New development in modeling of PVT SiC bulk crystal growth

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Key words: Numerical simulation, SiC crystal growth, growth prediction, stress and dislocations

Abstract

Numerical simulation provides an indirect, feasible way to reproduce the growth process by solving mathematical models. Most modeling approaches consider SiC crystal growth to be a steady-state process, however due to changes in some factors or properties can lead to variations in the system, non-stationarity is an inherent feature of the growth process. Here we use Virtual Reactor (VR) software to simulate the long-term growth of bulk SiC crystals. This software assumes that the transient times of all processes occurring in the system are much less than the growth duration, which means that actual growth with slowly varying parameters can be replaced by solving a series of steady-state problems at various discrete moments with constant parameters.

At each stage, based on user-defined model geometry, material properties, boundary conditions and processes (including system heating, inert gas pressure and coil motion), the heat transfer coupled with the reactive species transport is computed to obtain the crystal growth rate and the rate of formation of various deposits on the crucible walls, which are used to modify the geometry of the system. In this, the software takes into account parasitic deposition or etching on the crucible walls by equilibrium of all possible condensed phases in the SiC-C system with the initial graphite surface. Figure 1 shows the evolution of the crystal shape with time. Figure 2 shows the effect of different coil position on wall deposition, it can be seen that polycrystalline deposition is more pronounced at lower coils, while deposition on the wall at higher temperature is significantly suppressed at higher coils. Since polycrystalline deposition near the crystal strongly influences the evolution of the crystal shape, the prediction of the crystal shape will not be accurate enough without considering polycrystalline deposition. In addition, the software can characterize the reduction of graphite activity at high temperature by specifying the sticking coefficients of the different species on the graphite wall.

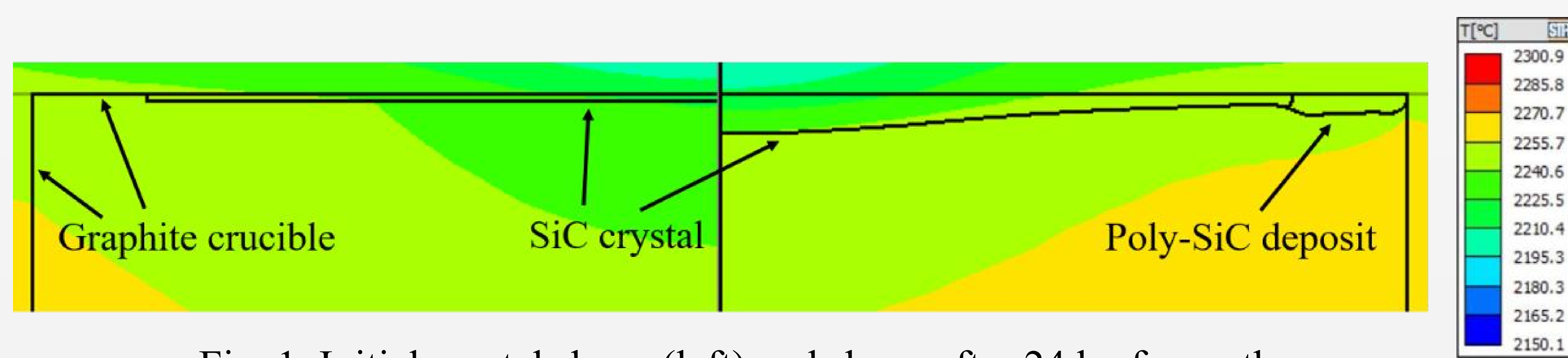

Fig. 1. Initial crystal shape (left) and shape after 24 h of growth

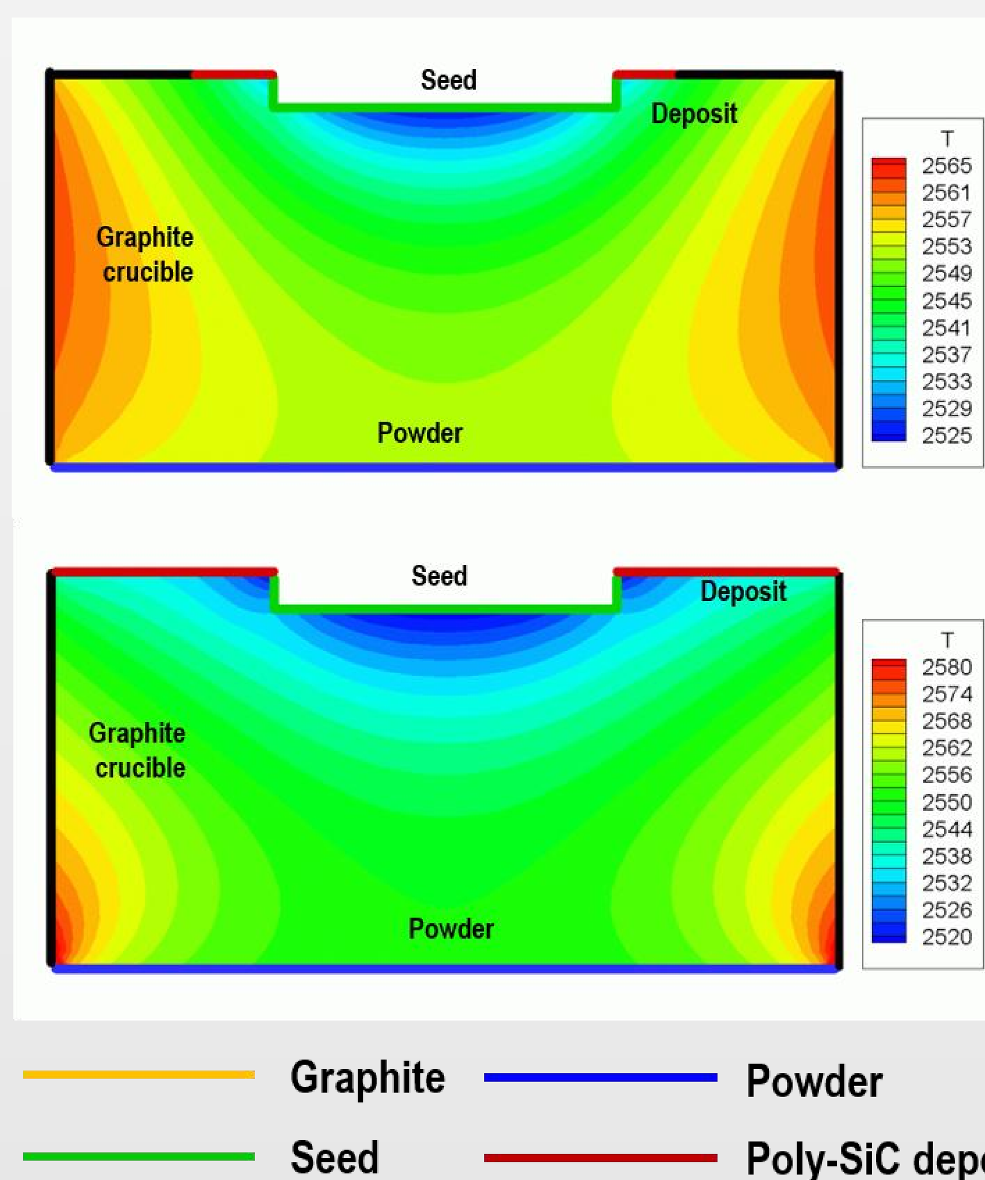

Fig. 2. Effect of coil position on the parasitic deposition: coil raised by 50 mm (top) and coil lowered by 50 mm (bottom)

The variation of powder properties is an important unstable aspect of the growth process. The VR software approximates the powder source as a continuous medium and uses the thermodynamic approach to model the chemical processes on the particles to obtain the variation of the powder parameters (local porosity, particle size and degree of graphitization) over time due to particle sublimation and recrystallisation. Figure 3 shows the distribution of the local porosity of the powder at different times.

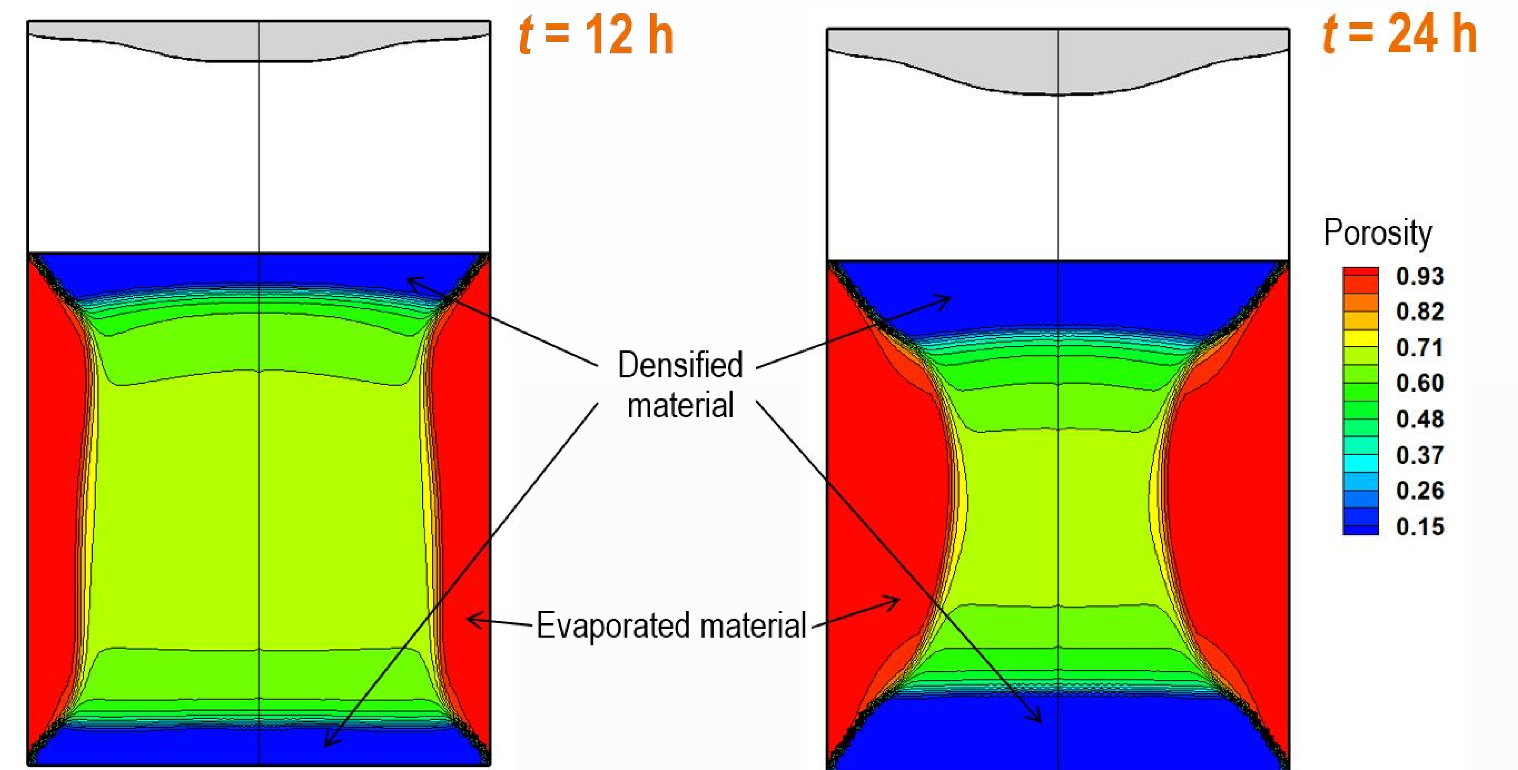

Fig. 3. Porosity distribution in the SiC powder source

The pressure of the gas mixture in the growth chamber is critical during growth, since the growth rate is directly dependent on the rate of species transfer to the growth surface by convection and diffusion. Generally, as the powder source sublimates and new species are added to the growth chamber, the pressure inside the chamber will differ from the external pressure, and will be linked to the pressure outside by mass exchange through the porous graphite. The VR software calculates the corresponding internal pressure and gas quality based on the pressure of the surrounding inert gas and the current temperature distribution, combined with the growth process and mass exchange between the internal and external of the crucible. Figure 4 shows the influence of the crystal temperature on the internal pressure and crystal growth rate. It can be seen that the internal pressure can change dramatically even if the external pressure remains constant.

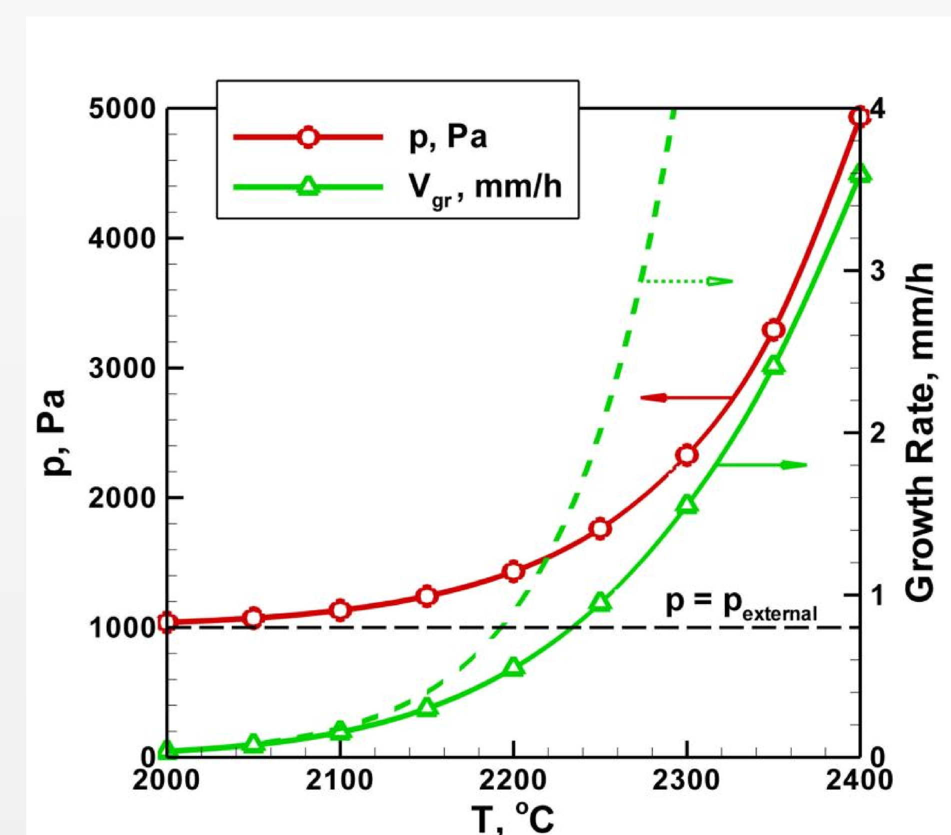

Fig. 4. Pressure inside the growth chamber (red line, circles) and the growth rate (solid green line, triangles) as functions of temperature. Dashed green line – growth rate computed as if the pressure in the chamber was equal to external pressure. External pressure = 1000 Pa

The VR software also allows the prediction of the thermoelastic stress as well as the dislocation distribution within the crystal during the growth. Generally, the SiC growth direction corresponds to the [0001] axis of the crystal, while hexagonal crystals have the characteristic of transverse isotropic, which means that the thermoelastic stress can be analyzed within the framework of a 2D axisymmetric model when the symmetry axis is [0001]. The computational domain is meshed using cylindrical coordinates and the absolute magnitude of the shear stress is considered to be the applied stress affecting the formation of gliding dislocations in the (0001) plane of the hexagonal crystal. Figure 5 shows the distribution of shear stress and dislocation density in the crystal. It can be seen that the maximum stress occurs at the periphery of the crystal and the dislocation density is proportional to the value of the shear stress. Software predicts also wafer bow based on the residual plastic strain in the layers located within the wafer cut out of the crystal. Information on the strain is based on the simulation of the crystal cooling. Figure 6 demonstrates plastic strain in the cooled crystal and predicted wafer warpage (wafer location is marked with dashed line).

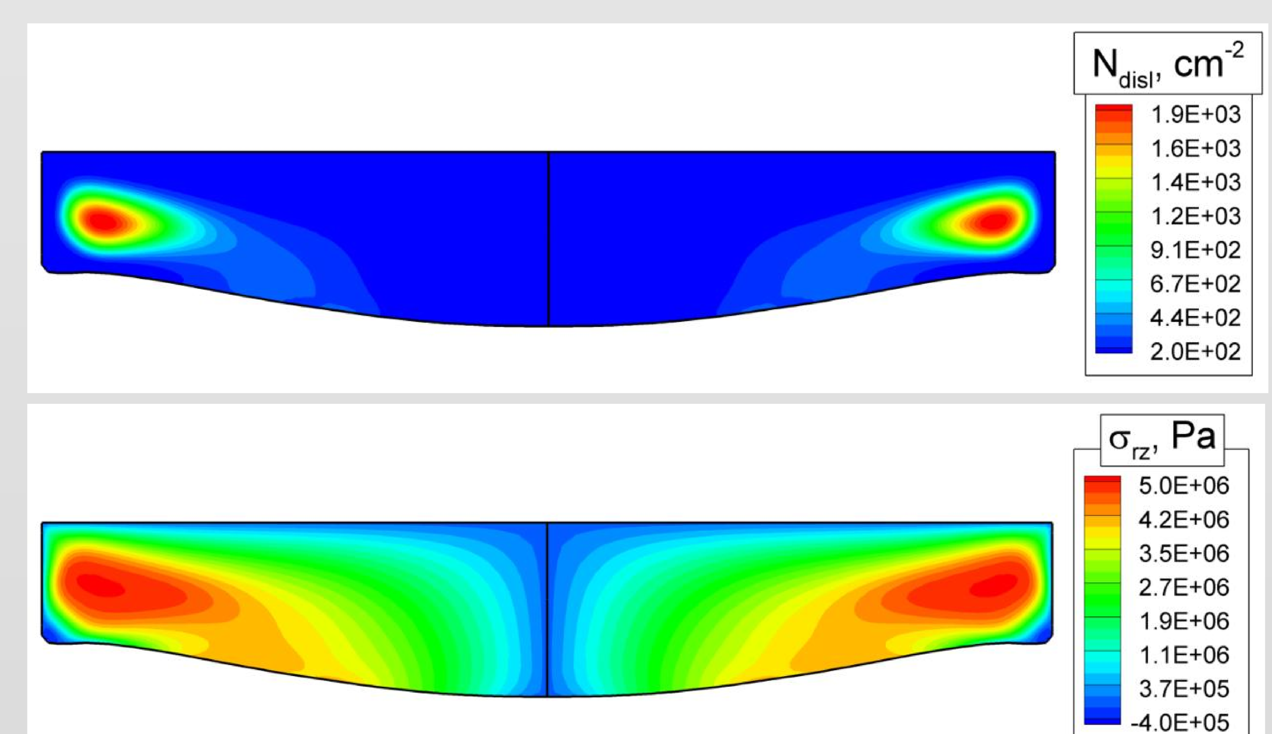

Fig. 5. Distribution of Basal Plane Dislocations density (top) and shear stress (bottom)

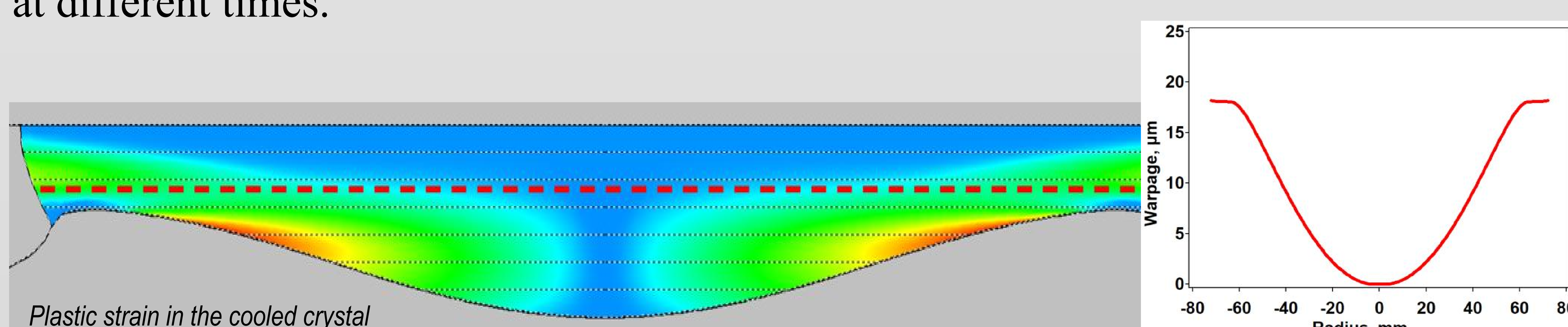

Fig. 6. plastic strain in the cooled crystal and predicted wafer warpage