実験より得た単結晶シリコン転位密度分布の解析に対する 3 次元 Alexander-Haasen モデルの優位性と限界

Potential and limitation of 3D Alexander-Haasen model in analyzing experimental dislocation-density distribution in single-crystal silicon

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Introduction

Experimental measurement is an important means for evaluating final quality of crystalline silicon, but it has its limitations. Dislocations in silicon are usually activated in more than one slip system. Identifying the dislocations activated by every slip system is a challenging task in experiments. Numerical simulation provides an effective supplement in analyzing the final quality of crystal. In this paper, we used a 3D Alexander-Haasen model [1,2] to compare and analyze experimental data. Two different crystal ingots, CZ crystal with axial line in [001] direction and FZ crystal with axial line in [111] direction, were used in both numerical simulations and experiments.

Results

A comparison of dislocation density in one slice of CZ crystal is given in Fig. 1. Numerical result shows good agreement with experimental data. For other slices in CZ crystal, numerical simulation using

the three-dimensional Alexander-Haasen (AH) model can always output consistent results with experimental data, and the details of activation of slip systems in experimental crystals can be well explained by numerical results. However, for FZ crystal with axial line in [111] direction, there are some difference between numerical and experimental data. The consistence in CZ crystal and inconsistence in FZ crystal indicates that the 3D Alexander-Haasen model has its potential and limitation. Furthermore improvement on the 3D Alexander-Haasen model is required.

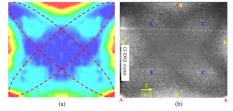


Fig. 1. Comparison of dislocation-density distribution between (a) numerical data and (b) experimental data in one slice of CZ crystal with axis in [001] direction.

References

- [1] B. Gao, S. Nakano, H. Harada, Y. Miyamura, K. Kakimoto, Cryst. Growth Des. 2013, 13, 2661–2669.
- [2] B. Gao, K. Kakimoto, J. Appl. Cryst. 2013, 46, 1771-1780.