Influence of Impurity Atoms on the Rate of Solid Phase Epitaxy: Molecular Dynamics Study

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ABSTRACT

In this study, we investigated the effect of arsenic atoms on the rate of Si SPE by using molecular dynamics simulation. In the case of non-doped Si, activation energy of SPE is found to be 2.1 eV±0.5eV, which shows good agreement with the experimental result (2.7 eV). It is also found that the energy barrier of crystallization in a/c interface amounts to be about 0.6eV, which corresponds to defect migration process. It indicates other processes such as defect formation also control the SPE process. The SPE rate increases by 2 times for 3 at% As doping and 100 times for 5 at% As doping and an activation energy remains to be constant. The increase in SPE rate would be enhanced by defect formation process in amorphous silicon, which reflects the increase in self-diffusion of silicon atoms caused by active As atoms.

1. Introduction

Solid phase epitaxy (SPE) of Si is one of the most fundamental processes in semiconductor fabrication techniques. Many experimental studies have been carried out for understanding the growth mechanism. However microscopic mechanism is not well understood. In this study, we investigated the effect of arsenic atoms on the rate of Si SPE by using molecular dynamics simulation.

2. Analysis Method

2.1. SPE simulation of non-doped silicon

For Si-Si interaction, Tersoff potential [1], which can describe amorphous silicon well, is employed. Here, a-Si/c-Si(001) interface is modeled as shown in Fig. 1. Amorphous silicon is well-relaxed through 10 ns annealing at 1600 K. Periodic boundary conditions are applied to all xyz directions. The system is annealed at constant volume and constant temperature conditions. In order to clarify the effect of temperature on the SPE rate, simulations at various temperatures ranging from 1500 K to 2300 K are carried out.
In order to detect the crystallized region, bond-angle deviation is employed as is proposed by our previous report [2].

2.2. SPE simulation of As-doped silicon

For As-As interaction, potential parameters proposed by Smith [3] are employed. For Si-As interaction, averaging rules proposed by the Tersoff and verified by Nakamura [4] is applied. As concentrations of 2, 3, and 5 at % are employed so as to see the dependence of impurity concentration on the SPE rate.

3. Result

3.1. SPE simulation of pure silicon

The dependence of SPE rate on temperature is shown in Fig. 2. The results are averaged over 3 samples. As can be seen, SPE rate shows thermal activation process. Its activation energies amount to 2.1eV±0.5eV at low temperature and 0.7eV±0.2eV at high-temperature region, which show good agreement with experimental results (2.7 eV and 0.7-1.1 eV, respectively). It also shows smooth transition from low to high temperature region. It is noted that a melting point of the Tersoff amorphous silicon is about 1900 K. Therefore, the epitaxy above 1900 K must be called as liquid phase epitaxy (LPE).
From nudged elastic band analysis, it is found that the energy barrier of crystallization in a/c interface amounts to be about 0.6eV. Since that barrier is close to that of LPE, it might correspond to defect migration energy in a/c interface. It also indicates that other processes such as defect formation also control the SPE process.

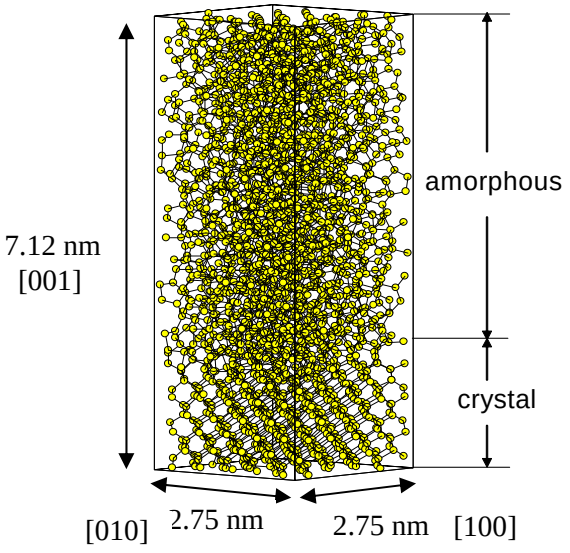

Figure1. Schematic view of a/c interface model

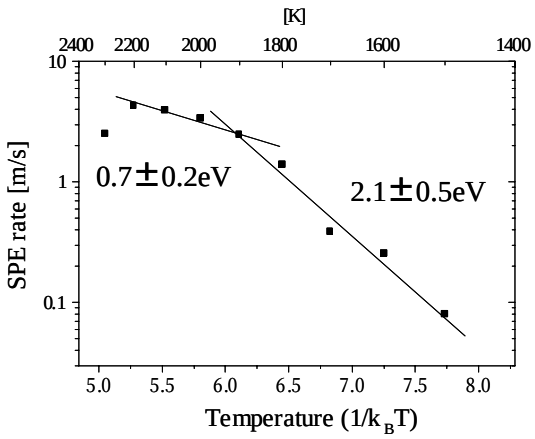

Figure.2 Dependence of SPE rate on temperature (average of three samples)

3.2. SPE simulation of As-doped silicon

SPE rate of As-doped silicon is shown in Fig. 3. The SPE rate increases by 2 times for 3 at% As doping and 100 times for 5 at% As doping and an activation energy remains to be constant. At each doped concentration, the deviation from the Arrhenius plot can be observed at high temperature region. Especially, SPE rate decreases in case of 5 at% above 1300K.

4. Discussion

Fig. 4 shows the dependence of self-diffusion constant of silicon atoms on As concentration. It can be seen that self-diffusion is significantly enhanced by As doping. Therefore, the increase in SPE rate would be enhanced by the defect formation process caused by active As atoms in amorphous silicon.

At high temperature region, self-diffusion constant of As doped silicon reaches that of undoped amorphous silicon at its melting point. Therefore, transition from SPE to LPE would induce the deviation from the Arrhenius plot. Moreover, in case of 5 at% over 1300 K, the self-diffusion of doped silicon exceeds that of undoped crystal silicon at its melting point. As a result, the competition between crystallization and melting appears in a/c interface. That would induce the decrease in SPE rate.

In Csepregi's experiment [5], SPE rate is enhanced about 10 times at 0.5 at% doping. That quantitative deviation might be caused by the accuracy in interatomic potentials, e. g. the accuracy in activation energy.

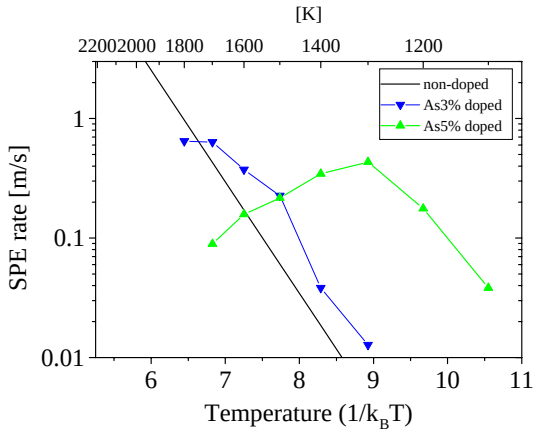

Figure.3 Dependence of SPE rate on temperature under various As-doping concentrations

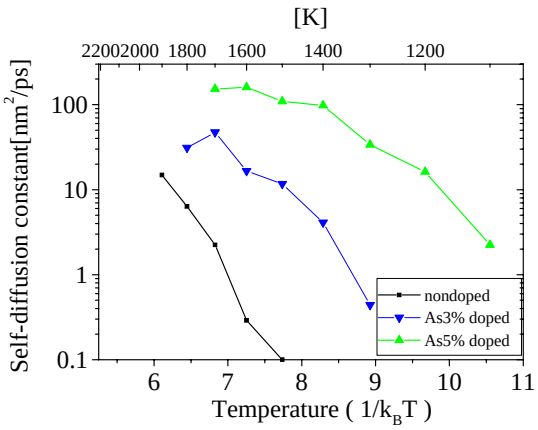

Figure.4 Dependence of self-diffusion constants of silicon atoms on As concentration

5. References

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