of the two defects changes in favor of negatively charged $\text{M}_i$ defects. The total incorporated concentration of vacancy species $\text{V} + \text{VM}_s$ will be then quickly reduced, which results in a suppression of voids.

Voronkov’s model – As void simulation – con’t

Measured and computed COP density vs [As], assuming that the measured COPs by SP1 represent a fraction F of the total voids. Data were fitted with F=0.14.

COP formation in heavily-doped silicon crystals
Summary

Void formation in 200mm diameter silicon wafers heavily doped with antimony, arsenic or phosphorus, respectively, in the range 1-50mΩ·cm was studied. A clear correlation between void density and dopant concentration is observed. Initially, void density increases with dopant concentration, but, at a higher dopant concentration, the void density drops sharply. For arsenic and phosphorus, the resistivity range covered was sufficient to identify the resistivity point of maximum void formation, at about 3.9mΩ·cm for arsenic and at about 2.4mΩ·cm for phosphorus. Above this resistivity, the void counts decrease slowly, while for lower resistivity values there is a sharp drop. For antimony, the explored range was not wide enough to identify the point of maximum. The observed impact of dopant concentration on void formation can be explained by assuming that the dopant atoms can trap both vacancies – forming a vacancy-dopant complex – and silicon interstitials – by exchange with dopant interstitial minority species. The total concentration of vacancy species is first increased by the contribution of trapped vacancies. At higher dopant concentration, the second mechanism – which produces interstitials - starts to dominate and the vacancy concentration is reduced.
Thank you!

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