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Modeling of growth kinetics of SiC single crystal in PVT process

Tomasz Wejrzanowski[1], Janusz Dagiel, Mateusz Grybczuk[1], Jakub Niescior[1],
Emil Tymicki[2], Krzysztof J. Kurzydlowski[1]

[1]Warsaw University of Technology, Faculty of Materials Science and Engineering (InMat)
Wołoska 141, Warszawa 02-507, Poland

[2]Institute of Electronic Materials Technology (ITME)
Warszawa 01919, Poland

Abstract

The present paper deals with the design of optimal process conditions for manufacturing of high quality SiC single crystal SiC. Different aspects of the technology have been taken into account. The geometry of the reactor was modified to obtain optimal mass transport and temperature profile and the influence of process conditions on the SiC crystal growth kinetics has also been studied. The results of modeling have been implemented in the SiC growth process developed for commercial use.
In this study the Finite Volume method was applied to understand the phenomena taking place in the PVT (Physical Vapor Transport) reactor during growth of bulk SiC single crystal.

Case study

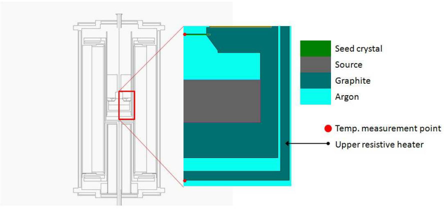

Figure 1.
PVT SiC reactor chamber with it's position in the furnace and main components described. Images obtained with Virtual Reactor.

Introduction

Influence of process conditions and reactor geometry on SiC single crystal growth was investigated. Virtual Reactor PVT SiC simulation software was used to study this subject. Furnace model (Figure 1) was based on reactor used by ITME ([2]). Purpose of this study was to determine the general behavior of the device and to predict optimal process conditions. Where available, results are compared with experimental data.

Temperature

Process conditions in the reactor chamber are controlled by fixing temperature at measurement points and forming insulator geometry over seed crystal. Heating is performed by two resistive heaters up to required temperatures. Reactor model was created to set the same process conditions.

Set of simulations for given temperature range were performed. Temperature distributions (Figure 3) and obtained crystal sizes were compared (Figure 2). The first conclusion is that higher temperature during the process produces bigger crystal [2]. It was found that changing lower measurement point temperature had little effect on crystal size which depends mostly on upper measurement point temperature. Simulations yielded bigger crystals, but are qualitatively consistent with experiment results. Discrepancy may be a result of modeling and omission of some growth hindering phenomena.

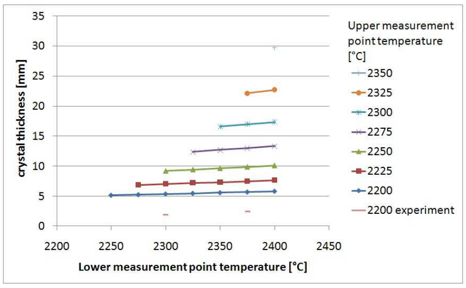

Figure 2.
Crystal thickness resulting from simulations for different temperature conditions. Results obtained with Virtual Reactor and compared to results from experiments.

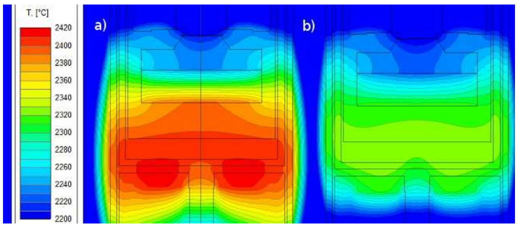

Figure 3.
Temperature distribution in the PVT SiC reactor for different temperatures at measurement points [°C]
a) 2200 and 2400; b) 2200 and 2300 ('upper' and 'lower'point respectively). Pictures from Virtual Reactor

Pressure

SiC crystal growth in PVT method is also governed by pressure and its influence has to be precisely studied. A set of simulations were performed to confirm that decreasing pressure in reactor chamber leads to increasing growth rate [2]. Simulation results were qualitatively consistent with experiment data (Figure 4). Partial pressure distributions of SiC thermal decomposition products in reactor chamber along with mass transport paths were also investigated (Figure 5).

Mass transport originated mainly from areas of the seed material bordering with reactor walls which can be explained by relatviely high temperature in this area.

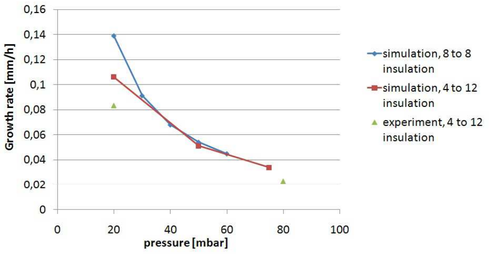

Figure 4.
Comparison of simulation and experiment about the pressure influence on crystal growth rate.
Simulations were performed for two insulation configurations: 8 to 8 and 4 to 12

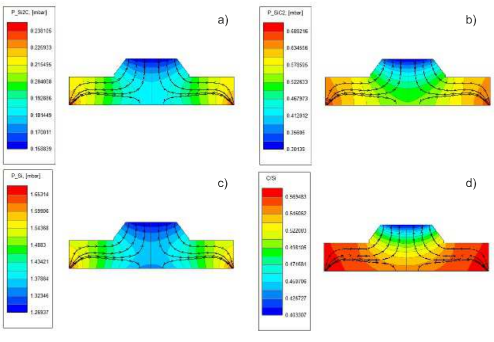

Figure 5.
Partial pressures distributions and mass transport streamlines inside reactor chamber.
a) Si_2C; b) SiC_2; c) Si; d) C to Si atom ratio
Pictures from Virtual Reactor

Insulation

Insulation geometry shapes temperature distribution over seed crystal. Figure 6 presents sample insulation geometries and figure 7 shows growth rate dependence on insulation geometry. Insulation geometry had some effect on crystal shape (figure 8) and geometries with less wide space area above seed made crystal more round at the edges.

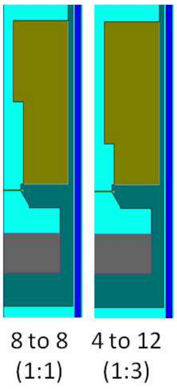

Figure 6.
Sample insulation geometries configurations. Pictures from Virtual Reactor

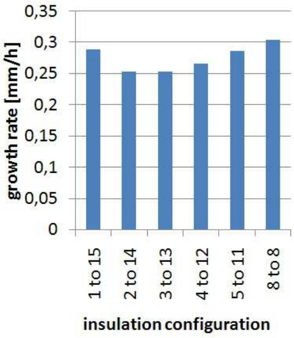

Figure 7.
Growth rate dependence of the insulation geometry. Data obtained with Virtual Reactor

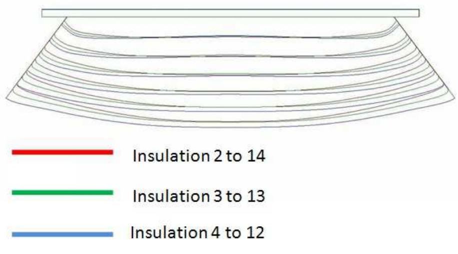

Figure 8.
Iinsulation geometry influence on crystal shape in subsequent simulation steps (timestep 10h). Data obtained with Virtual Reactor

Conclusion

Numerical simulations predict the temperature distribution and growth kinetics at satisfactory level. It was found that especially the early stage of crystal growth might be controlled by changing the insulation types. Apart from the thermal conditions, which can be controlled directly by setting up the temperature on the heaters or indirectly by modification of insulation geometry, the gas pressure in the chamber is of key importance for the growth rate of SiC bulk single crystal.

References

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Aknowledgements

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