Dynamic Simulation for Top-Seeded Solution Growth of SiC Single Crystal

Gangqiang Liang[1], Jie Zhou[1], Yuan Liu[2]
1. School of Materials Science and Engineering, Tsinghua University, Beijing 100084, China
2. Key Laboratory for Advanced Materials Processing Technology (Ministry of Education), Beijing 100084, China
*Corresponding address: e-mail: yuanliu@mail.tsinghua.edu.cn

Abstract: SiC-MOSFETs have partially replaced traditional Si-IGBT devices in high-voltage fields such as new energy vehicles and photovoltaics, but they still face the problem of high cost today. Solution method is a method capable of growing high-quality SiC single crystals at low cost, and numerical simulation is considered an effective way to probe its process parameters. The current research work reports the prediction of temperature, flow rate, and concentration distributions under initial steady-state conditions, however, detailed discussion on the kinetic coupling process of crucible corrosion and seed crystal growth during solution growth is limited. In this work, the prediction of the geometrical change of the interface between crucible corrosion and seed crystal growth is realized by using COMSOL software with the moving mesh module, and the effects of seed crystal rotational speed and temperature distribution on the stability of the growth interface are discussed.

Keywords: SiC single crystals; solution growth; numerical modeling

1 Introduction

Silicon carbide (SiC) power devices have found extensive applications in industrial equipment, including electric vehicles, photovoltaics and railways. As one of the IV-IV compound semiconductors, SiC is capable of applying to scenarios at high temperatures, high voltage and strong radiation attributed to its superior properties. The production of SiC substrate relies on SiC bulk growth technology. Most of the commercial N-type SiC substrates are produced by the physical vapor transport (PVT) method, while it is challenging to prepare P-type SiC ingots since the Al source is released excessively in the initial stage of sublimation, leading to large defect density. As an ideal alternative candidate, top-seeded solution growth (TSSG) was proved to be an effective way to fabricate P-type crystals with a low resistivity of 35mΩ cm [1]. Besides, micropipes can be easily eliminated induced by step flow, and most of the threading dislocation (TDs) can be converted into BPD or Frankel-type stacking faults, realizing the reduction of dislocation density in the grown crystals [2]. In the development of TSSG technology in the past 20 years, the crystal diameter has been enlarged from 4 mm to 15 mm by the meniscus growth [3], the maximum growth rate of 2 mm/h with a FWHM value of 20 arcsec [4] and 4H-SiC with ultra-low dislocation density have been reported [5]. TSSG therefore became a promising method to grow high-quality single crystal SiC ingots and the corresponding finite elements analysis (FEA) of SiC crystal growth process has been well established in previous investigations [6-10].

2 Experimental procedure

Figure 1 depicts the top-seeded solution growth system. A radiofrequency induction coil (1.8 kHz) with a power of 5 kW is employed to heat the graphite hot wall and graphite crucible under argon atmosphere at 50 kPa. The pure Si melt is 40 mm in height and 200 mm in diameter. The SiC seed crystal of 150 mm in diameter is mounted on the graphite seed holder connected by a graphite shaft and then dipped 1mm below the solution surface.

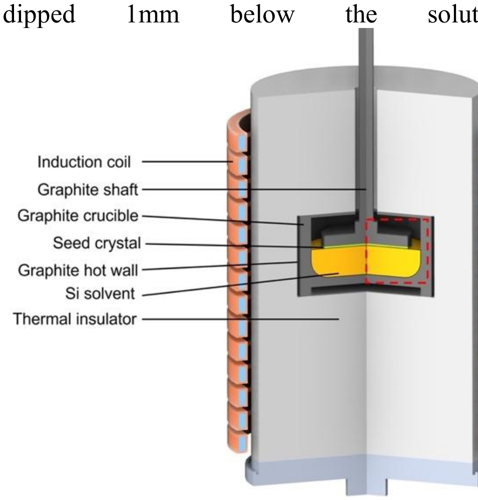

Figure 1 Schematic view of TSSG growth system

3 Result and discussion

Effect of crystal rotation rate on the corrosion of graphite crucible and grown crystal surface

The seed rotation brings the upward flow at the center of Si melt, enhancing the transport of carbon solute towards the growth surface. However, the rapid melt flow placed at the edge of the melt surface induced by seed rotation accelerates the local erosion of graphite wall, which may lead to leakage of the melt once crucible wall is cracked.

Effect of crucible rotation rate on the corrosion of graphite crucible and grown crystal surface

By employing the crucible rotation, the concentration distribution becomes uniform so that more carbon solutes are applied to the growth interface. The shape of the erosion area shifts from local erosion to uniform erosion at the interface between the solution and the graphite crucible wall.

4 Conclusion

In this work, we proposed a numerical model for predicting the geometrical change of the growth surface and graphite crucible during top-seeded solution growth of silicon carbide single crystals. The simulation results imply that seed rotation enhances the growth rate by facilitating the upward flow of carbon solute. Meanwhile, the melt leakage may occur under a long period of growth due to the local erosion of the crucible wall. This phenomenon is reduced by applying the crucible rotation since the erosion area expands. Higher growth rates are therefore obtained as well.

5 Acknowledgment

This work was financially supported by the Beijing Municipal Science and Technology Commission (Grant No. Z23111000270000).

References

[1] Shirai T, Danno K, Seki A, Sakamoto H, Bessho T. Solution growth of p -type 4H-SiC bulk crystals with low resistivity. 2014, 75–78.

[2] Harada S, Yamamoto Y, Xiao S, Koike D, Mutoh T. Dislocation conversion during SiC solution growth for high-quality crystals. Materials Science Forum, 2015, 821-823: 3–8.

[3] Danno K, Yamaguchi S, Kimoto H, Sato K, Bessho T. Trials of solution growth of dislocation-free 4H-SiC bulk crystals. Materials Science Forum, 2016, 85:19–22.

[4] Kado M, Daikoku H, Sakamoto H, Suzuki H, Bessho T, Yashiro N, Kusunoki K, Okada N, Moriguchi K, Kamei K. High-speed growth of 4H-SiC single crystal using Si-Cr based melt. Materials Science Forum, 2013, 73–76.

[5] Murayama K, Hori T, Harada S, Xiao S, Tagawa M, Ujihara T. Two-step SiC solution growth for dislocation reduction. Journal of Crystal Growth, 2017, 468: 874–878.

[6] Dang Y, Kutsukake K, Liu X, Inoue Y, Liu X, Seki S, Zhu C. A transfer learning-based method for facilitating the prediction of unsteady crystal growth. Advanced Theory and Simulations, 2022, 9(5): 2200204.

[7] Yu W, Zhu C, Tsunooka Y, Huang W, Dang Y, et al. Geometrical design of a crystal growth system. CrystEngComm., 2021, 23: 2695–2702.

[8] Sui Z, Xu L, Cui C, Wang R, Pi X, Yang D, Han X. Effects of solution height and crystal rotation on the solution flow behavior in the top-seeded solution growth of SiC single crystals. CrystEngComm., 2024, 2024, 26: 1022–1031.

[9] Liu B, Yu Y, Tang X, Gao B. Optimization of crucible and heating model for large-sized silicon carbide ingot growth in top-seeded solution growth. Journal of Crystal Growth, 2020, 533: 125406.

[10] Li F, He L, Yan Z, Qi X, Ma W, Chen J, Xu Y. Effects of crystal rotation on the carbon transport in the top-seeded solution growth of SiC single crystal. Journal of Crystal Growth, 2023, 607: 127112.