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CZ 法における炭素混入を考慮したシリコン原料融解過程の数値解析

Numerical Investigation of the Melting Process Including Carbon Contamination in a CZ-Si Crystal Growth

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CZ-Si process is invariably accompanied by transport of impurities, such as oxygen (O), carbon (C) and related resultants from reactions in high temperature range. C contamination can lead to a degradation of silicon wafers by the formation of C-induced defects. C and related gaseous CO species are always presented throughout the entire growth process due to the use of graphite components. Therefore, it's essential to investigate the C generation and accumulation from the melting stage of the CZ-Si growth.

O and C in the silicon melt and SiO and CO in the Ar gas are coupled by several reactions in the furnace. The coupled heat and mass transport model must be applied for numerical investigation of the impurity contamination. In the present study, a transient global model for melting process was developed, including the impurity transport in Ar gas and Si feedstock. The generation and accumulation of O and C during the melting process were predicted by the transient global simulation firstly.

Fig.1 shows the melting fronts for every 10 mins during the melting process. The arrow indicates the direction of melting front propagation. Si feedstock was melted by the heater from the lower part with the increase of heater power. Fig. 2 plots the total C and O in the feedstock according to the melting time. Once the melting front contacted with the Ar gas, the evaporated SiO was transported by the gas and reacted with the graphite components in the furnace. The increase of CO resultants enhanced the C contamination from the melt free surface. Meanwhile, the total O in the melt decreases dramatically due to evaporation of SiO. When the melting process finished, the total C in the feedstock attained to the maximum.

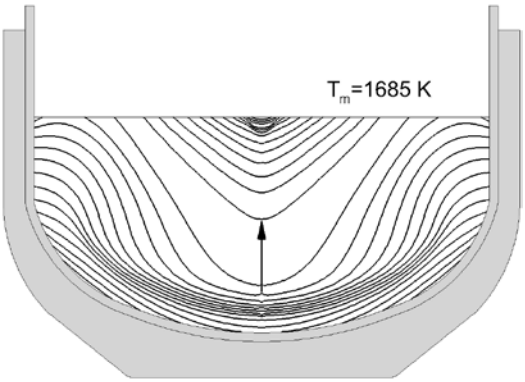

Fig. 1 Melting fronts during the melting process.

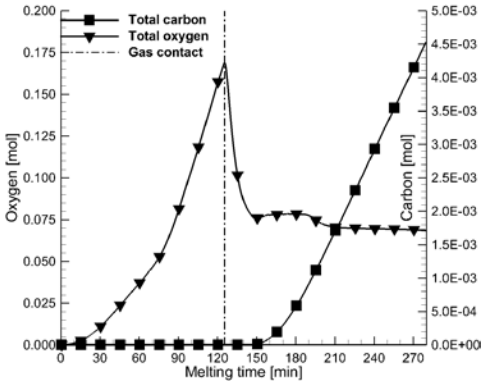

Fig. 2 Total O and C in the melting feedstock.