ON THE DIFFUSION MECHANISMS AND DIFFUSIVITY OF THE III AND V GROUP DOPANT IN SILICON MATERIAL

Vu Ba Dung
Faculty of Physics
Mining and Geology University, Hanoi

Abstract *Diffusion of impurity into silicon materials plays an important role in semic ductor device fabrication technology. The determination of diffusion mechanism is v difficult task. So far the diffusion mechanisms in silicon have been discussing. There three dominated main mechanisms of the III and V group impurity element diffused i silicon crystal such as interstitial mechanism, vacancy mechanism and interstitialcy me anism. In this report, the author estimated the diffusivities in three cases. An expressi of boron diffusitivity in silicon based on interstitialcy mechanism was presented. It shou that the diffusion mechanism affected strongly on diffusitivity of impurity in silicon.*

1. Diffusion and diffusion mechanism of atoms diffusion in silicon crystal

1.1. Fick theory of diffusion

The simple theory of the diffusion given by Fick in 1958 with basic contents co sisting two laws of Fick I and Fick II as following:

$$J = -D\frac{\partial C}{\partial x} \qquad (1)$$

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2}. \qquad (2)$$

The Fick I and Fick II laws describe only on basis of phenomenology. The F theory also indicates that the diffusivity D is constant. However, in fact, the diffusiv depends on many different factors. What does the Fick theory communicate about t dependence of the diffusitivity on the mechanism of diffusion?

1.2. Diffusion mechanisms in silicon

The diffusion of dopants into silicon may happen as following mechanism: Dir exchange mechanism, ring mechanism, interstitial mechanism, interstitialcy mechanis dumbbell mechanism crowding mechanism, vacancy mechanism and relaxion mechani (can be seen below in Fig.1) [1,2]. The diffusion mechanism of the III and V gro impurities are dominated by interstitial, vacancy and interstitialcy mechanisms.

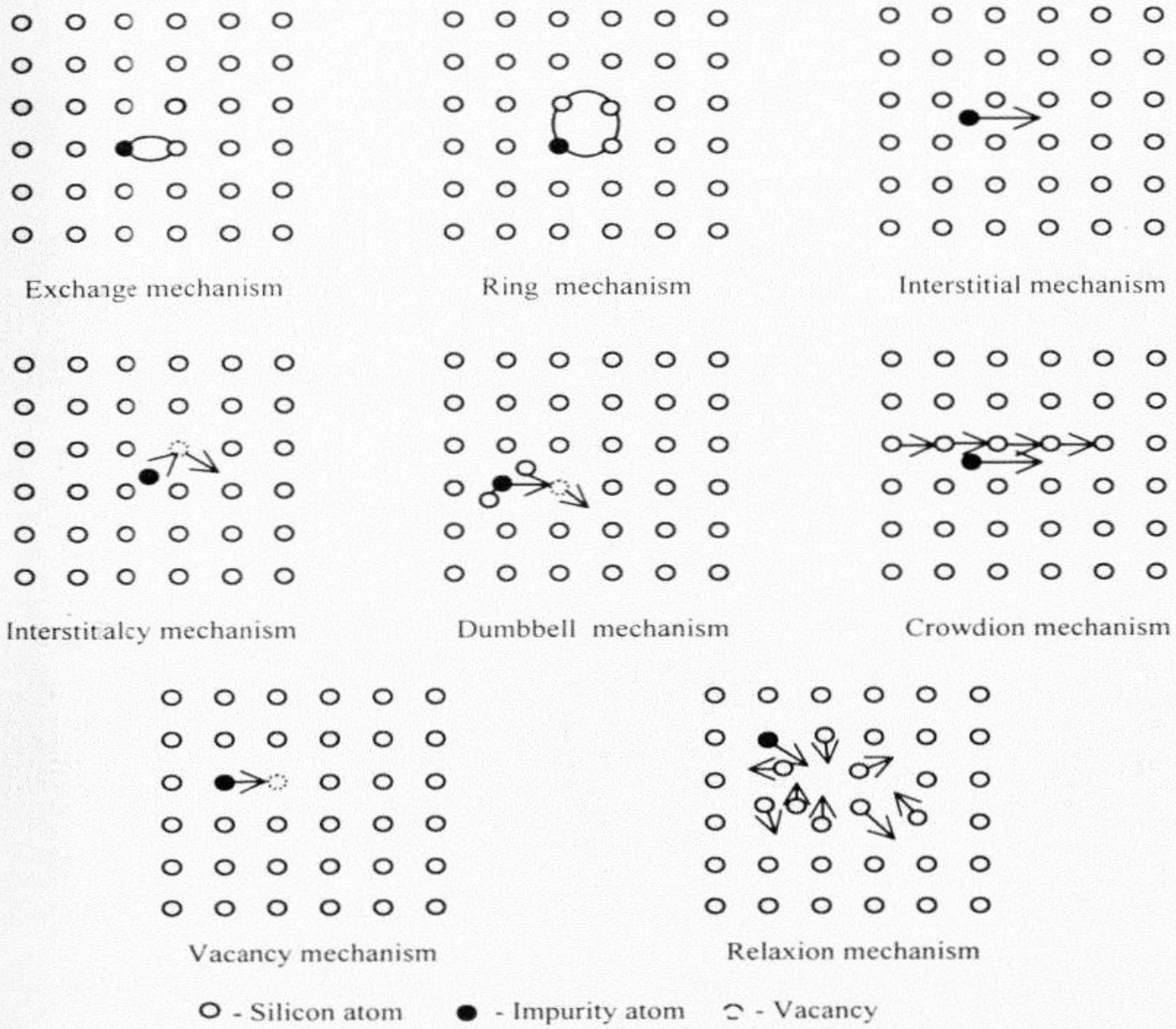

Fig.1: Some main mechanisms of diffusion in silicon.

2. Diffusivity of dopants in silicon

2.1. The general expression of the diffusivity based on jump theory

Jump steps based on jump theory carried out the diffusion of impurity atoms into ilicon crystal. Some authors showed that the general expression as following [1]:

$$D = c.D(C).h.f.\lambda^2.\nu. \tag{3}$$

We suppose that diffusivity is independent on impurity concentration $D(C) = 1$ hen we have

$$D = c.h.f.\lambda.\bar{\nu}.$$

where c is the typical constant of crystal ($c = 1/6$ for diamond lattice), ν is the jump frequency that estimated by the jum › theory, λ is the average distance between two jum $\bar{\nu}$ is the average velocity of diffused impurity atoms, ' is the correlation factor h is internal field enhanced factor [9].

$$h = 1 + \frac{1}{\sqrt{1 + 4\left(\frac{n_i}{N}\right)^2}}.$$

2.2. Diffusivity of the III and V group impurity element diffused i silicon crystal

If the impurities in silicon have been diffused in depth $d, by n_I$ jumping steps ba on the interstitial mechanism. The average distance of each jumping is λ, the time which the jump were happened is tI and the average velocity of diffused impurity is:

$$\bar{\nu}_i = \frac{d}{n\tau_I},$$

substitute into the Eq. (4) we have:

$$D_S^I = c.h.f.\lambda\frac{d}{n\tau_I}.$$

The Eq. (7) is the diffusivity of the pure interstitial mechanism.

If the impurities in silicon have been diffused in depth d by n_V jumping based the vacancy mechanism, the average distance of each jumping is λ, the time in which jump were happened is tV and the average velocity of diffused impurity is:

$$\bar{\nu}_V = \frac{d}{n\tau_V},$$

we have:

$$D_S^V = c.h.f.\lambda\frac{d}{n\tau_V}.$$

The Eq. (9) is the diffusivity of the pure vacancy mechanism.

If the impurity diffuse due to the interstitialcy mechanism in order to reac depth, the percentage of jumps due to the interstitial mechanism is f_I and that of to the vacancy mechanism is f_V. Therefore the number of jumps due to the intersti mechanism of impurity atoms is $n_I f_I$, the time in which the jumps realized is $n_I f_I$ Similarly, due to the vacancy mechanism the number of jumps of impurity atoms is n_V the time in which the jumps realized is $n_V f_V \tau_v$. The time in which the atoms w $n = n_I + n_V$ jumps to pass diffusion distance d is:

$$t_{IV} = nf_I\tau_I + nf_V\tau_V.$$

The average velocity in the interstitialcy mechanism will be $\bar{\nu}$. This can be written the following form:

$$\bar{\nu} = \frac{d}{t_{IV}} = \frac{d}{nf_I\tau_I + nf_V\tau_V}. \tag{11}$$

Substitute parameters into the Eq. (4), we have the diffusivity due to interstitialcy chanism:

$$D_S^{IV} = c.h.f.\lambda.\frac{d}{nf_I\tau_I + nf_V\tau_V}. \tag{12}$$

We suppose that $h = 1, f = 1$ and using equations (7), (9) and (12) yield them we ve:

$$D_S^{IV} = \frac{D_S^I D_S^V}{f_I D_S^V + f_V D_S^I}. \tag{13}$$

The Eq. (13) is the diffusivity of the pure interstitialcy mechanism.

Conclusion

1. The diffusion mechanism of impurities in semiconductor materials affects their fusivity very much.

2. In the interstitialcy mechanism, the diffusivity depends on percentage of the num- r of the jumps of atoms, due to the interstitial mechanism (f_I) and vacancy mechanism $_V$).

3. The velocity of the diffusion depends strongly on the mechanism of the diffusion.

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VỀ CƠ CHẾ KHUẾCH TÁN VÀ HỆ SỐ KHUẾCH TÁN TẠP CHẤT NHÓN III VÀ V TRONG VẬT LIỆU SILIC

Vũ Bá Dũng

Khoa Lý, Đại học Mỏ - Địa chất, Hà Nội

Khuếch tản tạp chất vào vật liệu bán dẫn là một khâu quan trọng trong công chế tạo các linh kiện bán dẫn. Xác định các cơ chế khuếch tán là một việc rất khó. tới nay cơ chế khuếch tán trong silic là vấn đề còn có nhiều tranh luận. Tuy nhiê tạp chất thuộc nhóm III và V khuếch tán trong silic theo ba cơ chế chủ yếu là co điền kẽ, cơ chế nút khuyết và cơ chế hỗn hợp. Trong bài báo này tác giả đã ước được các hệ số khuếch tán trong ba trường hợp. Biểu thức của hệ số khuếch tán the chế hỗn hợp cũng đã được đưa ra . Các kết qủa ước tính cũng chỉ ra rằng cơ chế kh tán ảnh hưởng nhiều đến hệ số khuếch tán của tạp chất trong silic