Molecular Dynamic Simulation on Boron Cluster Implantation for Shallow Junction Formation

Li Yuan[a], Wei Li[a], Min Yu[*a], Huihui Ji[a], Kai Zhan[a], Ru Huang[a], Xing Zhang[a], Yangyuan Wang[a], Jinyu Zhang[b] and Hideki Oka[c]
[a.] Institute of Microelectronics, Peking University, China 100871,
[b.] Fujitsu R&D Center Co. LTD , Room B1003, Eagle Run Plaza No.26 Xiaoyun Road Chaoyang District Beijing, China,
[c.] Fujitsu Laboratories LTD, 10-1 Morinosato-Wakamiya, Atsugi 243-0197,Japan
* Email: yum@ime.pku.edu.cn

INTRODUCTION

Boron cluster ion implantation is a potential technology for shallow junction formation in integrated circuits manufacture [1]. By cluster implantation, space-charge blow up of the beam can be minimized and more B atoms are implanted at the same beam current. Another advantage of using clusters is that it generates more defects to reduce channeling effect [2]. With the technology becoming more practicable, capability of simulating it for shallow junction formation becomes necessary, which is still difficult for full MD method. A localized molecular dynamic method [3] for simulating cluster implantation at normal dose, e.g. 10^{15} cm^{-2}, aimed at microelectronics application, is presented in this paper.

MODEL

In our MD simulation, a moving simulation box [3], composing of 3x3x3 unit cells (about 200 atoms), is applied to save computing time. Accurate geometry structures of boron clusters [4] are considered in the model by described accurate position of both B and H atoms as is illustrated in Fig. 1. In order to describe interactions between atoms in boron clusters, potential function in which the repulsive action term is ZBL potential function and attractive term has the form of SW [5] potential function is applied.

RESULTS

Simulation examples of $B_{10}H_{14}$ and $B_{18}H_{22}$ are performed. The snapshot of cluster implantation is shown in Fig. 2. Simulation results are shown in Fig. 3~6. It can be seen that range profiles from simulation agree well with the SIMS data. Specially, agreement of H profile is also shown for $B_{18}H_{22}$ implantation, where obvious deviation at near surface region exists maybe due to uncertainty of SIMS measurements at such shallow region. Simulation and SIMS data of B monomer implantation at equivalent energy and dose is also shown in Fig. 3 and 5 as comparison. It shows cluster implantation tends to generate shallower distribution profile. It is notable that with cluster model presented, the simulation can reproduce that difference well.

Fig.4, 6 also show that cluster implantation induces more Si interstitial defects than B monomer. These results agree with reference [2].

ACKNOWLEDGEMENT

This paper is supported by the National Natural Science Fund (No. 90207004)

REFERENCES

[1]Takayuki Aoyama, Masatoshi Fukuda, Yasuo Nara, Ext. Abs. the 5th International Workshop on Junction Technology (2005) S2-2
[2]Aoki T., Matsuo J., Takaoka G., Ion Implantation Technology. 2002. Proceedings of the 14th International Conference（2002） P560 - 563
[3]K. Norlund, Comput. Mater. Sci. 3 (1995) P448
[4]A.F. Wells, Structure Inorganic Chemistry Fourth Edition 870
[5] Paul B. Rasband, Paulette Clancy, Bruce W. Roberts, Journal Applied. Physics, V.84, P.2471 (1998)
[6]M. Ishibashi, Y. Kawasaki, K. Horita, Ext. Abs. the 5th International Workshop on Junction Technology (2005) S2-3
[7]Tanjyo M., Hamamoto N., Umisedo S., Solid-State and Integrated Circuits Technology, 7th International Conference (2004) V1 P434 - 438

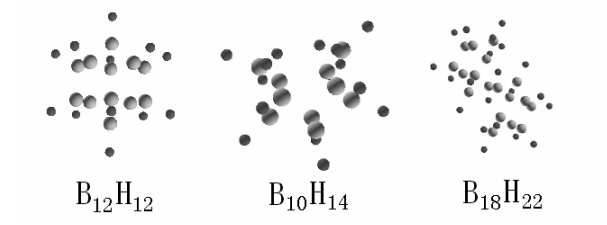

Fig. 1. The schematic representation of boron clusters ($B_{12}H_{12}$, $B_{10}H_{14}$ and $B_{18}H_{22}$). Structure of $B_{10}H_{14}$ and $B_{18}H_{22}$ is described based on that of $B_{12}H_{12}$.

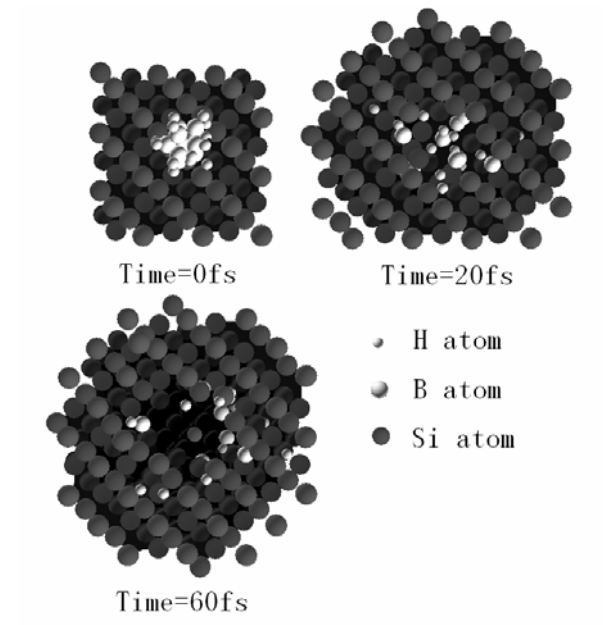

Fig. 2. Snapshots of B10H14 implantation at 1keV/molecular

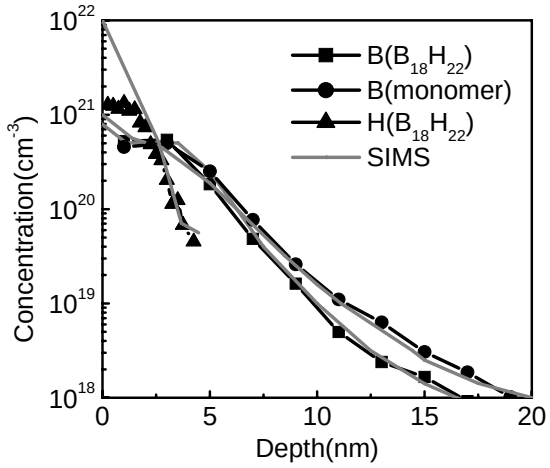

Fig.3 Concentration profiles of B atoms and H atoms for $B_{18}H_{22}$ implantation at 10keV/molecular and B monomer atom implantation at 0.5keV/atom. (Dose 3e14B/cm2)The SIMS data is from Ref. [6]

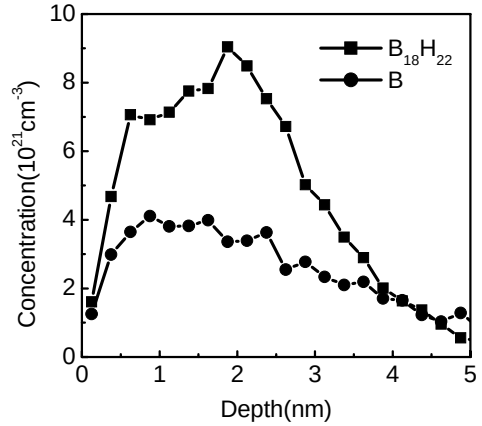

Fig.4 Concentration profiles of Si interstitials for $B_{18}H_{22}$ implantation at 10keV/molecular and B monomer atom implantation at 0.5keV/atom. (Dose 3e14B/cm2)

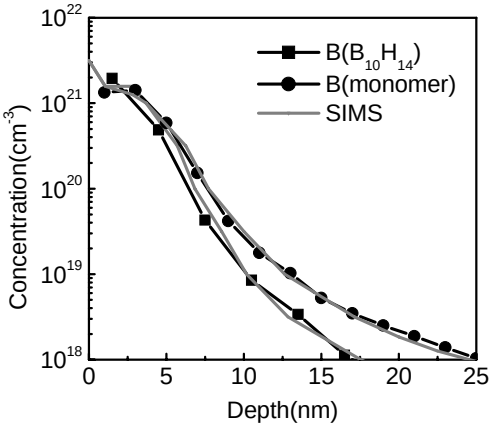

Fig.5 Concentration profiles of B atoms for $B_{10}H_{14}$ implantation (Dose 8.3e14B/cm2) at 5keV/molecular and B monomer atom implantation at 0.5keV/atom (Dose 8.1e14B/cm2). The SIMS data is from Ref. [7]

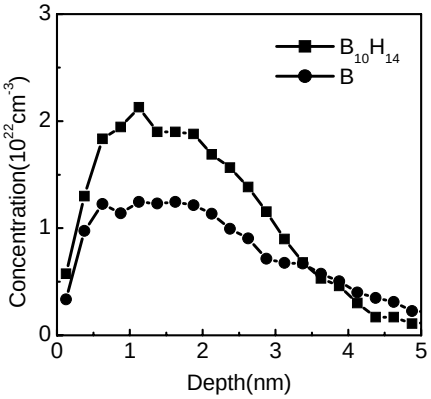

Fig.6 Concentration profiles of Si interstitials for $B_{10}H_{14}$ implantation (Dose 8.3e14B/cm2) at 5keV/molecular and B monomer atom implantation at 0.5keV/atom (Dose 8.1e14B/cm2).