Analysis of Dopant Diffusion in Si by a Pulsed Excimer Laser

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Dopant diffusion calculations explain well the mechanism of the non-equilibrium incorporation of boron atoms from the silicon surface into the molten silicon induced by a pulsed excimer laser. When a high-power laser causes the melt front to proceed into the substrate faster than 8 m/s, the doped region is formed only near the surface of the molten region because dopant atoms cannot diffuse sufficiently fast for the junction depth to reach the maximum melt depth.

1. Introduction

Ultra-shallow junctions have received much attention recently because submicron gate metal-oxide-semiconductor (MOS) transistors require a source and drain whose depth is on the order of 0.1μm. In order to form such a shallow junction, new doping techniques using a pulsed UV excimer laser have been developed1-3. We reported the laser-induced melting of predeposited impurity doping technique (LIMPID)4). This technique employs a radio-frequency glow discharge (rf-GD) to deposit a thin film uniformly on a silicon wafer by decomposition of a dopant gas, such as B₂H₆ and PH₃, followed by irradiation with a pulsed XeCl excimer laser (308 nm), leading to a superficial melting of the silicon and to diffusion of the dopant.

In this paper, we use computer simulation to examine the behavior of dopant diffusion during laser-induced melting. The fitting of calculated results to experimental data provides the diffusion coefficient of boron in molten silicon and the relation between melt depth and junction depth.

2. Melt behavior of surface region

The usual unidimensional heat-diffusion equation including the melting process was solved analytically5) in order to obtain the melt behavior of silicon surface region. We assumed that the photon energy was instantaneously converted into heat at the surface because the skin depth is as small as 20 nm at the wavelength of 308 nm. The solid phase changes to the molten phase when the region at the melting point absorbs the latent heat. Figure 1 shows the calculated melt-front profile of silicon on which transparent SiO₂ (1000 Å) and boron (100 Å) films were deposited. The melt front rapidly proceeded into the silicon substrate during irradiation with a laser pulse, and later moved back to the surface. The laser irradiation with a pulse width of 30 ns at 1.0 J/cm² and 0.55 J/cm² induced the surface melting for 200 ns and 50 ns, respectively6), in which the melt depth
reached 480 nm and 115 nm, respectively, as is shown in Fig. 1.

3. Analysis of dopant profile

The diffusion of dopant in molten silicon occurs with a coefficient on the order of $10^{-4}$ cm²/s [3], while the diffusion coefficient of dopant in solid silicon is as small as $10^{-11}$ cm²/s [4]. This allows us to ignore the diffusion of dopant in the solid region during laser treatment. We divided the melt-front profile into $N$ segments by a time interval of $At$. It was assumed that diffusion is stationary in the molten region within a step. For the time interval of $At$, the dopant diffusion equation at the $n^{th}$ segment can be solved using the image method [5] using the profile at the $(n-1)^{th}$ segment and the boundary planes of the melt front and the surface. The segregation coefficient of boron at the liquid-solid interface was assumed to be 1 [6]. The dopant concentration $C(n,x)$ at the $n^{th}$ segment and at $x$ nm is

$$x \leq X_m;$$

$$C(n,x) = \frac{A}{2\sqrt{\pi D_d At}} \int_0^{X_m} C(n-1,x') X$$

$$+ \sum_{k=-\infty}^{\infty} \exp[-(x+x'-2kX_m)^2/4D_d At] \int_{x'}^{X_m} dx'$$

$$x > X_m;$$

$$C(n,x) = C(n-1,x)$$

where $X_m$, $D_d$, $At$, and $A$ are the depth of the melt front at the $n^{th}$ segment, the diffusion coefficient of the dopant, the time interval of 1 ns, and an appropriate normalization factor, respectively. The dopant profile at the first irradiation of a laser beam is obtained by calculating eq. (1) from the first to the $N^{th}$ segment with a melt front whose depth changes at every step and using the initial condition in which dopant atoms are located at the surface before irradiation. In this way, we can obtain the evolution of the dopant profile during melt and solidification. Figure 2 (a) shows the calculated profiles with a diffusion coefficient of $2.5 \times 10^{-4}$ cm²/s at different stages of the melt induced by irradiation with a single pulse at 1.0 J/cm² and the boron profile obtained by the secondary ion mass spectrometry (SIMS). After 10 ns, laser irradiation was continuing and the melt front was proceeding at a velocity of 16 m/s into the substrate. The melt front moved faster than the boron atoms diffused. After 90 ns, the melt front came across the dopant profile. The part of the profile which the melt front passed through was frozen in the solid region. The good
agreement between the calculated result at 200 ns and the SIMS data indicates that the dopant profile is formed by a simple diffusion process in the molten region. The diffusion coefficient of \(2.5 \times 10^{-4} \text{ cm}^2/\text{s}\) agreed well with the value of boron in molten silicon found by Kodera\(^7\). The junction depth was 300 nm, which was smaller than the maximum melt depth of 480 nm, and the \(p^+\) layer was formed in the near surface molten region. To give another example, Fig. 2(b) shows the calculated result of the evolution of dopant profile during melt induced by laser irradiation at 0.55 J/cm\(^2\) and the boron profile obtained by SIMS. In this case, the melt front proceeded slowly at a velocity of 5.5 m/s during laser irradiation. As a result the dopant-profile front reached the melt front. Dopant atoms diffused throughout the molten region and the profile was more precipitous than that formed by laser irradiation at 1.0 J/cm\(^2\), as is shown in Fig. 2(a).

The calculation of the melt-front profiles and the dopant profiles shows us an interesting relation between maximum melt depth and junction depth. Figure 3 shows the dependence both of melt depth and junction depth on incident laser energy. The junction depth increased together with the melt depth below 0.6 J/cm\(^2\) because the velocity of the melt front was slower than 8 m/s and the dopant diffused throughout the molten region. On the other hand, the \(p^+\) region was formed in a part of the molten region above a laser energy of 0.6 J/cm\(^2\).

4. Electric properties of laser-doped region

Figure 4 shows the characteristics of a \(p^-n\) diode with a mesa structure fabricated using the LIMPID process with a single pulse at 0.85 J/cm\(^2\). The ideality factor and reverse bias current were 1.03 and 50 nA/cm\(^2\) (at -1 V), respectively. These results suggest that the rapid melt and regrowth of silicon on exposure to an XeCl excimer laser
beam does not result in any serious defects. A heavily doped region was successfully obtained using the LIMFID process. The 10-pulse irradiation by a laser operating at 1.1 J/cm² resulted in a boron-doped region with a peak concentration of $2 \times 10^{21} \text{cm}^{-3}$ and a dose of $4 \times 10^{16} \text{cm}^{-2}$, which was measured by SIMS. The measurement of Hall effect revealed that the doped region had a carrier concentration of $2 \times 10^{21} \text{cm}^{-3}$ and a hole mobility of 19 cm²/V.s. This indicates that all boron atoms must be activated during the rapid melt-regrowth process induced by the pulsed laser, even if the boron concentration exceeds the solubility limit in silicon ($6 \times 10^{20} \text{cm}^{-3}$).

5. Conclusion
Calculations of dopant diffusion in the molten region explain well the pulsed-laser doping process. Matching the experimental data and the calculated results provides a diffusion coefficient of $2.5 \times 10^{-4} \text{cm}^2/\text{s}$. When a laser pulse at an energy above 0.6 J/cm² causes the melt front to proceed into the substrate faster than about 8 m/s, $p^+$ region is formed near surface of the molten region because dopant atoms cannot diffuse sufficiently fast for the junction depth to reach the maximum melt depth. A $p^+\text{n}$ junction had an ideal I-V performance with an ideality factor of 1.03. This indicates that the rapid melt-regrowth of silicon does not result in any serious defects.

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7. References