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Diffusion Coefficient of Boron in Tungsten Silicide

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Abstract

We developed a method of determining the impurity diffusion coefficient in WSi_2. We modeled the lateral diffusion profiles in the CMOS gate WSi_2 wire, which enabled us to determine the diffusion coefficient of boron from the three dimensional SIMS impurity profiles as to be of the order of 10^{-9} cm^2/s at 800°C. This value was more than 1 million times larger than that in silicon.

Introduction

The degradation of threshold voltage in polycide dual gate CMOS was caused by impurity diffusion through polycide(1)-(3). However, little characterization of this phenomenon has been done, and we have had no clear guide to suppressing this degradation. We must determine the diffusion coefficient in silicide to simulate this process. The difficulty exists in the very large impurity diffusion coefficient in silicide. The profiles after thermal process are always flat for the practical silicide film thickness (about 500 nm), and it is impossible to determine the diffusion coefficient from this.

Three dimensional SIMS analysis gives us a lot of information on diffusion in silicide(3), because we can diffuse impurities over 1 mm region, and can observe the lateral image of the impurity concentration profile variation during thermal processing.

We modeled diffusion in a silicide wire and determined the diffusion coefficient in silicide from the three dimensional SIMS profiles.

Experimental

Figure 1 shows the test structure. After 100 nm of polysilicon was deposited on SiO_2 film, 400 nm of WSi_2 was deposited at 360°C by CVD. The polysilicon was inserted to prevent the removal of the WSi_2 during following thermal process, and we made the polysilicon as thin as possible to neglect the amount of impurities that could diffuse into it. The WSi_2 and polysilicon was patterned by reactive ion etching to be 2 mm long and 30 μm wide, and boron was selectively implanted into the 20 μm-long window with a dose of 5×10^{14} cm^{-2} at 80 keV. Diffusion is strongly affected by solid solubility limit (about 10^{19} cm^{-3})(4), so we chose ion implantation conditions so that the boron concentration was less than the solid solubility limit for simplicity. After the WSi_2 film was covered with SiO_2 film, thermal processing was performed in dry nitrogen.

Three dimensional SIMS analysis was carried out with Perkin Elmer Atomica 6500 ion microprobe. The O_2^+ primary ion was focused to a 2 μm diameter to improve lateral resolution, and the positive boron ions were collected for their high sensitivity.

Theory

The diffusion coefficient of boron in WSi_2 is large enough to regard the diffusion depth profile as uniform, although we do not know its precise value. We suppose that the outdiffusion of boron to SiO_2 and polysilicon film is negligible. Consequently, this diffusion process is a simple one dimensional problem (Fig. 2), and is given by the Fick equation

$$\frac{\partial n(x,t)}{\partial t} = D\frac{\partial^2 n(x,t)}{\partial x^2}$$

with an initial condition of ,

$$n(x,0) = \begin{cases} n_0 & |x| < \frac{L_0}{2} \\ 0 & |x| > \frac{L_0}{2} \end{cases}$$

where L_0 is the length of the implanted region and n_0 is the initial doping concentration and can be defined as the division of boron dose Φ by the WSi_2 thickness d as $n_0 = \Phi/d$. The solution of the differential equation is

$$n(x,t) = \frac{n_0}{2}\left[\mathrm{erf}\left(\frac{x + L_0/2}{2\sqrt{Dt}}\right) - \mathrm{erf}\left(\frac{x - L_0/2}{2\sqrt{Dt}}\right)\right]$$

Consequently, the unknown parameter is the diffusion coefficient, and we can compare this theory and measurements using the diffusion coefficient as a fitting parameter.

Discussion

Figures 3 (a) and (b) are the lateral boron concentration images of the three dimensional SIMS boron profiles. We can clearly see the variation of the as-implanted boron profile during thermal processing at 800°C.

To do quantitative analysis, the beam was line scanned, and the lateral impurity concentration profile were observed.

Figure 4 is the profile just after the boron was implanted into the WSi_2. We used this profile to calibrate the impurity concentration, and determined that n_0 corresponds to 1050 counts. The bold line corresponds to theory. The lateral resolution of this SIMS is evaluated by comparing the theory and the data at about 5 μm.

Figure 5 is the lateral SIMS impurity profile after 800°C for 60 minutes annealing. Theory and experiment were in agreement at near diffusion coefficients of 5×10^{-9} cm^2/s. The value is about one million times larger than that in silicon(5), and about ten thousands times larger than that in polysilicon(6). The difference between theory and experiment may suggest that the diffusion coefficient depends on boron concentration.

Conclusion

We modeled the lateral diffusion profiles in WSi_2 wire and determined the diffusion coefficient of boron, which enables us to design the thermal process for half micron dual gate CMOS.

Acknowledgements

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References

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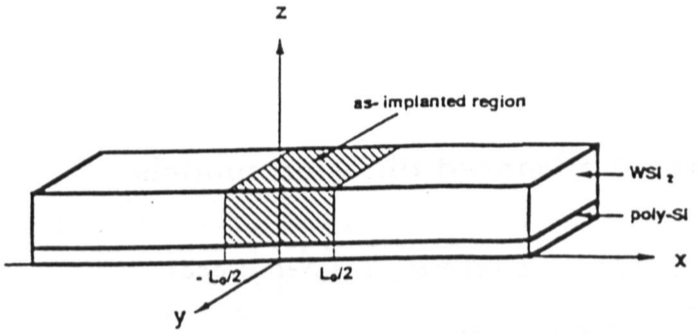


Fig. 1 Test structure. Boron was implanted into $-L_0/2 < x < L_0/2$.

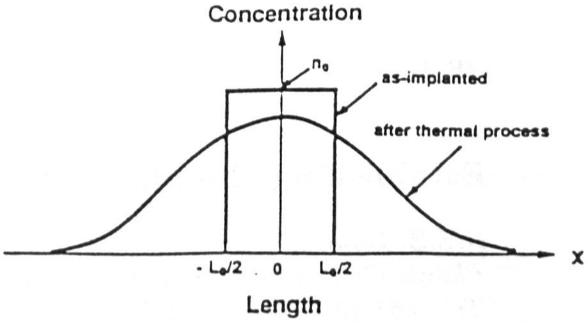
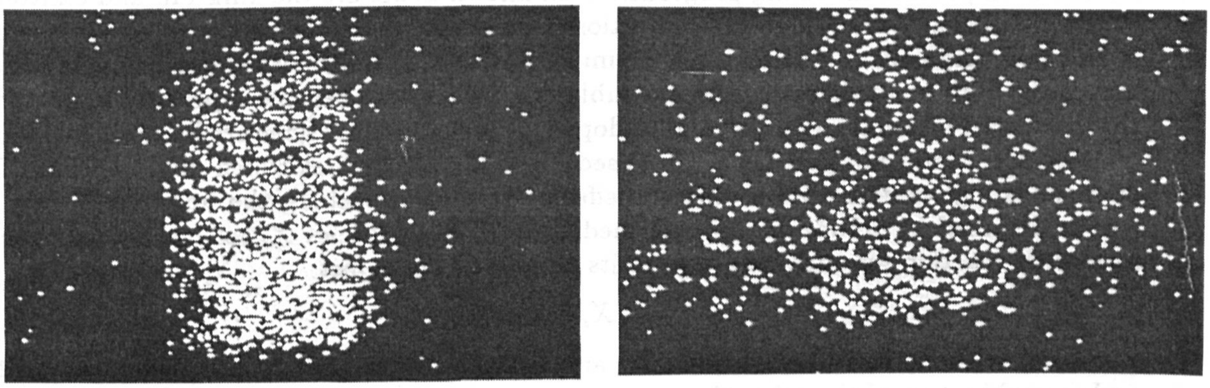


Fig. 2 Lateral diffusion profile. We assume the profile in y and z direction in Fig. 1 to be uniform and neglect the outdiffusion from the WSi_2 film to SiO_2 and polysilicon films.



(a) as-impanted

(b) 800°C 30 min

Fig. 3 Lateral diffusion boron concentration images of the three dimensional SIMS.

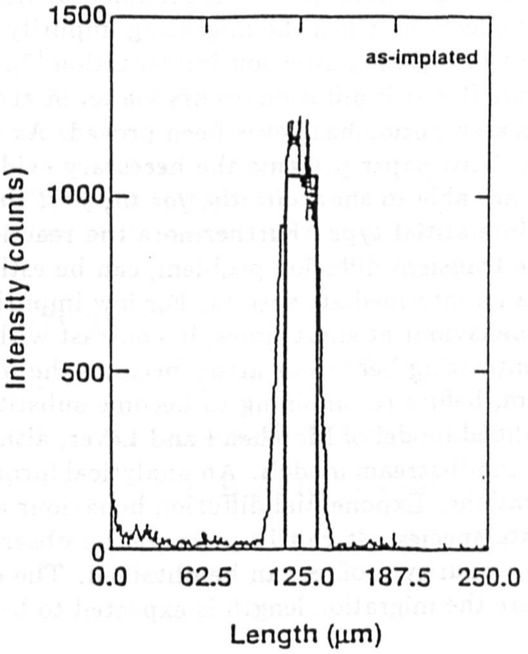


Fig. 4 Lateral boron concentration profile of as-implanted sample. The bold line is calculated.

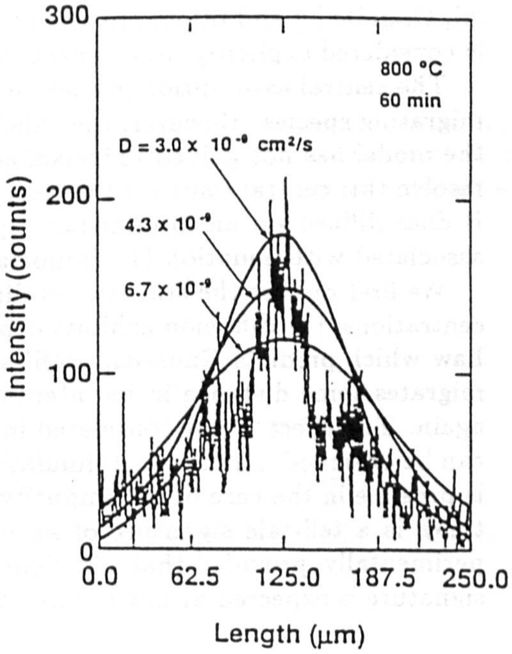


Fig. 5 Lateral boron concentration profile of samples annealed at 800°C for 60 minutes. The bold lines are the theory with various diffusion coefficients.