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Simulation of plasma doping process by using the localized molecular dynamics method*

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Plasma doping is the candidate for semiconductor doping. Accurate simulation of the doping technology is needed for the advanced integrated circuit manufacturing. In this paper, the plasma doping process simulation is performed by using the localized molecular dynamics method. Models that involve the statistics of the implanted compositions, angles and energies are developed. The effect of the model on simulation results is studied. The simulation results about the doping concentration profile are supported by experimental data.

Keywords: plasma doping, simulation, molecular dynamics

PACC: 7115Q, 5240H

1. Introduction

The plasma doping (PLAD) technique is a leading candidate for the next generation shallow junction technology in integrated circuit (IC) manufacturing.[1,2] With the development of the PLAD technique,[3] its application in IC manufacturing is becoming more and more promising. Thus the accurate simulation of PLAD is needed, which cannot only support the development of the technology but also improve its application.

There has been a lot of simulation investigations of plasma formation.[4−8] The fluid model, the particle-in-cell model and the Monte Carlo method are the main calculation methods in the simulations. Such simulations provide a reliable description for plasma sheath and ions. On the other hand, the simulation of PLAD induced ion distribution in solids has seldom been carried out and the simulation of concentration profile is less verified by experimental data.

TRIM, which is the beam ion implantation simulator and based on the binary collision approximation (BCA), has been applied in PLAD simulation.[8,9] For ultra-low energy (e.g. less than 500 eV), the localized molecular dynamics (MD) method has been proved to be the accurate simulation model.[10,11] To the best of our knowledge, the localized MD method has not been used in the PLAD simulation so far.

In this paper, the simulation study on PLAD is carried out by using the localized MD method. Several physical effects in the PLAD process are involved. Different ionic species involved in the PLAD are modelled and discussed. The ion injection angle perturbed by the plasma sheath around the wafer[12,13] is included. Both the biased voltage applied to the wafer and the plasma potential[14] are considered in determining the implanted ion energy, and the statistic distribution of ion energies is modelled. Simulation results show that the model has a notable effect on the simulated dopant profiles, and more reasonable simulation results can be achieved with the models presented here. The simulation results are supported by experimental data. Agreement between simulation and experimental results of dopant concentration profile is achieved.

2. Physical models

In this work, the Ziegler–Biersack–Littmark (ZBL) potential[15] is used for describing the interaction between implanted ions and target atoms, the SW potential[16] is applied to the interaction among target atoms and David Cai's model[17] is used to de-

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scribe the electronic stopping power.[11] A free parameter, i.e. the single electron radius, exists in the David Cai's model. The full MD method is accurate because it considers interactions in the whole simulation space. However, its computational efficiency is too low to simulate the shallow junction technology, where the implantation dose is always as high as $10^{15}\,\mathrm{cm}^{-2}$. Thus a method of moving box that contains 3^3 unit cells (about 200 atoms), which restricts the MD method to a local area around moving ions, is used to increase the simulation efficiency.[10]

In the traditional beam ion implantation, there is only one ionic species, while in the PLAD there are always several different ionic species. For example, in the plasma of B_2H_6, there may exist BH_x, B_2H_x, and even B_2H_6 ionic species.[18] In the PLAD process, the plasma is in a stable state, thus the ratios among different ionic species are constant.

In the beam ion implantation, the direction of ion injection is well controlled by the tilt angle and rotation angle of beam line. In the PLAD, however, the direction of ion injection in PLAD is not so well controlled. As illustrated in Fig.1, the flying direction of ions is random in the plasma body due to lack of acceleration electric field inside the plasma body. Thus the injection directions of ions in PLAD are randomly distributed. In this figure, $\boldsymbol{V}_1$ corresponds to the ion velocity in plasma body and $\boldsymbol{V}_2$ corresponds to the ion velocity when the ion moves into the plasma sheath. It is assumed here that the statistical distribution of injection angles in the PLAD can be described by the Gaussian distribution function as follows:

$$N(A) = \frac{1}{\sigma\sqrt{2\pi}} \mathrm{e}^{-\frac{(A-A_0)^2}{2\sigma^2}}, \qquad (1)$$

where the value of the deviation σ and the mean value A_0 are determined by PLAD experimental conditions. The implanted angle is defined as the angle of ion velocity with respect to the axis that is vertical to substrate surface. For an implantation into planar wafer, the rotation angle which corresponds to the velocity with respect to the horizontal axis is expected to be in a uniformly random distribution while A_0 is zero due to vertical electric field on the wafer surface. The parameter σ is set to be 1 degree for planar plate considered in this paper.

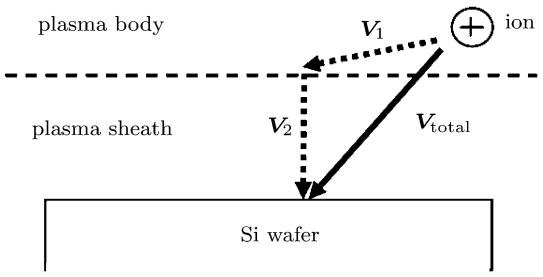


Fig.1. The implanted angle of the chosen molecular ion in the plasma doping process.

The energy of ion is determined by the biased voltage and the plasma potential. In the PLAD process, ions are attracted by the negatively biased wafer. The biased voltage (V_b) is always pulsed at a frequency up to hundreds of kHz. The rising and falling of voltage pulse results in the deviation of ion energy. At the same time, the existing plasma potential (V_p) supplies an additional energy to dynamic ions. This is illustrated in Fig.2. Besides, the random distribution of ion flying directions results in collisions among ions, which also contribute to the random distribution of ion energy.

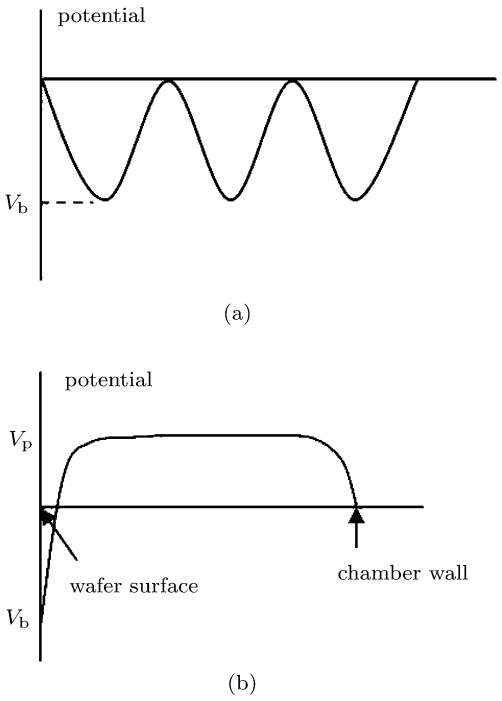


Fig.2. The biased voltage applied to the wafer (a) and the biased voltage and the plasma potential in the chamber (b) in the plasma doping process.

Thus two Gaussian functions are applied to describing the random distribution of ion energies determined by the biased voltage and the plasma potential, expressed as

$$N(E) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(E-E_{b0})^2}{2\sigma_1^2}} + \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(E-E_{p0})^2}{2\sigma_2^2}}, \quad (2)$$

where σ_1 and σ_2 are the deviations, E_{b0} and E_{p0} are the mean energies obtained from the biased voltage and the plasma potential respectively. In this paper, σ_1 and σ_2 are set to be $E_{b0}/3$ and $E_{p0}/6$ respectively when considering the numerical simulation results of plasma formation.[9]

In plasma doping, ion species are always molecular ions such as BH_x, B_2H_x, etc. The energy of B atom within molecules is determined by the ratio of its mass to the mass of ionic molecule. The breakdown of molecules consumes dynamic energy during injection due to the breaking of bonds within the molecules. This effect has been investigated in our previous work.[19] In this study the interaction within an ionic molecule is neglected because of its little effect.

3. Discussion

In the following simulation study, the source gas of plasma is chosen to be B_2H_6. In plasma body, the possible ionic species could be grouped into BH_x and B_2H_x and ratios of their species depend on experiment conditions.[18] To illustrate the effect of different species on doping profile, the ionic species in the plasma body are assumed to be B^+, BH_5^+, B_2^+ and $B_2H_5^+$[18] and the biased voltage applied to the wafer is 60 eV. The B dose of each ionic species is assumed to be the same in order to make a comparison between the depths of concentration profiles. In Fig.3, the profiles of each typical species as well as the total species are shown. It shows that with the increase of the mass of species, the doping profile becomes shallower due to the lessening of equivalent B energies.

It is found that the profiles of B^+, BH_5^+, B_2^+ and $B_2H_5^+$ shows graded doping depths which correspond to the graded molecular weights of 10, 15, 20 and 25. Besides, the profile of BH_5^+ is obviously shallower than that of B^+ and the profile of $B_2H_5^+$ is shallower than that of B_2^+. The reason is that H atoms in the molecules consume some dynamic energy which cannot be neglected in the PLAD simulation. Thus different ionic species should be considered in the PLAD process simulation.

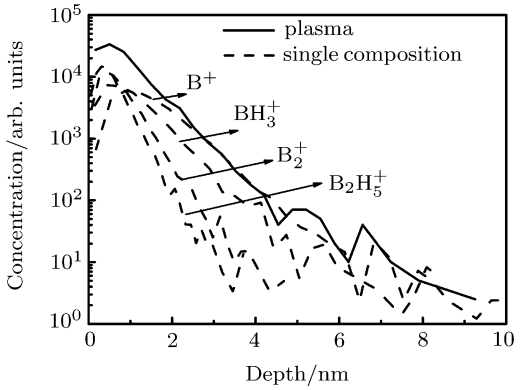


Fig.3. Simulation results with the composition model, showing obvious deviations of depth profile for different species.

In the simulation, parameter E_{b0} is set to be the biased voltage and E_{p0} is the plasma potential. To achieve a shallow junction, the biased voltage can be as low as 60 V,[20] which is compatible with the plasma potential which is about 30 V.[20] Thus the plasma potential must be considered in order to simulate the PLAD process accurately. Figure 4 shows the simulation results with (w/) and without (w/o) using the plasma potential model.

It is shown from Fig.4 that without the plasma potential, the simulation result underestimates the depth of concentration profile notably. In the figure, simulation without energy deviation is also shown for comparison. Figure 4 shows that the plasma potential and the energy deviation play a notable role in predicting the doping profiles of PLAD.

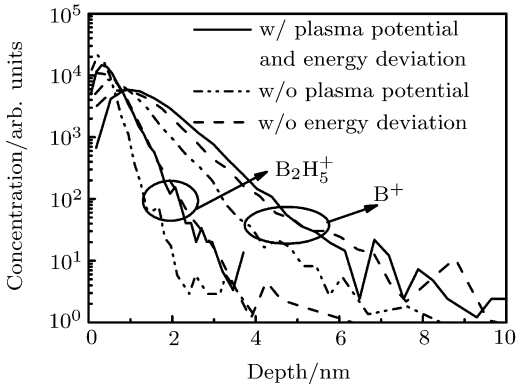


Fig.4. Effects of plasma potential and energy deviation on simulation results.

The angle model is included in the simulation. Simulation indicates that such an angle deviation has little effect on simulation results. It is expected that

the angle model is necessary for simulate the PLAD on a complex substrate structure.

To further verify the above models, PLADs are simulated and their results are compared with experimental results.[21] Because of the exact ratio of plasma species unavailable, two ratios are adopted for this simulation. One is 0.91:0.03:0.03:0.03 and the other is 0.03:0.03:0.03:0.91 for the species of B^+, BH_5^+, B_2^+ and $B_2H_5^+$. The former ratio is for the B^+ dominated case and the second for the $B_2H_5^+$ dominated case. Figure 5 shows the simulation results of PLAD with a zero biased voltage.

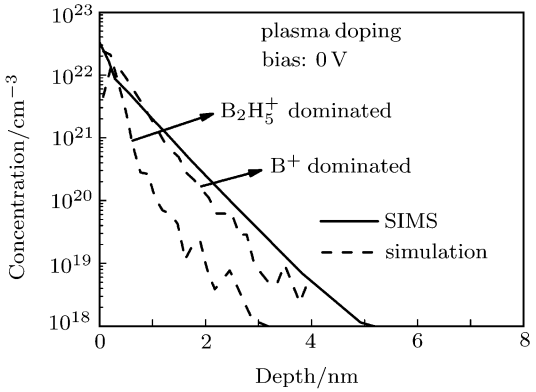


Fig.5. Simulation results of PLAD with plasma potential only and their comparison with experimental data.[21]

Figures 6 and 7 correspond to the cases of PLAD with biased voltages of 60 V and 200 V, respectively.

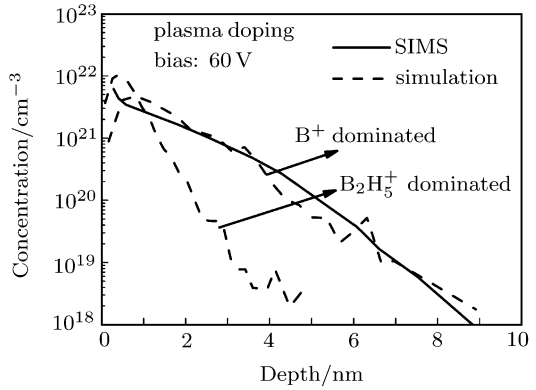


Fig.6. Simulation results of PLAD at a 60 V bias voltage and their comparison with experimental data.[21]

The figures show clearly that the $B_2H_5^+$ domination underestimates the measurements seriously while the B^+ domination is closer to measurements. This indicates that the plasma is more likely to be dominated by lighter species.

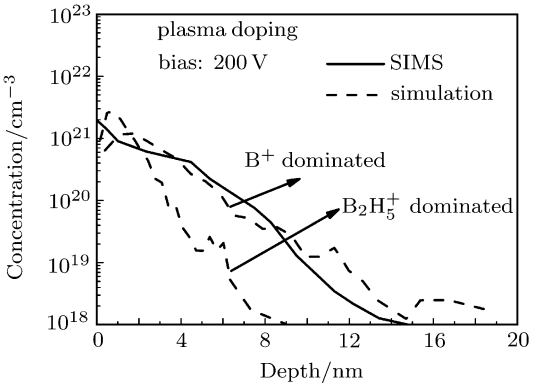


Fig.7. Simulation results of PLAD at a 200 V bias voltage and their comparison with experimental data.[21]

4. Conclusion

The localized MD method is applied to the PLAD simulation for the first time. By using this method, the species, angle and energy models have been built to investigate the special characteristics of the plasma doping process. The simulation results show that the models have a notable influence on doping profile simulation and more reasonable simulation results could be obtained with the present models. Simulation of concentration profile is supported by the experimental data.

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