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Review

Growth of semiconductor silicon crystals

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Abstract

This paper focuses on the recent developments in Czochralski (CZ) crystal growth of silicon for large-scale integrated circuits (LSIs) and multi-crystalline silicon growth using a directional solidification method for solar cells. Growth of silicon crystals by the CZ method currently allows the growth of high-quality crystals that satisfy the device requirements of LSIs or power devices for electric cars. This paper covers how to obtain high-quality crystals with low impurity content and few point defects. It also covers the directional solidification method, which yields crystals with medium conversion efficiency for photovoltaic applications. We discuss the defects and impurities that degrade the efficiency and the steps to overcome these problems.

Keywords: silicon; convection; defect; impurity; stress

1. Introduction

Silicon crystals are required for the continuous development of large-scale integrated circuits (LSIs), which are used in several electronic devices, solar cells, and power devices for electric cars and in the fields of information, energy production, and energy conservation. Single crystals of silicon constitute a key material for such development. In order to realize these developments, silicon crystals must be grown with a low concentration of impurities such as oxygen and carbon, and few dislocations and point defects. The melt, which is the raw material for growing crystals, is supported by a quartz crucible and is easily contaminated with oxygen and heavy metals. During crystal growth, defects are easily introduced. The novel Czochralski (CZ) method, however, leads to growth of crystals with low defects [1]. Furthermore, by leveraging the necking process of the seed crystal, Teal and Little [2] extended the CZ method by developing a new growth method that does not lead to the formation of dislocations. The absence of dislocations means that large crystal-growth speeds and rapid cooling are possible, which allows crystal growers to increase the crystal yield [3]. The growth and cooling rates of dislocation-free crystals can be increased compared to those with dislocations because the deformation is elastic, and at room temperature, the final residual stresses in the crystals are reduced to almost zero.

Another critical issue in crystal growth is the formation of point defects such as vacancies and interstitials in the crystal. During the cooling process after solidification of the melt, vacancies and interstitials form voids or dislocation loops, respectively, which degrade the properties of the oxide layer in LSIs, thereby reducing the lifetime of minority carriers in power devices [4]. Recent advances in information technology could not have been achieved without a reduction in the concentration of voids and/or dislocation loops. Therefore, during crystal cooling, the distribution and concentration of point defects should be controlled with precision.

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Because of their relatively high conversion efficiency and reasonable production costs, silicon single crystals have now become one of the main materials in the photovoltaic market.

The CZ method is a well-established technique for large-scale production of silicon single crystals. However, the critical issues of controlling light-element impurities and point-defect concentrations in order to increase the lifetime of carriers such as electrons and holes still remain. Oxygen and carbon are the main light-element impurities in these crystals; therefore, effective control of oxygen and carbon concentrations in a crystal is required for the mass production of high-quality single crystals. Because of the chemically reactive melt inside the furnace, experimental investigation of these issues is difficult. Developments in computer technology, including hardware and algorithms, have allowed quantitative simulations of the global environment of crystal growth, which facilitate the search for techniques to ensure crystal purity during growth.

Although many studies have focused on simulating impurity transport [5–16], most of them used the local model [5–11], which neglects the transport of impurities in the gas and in the melt in a furnace. A few studies have used global simulations [12–15], but Ref. [12] neglected oxygen and carbon impurities in the silicon melt in their simulation, and carbon impurity in both gas and silicon melt was neglected in the simulation in the other studies [13–15]. No simulations have addressed the transport of oxygen and carbon impurities in both gas and the silicon melt. Bornside and Brown [12] conducted the first analysis that incorporated oxygen and carbon transfer in both the silicon melt and ambient gas.

In the directional solidification (UD) method, as in the CZ method, contamination by light elements is governed by impurity transport [16]. Carbon is one of the major impurities in a crystal of multi-crystalline silicon; its concentration can affect the density and electrical activity of dislocations in multi-crystalline silicon [17]. When the carbon concentration exceeds its solubility limit in silicon, it precipitates to form silicon carbide (SiC) particles, which can lead to Ohmic shunts in solar cells and to nucleation of new grains in silicon ingots [18]. Carbon, oxygen, and SiC and Si_3N_4 particles in a solidified silicon ingot cause significant deterioration in the conversion efficiency of solar cells. If the carbon concentration in the melt exceeds 4×10^{16} atoms/cm^3, which equals the solubility limit of carbon in the melt, it markedly influences the precipitation of oxygen during thermal annealing of crystals and during device processing of wafers cut from these crystals [19–24]. Oxygen precipitation is known to act as intrinsic gettering sites for heavy-metal impurities and to affect the mechanical strength of wafers [25,26]. Therefore, effective control of carbon concentration in a crystal is required to produce high-quality crystals. Experimental explorations [27–30] and numerical simulations [31–34] have been performed to find techniques for improving the crystal purity. The C and O concentrations in the multi-crystalline Si crystals can be significantly affected by using a specially designed gas-flow system [30]. Using a tungsten crucible cover in a UD furnace reduces the C impurity concentration to a reasonable level and markedly reduces the O concentration; however, it is easy to corrode with Si vapor [26]. Because of the problems linked with chemical reaction between tungsten and silicon vapor, coating with materials such as carbon or carbon with SiC is preferred.

2. Light-element transfer in a CZ furnace

Fig. 1 shows typical configuration of a CZ furnace. The left half of the figure shows a furnace structure from the 1970s, and the right half is a furnace structure from the 1980s. The heat shield plays the important role of

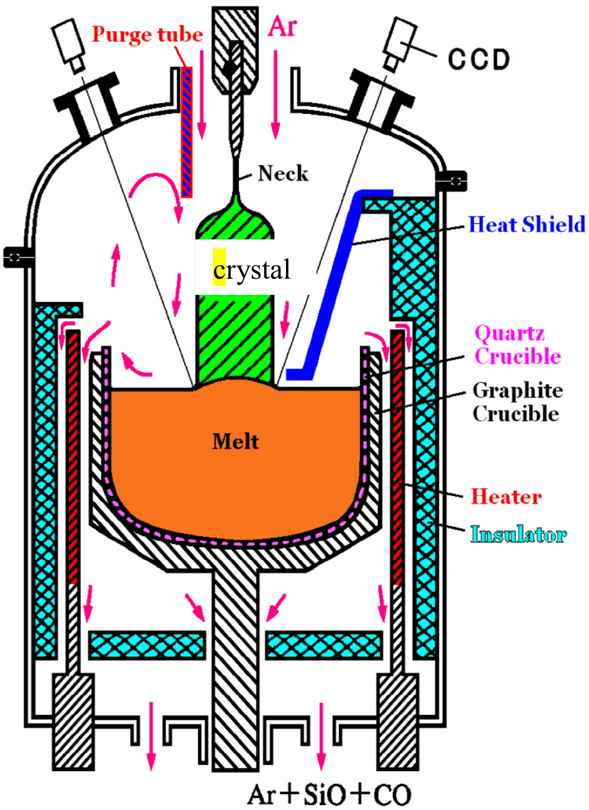

Fig. 1. Typical configuration of CZ furnace. Left (right) half shows furnace structure from the 1970s (1980s).