

Method For Producing Semiconductor Wafers From Monocrystalline Silicon

The invention provides a process for producing semiconductor wafers from monocrystalline silicon.

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Single crystals are produced from silicon in the majority of practical cases in a crucible pulling method (called the Czochralski process or CZ method) or a crucible-free pulling method (called zone melting process or FZ method). The single crystals in the form of rods with diameters of typically 100 to 300 mm serve primarily as base
10 material for production of wafers, from which electronic components are manufactured in turn.

The Czochralski method comprises the pulling of a single crystal from a melt present in a crucible. The single crystal is pulled out of the melt suspended from a seed
15 crystal. In general, a neck is first crystallized at the lower end of the seed crystal, in order that dislocations move to the edge of the neck and are eliminated in that way. The further pulling of the single crystal of silicon is continued in a customary manner, specifically by the pulling of a conical section, a cylindrical section and an end cone of the single crystal. Toward the end of the pulling operation, the single crystal tapers
20 conically to a small diameter. This prevents sliding or dislocations in the single crystal that arise(s) in the separation of the single crystal from the melt from running back into the single crystal to any extent, especially into the cylindrical section. Monocrystalline semiconductor wafers of silicon are cut off from the cylindrical section of the single crystal and processed further.

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Of particular significance in the pulling of a single crystal of silicon by the CZ method is control of the V/G ratio of pulling speed V and axial temperature gradient G at the crystallization boundary.

30 The pulling speed V is the speed with which the growing single crystal is raised upward away from the melt, and the axial temperature gradient G is a measure that indicates the change in temperature at the crystallization boundary in the direction of crystal displacement.

If the ratio V/G is above a critical value k_1 , predominantly vacancies will occur, which can agglomerate and then be identified as COPs (crystal originated particles).

Depending on the detection method, they are also referred to as LPD (light point defects) or LLS (localized light scatterers).

If the ratio of V/G is below a critical value k_2 , which is less than k_1 , predominantly intrinsic point defects will be manifested in the form of interstitial lattice atoms (silicon self-interstitials), which can likewise form agglomerates and appear macroscopically as dislocation loops. Agglomerates of interstitial lattice atoms form local crystal dislocations which, on account of the detection method applied, are also referred to as LPITs (large etch pits).

In the broadest sense, the region in which no agglomeration of defects or of interstitial lattice atoms takes place, i.e. in which V/G is between k_1 and k_2 , is referred to as the neutral zone or perfect region. The value of V/G at which the crystal changes from an excess of defects to interstitial lattice atoms is naturally between k_1 and k_2 .

The axial temperature gradient G at the crystallization boundary and the radial profile thereof are determined by heat transfer from and to the crystallization boundary. Heat transfer is in turn influenced significantly by the thermal properties of the environment of the growing single crystal, called the hot zone, and by the supply of heat through one or more heating devices.

The axial and radial profile of the axial temperature gradient G at the crystallization boundary can be determined by simulation calculations that take account of the heat balance.

In order to keep the quotient V/G within an intended range in axial direction as well, it is necessary to compensate for the change in the axial temperature gradient G over time by a corresponding change in the pulling speed V . By controlling the pulling speed V , it is also possible to control the quotient V/G .

Oxygen plays an important role in the formation of BMDs (bulk microdefects). BMDs are oxygen precipitates that form nuclei from BMDs in a heat treatment. BMDs act as internal getters, i.e. as energy sinks for impurities, and are therefore fundamentally advantageous.

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US 2020/199776 A1 discloses a process for producing a single silicon crystal in which – if dislocations occur during crystal pulling – pulling is continued at the same pulling speed until the starting point of the dislocations passes through a temperature zone in which BMD nuclei are formed. The aim of the process is thus to not influence the thermal history in the nondislocated region by changes in the pulling process, and to enable the formation of BMDs in later thermal treatments of these wafers.

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EP4025726A1 discloses a method of producing semiconductor wafers from monocrystalline silicon by CZ, in which the direction of the rotation of the crucible is changed continually. This makes it possible to more than halve axial fluctuations in the concentration of oxygen in the cylindrical section of the single crystal, expressed as the differential of greatest concentration and smallest concentration.

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In the study of wafers divided from the cylindrical section of a single crystal in the range from 75% to 95% of the rod length, an increase in LLS with a size of less than 19 nm was found. LLS of this size can be detected by scattered light measurement with the SP5 particle measurement device from KLA Corp.

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It was an object of the invention to reduce the LLS contamination of the wafers.

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The object of the invention is achieved by a process for producing semiconductor wafers from monocrystalline silicon, comprising the pulling of a cylindrical section and subsequently of an end cone of a single crystal of silicon from a melt present in a crucible;

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wherein the pulling speed in the pulling of the end cone remains essentially constant compared to the pulling speed in the pulling of the cylindrical section; the rotating of the crucible with a speed of rotation and in a direction of rotation during the pulling of the cylindrical section and the end cone of the single crystal; and

the dividing of the semiconductor wafers of monocrystalline silicon from the cylindrical section of the single crystal, wherein the pulling speed during the pulling of the end cone is at least greater than 0.46 mm/min, while the direction of rotation of the crucible is constantly changed and an amplitude of the speed of rotation before and after the change in the direction of rotation is not less than 6 rpm.

The process of the invention makes it possible to distinctly reduce the level of LLS with a size of less than 19 nm in wafers divided from the cylindrical section of the single crystal in the range from 75% to 95% of the rod length.

In the view of the inventors, this is associated with the fact that the process reduces the dwell time in this section (75% to 95% of the rod length). This will be shown later in the examples.

Preferred embodiments of the invention are set out in the description that follows and in the claims.

The melt, at least during the pulling of the cylindrical section of the single crystal, is preferably subjected to a horizontal magnetic field. The horizontal magnetic field, in the region of the phase boundary between the growing single crystal and the melt, has an intensity of preferably not less than 0.2 T and not more than 0.4 T.

The process of the invention is particularly suitable for production of monocrystalline semiconductor wafers of silicon having a diameter of at least 200 mm, especially having a diameter of at least 300 mm.

The growing of the cylindrical section of the crystal preferably adjusts v/G such that the rod is free of agglomerates of defects and interstitial lattice atoms, i.e. the wafers produced therefrom do not contain any L-Pits and COPs.

In one embodiment, no dislocations occur in the pulling of the cylindrical section of the single crystal.

The changing crucible rotation in the creation of the end cone leads to a more stable shape of the end cone. It was possible to reduce the dislocation frequency of the end cone by 2%.

- 5 The features that have been specified with regard to the above-detailed embodiments of the process of the invention can be implemented either separately or in combination as embodiments of the invention. In addition, they may describe advantageous executions that are protectable independently.

10 **Examples**

The simulation of the thermal history of the CZ process shows a high dwell time in the temperature range between 600°C and 700°C in the rod region (75-95%) in which the LLS defects have also been observed.

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An increase in the pulling speed in the end cone and a high degree of changing crucible rotation allows the dwell time to be reduced such that the defects are distinctly reduced.

- 20 Various pulling speeds were simulated and tested experimentally.

Comparative example:

Lower pulling speed of end cone (-10%)

25 **Example 1:**

Lower pulling speed at rod end, then constant from rod end to end cone

Example 2:

Higher pulling speed from rod end to end cone

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(Inventive) example 3:

Higher pulling speed from rod end to end cone and changing crucible rotation for end cone

Table 1 shows the minimum and maximum dwell times for **comparative example** and **examples 1 to 3**, ascertained by numerical simulations.

5 **Table 1**

	Minimum dwell time / min	Maximum dwell time / min	Ratio
Comparative example	241	558	2.3
Example 1	241	496	2.1
Example 2	241	502	2.1
Example 3	241	459	1.9

Examples 1 to 3 lead to a distinct reduction in LLS < 19 nm, as shown by **table 2**.

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Table 2

	LPD counts / wafer < 19 nm	COPs / LPits
Comparative example	71.8	none
Example 1	19.2	none
Example 2	18.1	COPs at rod end
Example 3	11.3	none

However, in **example 2** (without changing crucible rotation), COPs are found at the rod end.

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Only **example 3** with elevated pulling speed and changing crucible rotation leads to an even more distinct reduction in LLS (compared to **examples 1 and 2**) and simultaneous avoidance of COPs.

The above description of illustrative embodiments should be considered by way of example. The disclosure thus made firstly makes it possible for the person skilled in the art to comprehend the present invention and the associated advantages, and the
5 understanding of the person skilled in the art secondly also encompasses obvious alterations and modifications of the structures and methods described. Therefore, all such alterations and modifications and equivalents shall be considered to be covered by the scope of protection of the claims.

Claims

1. A process for producing semiconductor wafers from monocrystalline silicon, comprising the pulling of a cylindrical section and subsequently of an end cone of a single crystal of silicon from a melt present in a crucible;
5 wherein the pulling speed in the pulling of the end cone remains essentially constant compared to the pulling speed in the pulling of the cylindrical section end region;
the rotating of the crucible with a speed of rotation and in a direction of rotation
10 during the pulling of the cylindrical section and the end cone of the single crystal; and
the dividing of the semiconductor wafers of monocrystalline silicon from the cylindrical section of the single crystal, wherein the pulling speed during the pulling of the end cone is at least greater than 0.46 mm/min, while the direction
15 of rotation of the crucible is constantly changed and an amplitude of the speed of rotation before and after the change in direction of rotation is not less than 6 rpm.
2. The process as claimed in claim 1, wherein the pulling speed during the pulling
20 of the end cone is at least greater than 0.5 mm/min.
3. The process as claimed in either of claims 1 and 2, wherein the dwell time of a range from 75% to 95% of the rod length of the cylindrical section within the temperature range of 600-700°C is less than 460 min.
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4. The process as claimed in any of claims 1 to 3, wherein the divided semiconductor wafers are free of COPs and LPits.
5. The process as claimed in any of claims 1 to 4, wherein no dislocations occur
30 in the pulling of the cylindrical section of the single crystal.
6. The process as claimed in any of claims 1 to 5, wherein the melt is subjected to a horizontal magnetic field.