Study of oxygen atom diffusion coefficient in silicon melts

K.Terashima, S.Nishimura and D.Kitamura

Materials Science and Technology, Shonan Institute of Technology
1-1-25 Tsujido-Nishikaigan, Fujisawa, Kanagawa, Japan

Abstract

The oxygen diffusion has been studied by using the capillary technique. As the initial stage of quartz dissolution into silicon melts causes an experimental error, the holding time of more than 30 minutes was needed to analyze the diffusion constant. The analyzed diffusion constant of oxygen atoms in silicon melts is suggested to be $2x10^{-4}$ cm^2/sec.

1. Introduction

Oxygen atoms in silicon crystals generate extended defects in silicon substrates. In silicon substrates they may capture the heavy metal ions which are detrimental for the drive of Si device. These oxygen atoms are incorporated into silicon crystals from the quartz crucible in the pulling process of single crystals. The solubility of oxygen atom into silicon melts is about $2\sim3x10^{18}$ $atoms/cm^3$ which is slightly affected by the presence of doping impurity. The transport of oxygen atoms are thought to be dominated mainly by the melt convection in a crucible. Up to date the natural convection and forced convection have been well studied to control the oxygen distribution in the substrates. Therefore, the diffusion of oxygen atoms is thought to be low enough to be neglected in former days. However, the recent advanced IC technologies have been requiring silicon substrates with low oxygen content. For the production of such low oxygen substrates, it is necessary to control the behavior of oxygen atoms in melts strictly. Therefore, it is extremely important to obtain the precise knowledge of the physical properties of silicon melts, such as diffusion constant of oxygen in silicon melts.

We have studied the behavior of oxygen atoms in silicon melts. The diffusion constant has been studied by using a capillary technique. The approximate value is $2x10^{-4}$ cm^2/sec at 1743K. This report describes the experimental procedures and the analyzed values of oxygen diffusion coefficient in silicon melts.

2. Experimental

The BN container with two capillaries was employed to contain silicon melt. Quartz rods(fused quarts rod) with 1.5 mm diameter was used as an oxygen source. In the capillary was put a couple composed of this quartz rod and the polycrystalline silicon rods with 1.5mm diameter. The BN container was evacuated. The samples were melted and kept at 1703, 1723

and 1743K in a vertical furnace for 5-60minutes. The silicon rod was melted by keeping its contact with the quartz rod during these heating treatments. After the heat treatments, the samples were quenched by flowing nitrogen gas into the furnace. The solidified silicon rods were well wetted to the quartz rods. The silicon rod samples were detached and, then, the concentration profile of oxygen atoms in this silicon rod was detected by the SIMS.

3. Results and discussion

The concentration profile of oxygen atoms was measured by the SIMS along the silicon rod axis. The diffusion constants were analyzed in terms of this oxygen profile. The analyzed diffusion constants are summarized in Fig.1 as a function of the distance of oxygen profile from the interface which corresponds to the heating period. The analyzed diffusion constant increases with increasing the heating period and reaches a constant value of about $2x10^{-4}cm^2/sec$. This variation is due to the dissolution mechanism of SiO_2 into silicon melt. The first stage of SiO_2 dissolution continues at the SiO_2-Si melt interface until the oxygen concentration in this interface reaches the solubility limit of about $2x10^{18}$ atoms/cm^3. This highly concentrated oxygen layer is called as the diffusion layer. It takes about 15 minutes to form such a layer around the interface. The oxygen atoms diffused from this diffusion layer into silicon melts due to the gradient of oxygen atom distribution. So, the analyzed diffusion constants are markedly small at the early stage of heating process. The analyzed diffusion constants increased to the saturation level, $2x10^{-4}cm^2/sec$. The real oxygen diffusion constant value may be slightly above the saturation level in Fig.1. The diffusion constant of oxygen atoms in silicon melts will be $2x10^{-4}cm^2/sec$ from the results in Fig.1.

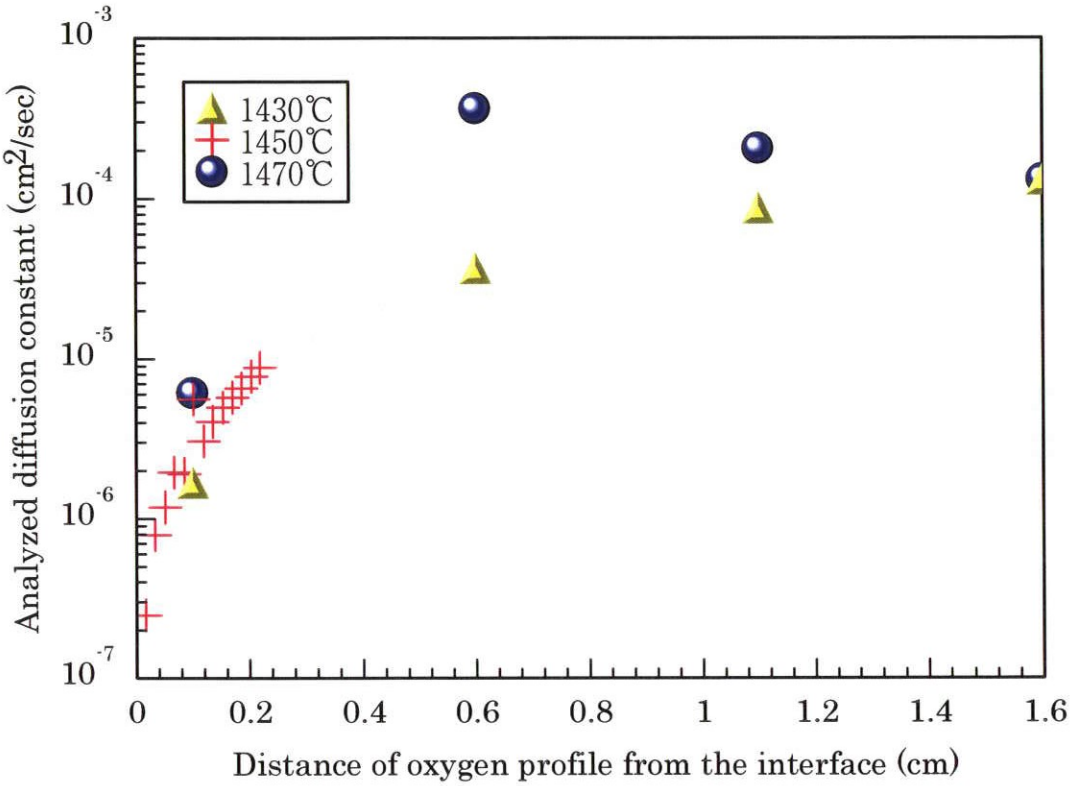

Fig.1 Analyzed diffusion constant (Closed circles and triangles were heat treated more than 30minutes)

4. Summary

The oxygen atom behavior in silicon melts has been studied by the capillary technique. The BN containers were used to hold silicon melts in contact with the quartz rod. The analyzed diffusion constant of oxygen atom in silicon melt is estimated to be about $2x10^{-4}cm^2/sec$. A large error may be included due to the quartz rod dissolution process in the initial stage.