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数値計算を用いた円筒状単結晶における転位発生に対する冷却フラックスの影響

Influence of cooling flux on the generation of dislocations for cylindrical single crystal silicon by numerical modeling

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Introduction

Seeded-growth monocrystalline silicon has recently become popular due to its potential advantages of low cost and high quality technique. However, the evolution of the casting technique in producing mono-like silicon has encountered some problems due to extra-large dislocations generated between grains. To further make the casting technique progress in producing mono-like Si, the dislocations have to be reduced. A good control of cooling flux can dramatically reduce the generation of dislocations. However, in order to effectively control the cooling flux for the reduction of dislocations, it is a prerequisite to first know how the dislocations are affected by cooling flux inside the crystal.

Calculation method

Alexander and Haasen mode is extended to a multi-axis stress state. The generation of dislocation is attributed to the slip on 12 possible slip directions and the cross-slip between different slip systems; the immobilization of mobile dislocation and the annihilation of dislocation are also included.

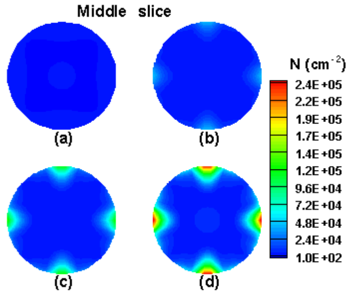

Fig 1. Distribution of dislocation density of the middle and bottom slices of crystals with a fixed diameter of 10.6 cm and with a maximum radial cooling flux of (a) 100 K/m, (b) 300 K/m, (c) 500 K/m, and (d) 700 K/m.cooling rate, (b) slow cooling rate

Results

Both radial cooling flux and axial cooling flux can affect the generation of dislocations. Radial cooling flux can directly determine the generation of dislocations; however, axial cooling flux needs a gradient to determine the generation of dislocations. In the radial direction, it is the total radial cooling flux passing through the cylindrical surface determining the generation of dislocations; however, in the axial direction, it is the cooling flux difference between the bottom and top surfaces determining the generation of dislocations. The generation of dislocations is very sensitive to the cooling flux. A linear increase of the total radial cooling flux passing through the cylindrical surface or the cooling flux difference between the bottom and top surfaces can cause a square increase of the maximum dislocation density.