

Methods and Solutions for Reducing Defects in Semiconductor Crystals

Sobirova Tursunoy Abdipatto qizi

Andijan State Technical Institute, Assistant of the Department of Automation of Mechanical Engineering Production
tursunoy.sobirova.1993@mail.ru

Annotation

This article discusses the types of defects in semiconductor crystals, the causes of their formation, as well as modern methods for reducing these defects. In addition, an analysis of the effectiveness of the results of these methods in real industrial and scientific practice is presented.

Keywords: semiconductors, microchips, diodes, transistors, solar panels, defects, impurities, crystal growth, epitaxy.



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Introduction

Semiconductors are the basis of modern electronic technologies. Without them, microchips, diodes, transistors, solar panels and many other devices are unthinkable. Therefore, the quality of semiconductor materials, especially the level of defects in their crystal structure, directly affects the efficiency of the device. Any crystal growth process is accompanied by a certain amount of defects. These defects can negatively affect the electrical, thermal and optical properties.

Semiconductors are materials that are between insulators and conductors in terms of their electrical conductivity, the most popular of which are silicon (Si) and germanium (Ge). These materials are mainly used in the following areas:

1. Electronics: Transistors, integrated circuits and sensors.
2. Photovoltaics: Solar cells.
3. Optoelectronics: LEDs, lasers and infrared detectors.
4. Telecommunications: Components used in microchips.

The reliability and efficiency of semiconductor devices largely depend on the perfection of the crystal structure. Perfect crystals have highly stable electrical properties, which is essential for modern technologies. Defects in crystals are divided into two categories: defects and impurities.

Main types of defects:

Point defects: Vacancies, interstitials, substitutional defects

Linear defects (dislocations): Drilling dislocations, edge dislocations

Surface and plane defects: Grain boundaries, stacking faults

Bulk defects: Inclusions, foreign phases.

Impurities: Impurities (such as phosphorus or boron) added to a crystal are important in controlling the properties of a semiconductor, but they are also considered defects if they are in the wrong concentration [1].

Defects in crystals negatively affect the electrical, thermal, and optical properties of a material. From an electrical perspective, defects hinder the movement of electrons and holes, resulting in reduced conductivity. In thermal properties, dislocations reduce thermal conductivity, which causes the device to heat up more quickly. Regarding optical properties, surface defects change the light absorption, which is important in optoelectronic devices. Therefore, minimizing the number of defects in semiconductor crystals is a key requirement for producing high-quality devices.

METHODS AND ANALYSES

Crystal growth is an important stage in the preparation of semiconductors, where various technological methods are used to determine the amount of defects.

Some of the most effective technologies include [2].

Czochralski (CZ) method - Silicon crystals are grown from a melt by slow spinning and stretching. Crystalline materials, especially semiconductors, are the basis of the modern electronics and optoelectronics industry. The technology for growing high-quality crystals of these materials directly affects the performance of the devices made from them. The Czochralski (CZ) method is currently one of the most widely used methods for growing crystals, in particular materials such as silicon (Si), germanium (Ge), gallium arsenide (GaAs). The advantage of this method is that the crystal is large. The disadvantage is that there are more dislocations. This method, discovered by the Polish scientist Jan Czochralski in 1916, allows the gradual addition of several atomic layers from a melt to form a single crystal. The process consists of the following main steps:

- ✓ Obtaining a melt (usually Si is melted at 1414°C)
- ✓ Lowering a single crystal seed (particle) into the melt
- ✓ Gradually stretching it upwards
- ✓ Constantly controlling the temperature and rotation speed

As a result, a cylindrical crystal elongated along its axis is obtained [3].

To implement the CZ method, special furnaces and control systems are required. They are as follows: Quartz crucible - the solution is placed in it. Induction furnace - needed to melt silicon. Seed crystal holder - to start crystal growth. Rotating and lifting mechanism - to rotate and pull the crystal. Strong vacuum or inert gas environment (argon) - to prevent oxidation. The process requires very fine adjustments. For example, a temperature difference of several degrees can seriously affect the quality of the crystal.

The above method has many advantages. Single crystals grown by the CZ method have a highly ordered lattice. This method allows you to obtain crystals with a large diameter (up to 200–300 mm). CZ technology is implemented in semi-automatic or fully automated lines.

There are also several disadvantages of this method. Small amounts of oxygen or other elements can enter the crystal from the crucible materials and the furnace environment. The process of

stretching the crystal from the solution requires high energy. Due to temperature changes, defects in the crystal lattice can occur.

The CZ method is mainly used to grow Si crystals. Such crystals serve as the basis for integrated circuits, solar cells, diodes and transistors. Si crystals used in solar panels are grown using CZ technology. Optical materials such as sapphire (Al_2O_3) and lithium niobate (LiNbO_3) are also grown using the CZ method.

In modern production, the CZ method is being combined with several new technologies:

Magnetic-controlled CZ (MCZ): controlling the movement of the melt using a magnetic field to improve crystal quality.

Impurity reduction: preventing oxide inclusion by changing crucible materials or combining with float-zone methods.

Process optimization through artificial intelligence: controlling temperature and rotation speed in real time [4].

Float Zone (FZ) method – No solution is used, high-purity silicon is obtained by zone purification. This method produces a crystal with very few defects. Only this method is complex and quite expensive to manufacture. The semiconductor materials that are the basis of modern technologies – especially silicon (Si) crystals – require a high level of purity. Silicon in the monocrystalline state is the basis for many electronic devices such as integrated circuits, solar panels, diodes and transistors. The Float Zone (FZ) method is one of the most advanced and low-pollution technologies for obtaining such pure and perfect crystals. The FZ method is based on the principle of forming a crystal by melting the crystal and moving the melting zone downwards. In this method, a silicon rod (rod) is melted locally (only in the zone) using a high-frequency induction furnace. The melted zone is gradually moved downwards, and a new crystal grows from above.

This method involves several steps in crystal growth. First, a well-cleaned silicon rod is prepared. Then, a portion of the rod is melted using an induction ring. A single-crystal seed is ignited from above. Then, the molten zone is moved downwards and the crystal is stretched. The process is carried out under an inert gas atmosphere (usually argon) [5].

Although the FZ technology is more expensive than the Czochralski (CZ) method, it has a number of important advantages: In the FZ process, silicon does not come into contact with the crucible, i.e. the crystal does not touch any crucible or container. As a result, impurities such as oxygen or carbon do not migrate to the crystal. Crystals with extremely low concentrations of impurity elements can be obtained (up to 10^{12} atoms/cm³).

Crystals grown using the FZ method have very high electrical resistance. This makes them suitable for use in: High-power high-voltage devices. Radiation-resistant electronics (space technology, nuclear devices). Due to the low dislocation density in the crystal lattice, the devices operate reliably and the problem of electromigration is reduced. Crystals grown using the FZ method have led to a number of technological advances: FZ silicon crystals serve as the basis for microcircuits used in VLSI (Very Large Scale Integration) systems. Because they emit little heat, operate quickly, and are low-noise. Silicon panels obtained using the FZ method absorb sunlight much better and increase the photoelectric conversion efficiency to 22–24%. FZ crystals are widely used in electronic components designed for nuclear power plants, space probes and satellites.

The FZ method, while providing high accuracy and purity, also has a number of technical and economic problems: it is quite expensive due to energy consumption and the need for special equipment. Usually crystals with a diameter of up to 150 mm are obtained (300 mm and more in CZ). Control of the molten zone is complex and depends on the operator's skills. Modern

technologies are developing towards further improving the FZ method. Using Multiple Pass FZ (multiple melting), impurities can be completely eliminated. The speed and temperature of the zone are precisely controlled with artificial intelligence. Radiation-resistant FZ crystals are special modifications for operation in a radiation environment.

Bridgman technique - a crystal is formed by cooling the solution in a temperature gradient. Useful for reducing dislocations.

Epitaxial growth - Atoms are deposited layer by layer on a prepared substrate.

Epitaxial layers are usually less defective [6].

Annealing is the process of reducing defects within a crystal by heating a semiconductor material to high temperatures. This process helps to align point and line defects and reduce dislocations. There are several types of thermal treatment:

1. Low-temperature annealing. It is carried out at temperatures of 400–600°C. It is used to restore a damaged lattice after the ion implantation process. It helps to activate the electrical.
2. High-temperature annealing. It is carried out at 800–1200°C. It is used to reduce deep defects and "correct" dislocations by moving them.
3. Rapid Thermal Annealing (RTA). It is heated at high temperatures for a very short time (a few seconds). The main advantage: high-precision control and energy efficiency.

As a result, the crystal lattice is restored, electrical conductivity is improved, and impurities are activated (for example, implanted dopants). Ion implantation is a method of introducing ions of the necessary elements into a semiconductor crystal at high speed. This method is more accurate and efficient than the traditional diffusion method. The concentration and depth of dopants can be precisely controlled. Local doping (through masks) is possible. It is widely used in scaling and microchip design. However, it impacts the crystal lattice and creates defects. For this reason, it is always used in conjunction with thermal treatment [7].

Epitaxy is the process of growing a new crystal layer on an existing crystal substrate by adjusting it at the atomic level. Gas phase epitaxy (VPE) — gases react to deposit a layer on the substrate. Molecular beam epitaxy (MBE) — atoms are deposited layer by layer in a vacuum. The crystal lattice is continuous - minimal defects. Layers can be arranged in a coherent manner (hetero-surfaces can be created). Allows the production of high-quality microcircuits.

The properties of semiconductor materials, especially the electrical properties of silicon, are directly dependent on its chemical purity. Even a 1 ppm (one part per million) impurity can cause significant changes in electrical properties.

There are several purification steps:

1. Raw material preparation (sand → metallurgical silicon): SiO_2 (silicon oxide) is converted into Si metal in an electric furnace. Metallurgical silicon (~98% pure) is obtained.
2. Zone refining: A silicon ingot (rod) is slowly heated and moved through a molten zone. Impurities are left in solution → the crystal remains pure. The result is silicon that is 99.9999% (6N) or purer.
3. Acid cleaning: Surface impurities are removed with HF, HCl, and other acids. As a result, electrical conductivity is dramatically improved. The number of defects is reduced. Crystal symmetry is maintained at a high level → which increases the reliability of microcircuits [8].

Conclusion

The above-mentioned Czochralski method is currently one of the main technologies for the production of single-crystal materials, which are important for high-precision electronic and

optical devices. It surpasses other methods in terms of crystal quality, size, and industrial adaptability. At the same time, scientific research is still ongoing on the issue of energy efficiency and defects. In the near future, this technology will be further improved and can be used to produce new materials. Crystal growth using the Float Zone method is characterized by high purity, electrical stability, and physical quality. This technology is especially important in the production of high-quality semiconductors, radiation-resistant devices, and solar cells. The complexity and cost of the FZ method make it ideal only for strategic areas, but its results are very important for technological advances.

In recent years, a lot of scientific research has been conducted to reduce defects and create an ideal crystal. Laboratories at MIT and Intel (USA) have managed to reduce the dislocation density in epitaxial silicon layers to 10^4 cm^{-2} . Japan (Hitachi Research) has eliminated up to 95% of implantation defects through thermal cycling. Radiation-resistant semiconductors developed by CERN (Europe) are used in high-energy physics. Companies such as Intel, AMD, TSMC use substrates with the highest purity and fewest defects for 7 nm and 3 nm technological processes. Due to the use of mono-crystalline silicon in solar panels (photovoltaics), the efficiency has been increased to 23–25%. Defects in semiconductor crystals are an important factor that negatively affects the performance of the device. This article analyzes the types of defects, methods for their reduction, and practical results. Therefore, the reduction of defects must be controlled at each stage of the technological processes. Thermal treatment combined with epitaxial growth and ion implantation is an effective strategy. The degree of purification and crystal quality are crucial for high-tech devices.

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