論 文 の 内 容 の 要 旨

Reaction Pathway Analysis for the Mobility of Partial Dislocation in 3C-SiC and Shuffle-set Perfect Dislocation in Silicon

(3C-SiC の部分転位とシリコンのシャフルセット完全転位の移動度に関する反応経路解析)

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Dislocations are linear defects that carry out the plastic flow at the microscopic scale, and have strongly influence on semiconductor materials' electric and mechanic properties. During the wafer growth of the semiconductor materials by CVD, dislocation propagation is thought to be one of main factors that cause the wafer warpage. With the purpose of obtaining a high quality of wafer, the reaction pathway analysis is performed for a good understanding of the dislocation propagation in wafer.

In this paper, the mobility of Shockley partial dislocations in 3C-SiC and Shuffle-set perfect dislocation in silicon have been investigated by reaction pathway analysis. For 3C-SiC, there are two types of dislocations according to which kind of atom, Si or C, comprises the core edge of the dislocation line. 3C-SiC is represented by Vashishta potential function, and the reaction path of kink pair nucleation and kink migration are investigated by NEB. The dependence of the activation energy on the driving shear stress has been obtained. The results show that during kink migration, 30° partial dislocations have a lower activation energy barrier than 90° partial dislocation. And, C-core partial dislocations have a higher activation energy barrier than Si-core dislocations for both degrees of partial dislocations during kink migration and nucleation. This conclusion is consistent with the experimental result that Si-core dislocations migrate more readily than C-core dislocations. Besides I have found that the partial dislocation with a larger distance between the dangling bond atoms along the dislocation line also has a higher activation energy barrier for both 30° and 90° partial dislocations. Moreover, based on the activation energy barrier calculation, new models are proposed to explain the morphological character of different partial dislocation lines that the 30° partial dislocation lines prefer to be smooth because of the large activation energy difference between kink nucleation and kink migration. And the 90° partial dislocations lines prefer to be zigzagged for the reason that the 90° partial dislocation lines have the possibility to migrate and nucleate simultaneously. Based on our mobility analysis, the stacking fault morphologies have been discussed. Our consultations agree well with previous experiment data.

For the shuffle-set perfect dislocation analysis in silicon, the EDIP potential function is employed for representing the silicon. There are three possible shuffle-set dislocation core structures named as S1, S2 and S3. Here, the activation energy barriers of the kink migration and nucleation in S1and S2 types are investigated by NEB method. The simulation results show that the resolved shear strain of the shuffle-set dislocation in S1 type is around 5%, and the S1 type is the dominate one in the shear strain of 0% to 5%. I also have found that the activation energy barriers of the two sides kink migration is nearly two times than that of the one side kink migration. More interestingly, the kink nucleation path is accomplished by the motion of two atoms simultaneously. These phenomena could be responsible for the missing long segment of shuffle-set perfect dislocation in the experiment observation. I am guessing whether it is possible that the dislocation propagation and the movement of shuffle-set perfect dislocation segment have different mechanisms. During the shear strain from 5% to 12.5%, the dislocation can move as the S1 core kink nucleation and migration and the S1 dislocation core is in process of transforming into S2. The S2 dislocation core structures begin to appear along the S1 dislocation line since the shear strain is larger than 5% shear strain, and the transition is ended around the shear strain

12.5%. The kink structures are asymmetric in S2 dislocation and both the LK and RK migration process have been studied. In the RK migration process with S2 dislocation we find that both the shuffle-set and glide-set bond breaking and forming are involved. This may imply that there could be a possibility that the shuffle-set dislocation core can translated into a glide-set dislocation core. The high activation energy barrier indicates that this transition could only happen in high temperature. S3 dislocation motion is not considered here for the bad representation of kink structures.

We believe that our dislocation reaction pathway analysis can improve our understanding of dislocation motion in 3C-SiC and silicon and provide more evidences for solving the unclear issues in both of them.