

Coupled Numerical Modeling and Thermodynamic Approach for SiC Growth Process

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Abstract

Silicon carbide (SiC) single crystals are industrially produced by the physical vapor transport technique. Apart from the geometry of the growth setup, there are two main process parameters that can be controlled: temperature and pressure. To support the development of the process, numerical simulation has imposed as the only tool able to describe the process itself, providing a good evaluation of physical parameters and their distribution inside the growth chamber [1-2]. Although the computation of heat and mass transfers in real growth geometry (2D axisymmetric or 3D) is now accurate enough to be predictive, there are still some strong issues which are not considered in a satisfactory way. This is the case for instance for the thermochemistry of the Si-C system and its coupling to mass transfer. Recently, it has been reconsidered and a better comprehension of the solid-vapor interface was reported [3-4]. But two essential questions are still open: i) how to treat the thermochemistry of the solid SiC crystal? ii) How the latter could be coupled to the numerical modeling of the process?

In this work, we present a method to assess the chemistry of solid SiC crystal, i.e. the activities of both Si and C atoms in the crystal during the PVT growth process by using the coupled numerical modeling of heat and mass transfer (Fig. 2 and 3) and the thermodynamic calculations approach. The numerical modeling for the induction heating, heat and mass transfer was done by Finite Element Method computed in a 2D axisymmetric space dimension with COMSOL Multiphysics. A typical geometry and computed temperature distribution are shown in Fig.1. The thermodynamic calculation was done by treating SiC as a solid solution using the thermochemical properties taken from the JANAF database [5].

The link between the applied growth conditions and the SiC crystal thermochemistry (Fig. 4) could be one of the key issues that will allow first to link the growth and the occurrence of cubic or hexagonal polytypes, and second to describe quantitatively doping incorporation.

Reference

[1] M. Pons, E. Blanquet, J.M. Dedulle, I. Garcon, R. Madar, C. Bernard, J. Electrochem. Soc. 143 (1996) 3727.

[2] A. S. Segal, A.N. Vorob'ev, S.Yu. Karpov, Yu. Makarov, E.N. Mokhov, M.G. Ramm, M.S. Ramm, A.D. Roenkov, Yu.A. Vodakov, A.I. Zhmakin, Mater. Sci. Eng. B61-62 (1999) 40.

[3] G. Honstein, C. Chatillon, F. Baillet, J. Eur. Ceram. Soc. 32 (2012) 1117.

[4] T. Fujimoto, N. Ohtani, H. Tsuge, M. Katsuno, S. Sato, M. Nakabayashi, T. Yano, J. Electrochem. Soc. 2(8) (2013) N3018.

[5] M. W.Chase, NIST-JANAF thermochemical tables. American Chemical Society, Washinton, D.C. and Woodbury, N.Y., 1998.

Figures used in the abstract

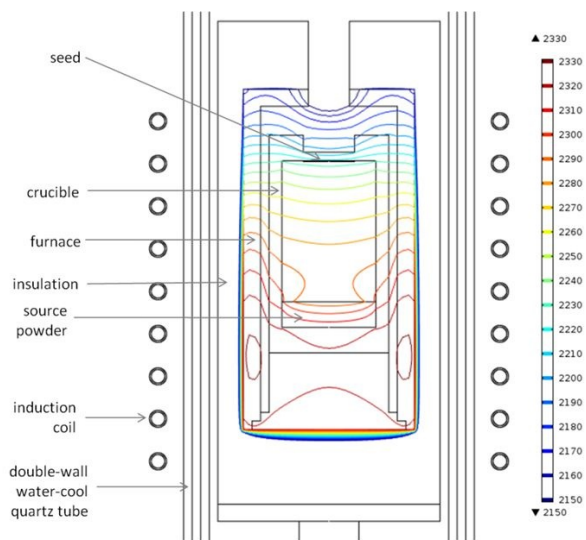


Figure 1: Fig. 1. Geometry and temperature distribution (°C) in the PVT growth reactor

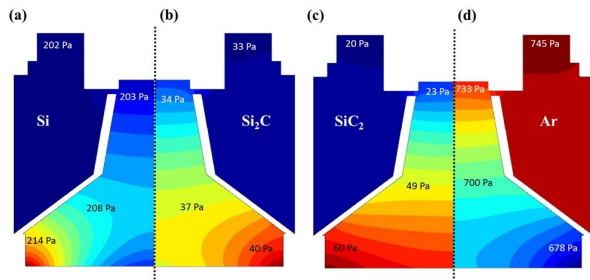


Figure 2: Fig. 2 Distribution of species partial pressure in the growth chamber: (a) Si, (b) Si₂C, (c) SiC₂, and (d) Ar

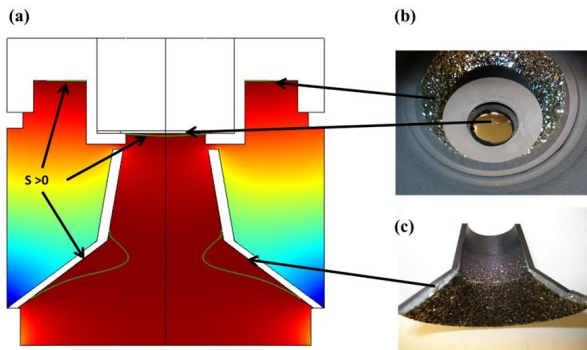


Figure 3: Fig. 3 (a) Distribution of supersaturation (S) in the growth chamber and the experimental observations (b) at the seed holder, and (c) at the graphite guide

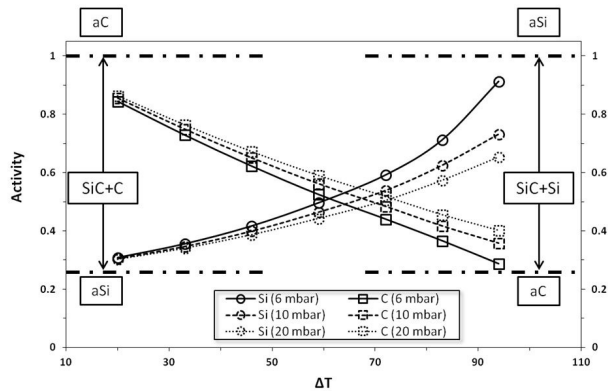


Figure 4: Fig. 4. Activity of Si and C in solid SiC crystal with varying seed-source temperature difference and the effect of total pressure. The seed temperature is fixed at 2225 °C (± 2 °C). The dashed-dotted lines show the limit of activity at the SiC-Si and SiC-C phase boundaries