# Analysis of Macrostep Interaction via Carbon Diffusion Field in SiC Solution Growth

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In solution growth of SiC, a high-quality crystal can be grown due to the dislocation conversion phenomenon by macrosteps. However, over-developed macrosteps lead to the formation of macro defects, so forming and controlling macrosteps of moderate height is important. Chernov theoretically demonstrated the instability of steps due to solution flow [1]. However, few studies have focused on macrostep instability other than flow direction and velocity. In this study, the effect of both step spacing and solution flow on macrostep instability is analyzed numerically. The 3D solution flow and carbon concentration around macrosteps were calculated by the upwind difference method. The computational model was based on the boundary layer model developed by Dang et al [2]. The macrostep is assumed to consist of 20,000 elemental steps. As a boundary condition at the macrostep, the amount of carbon incident on the macrostep was equal to that absorbed by the macrostep moving at a velocity proportional to the local supersaturation. The calculations were performed under a variety of flows, with macrosteps equally spaced and the position of the middle macrostep varied.

Fig. 1 (a)-(c) show carbon concentration under each flow when the step spacing is 0.5 mm. The blue dots represent macrostep positions. The step velocities($V_u, V_m, V_d, etc.$) at each step position were calculated, and macrosteps move in the right direction. In (a) and (c), where there is flow, carbon concentration is tilted in the direction of the flow. Fig. 1 (d) shows relative step velocity(defined as $V_m - 1/2(V_u + V_d)$) for each step spacing. If it is positive, it means that the macrostep is pulled relatively forward(to the right), leading to bunching. If it is negative, the opposite is true. From the plots of (a)-(c), there is bunching under parallel flow and debunching under anti-parallel flow. This is because carbon diffusion field extends downstream of the flow. In addition, relative velocity can be seen to vary with the step spacing. When macrosteps are equally spaced(the step spacing$= 1.0\ mm$), the relative velocity is zero, but as the step spacing decreases, the change of the velocity increases. This is due to the larger step interaction. These analyses will allow us to estimate the appropriate step spacing and solution flow.

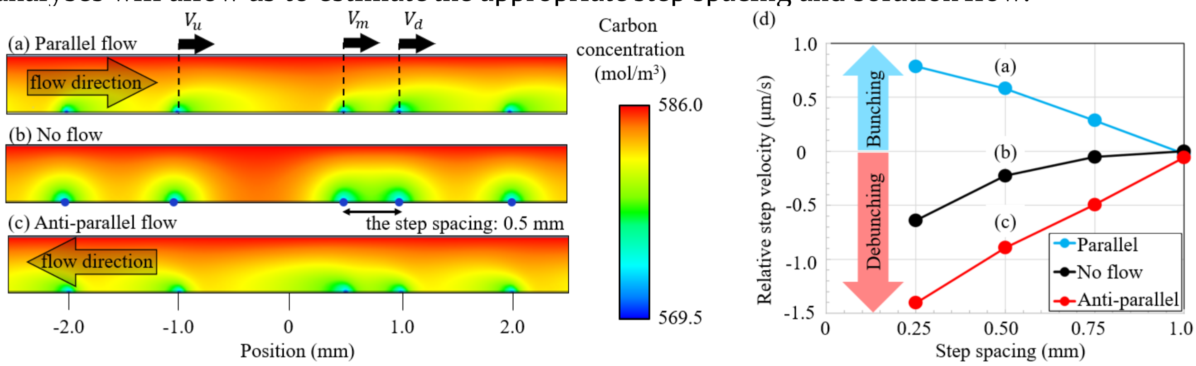


Fig. 1. Carbon concentration under (a) parallel flow, (b) no solution flow and (c) anti-parallel flow. (d) Relative step velocity changes with step spacing and solution flow.

**References**
[1] A.A. Chernov. J. Cryst. Growth 1992, 118, 333-347.
[2] Y. Dang, et al. Cryst. Growth Des. 2023. doi:10.1021/acs.cgd.2c01194.