Elucidating the Step Propagation Mechanism in SiC Solution Growth Using the Phase-Field Method

Seiya Harada[1]*, Kentaro Kutsukake[1,2], Shunta Harada[1,2], Toru Ujihara[1,2].
1 Graduate School of Engineering, Nagoya University, Japan
2 Institute of Materials and Systems for Sustainability (IMaSS), Nagoya University, Japan
*E-mail :harada.seiya.z3@s.mail.nagoya-u.ac.jp

Introduction

In the solution growth of SiC, crystal grow via a step-flow mechanism, where macro-steps formed by the bunching of multiple monoatomic steps contribute to the production of high-quality crystals with low dislocation density. However, this growth method can also lead to the formation of defects known as inclusions, which remain a significant challenge.

Recent experimental observations using cross-sectional SIMS analysis of 4H-SiC crystals have reported linear regions with low concentrations of impurities such as aluminum (Al) and nitrogen (N) [1,2]. These features are hypothesized to represent the traces of propagating macro-steps, and discussions based on this assumption are ongoing. Nevertheless, the mechanism behind their formation has not yet been fully elucidated.

Therefore, the aim of this study is to clarify the step propagation mechanism in SiC solution growth by employing the phase-field method, with particular emphasis on understanding how multi-level steps influence impurity distribution and contribute to defect formation.

Experiment Procedures

A phase-field model was constructed in which the step was defined as an interface through an order parameter, and its propagation was reproduced by coupling the model with a diffusion field representing the solution environment inside the crucible [3].

Furthermore, to account for the role of impurities, a stochastic model was implemented in which impurity atoms randomly adsorb and desorb on the terrace regions during growth. This enabled us to analyze how the passage of multi-level steps influences impurity incorporation.

The proposed model was applied to the case of 4H-SiC solution growth, and numerical simulations were carried out to evaluate the impurity distribution in the crystal under different growth conditions. As a result, the quantitative relationship between macro-step propagation and impurity concentration distribution was clarified.

Results and Discussion

As a result of the simulation, it was confirmed that the macrostep repeatedly undergoes bunching and debunching and propagates more slowly compared to a single step.

Furthermore, Fig. 1(A) shows that a low-supersaturation region is formed at the upper edge of each step position, and that the macrostep region forms a significantly lower supersaturation region compared to its surroundings. In Fig. 1(B), the red circles represent impurities adsorbed on the terrace, while the blue circles represent impurities incorporated into the crystal. When both the adsorption and desorption probabilities of impurities were set to 0.000001, the impurity concentration distribution shown in Fig. 1(B) appeared. This indicates that the trajectory of the macrostep is linear and inclined due to the effects of debunching and bunching. The adsorption probability and desorption probability of 0.000001 indicate that once adsorbed, desorption is unlikely. In the macrostep region, where adsorption sites are scarce, impurity uptake is minimal. Conversely, in the microstep region, where adsorption sites are abundant, impurity uptake occurs frequently, leading to the observed impurity concentration distribution.

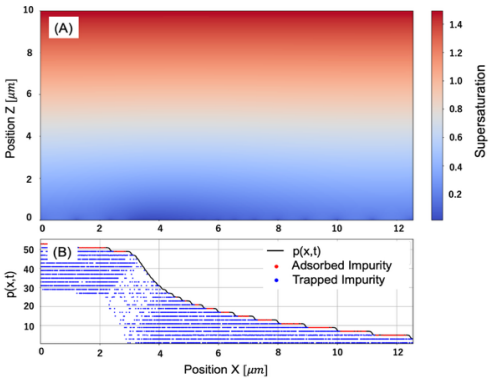

Figure1 Phase-field simulation result with impurity adsorption and desorption

References

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