diffusion-fundamentals

The Open-Access Journal for the Basic Principles of Diffusion Theory, Experiment and Application

Formation Mechanism of Plateau, Rapid Fall and Tail in Phosphorus Diffusion Profile in Silicon Based on the Pair Diffusion Models of Vacancy Mechanism and Interstitial Mechanism

Masayuki YOSHIDA, Masami MOROOKA, Shuji TANAKA and Manabu TAKAHASHI

Yoshida Semiconductor Laboratory, 2-2-37 Kusagae, Chuo-ku, Fukuoka 810-0045, Japan
E-mail: myoshida@ws.ipc.fit.ac.jp

1. Introduction

Experimental P diffusion profile in Si with the P surface concentration of 3×10^{20} cm^{-3} at 900℃ under an inert atmosphere has unique features of the plateau, rapid fall and tail as shown in Fig. 1.[1] Yoshida *et al.* [2,3] studied P diffusion in Si based on the pair diffusion models of the vacancy mechanism and the interstitial mechanism. They obtained the effective P diffusion coefficient from the P diffusion equation, then proposed the limiting process of P diffusion. Based on these, the formation mechanism of the plateau, rapid fall and tail is studied. [3,4]

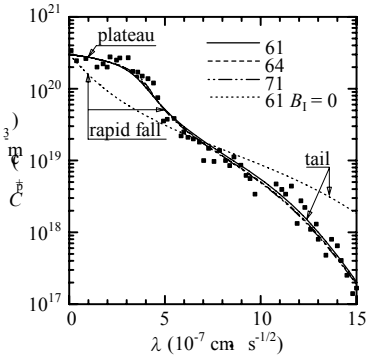

Fig. 1: Experimental P diffusion profile and its simulation. [1,3]

2. Pair Diffusion Model

Based on the vacancy potential energy in the vicinity of P shown in Fig. 2, [5] there is a strong attractive force between P and V, vacancies. By this force, a P-V pair can diffuse over a long distance without complete dissociation to P and V. This is the pair diffusion model of the vacancy mechanism.[1]

At high P concentration, C_{P^+}, the vacancy

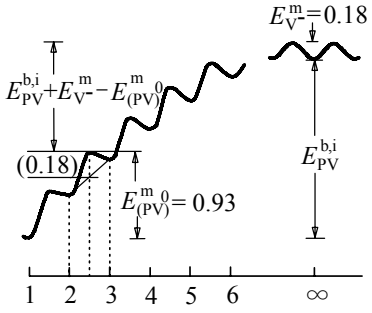

Fig. 2: Vacancy potential energy in eV in the vicinity of P atom.

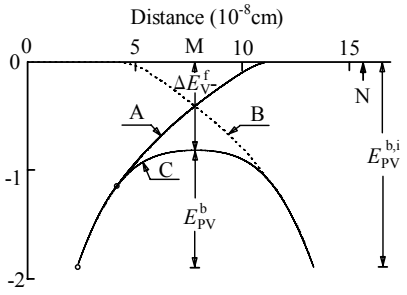

Fig. 3: Decrease in quasi vacancy formation energy.

potential energies generated by two adjoining P atoms overlap each other and the decrease in quasi vacancy formation energy, $\Delta E^{\mathrm{f}}_{\mathrm{V}^-}$, occurs.[6] The case of $C_{\mathrm{P}^+} = 5\times10^{20}$ cm^{-3} is shown in Fig. 3. The overlapping is seen in Fig. 3.

The vacancy potential energy shown in Fig. 2 is the basic condition for the pair diffusion model of the vacancy mechanism and $\Delta E^{\mathrm{f}}_{\mathrm{V}^-}$. Therefore, if the pair diffusion model of the vacancy mechanism is adopted, $\Delta E^{\mathrm{f}}_{\mathrm{V}^-}$ should also be adopted.

Applying the idea mentioned above to the interstitial mechanism, we have the pair diffusion model of the interstitial mechanism and the decrease in quasi self-interstitial formation energy, $\Delta E^{\mathrm{f}}_{\mathrm{I}^-}$. If the pair diffusion model of the interstitial mechanism is adopted, $\Delta E^{\mathrm{f}}_{\mathrm{I}^-}$ should also be adopted.

3. Conclusion

P diffuses predominantly by the interstitial mechanism.[7] Therefore the basic process of P diffusion is the diffusion of (PI), where I and (PI) denote self-interstitials and P-I pairs.

In the high C_{P^+} region, excess I is generated by the dissociation of (PI) and the limiting process of P diffusion depends on whether or not excess I is controlled. That is, 1) if the concentration of excess I decreases relatively due to the effect of $\Delta E^{\mathrm{f}}_{\mathrm{I}^-}$, or 2) if excess I is removed by the recombination with vacancies, P diffuses fast and the plateau is formed; if not, P diffuses slowly and the rapid fall is formed.

In the tail region, C_{P^+} is low and the limiting process of P diffusion is the basic process of P diffusion or the diffusion of (PI). Excess I generated in the high C_{P^+} region diffuses into the tail region and I is supersaturated there. Therefore the concentration of (PI) increases, resulting in the fast diffusion of P and the formation of the tail.

Two methods, 1) and 2), were described above for the control of excess I. Investigating which of them actually occurs is a problem in the future.

References

[1] M. Yoshida, E. Arai, H. Nakamura and Y. Terunuma: J. Appl. Phys. **45** (1974) 1498.

[2] M. Yoshida, M. Morooka, M. Takahashi and H. Tomokage: Jpn. J. Appl. Phys. **39** (2000) 2483.

[3] M. Yoshida and S. Tanaka: Jpn. J. Appl. Phys. **41** (2002) 5493.

[4] S. Tanaka, M. Yoshida, M. Morooka and M. Takahashi: Res. Bull. Fukuoka Inst. Tech. **36** (2004) 207.

[5] G. D. Watkins and J. W. Corbett: Phy. Rev. **134** (1964) A1359.

[6] M. Yoshida: Jpn. J. Appl. Phys. **32** (1993) 5523.

[7] T. Shimizu, T. Takagi, S. Matsumoto, Y. Sato, E. Arai and T. Abe: Jpn. J. Appl. Phys. **37** (1998) 1184.