Coupled Numerical Modeling And Thermodynamic Approach For SiC Growth Process

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Introduction: SiC single crystals are industrially produced by the PVT. 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 [1].

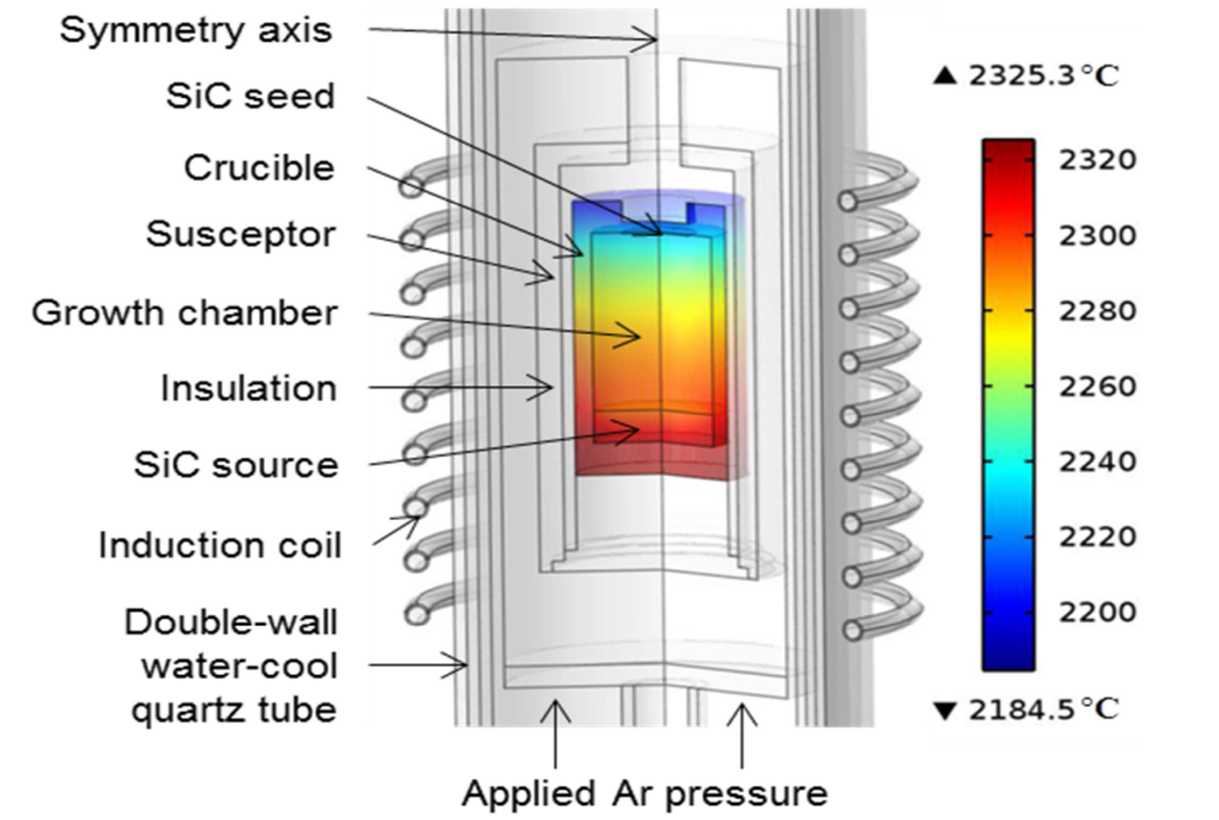

Figure 1. Geometry and temperature distribution (Celsius) in the PVT growth reactor.

Computational Methods: We developed 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. Using the temperature distribution presented in Figure 1, we computed the mass transport with the set of boundary conditions.

Results: At constant seed temperature, the effect of the pressure and of the ΔT on the activities of Si and C in solid SiC is shown and compared to the limit of Si and C activities at the SiC-Si and SiC-C phase boundaries (Figure 2).

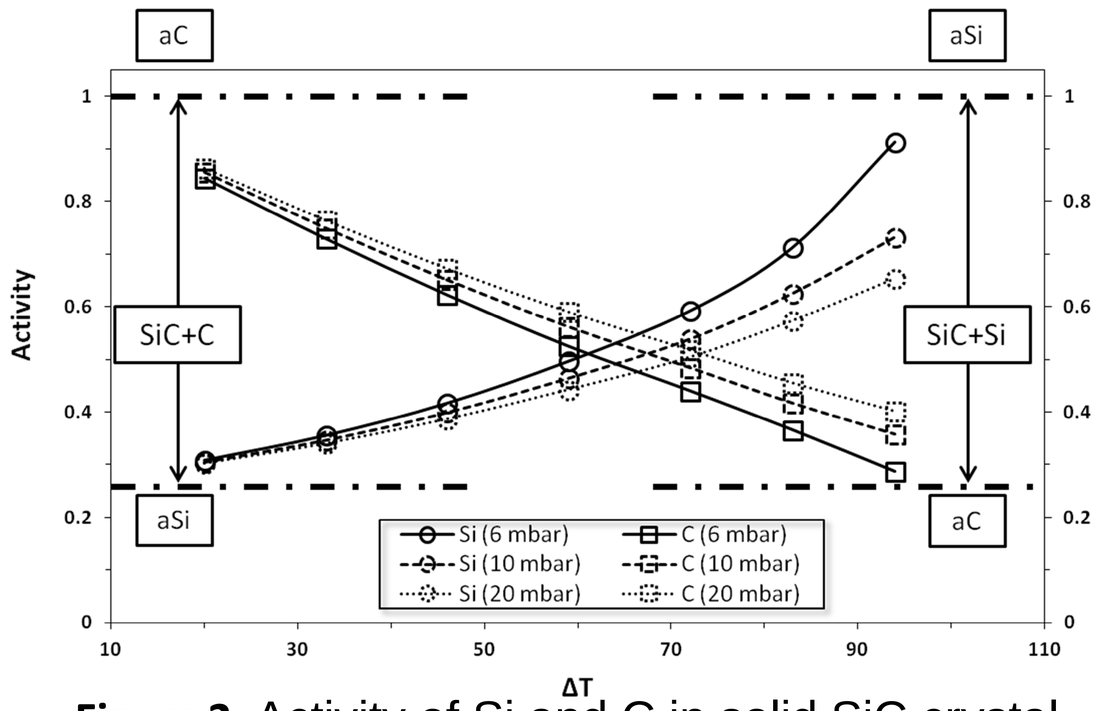

Figure 2. Activity of Si and C in solid SiC crystal

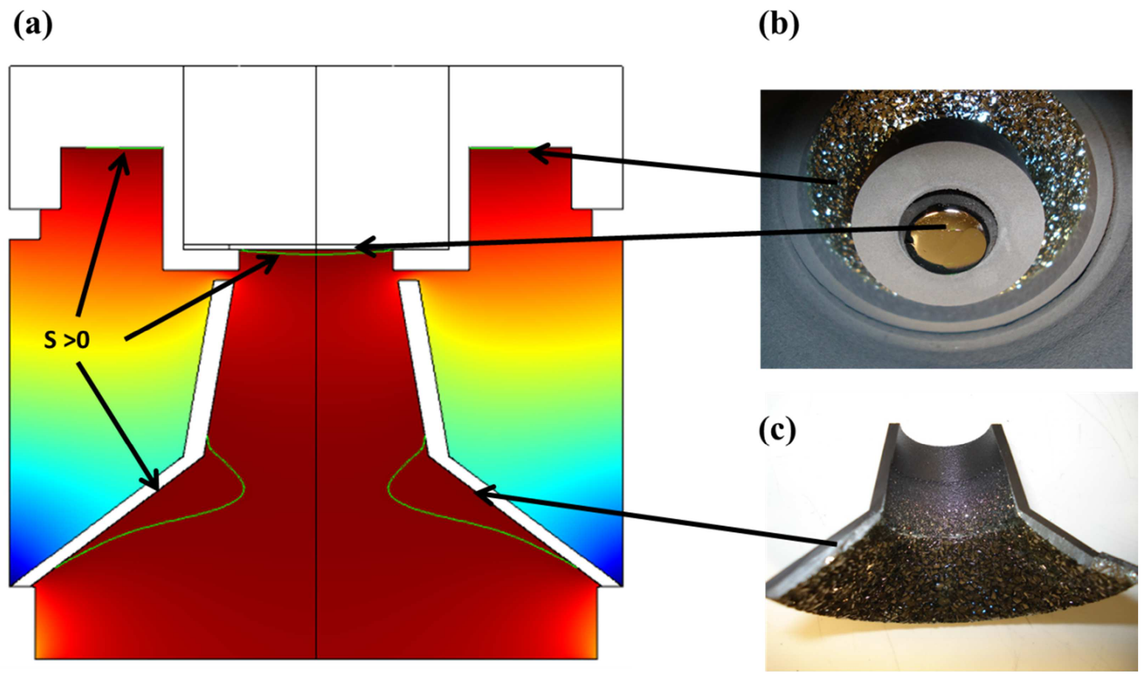

Figure 3. (a) Distribution of supersaturation in the growth chamber and the experimental observations (b) at the seed holder, and (c) at the graphite guide

Conclusions: The link between the applied growth conditions and the SiC crystal thermochemistry (Fig. 3) 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.

References:

1 A. S. Segal, and al, Mater. Sci. Eng. B61-62 (1999) 40.