A thermodynamic interpretation for PVT growth of SiC Single Crystals and challenges for the reduction of the dislocation density

T. Fujimoto, S. Ushio, S. Sato, K. Tani, M. Katsuno, H. Tsuge, H. Yashiro, H. Hirano, and T. Yano

Advanced Technology Research Laboratories,
Nippon Steel & Sumitomo Metal Corporation
20-1 Shintomi, Futtsu, Chiba 293-8511, JAPAN

There has been remarkable progress in the research field of silicon carbide (SiC) power devices, a key technology by which it is expected that more efficient systems for utilization of electric power can be possible. SiC single crystals are a key material for a wide variety of power device applications, and physical vapor transport (PVT) method, which is so-called the modified Lely method, is now a widely adopted method for fabricating SiC crystals. Up to now, the PVT method has also been developed markedly, giving rise to the realization of larger diameter SiC crystals up to 150 mm, thereby stimulating intense research in order to improve crystallinity, i.e., the reduction of the dislocation density as well as the micropipe (MP) defect density. As a result, 100 mm-diameter 4H-SiC single crystal wafers with MP densities less than 1/cm^2 have become commercially available [1].

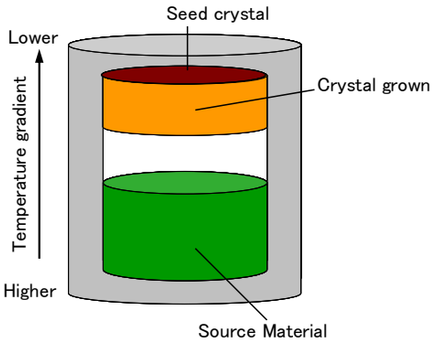

Fig. 1 Schematic of typical growth configuration of PVT method for SiC single crystals

Fig. 1 shows schematic of a basic setup for SiC growth by the PVT method, in which a SiC single seed crystal and source materials such as SiC powders are placed in a graphite crucible. At higher temperatures exceeding around 2300K with an appropriate temperature gradient, the SiC source material starts subliming, followed by being transported by diffusion to the seed crystal. The SiC vapor becomes over-saturated, leading to recrystallization of solid SiC onto the seed surface. Until recently, the elemental processes occurring during the PVT growth were mainly discussed by means of numerical thermodynamic calculations because the process temperature is too high to experimentally elucidate details of the processes. However, combining with a number of results obtained by observations of the phenomena in actual growths of SiC, we have succeeded in deducing a pressure-dependent phase diagram of Si-C binary system which is very important for realizing accurate control of the growth phenomena. It can be shown that the phase diagram obtained allows us to give possible explanation for almost all the elemental processes in PVT by assuming that the effect of the graphite crucible is smaller although it was shown experimentally that it definitely exchanges carbon with sublimed gaseous species [2]. In other words, the PVT method does comprise of phase transitions between stable Si-C phases at high temperatures. In addition, the formation mechanism of various macro-defects such as Si-droplets and hexagonal defects will be explained by means of the phase diagram obtained [3, 4].

Macro-defects in SiC single crystals such as the MP defect are in general formed mainly due to insufficiently optimized crystal growth conditions such as unwanted disturbance of SiC growth mode caused by foreign phases such as silicon droplets or foreign polytype formation during 4H-SiC growth. Based upon the phase diagram described above, we can provide quasi-quantitative explanation for suppressing the growth disturbances, and thus gain deeper insight into actual process of the PVT for SiC in order to establish the accurate process control. Such understanding is also important for reducing other crystal imperfections such as dislocations or stacking faults with various structures. Although these defects are not a form of stable phases, the process control for realizing growth stability is undoubtedly necessary from viewpoints of both constituent chemical reactions in the PVT process and thermo-mechanical effects on the crystal grown.

In particular, basal plane dislocations (BPDs) have drawn much attention with respect to high-power bipolar device applications because it leads to the formation of Shockley-type stacking faults in forward operations of the devices of particular structures, resulting in severe deterioration of device properties [5]. The BPD is known to generate due to inappropriately large internal shear stresses caused by the temperature gradient inside crystals grown, suggesting that optimizing growth conditions in viewpoint of the residual stress inside the crystal will lead to the reduction of the BPD [6].

In the ECS symposium, a possible mechanism for the SiC growth in PVT based upon the Si-C binary system is firstly introduced, and then recent progress of SiC crystals with much reduced defect densities is reported, specifically on the reduction of the BPD density in SiC single crystal wafers.

References

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This work is partly supported by New Energy and Industrial Technology Development Organization (NEDO) under the project of "Novel Semiconductor Power Electronics Project Realizing Low Carbon Emission Society".