IWMCG-8 国际晶体生长模型化会议报告

——单晶硅提拉法生长工艺，熔体碳杂质的下降

Czochralski (CZ) crystal growth of single crystalline silicon (Si) is invariably accompanied by transport of impurities such as carbon (C), oxygen (O), and related products from chemical reactions in the high temperature range. C contamination in the growing crystal is detrimental for the minority carrier lifetime, which is one of the critical parameters of wafer for power device [1]. Reduction of C contamination in the CZ-Si crystal is required for the production of high performance Si wafer.

Contamination of C in Si crystal mainly originates from carbon monoxide (CO) generation on the graphite components. And, incorporation of C occurs prior to the growth stage [2]. The reason is the CO generation starts from the preheating stage, and reaches the maximum in the melting stage of the CZ-Si crystal growth. The generated CO incorporated into the Si feedstock and accumulated in the melt. Thus, C prediction with quasi-static assumption is not sufficient to account for C accumulation in CZ-Si crystal growth [3]. Therefore, transient global simulations of heat and mass transport were performed for the melting process of CZ–Si crystal growth. A virtual PID controller for the temperature was introduced to realize the power control of the heater. Accumulation of C in Si feedstock was predicted for the entire melting process, which consists of preheating, melting and stabilization stages.

To reduce the C contamination effectively, it is essential to control the C transport from its generation, incorporation and accumulation in the growth. Besides the CO generation by the reaction between graphite and SiO, the reaction between quartz crucible and graphite susceptor was also taken into account as another CO source [4]. Since softening crucible contacts with susceptor, this reaction is actively involved at the high temperature. The contact reaction process is shown schematically in Fig. 1. The generated SiO and CO could be transported from the narrow gap to the gas domain. Back diffusion of CO may affect C contamination in Si feedstock.

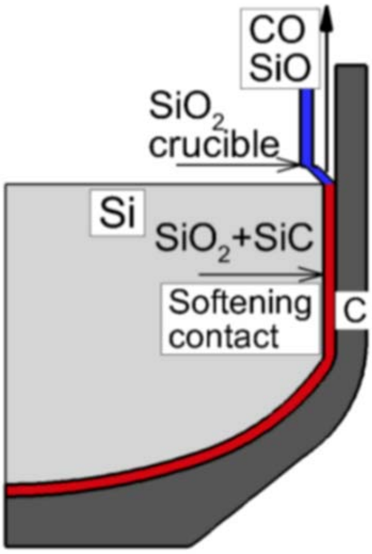
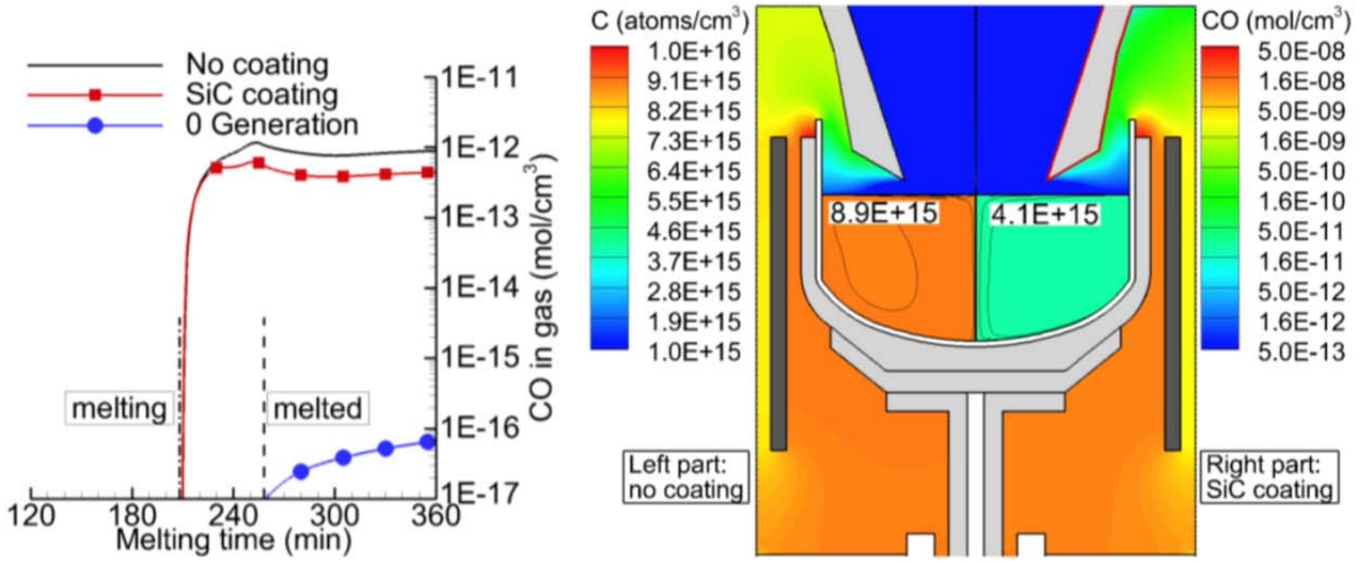


Fig. 1 Contact reaction between crucible and susceptor

To suppress the CO generation, silicon carbide (SiC)□coating could be applied conventionally to the gas-guide above the melt surface. Three cases, including no coating, SiC coating and no reaction, were compared for CO concentrations above the melt surface, as shown in Fig. 2(a). Without the consideration of coating reaction, hardly any CO could be incorporated into the Si melt as C contamination. This is inconsistent with the practical process. Even the reactivity of SiC is lower than graphite, reaction between SiC and gaseous SiO must be taken into account due to the short distance between gas-guide and Si feedstock. Actually, SiC coating with low CO generation could only reduce the C incorporation partially in real growth, as shown in Fig. 2(b). Therefore, these two extra CO sources were introduced in the present study, and implemented as boundary conditions of the transient global simulation of melting process of CZ-Si growth.



(a) CO evolution above the melt surface (b) CO and C at final state of melting process
Fig. 2. Effect of SiC coating on CO and C transport

According to the physical properties of□argon (Ar) gas, the Péclet number of□CO transport in the typical gas flow of□CZ-Si growth is very high, around□2000 [5]. This indicates the□enhancement of the Ar flow above the□melt could reduce the incorporation□rate of C efficiently. Parameter studies□of furnace pressure and gas flow rate□were conducted on the accumulation of□C during the melting process.□Convective transport of SiO and CO□dominated at the higher flow rate. Thus,□generation and back diffusion of CO□were both suppressed by the intense gas□flow. Because of the combination of these two positive effects, the increase in flow rate could reduce the C contamination by logarithm, as shown in Fig. 3. According to the accumulation of C, the final C content depends on the growth duration and contamination flux at the gas/melt interface.

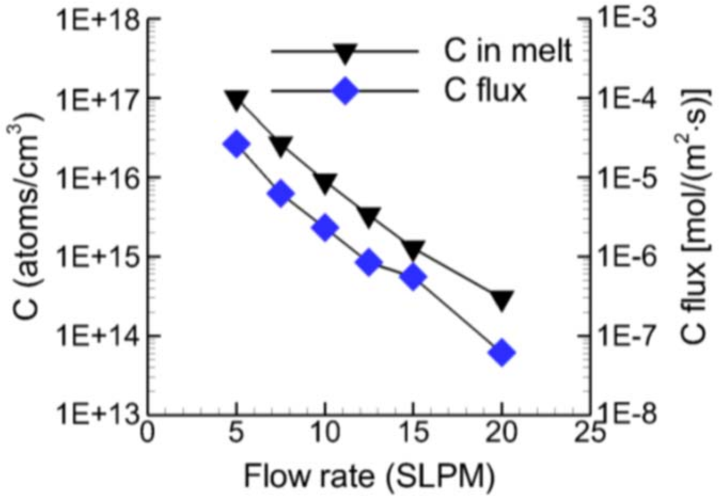


Fig. 3 Effect of Ar gas flow rate on C contamination in Si melt

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