3D analysis of dislocation density in a Ga_2O_3 crystal grown by a vertical Bridgman method

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This paper reports recent development of numerical modeling in crystal growth process including defect analysis. study of dislocation-density distribution in a β-gallium oxide (β-Ga2O3) by using three-dimensional analysis. We used Alexander-Haasen (AH) model [1] in the time-dependent numerical analysis. Growth system used in the present study is vertical Bridgman (VB) method.

Temperature distribution and the interface shape were obtained by transient calculation as a function of time [3]. The calculation was carried out in two-dimensional configuration. The furnace contains a growing crystal, a crucible, resistive heaters, a pedestal, and thermal shields. The temperature distribution in a crystal is dense while that in the melt is space. This is due to convection of the melt which homogenize temperature distribution in the melt.

We used three different orientations of a seed crystal as [010] and [001]. We imposed barrier height of dislocation motion as 2.9 eV in this case although the value is not reported so far. Slip systems used in this study is based on the result published by Yamaguchi et al. [3]. The main slip systems used in this calculation are {-201}/<010>, {-201}/1/2<112>, {101}/<010>, and {101}/<10-1> [3]. Figures 1 (a) and (b) show calculated distributions of dislocation density of [010] and [001] grown crystals, respectively. The maximum dislocation density in both [010] and [001] grown crystals are observed in [100] direction.

References
[1] P. Haasen, (1962), Z. Phys., 167, 461-473.
[2] B. Gao, K. Kakimoto, (2014), J. Crystal. Growth., 386, 215-.
[3] H. Yamaguchi, Akito Kuramata, Takekazu Masui, (2019), Superlattices and Microelectronics, 130, 232-232.

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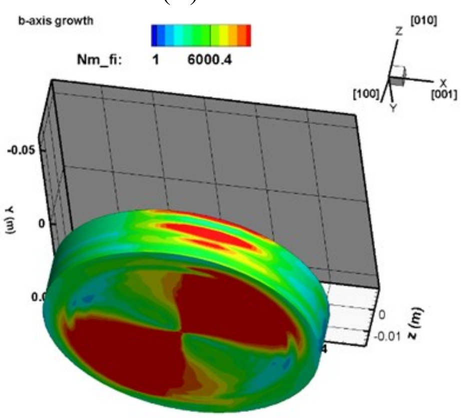

Fig. 1 Dislocation density distribution in a [010] grown crystal.

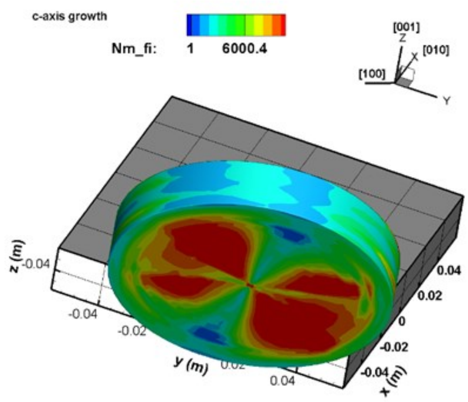

Fig. 2 Dislocation density distribution in a [001] grown crystal.