Numerical simulation of plasma implanted nitrogen depth profiles in iron

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Abstract

Plasma immersion ion implantation (PIII) is a relatively complex process. Utilizing plasma and TRIM simulation, plasma implanted nitrogen depth profiles in iron are simulated in this work. Many factors such as the high voltage pulse rise time, voltage amplitude, pulse duration, plasma composition, etc. have a critical influence on this depth profiles. Our results confirm the broader distribution as well as shift of the implant peak toward the surface. Compared to the pulse duration and plasma composition, the rise time of the high voltage pulse has a more predominant effect on the shape of the profile. At higher implantation voltage, the nitrogen profile resembles that of multiple energy implantation in the beam-line mode. From this perspective, broadening of the ion energy spectrum in PIII is favorable since a single process can achieve the results of multiple energy ion implantation. This is particularly useful for processes such as shallow junction formation in microelectronics.

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1. Introduction

Plasma immersion ion implantation (PIII) excels in niche applications such as the treatment of objects with an irregular geometry, synthesis of silicon-on-insulator (SOI), and plasma doping of semiconductors [1–3]. In this technique, the entire surface of the specimen is implanted simultaneously without the need for complex beam and sample scanning. In general, PIII has the following features compared to conventional beam-line ion implantation: (1) All ion species in the plasma are co-implanted into the sample. (2) Ion acceleration is achieved through the plasma sheath and its shape depends on the sample holder configuration as well as processing conditions. Conformal implantation is sometimes difficult due to uneven propagation of the plasma sheath. (3) The ions are not mono-energetic due to three factors: plasma sheath expansion during ion transit to the target surface, effects of the ion-matrix sheath, and the finite rise and fall times of the implantation voltage pulses [4]. Hence, the ion flux and ion trajectory in PIII are largely determined by the sample voltage, pulse duration, plasma density, and other plasma parameters [5]. It can be speculated that the ion distribution is complex due to the broader energy...
spectrum of incident ions and multiple ion species in the plasma. Our previous investigation demonstrates that the rise-time of the voltage pulse has a great influence on this spectrum [6]. For instance, the low-energy (less than $eV_0$, $V_0$ being the applied potential) ions occupy nearly 30% of all the implanted ions for a pulse width of $t_p = 10 \mu s$ and rise time of $t_r = 3 \mu s$ according to Child–Langmuir law [7]. In this work, we numerically simulate the depth profiles of plasma-implanted nitrogen in iron under different conditions to investigate the effects of experimental parameters on the nitrogen in-depth distribution.

2. Numerical simulation

In our simulation, an analytical model, which has been described elsewhere in details [6], was employed to simulate the energy spectrum of the implanted ions. Subsequently, TRIM [8] was used to simulate the ion distribution in the substrate. To confirm the effectiveness of the numerical simulation, experimental investigation was also conducted and the results exhibit consistency [9]. For simplification, the full energy of the incident ions was divided into 10 energy spectra. The ion distributions with different energies were summed to yield the final atom distribution. It should be mentioned that ions with low energies (e.g. less than 1 keV) also induce sputtering which leads to a thin modified layer. However, due to the small $\delta$ (e.g. $\delta_{<1\text{keV}} \sim 2\%$ for 20 keV implantation with a rise-time of 1 and 20 $\mu s$ pulse-duration [6]), its effect was not considered in our simulation for simplification.

3. Results and discussion

3.1. Rise time and pulse duration

Figs. 1 and 2 demonstrate the effects of the sample voltage rise time and pulse duration on the depth profile under the following implantation conditions: $N_2^+$ plasma, implantation voltage of 20 kV, and implant dose of $1.0 \times 10^{17}$ cm$^{-2}$. The near-Gaussian distribution observed for conventional beam-line ion implantation is no longer valid in PIII even in the case of a very short rise time. The PIII profile is characterized by a slant-plateau distribution. The projected range shifts towards the surface resulting in shallower ions. The phenomenon can be explained by the relatively large ion current determined by Child law and lower acceleration voltage during the rise time of the voltage pulse. In contrast, the influence of the pulse duration is relatively small. For instance, very little
changes in the depth profiles can be observed changing the pulse duration from 10 to 40 μs for a fixed rise time of 1 μs. Our results thus show that control of the rise time of the voltage pulse is crucial since the tribological properties of the implanted materials have been found to be very sensitive to the implanted nitrogen distribution [10], which depends very much on the rise time.

3.2. Voltage

As shown in Fig. 3, the nitrogen depth profile is affected by the implantation voltage. As expected, a higher implantation voltage leads to a larger projected range and a lower peak concentration. It can be observed that at lower implantation voltages, the changes in the profile are more evident. The peak concentrations differ significantly. On the other hand, at higher implantation voltages, the changes are smaller and the plateau becomes flatter. Our results are similar to that obtained by multiple energy beam-line ion implantation [11,12]. Such a profile shape is beneficial to some applications such as plasma doping of semiconductors. In PIII, such a distribution can be obtained in one single process whereas multiple steps are required for conventional beam-line ion implantation. This unique feature makes PIII more efficient and economically in some applications.

3.3. Ion species

In addition to the attributes of the voltage pulse such as pulse shape and amplitude, the existence of multiple species in the plasma affects the depth profile. For example, a nitrogen plasma is usually composed of N⁺ and N²⁺. Upon impact, each atom in the N⁺ ion receives only half of the original energy and is implanted to a shallower depth than N²⁺. Our simulation data using the following conditions: rise time of 1 μs, pulse duration of 10 μs, implantation voltage of 20 kV, and dose of 1.0 x 10¹⁷ atoms/cm², show unexpectedly that the plasma composition has a small influence on the depth profile (Fig. 4). The nitrogen concentration decreases precipitously after the depth corresponding to the projected range of N²⁺. The discrepancy induced by the different plasma composition manifests more at the position corresponding to the position of N⁺. In this vicinity, the nitrogen concentration increases slightly, accompanied by a small concentration decrease in the zone between the surface and the N²⁺ projected range.

4. Conclusion

The rise time of the high voltage pulse is finite in PIII due to the equivalent capacitance effects of the
PIII hardware and plasmas. Consequently, even under collisionless conditions, the ion energy is not singular. The implantation energy is influenced significantly by the ratio of the pulse duration to the rise time. Due to the broadening of the incident energy, the depth profile of the implanted particle deviates significantly from a Gaussian. The implanted layer is shallower due to these low energy ions. However, this feature bodes well for applications in which multiple energy implantation is required. Our simulation results suggest that depth profiles with a plateau can be readily generated using the appropriate plasma parameters.

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