

Simulation of V/G During $\Phi 450$ mm Czochralski Grown Silicon Single Crystal Growth Under the Different Crystal and Crucible Rotation Rates

X J GUAN^{1,2,a,*} and X Y ZHANG^{1,2,b}

¹School of Materials Science and Engineering, Shandong University, Jinan 250061, China

²Institute of Crystal Materials Shandong University, Jinan 250100, China

^axjguan@sdu.edu.cn, ^bzhangxiangyu0012@163.com

Abstract. For discovering the principle of processing parameter combination for the stable growth and better wafer quality of $\Phi 450$ mm Czochralski grown silicon single crystal (shortly called Cz silicon crystal), the effects of crystal rotation rate and crucible one on the V/G ratio were simulated by using CGSim software. The results show that their effect laws on the V/G ratio for $\Phi 450$ mm Cz silicon crystal growth are some different from that for $\Phi 200$ mm Cz silicon one, and the effects of crucible rotation rate are relatively smaller than that of crystal one and its increasing only makes the demarcation point between two regions with different V/G ratio variations outward move along radial direction, and it promotes the wafer quality to weaken crystal rotation rate and strengthen crucible one.

1 Introduction

Since the 21th century, information industry has been quickly developing and the new generation of silicon wafer shows a trend of the biggest diameter of 450 mm, high uniformity and high detgency. In 2008, an agreement for a pilot line of the new silicon wafer was entered into Intel Corp, Samsung Electronics, and TSMC [1]. But, this goal has been postponed indefinitely due to the enormous input, and it is necessary to carry out the related simulation researches in advance.

The ingot of $\Phi 450$ mm silicon crystal is more than 2000 mm long and 800 kg heavy. The hot zone of furnace is estimated to be $\Phi 40$ in. or even larger [2], which results in bigger deflection of melt/crystal interface and thermal stress. Moreover, the crystal rotation rate and crucible one are relatively low than that in the smaller diameter ingot growth. It is of great interest to investigate the V/G ratio and the microdefect distribution under different combinations of crystal rotation rate and crucible one. A ingot of $\Phi 450$ mm silicon crystal was successfully grown by MEMC [3] and the change law of hot zone along with increasing crystal diameter had been preliminary discussed. E Kamiyama et al [4] investigated the size and density of voids formed with Voronkov criterion conditions and

*Corresponding author: xjguan@sdu.edu.cn

proposed several possible solutions for wafer surface inspection tools. Liu [5] successfully established 2D model of small silicon crystal growth to simulate the evolution of interface shape with different crystal and crucible rotation rates. In this paper, we carried out a 2D modeling for $\Phi 450$ mm Cz silicon crystal ingot growth, and simulated the change law of V/G ratio at different combinations of crystal/crucible rates to demonstrate their optimal combination for improving the processing technology.

2 Model Description

A 2D model of $\Phi 450$ mm Cz silicon crystal ingot growth was successfully constructed by using a commercial software, CGSim, using quasi-steady approximation. Previous experiments confirmed the correct predictions simulated by the software [6-8]. The main structure of the furnace is showed in Fig. 1. For the modeling, all heat transfer phenomena such as conduction, melt/gas convection, heat radiation and heat release were considered. Melt flow calculation adopted one equation of turbulence model based on RANS approaches. The exterior temperature was set to 300 K and shielding gas Ar was blown at a constant rate. The energy balance equation of melt/crystal interface is shown as following [6]:

$$k_{\text{crys}} \frac{\partial T}{\partial n} \Big|_{\text{crys}} - k_{\text{melt}} \frac{\partial T}{\partial n} \Big|_{\text{melt}} = \rho_{\text{crys}} \cdot L_H \cdot V_n, \quad (1)$$

where T is the temperature; n is the normal vector at the crystallization front; L_H is the silicon latent heat and V_n is the local crystallization rate normal to the melt/crystal interface; k_{crys} and k_{melt} is the crystal conductivity and melt one, respectively.

All of the performed simulations were at middle stage of crystal growth corresponding to the crystal height of 500 mm. The process parameters used in the simulations for controlling growth are given in Table 1, which are constant except for crystal rotation rate and crucible one. And the physical properties of the materials used in the simulations are same as that in References [9, 10].

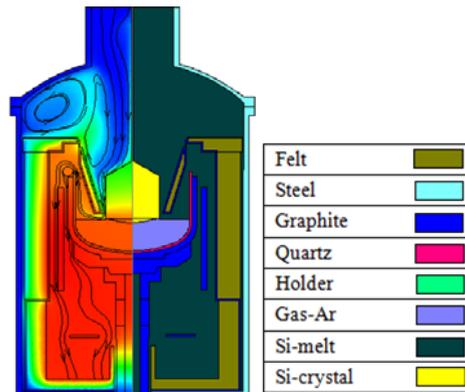


Fig. 1 Furnace geometry at the crystal height of 500 mm

Table 1 Operational Parameters Used In The Simulations

Parameter [unit]	value
Crucible diameter [in.]	40
Crystal high [mm]	500
Pulling rate [mm·min ⁻¹]	0.3
Silicon charge [kg]	400
Crystal rotation rates [rpm]	1~20
Crucible counter rotation rates [rpm]	1~5
Average heat power [kW]	120
Atmosphere pressure [Pa]	1000

3 Results Discussions

Fig. 2 shows the V/G ratio curve at different crystal rotation rates and crucible rotation one of 1 rpm, 3 rpm, and 5 rpm. It is shown in this figure that the effect laws of crystal rotation rate on V/G ratio are all same at the three crucible rotation rates, that is, when crystal rotation rate is less than 4 rpm, V/G ratio in the area near by crystal ingot axis increases and V/G ratio in the area far from crystal ingot axis decreases with speeding crystal rotation; when crystal rotation rate is larger than or equal to 4 rpm, V/G ratio monotonically decreases and the decreasing amplitude diminishes from inside to outside with accelerating crystal rotation, except for the side surface and its adjacent area. However, the crucible rotation rate also affects the law mentioned above in some degree. With crucible rotation rate increasing, the demarcation point of the two regions outward moves along radial direction, and V/G ratio decreases as the crystal rotation rate is less than 4 rpm and V/G ratio increases when the crystal one is greater than or equal to 4 rpm.

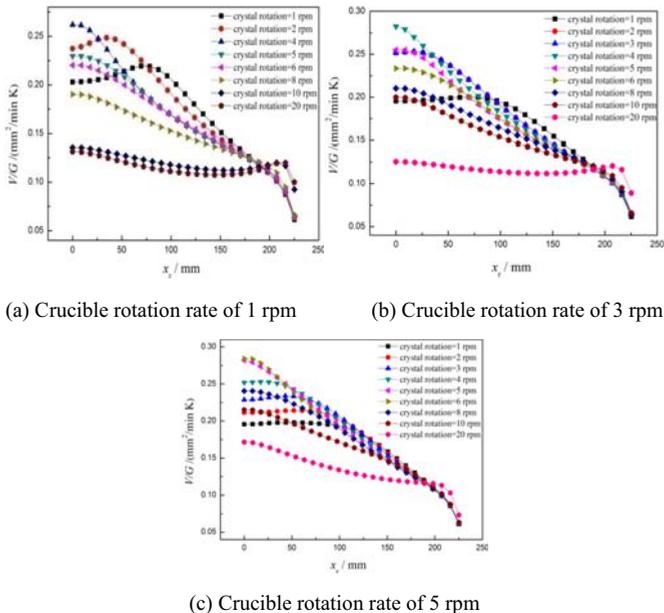


Fig. 2 The changes of V/G along radial direction under the different crystal rotation rates and crucible one

The laws of radial V/G ratio variation within the outer portion of $\Phi 450$ mm Cz silicon crystal are same as that in $\Phi 200$ mm Cz silicon crystal [9], and the corresponding V/G values synchronously reduce with the increase of crystal rotation rate except for the outer layer. But, when the crystal rotation speed is less than 4 rpm, the laws of radial V/G ratio variation within the core portion of $\Phi 450$ mm Cz silicon crystal are exactly opposite with that in $\Phi 200$ mm Cz silicon one [9]. The above results mainly attributes to the combined effect of two different mechanisms which makes the temperature gradient at the crystal side of melt-crystal interface, G , vary. On the one hand, with the increase of crystal radius, the region of raising G outward moves along radial direction due to the heat exchange between the side surface of crystal ingot and the furnace chamber atmosphere. On the other hand, with the increase of crystal rotation rate, the suction effect of melt below the interface enhances and the tendency that G decreases with increasing the radius weakens. Obviously, when the crystal rotation rate is less than 4 rpm, the later effect is stronger than the former one within the core portion of ingot, so that the V/G ratio decreases with the increase of radius, but the other circumstances is just the opposite. It is seen that the increase of crystal radius promotes the effect caused by its rotation accelerating, so that the radial V/G ratio variation of 450 mm Cz silicon crystal has some differences compared with that of 200 mm Cz silicon one.

The mechanisms for the effects of crucible rotation rate on the radial V/G ratio variation is that its acceleration not only effectively strengthens the stability of hot field and flow one of melt, but also weakens the suction effect resulted from the crystal rotation below the interface [10], so that with the increase of crystal radius, the tendency of decreasing G strengthens resulting in the expand (shrink) of crystal outer portion (core portion) and the increase (decrease) of the related V/G ratio. It is clear that the change of crucible rotation rate does not alter the effect laws of crystal rotation rate on the radial V/G ratio variation and only makes their influence extent and the sizes of corresponding areas be different. Therefore, the effect of crystal rotation rate on the radial V/G ratio variation of $\Phi 450$ mm Cz silicon crystal is larger than that of crucible rotation rate under the simulating conditions of this paper.

Obviously, the core region near by the axis of ingot has higher probability to cause V/G ratio over its lowest critical value of $0.13 \text{ mm}^2 \cdot (\text{min K})^{-1}$, which makes vacancy-type defects exist. Hence, when the smaller is crucible rotational rate and the larger is crystal one, the smaller is the region, and the smaller is the crystal defect type transition radius, r_c , in front of crystallization and the greater is the concentration of interstitial defect. It is seen in Fig. 2 that when the crucible rotation rate is 1 or 3 rpm, and crystal one is 10 and 20 rpm or 20 rpm, the V/G ratios in the entire front of crystallization are nearly less than the threshold value, which causes self-interstitial defect to dominate in the ingot, so that oxidation induced stacking fault ring (OSF-ring) and oxygen precipitate increase in the process of following annealing to damage the performances of monocrystalline silicon wafer.

For plain studying the point transformed from void defects to interstitial one in the crystal ingot, the transfer radius, r_c , under the different combinations of crystal rotation rates and crucible one are showed in Fig. 3. It is known that r_c increases with crystal rotation rate decreasing and crucible one increasing, in other words, slower crystal rotation and faster crucible one help to the increase of r_c . In industry production, the bigger r_c is desired for improving the quality of silicon single crystal wafer. However, considered their effects on the melt field and melt/crystal interface [10], the reasonable combination of crystal rotation rate and crucible rotation one is significant, i.e., neither crystal rotation rate could be too slow, nor crucible rotation rate should be too fast.

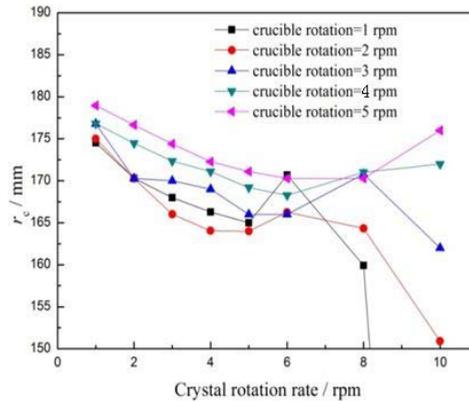


Fig. 3 Defect transition radius, r_c , under the different combinations of crystal/crucible rotation rates

4 Conclusions

The evolution of V/G ratio during 450 mm Cz silicon crystal growth has been investigated under the different combinations of crystal rotation rates and crucible one, which shows a few differences from that during 200 mm Cz silicon one. The effect laws of crystal rotation rate on V/G ratio are that when it is less than 4 rpm, the V/G ratio in the area near by the axis of ingot increases and the V/G ratio in the region far from the axis decreases with accelerating crystal rotation; when crystal rotation rate is larger than or equal to 4 rpm, V/G ratio monotonically decreases and the decreasing amplitude diminish from inside to outside with crystal rotation strengthening, except for the side surface of ingot and its adjacent area. The effects of crucible rotation rate on V/G ratio are relatively smaller than that of crystal one and its increasing merely makes the demarcation point between two regions there are different V/G ratio variations in outward move along radial direction, but the law of V/G ratio change still relates to the setting crystal rotation rate. The crystal rotation rate weakening and crucible one strengthening promote the increases of defects transition radius which improves the wafer quality, and the determination of their reasonable combination needs to consider the related effects on the melt field and melt /crystal interface.

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