Investigation of $\Sigma 3$ Generation on Random Grain Boundary in Multicrystalline Silicon

Xianjia Luo, Jun Chen, Takashi Sekiguchi

(1. MANA Nano Electronics Materials Unit, National Institute for Materials Science, Tsukuba Ibaraki 305-0044, Japan)

E-mail: LUO.Xianjia@nims.go.jp

Fundamental investigation of crystal growth in multicrystalline Si (mc-Si) is important in order to improve the crystal quality and device performance. However, $\Sigma 3$ generation is unavoidable in crystal growth of mc-Si. Thus, it is necessary to understand the effect of $\Sigma 3$ generation on device performance. In this work, we investigated the effect of $\Sigma 3$ generation on random (R) grain boundaries (GBs) by means of electron-beam-induced current (EBIC) and electron-back-scatter diffractions (EBSD). The EBIC result indicates that $\Sigma 3$ generation affects the electrical activity of R GBs at the initial stage of crystal growth, while does not impact on it at the steady stage. The reason of EBIC contrast variation of R GBs was studied. R GBs refer to large angle (LA) GBs except $\Sigma 3$, $\Sigma 9$ and 27. Fig. 1(a) shows that one LA grain boundary (GB) change to another LA GB after $\Sigma 3$ generation and misorientation change between two LA GBs is about 7°. Fig. 1 (b) and (c) show that the EBIC contrast variation is large after $\Sigma 3$ generation at the initial stage, while almost the same at the steady stage. High misorientation change had large EBIC contrast variation at the steady stage, whereas large EBIC contrast variation of high misorientation change was found at the initial stage. This result reveals that the structure of R GB is inclined to change after $\Sigma 3$ generation at the initial stage. On the other hand, the structure of R GB tends to be stable after $\Sigma 3$ generation at the steady stage. We also found that large EBIC contrast variation corresponded to high angle $\theta$ which was the angle between original R GB and new R GB after $\Sigma 3$ generation. In conclusion, the structure of R GB is unstable at the initial stage and tends to change through $\Sigma 3$ generation, which results in large EBIC contrast variation and high angle $\theta$. High angle $\theta$ leads to high possibility of annihilation with other GB. After crystal growth to the steady stage, most of unstable R GB annihilated. Thus, at the steady stage $\Sigma 3$ generation almost does not change the structure of R GB, namely its EBIC contrast.

Fig. 1. (a) EBSD image when one LA GB changes to another LA GB after $\Sigma 3$ generation, (b) and (c) EBIC contrast variation and number with respect to misorientation change at the initial stage and steady stage.