

# Alexander-Haasen model を用いたサファイア単結晶における基底面転位のモデル化 Modeling basal plane dislocations in single-crystal sapphire by Alexander-Haasen model

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## Introduction

Single-crystal sapphire has recently garnered significant attention as an important substrate material for fabricating gallium nitride light-emitting diodes (LEDs). High-quality gallium nitride requires high-quality sapphire substrates. To enhance the quality of crystalline sapphire, the density of dislocations must be controlled and reduced. To reduce the generation rate of dislocations during the growth of crystalline sapphire, a model that relates dynamic dislocation generation to the practical growth conditions is required. However, no such model, which can describe the plastic deformation of sapphire, currently exists. To address this shortfall, the dislocation density-based Alexander-Haasen (AH) model[1], which was originally used for crystalline silicon, is applied to crystalline sapphire.

## Results

Figure 1 shows the dislocation density distribution before and after cooling. Before cooling [Figure 1(a)], i.e., just after the heating process, the BPD density increases only at the bottom; however, after cooling [Figure 1(b)], the BPD density increases at both the bottom and at the side of the crystal. Therefore, the cooling process is a significant factor affecting the generation of BPDs during the growth of single-crystal sapphire.

Figure 2 shows the distributions for different cooling rates. Fastest cooling rate [Figure 2(c)] results in the largest BPD density, whereas the slowest cooling rate [Figure 2(a)] results in almost no increase in dislocation density relative to that before cooling [Figure 1(a)]. Because the main difference between 3 cases is the cooling rate in the high-temperature region, it is essential to use a slow cooling rate at high temperatures in order to reduce the rate at which dislocations are generated.

## References

[1] P. Haasen, *Z. Phys.* 167, 461–467, 1962.

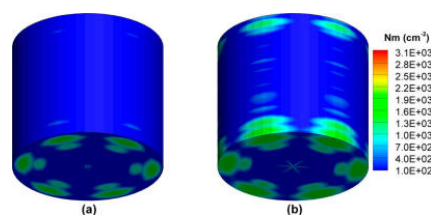


Fig. 1. The comparison of BPD distribution (a) before cooling and (b) after cooling.

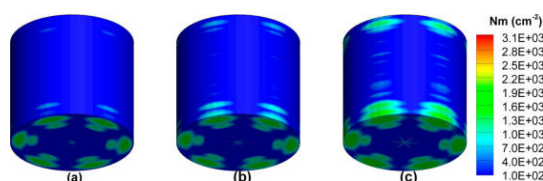


Fig. 2. The comparison of BPD distribution after cooling process for (a) slowest cooling, (b) middle cooling, and (c) fastest cooling rate.