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Crystal Growth of CZ-Si and Relationship between Carrier Lifetime and Defects

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Abstract

A Czochralski (CZ) growth of single silicon (Si) crystals is in variably accompanied by transport of impurities such as carbon (C), oxygen (O), and related compounds produced by reactions at high temperature. To study the generation and accumulation of C during the melting process, a transient global model was developed that included coupled O and C transport. Transport phenomena of C, O, and related compounds were predicted by considering five chemical reactions in the furnace. The dynamic behavior of impurities was revealed during the melting process of the Si feedstock. The effect of thermal donors on lifetime of carrier was investigated by growing crystals with high purity. The results indicated that thermal donors do not act as lifetime killers.

1. Introduction

One of the main defects is oxygen precipitates in silicon crystals. The minority carrier lifetime of silicon (Si) wafers is one of the most important parameters in fabrication of solar cells as well as power devices. The bulk lifetime of Si crystals is shortened by oxygen (O) precipitates, which are enhanced by carbon (C) contamination [1,2]. Therefore, reduction of C contamination in Czochralski silicon (CZ-Si) crystal growth is required for production of Si wafer with a long carrier lifetime. Contamination of C in Si crystals mainly originates from carbon monoxide (CO) generation on the graphite components, which reaches a maximum in the melting stage [3]. It is essential to control CO generation and C incorporation from melting to tailing.

Loading a crucible with poly-Si feedstock includes many technical details for optimization of the melting and growth processes [4]. In the CZ-Si process, poly-Si in the form of granules, chunks, or a mixture of chunks and granules is first loaded into a quartz crucible. The packing density of poly-Si within the crucible is greater than about 0.7. For the melting of packed Si chunks, the packing structure can affect the heat transport by the effective thermal conductivity (ETC), which is different from the thermal conductivity of bulk Si. The ETC is a function of many parameters, including the conductivities of the solid and the fluid, porosity, emissivity, temperature, and chunk size [5]. Many researchers have proposed ETC models according to different modeling principles [6].

Bornside et al. [7] derived a chemical model for coupled CO and SiO from thermodynamic analysisof their reactions in the high temperature range. Based on this chemical model, Gao et al. [8] developed a coupled transport model for SiO and CO in argon (Ar) gas, and C and O in a Si melt. However, the C content predicted under the quasi-static assumption does not account for C accumulation during CZ-Si crystal growth [9]. Transient global simulations of heat and mass transport have been performed for C accumulation in the melting process of CZ-Si crystal growth [16, 17]. However, in these studies, packed Si chunks were modeled with the thermal conductivity of bulk Si. The difference between the thermal conductivities of packed Si chunks and bulk Si can result in unreliable prediction of the thermal history of the melting process. The present study focuses on evolution of C contamination during the melting process of packed Si chunks in CZ-Si crystal growth.

Formation of thermal donors is the other important issues of growing crystals during crystal growth, especially for formation of nuclei of oxygen precipitates in the crystals.

This paper focused on reduction of carbon concentration during silicon crystal growth as well as melting process of raw materials since main process of contamination is in melting process of raw materials, not process of crystal growth. This paper also discussed on thermal donors act as recombination centers or not.

2. Carbon reduction by numerical investigation

The melting process proceeded until all the Si feed stock melted. The concentrations of O, C, SiO, and CO equilibrated at the gas/melt interface after the melting process was complete.

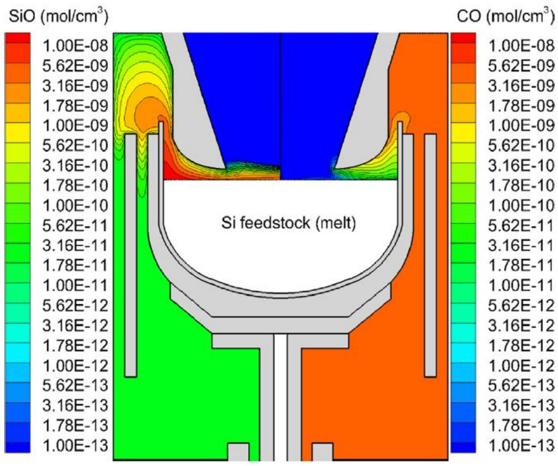

Fig. 1 Concentrations of SiO and CO in the Ar gas domain during the third stage of the melting process.

The distributions of SiO and CO in the gas domain of the third stage (time = 300min) are presented in Fig. 6. The maximum concentrations of SiO and CO in the gas were both of the order of 10^8 mol/cm^3. Evaporation of O and contamination with C at the gas/melt interface also reached equilibrium.

Flux and concentration of C in the melt side are ploted as a function of flow rate in Fig. 2. C flux and C concentration both decreased rapidly as the flow rate increased.

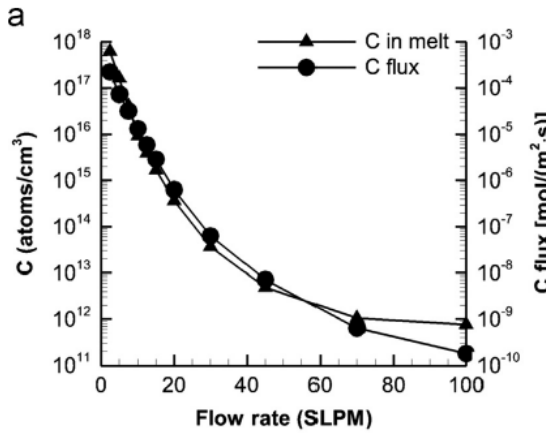

Fig. 2. Effects of gas flow rate on C transport. C concentration and C flux at the monitored location in the melt.

2. Carbon reduction by numerical investigation

We performed experiment to growth the two different processes to form thermal donors. Crystal-II and –I show the two different crystals with and without thermal donors. The position with thermal donors is indicated by an arrow.

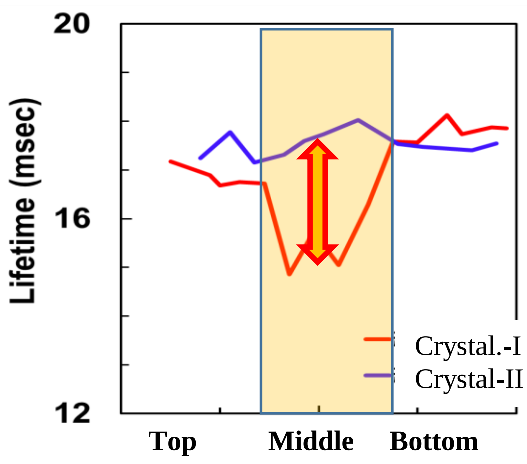

Fig. 3. Relationship between lifetime of carriers and crystal positions. Crystal-I and –II; without and with thermal donors.

Figure 3 shows decrease of lifetime is observed at the position with thermal donors indicated by an arrow. The lifetime is also dependent of carrier concentrations. To clarify the effect of carrier concentration the relationship between carrier concentration and lifetime is plotted as shown in Fig. 4. The result makes clear that lifetime with thermal donors indicated by crystal-II is in the series of crystal-I. This means that thermal donors do not act as lifetime killer.

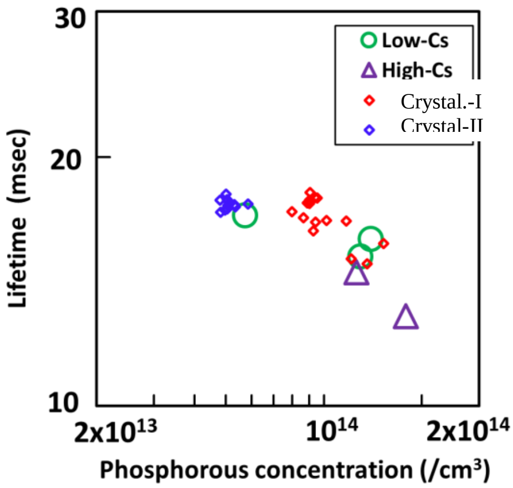

Fig. 4. Relationship between phosphorous concentration and carrier lifetime.

3. Conclusions

Reduction of carbon which is harmful for lifetime of carrier in silicon crystals for solar cells during crystal growth process was discussed by using numerical method. Melting process is the most important process for the reduction. Investigation of the effect of thermal donors on lifetime was carried out. The conclusion is thermal donors do not act as lifetime killer.

Acknowledgements

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