Effects of surface size and shape of polycrystalline powder on the silicon carbide crystal growth by PVT method

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P35

ABSTRACT

Silicon carbide (SiC) polycrystalline powder, as the raw material for SiC single crystal growth by Physical Vapor Transport (PVT) method, its surface size and shape have great influence on growth of crystal. In this paper, the surface size and shape of polycrystalline powder were investigated by numerical simulation. Firstly, the temperature distribution and deposition rate distribution for the PVT system were calculated by global numerical simulation method, the optimal ratio of polycrystalline powder surface diameter to seed crystal diameter was determined to be 1.6~1.7. Secondly, the surface of the SiC polycrystalline powder was covered by a graphite ring and a graphite disc respectively to change its surface shape. Finally, the results show that adjusting surface size and shape of polycrystalline powder is an effective method to control the growth rate, growth stability and growth surface shape of the single crystal.

MODEL

Numerical simulation of single crystal growth with an axisymmetric global numerical model.

The SiC PVT growth reactor has many parts, such as seed, polycrystalline powders, crucible, and induction coils, as shown in Fig. 1. In a closed graphite crucible, the elements Si and C are sublimated from the SiC polycrystalline powder on crucible bottom, transported to SiC single crystal at crucible top for crystallization.

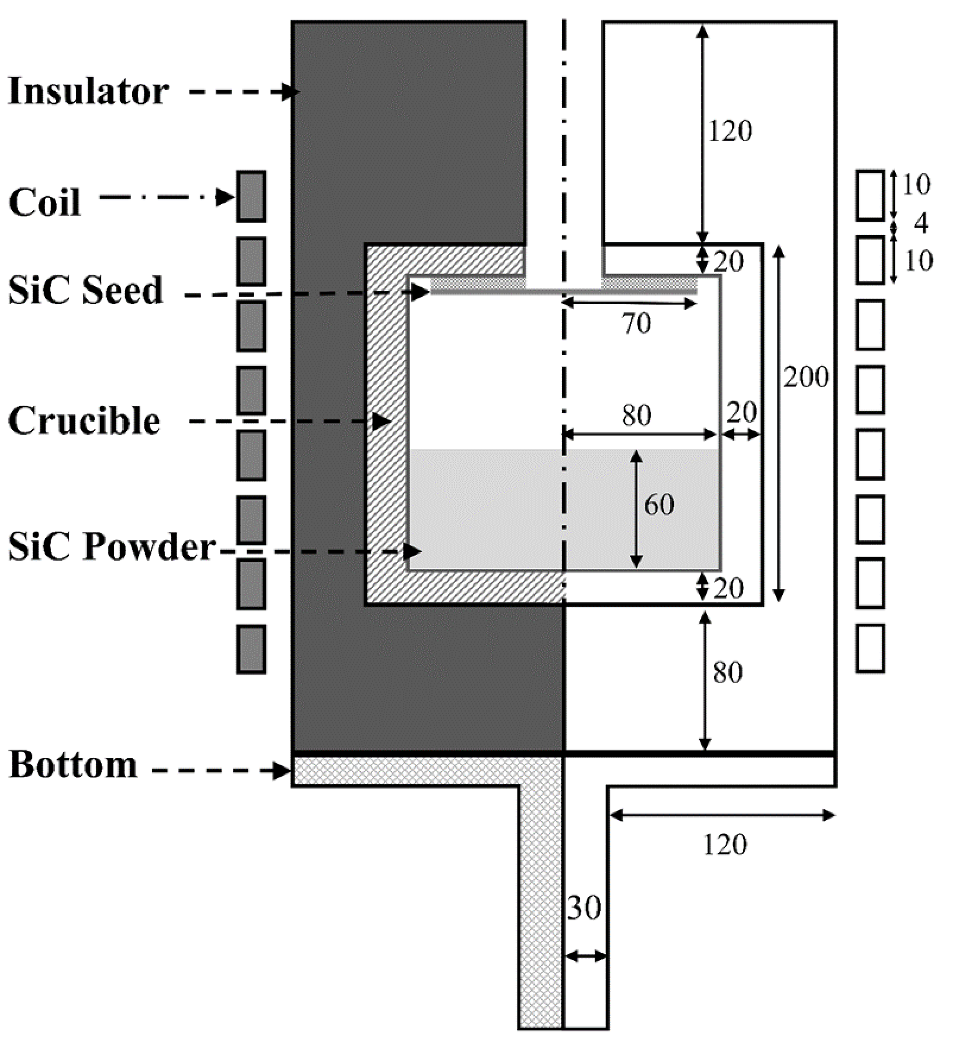

Fig.1. Reactor for PVT SiC single crystal growth (mm)

RESULTS AND DISCUSSIONS

1. Effects of ratio of polycrystalline powder diameter to seed crystal diameter.

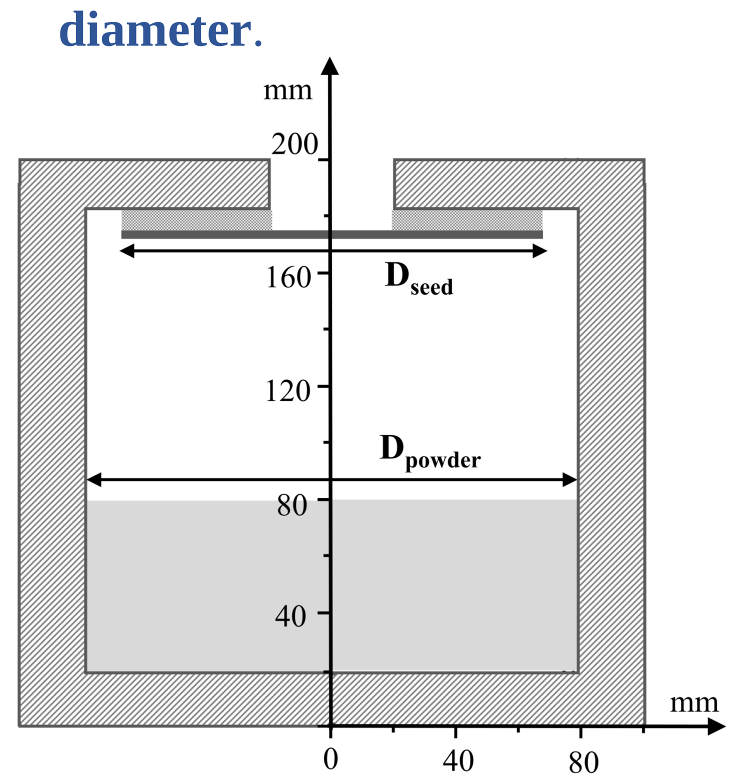

Fig. 2. Cross section diagram of crucible for growing SiC

The ratio of polycrystalline powder diameter to seed crystal diameter can be expressed as:

$$D = D_{powder}/D_{seed}$$

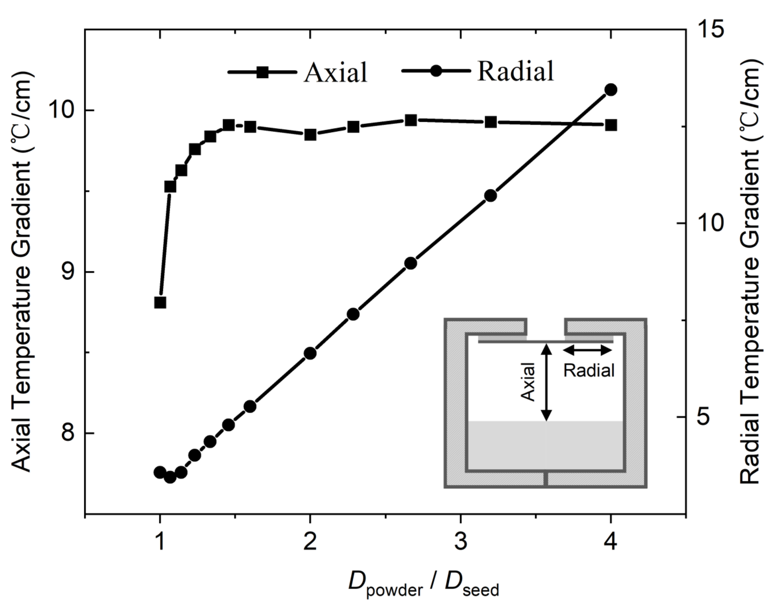

Fig. 3. Temperature gradient distribution at different values of D

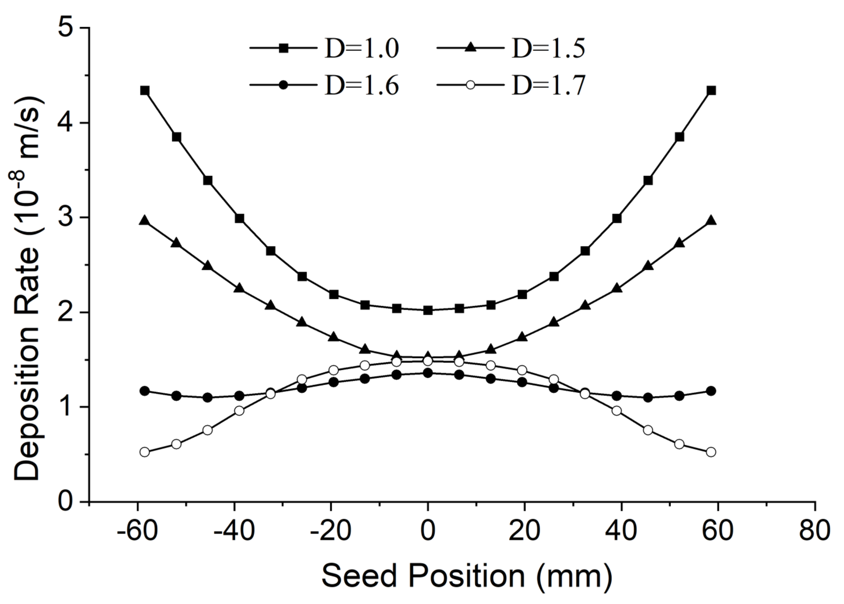

Fig. 4. Deposition rate distribution at different values of D

The optimal cover ratio was researched, combining temperature distribution and deposition rate distribution. Axial temperature gradient is small at a ratio of polycrystalline powder diameter to seed crystal diameter of less than 1.5, which leads to a lack of mass transfer power. At D>1.7, linear increase in radial temperature gradient, high radial temperature gradient increases thermal stress, thus causes crystal defects. At D<1.5, the surface shape is concave, which tends to generate stress. At D>1.5, the surface shape is slightly convex. According to the results of the researches, $D = D_{powder}/D_{seed} = 1.6\sim1.7$ is more suitable for the growth of crystal.

2. Effects of ratio of polycrystalline powder diameter to seed crystal diameter.

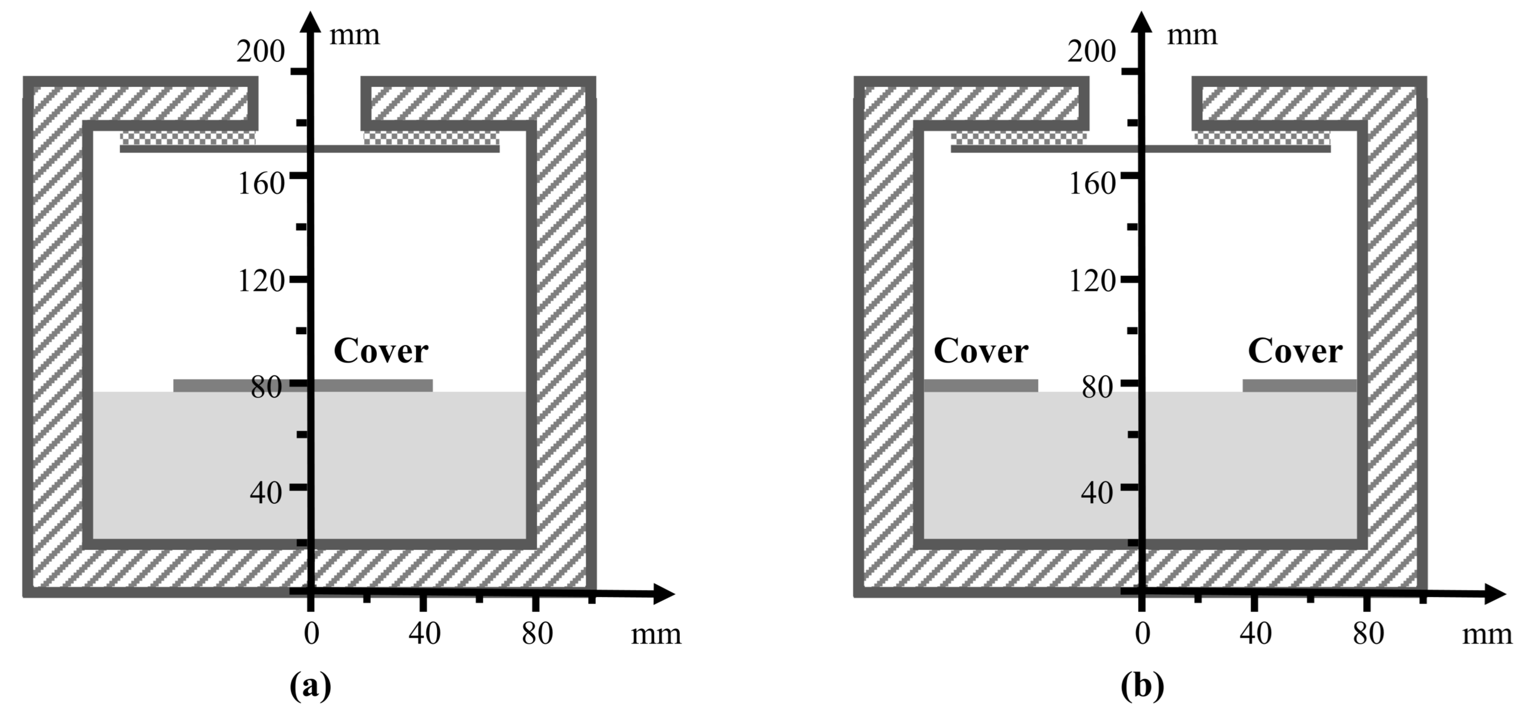

Fig. 5. (a) graphite disc cover, (b) graphite ring cover

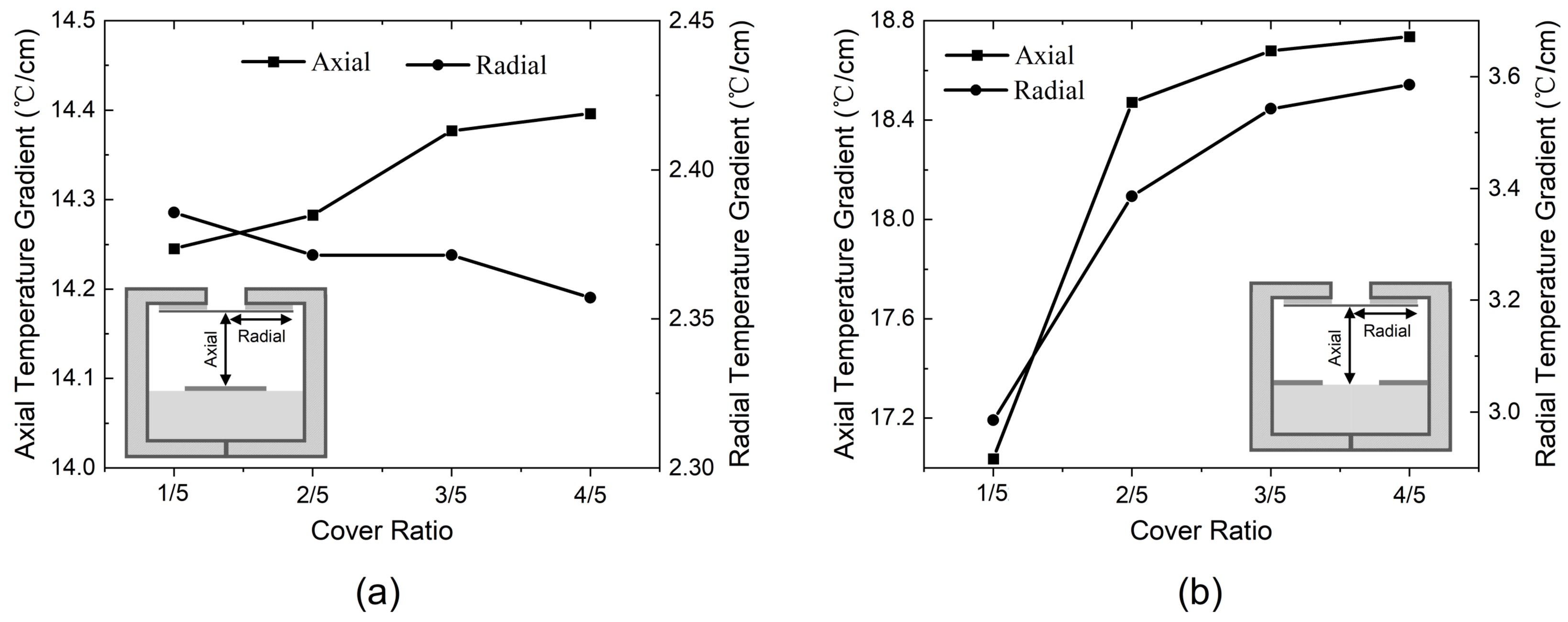

Fig. 6. Temperature gradient distribution (a) graphite disc cover (b) graphite ring cover

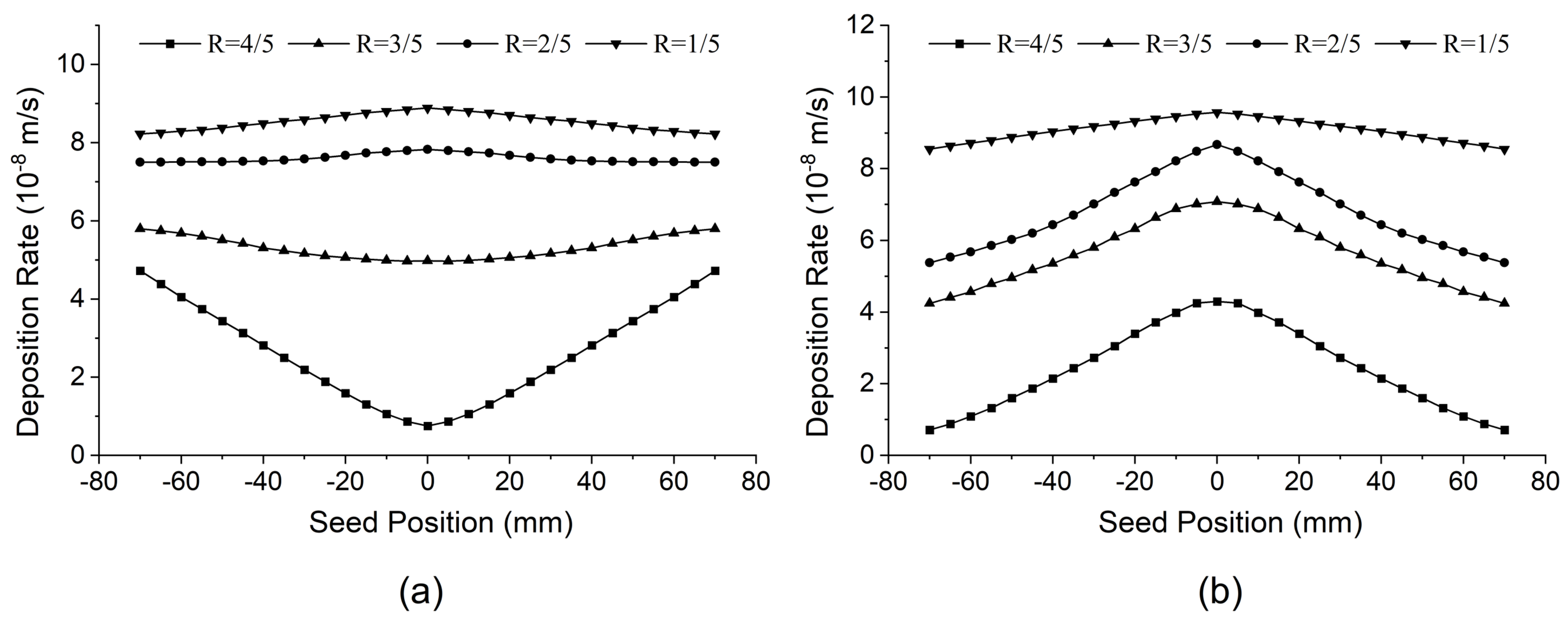

Fig. 7. The deposition rate distribution at different cover ratios (R) (a)graphite disc cover, (b)graphite ring cover

For graphite disc, at cover ratios of less than 2/5, the center deposition rate is slightly higher than that of the edge, slightly convex shape of single crystal growth surface, which means that the single crystal growth quality is high.

For the graphite ring, difference between center deposition rate and edge deposition rate gradually increases with increase of the cover ratio, more serious convexity in the shape of the growth surface.

CONCLUSIONS

1. Polycrystalline powder structures with cover are proposed and investigated after optimizing the size of the polycrystalline powder.
2. The optimal ratio of polycrystalline powder diameter to seed crystal diameter was found to be 1.6~1.7.
3. The single crystal growth surface uniformity can be improved by changing the shape of the polycrystalline powder surface.

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