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# Reusability of contaminated seed crystal for cast quasi-single crystalline silicon ingots

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ABSTRACT

Reusing seed crystal is beneficial for reducing the production costs for cast quasi-single crystalline (QSC) silicon ingots. We numerically investigate the reusability of seed crystal in the casting processes with quartz crucible and silicon feedstock of different purities. The reused seed crystal is recycled from the standard QSC ingot and has been highly contaminated by iron impurity. Transient simulations of iron transport are carried out and special attention is paid to the diffusion and distribution characteristics of iron impurity at the ingot bottom. The heights of the bottom iron contaminated region are compared for silicon ingots grown from normal and recycled seed crystals. The results show that the purity of quartz crucible can influence the reusability of seed crystal more significantly than that of the feedstock. The recycled seed crystal with high iron concentration can be reused for casting processes with standard crucible, whereas it is not recommended for reusing for processes with pure crucible.



## 1. Introduction

Reuse of seed crystal is a hot topic for cast quasi-single crystalline (QSC) silicon ingots for solar cells, as it is beneficial for reducing production costs [1,2]. The normal seed crystal is prepared from Czochralski silicon rods, which has no grain boundaries and low dislocation density. After the casting process, the dislocation density in the seed crystal is still low, whereas the impurities, such as oxygen, nitrogen and iron, are enriched in the seed crystal owing to the contact with quartz crucible and silicon melt at high temperature. Reuse of the contaminated seed crystal may increase impurity content in the ingot bottom region and reduce the ingot quality. Therefore, it is necessary to evaluate whether the contaminated seed crystal can be reused.

Iron is an important metallic impurity in crystalline silicon ingots and it has been proved to be an important minority carrier lifetime killer [3]. Recent study shows that the iron transport during casting process can lead to a large region enriched with iron impurity at the bottom of a QSC silicon ingot, which corresponds to the low lifetime region in this location [4]. The seed crystal is also highly contaminated during the casting process. However, it is unknown whether the iron contaminated seed crystal can be reused. One simple method to evaluate the reusability of seed crystal is to compare the bottom iron enriched regions for the QSC silicon ingots grown from normal and recycled seed crystals. The contaminated seed crystal can be reused if there is no significant increase of the height of iron enriched region at the ingot bottom.

Some studies have been carried out to study the transport and contamination of iron impurity in the casting process for QSC silicon ingots [4–6]. The results show that iron contamination is the main factor for the large low lifetime region at the ingot bottom and the total iron concentration in the seed crystal is more than $10^{14}$ atoms/cm$^3$after solidification. Zhong et al. [7] carried out experiments to investigate the reusability of iron contaminated seed crystal with standard crucible and standard feedstock. They found that the heights of the bottom low lifetime region are similar for two silicon bricks with normal and recycled seed crystals. This means the contaminated seed crystal does not increase the iron enriched region at the ingot bottom significantly and therefore it can be reused. However, the purity of quartz crucible and that of silicon feedstock are always varied in the production process. The above experiments are not sufficient to reveal the reusability of contaminated seed crystal under these conditions comprehensively. In addition, it is difficult to carry out large-scale experiments due to the high costs. Therefore, numerical simulation becomes an effective method to study the conditions for the reusability of iron contaminated seed crystal.

## 2. Model description

The configuration and dimensions of the casting furnace for QSC silicon ingots have been introduced in a previous study [8]. The schematic diagrams of the seed crystal, silicon melt, and iron

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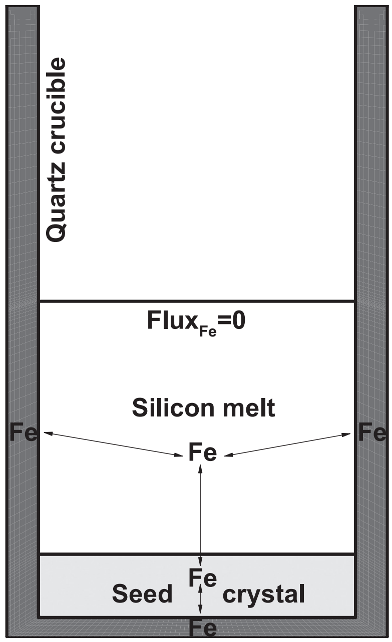


**Fig. 1.** Schematic diagram of seed crystal, silicon melt, and iron transport in the quartz crucible.

transport in the quartz crucible are shown in Fig. 1. The crucible diameter and the silicon ingot height are 100 mm. A single-crystalline silicon seed of 20 mm thickness is placed at the base of the crucible. The iron comes from the crucible walls, the silicon feedstock and the contaminated seed crystal, and it is transported by convection, diffusion and segregation.

Transient simulations of global heat transfer and iron transport for the casting process are carried out. The algorithms for the global modeling of heat transfer have been published elsewhere [8]. The equations governing iron transport in the silicon melt and crystal are

$$\frac{\partial(\rho_{Si}\omega_{Fe})}{\partial t}+\nabla\cdot\left(\rho_{Si}\omega_{Fe}\vec{u}_{Si}\right)=\nabla\cdot\left[\rho_{Si}D_m\nabla\omega_{Fe}\right], \quad (1)$$

$$\frac{\partial(\rho_{Si}\omega_{Fe})}{\partial t}=\nabla\cdot\left[\rho_{Si}D_c\nabla\omega_{Fe}\right], \quad (2)$$

where $\rho_{Si}$ is the silicon density, $\omega_{Fe}$ is the mass fraction of iron atoms in the silicon and $\vec{u}_{Si}$ is the velocity vector of the silicon melt. $D_m$ and $D_c$ are the diffusivities of iron atoms in silicon melt and crystal. Their values are expressed as [9]

$$D_m=1.0\times10^{-3}\ \mathrm{cm^2/s}, \quad (3)$$

$$D_c=\exp\left[-(3.028+3286/T)\ \ln 10\right]\ \mathrm{cm^2/s}, \quad (4)$$

where the subscript symbols $m$ and $c$ denote the melt and the crystal, respectively.

At the crystallization front, iron is segregated into the crystal, and the law of mass conservation is expressed as

$$D_m\frac{\partial C_m}{\partial n}+V_gC_m(1-k_{Fe})=D_c\frac{\partial C_c}{\partial n}, \quad (5)$$

where $C_m$ and $C_c$ are iron concentrations in the melt and crystal, respectively. $n$ is the normal direction of the melt–crystal interface and $V_g$ is the growth velocity. $k_{Fe}$ is the segregation coefficient and it is set to $8.0\times10^{-6}$.

A seed preservation process always exists after the complete melting of feedstock and before the start of crystal growth. The growth velocity $V_g=0$ and there is no segregation during this process. Therefore, the relationship of iron concentrations between the two sides of the melt–seed interface is

$$C_c=C_m. \quad (6)$$

For the crystal growth process, segregation should be taken into account and the relationship of iron concentrations between the two sides of the melt–crystal interface is

$$C_c=k_{Fe}C_m. \quad (7)$$

As the iron concentration in the quartz crucible and that in the silicon feedstock influence the transport of iron impurity and contamination of seed crystal, the reusability of contaminated seed crystal for crucibles and feedstock with different iron contents will be studied comprehensively. The quartz crucible is an important iron source and it can lead to the contamination of ingot border region. The iron concentrations on the walls of standard and pure crucibles are $2.0\times10^{15}$ and $1.0\times10^{14}$ atoms/cm$^3$ [9,10], respectively. The silicon feedstock is another iron source and the iron concentrations for the standard and pure feedstock are $2.0\times10^{15}$ and $1.0\times10^{13}$ atoms/cm$^3$ [9,10], respectively. As there is no iron evaporation at the melt free surface, we assume that the initial iron concentration in the silicon melt is the same as that in the feedstock. The iron concentration in the normal seed crystal is 0.

For the recycled seed crystal, it is not easy to determine the iron contamination level. The more realistic situation is that we consider using the iron profile obtained from an ingot with a normal seed as the initial iron concentration in the recycled seed crystal. However, there are many cases, and not all of them are representative. The recycled seed crystal can come from solidification process with different purities of crucible and feedstock, and it can also be used in solidification process with different purities of crucible and feedstock. There will be 16 cases in this study and not all of them are representative. So, a typical case should be chosen to represent the situations that often happen in the real production process. In the production process, the recycled seed crystal usually comes from the solidification process with standard crucible and standard feedstock, which leads to the typical iron concentration in the seed. Therefore, the paper mainly studies if the recycled seed crystal with typical iron concentration can be reused. For the solidification process with standard crucible and standard feedstock, the iron profile in the recycled seed crystal varies around the value of $1.0\times10^{15}$ atoms/cm$^3$, as shown in our previous study [4]. However, the profile is not unique and it varies with the change of preservation time. On the other hand, the iron profile in Ref. [4] is just at the end of full solidification. There will be annealing and cooling processes after solidification, and the iron diffusion will lead to the iron distribution in the seed more uniform to some extent. Therefore, we finally choose $1.0\times10^{15}$ atoms/cm$^3$ to represent the iron contamination level in the recycled seed crystal.

## 3. Results and discussion

The seed preservation process lasts from the end of feedstock melting to the beginning of crystal growth. There is no iron segregation during this process and Eqs. (5) and (6) hold for the iron diffusion at the melt–seed interface. During the crystal growth process, segregation occurs and Eqs. (5) and (7) hold for the iron transport at the melt–crystal interface. Iron keeps on diffusing along the seed–crystal interface at the same time. The iron diffusion during seed preservation and crystal growth is the main factor for the large iron enriched region at the ingot bottom [4,5]. Therefore, we will study the diffusion and distribution characteristics of iron impurity in the casting process for QSC silicon ingots, and evaluate the reusability of contaminated seed crystal with different quartz crucibles and silicon feedstock.