

**PVT 成長法における Alexander-Haasen モデルを用いた
4H-SiC 単結晶の転位密度塑性挙動モデル化**

**Dislocation density-based modeling of plastic deformation of 4H-SiC single crystals by
the Alexander-Haasen model during PVT growth**

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Introduction

Numerical modeling of plastic deformation of elemental and III-V compound semiconducting materials has been extensively studied in a wide range of stress and temperature by using the Alexander-Haasen (AH) model; however, the numerical modeling of plastic deformation of IV-IV compounds, such as SiC, has been rarely implemented due to the complexity of dislocations in IV-IV compounds and also due to the lack of experimental data. Since the Alexander-Haasen model well describes the plastic behavior of elemental and III-V compound semiconductor materials, and its applications in global modeling of crystal growth already demonstrate extraordinary ability for the optimization and reduction of dislocations in those materials, it would be very useful to determine whether the AH model can be extended to SiC material.

Calculation method

Alexander and Haasen model is extended to SiC single crystal. Global simulation of PVT growth of SiC was performed and the dislocation density was calculated by Alexander and Haasen model during the total crystal growth and cooling process.

Results

In this paper, we demonstrate that the AH model can be used to SiC material if only the carbon-core dislocation and silicon-core dislocation can be dealt with at different temperatures. Our simulations show good agreement with experiments in wide temperature range. The effect of cooling process on the final dislocation of SiC in PVT growth was also studied. Results show that the cooling rate has a large effect on the generation of dislocations. The optimized design of cooling process is very important for the reduction of dislocations.

The region of stacking fault formed during the growth was also disclosed by numerical simulation. The stacking fault region can be effectively tracked by numerical simulation, thus, it is possible to reduce the stacking fault by optimizing the cooling process.