

BORON AND PHOSPHORUS DIFFUSION IN SILICON: PRESSURE DEPENDENCE

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Abstract. *The effects of pressure on diffusion of impurities in silicon crystal are investigated by using the statistical moment method (SMM). Pressure dependence of diffusion coefficient, D , is characterized by an activation volume, V^* . Numerical results for B and P diffusion in silicon are performed and compared to experimental data showing the good agreement.*

I. INTRODUCTION

Dopant diffusion is an elementary physical process in microelectronic device fabrications. As device sizes become smaller and smaller, the role of atomistic dopant diffusion modeling is becoming more important. B and P are important p-type and n-type dopants in silicon, and their diffusion properties in silicon have been extensively studied. Both experimental observations and theoretical calculations indicate that diffusion of B and P in silicon mediated by an interstitialcy mechanism [1, 2, 3, 4]

A study of the dependence of the atomic diffusivity on pressure(p) can provide valuable information to help elucidate atomistic diffusion mechanisms.

In the present study we used the moment method in statistical dynamics within the fourth order moment approximation, to calculate the activation volume, V^* , at temperature T and diffusion coefficient, D , of B and P in silicon at temperature T and at pressure p . We find that both B and P diffusion in silicon via an interstitialcy mechanism. The diffusivity of B in silicon is enhanced by pressure, while the diffusivity of P in silicon is retarded by pressure and almost independent of pressure. These results are in agreement with conclusions by Aziz[8] and Zhao[7]. We also compare the calculated results with the experimental data and previous theoretical calculations.

II. EFFECT OF PRESSURE ON THE DIFFUSION IN SILICON

The pressure-dependence of the diffusivity is characterized by the activation volume, V^* , [5, 6, 7, 8]

$$-k_B T \frac{\partial \ln D(p, T)}{\partial p} = V^*, \quad (1)$$

where k_B is the Boltzmann constant and T is the absolute temperature. From Eq. (1) it is easy to obtain the expression of the diffusion coefficient

$$D_{(p,T)} = D_{(0,T)} \exp\left\{-\frac{pV^*}{k_B T}\right\}, \quad (2)$$

In the equation (2), $D_{(0,T)}$, is the diffusion coefficient at a zero pressure and temperature, T , [9]

$$D_{(0,T)} = D_0 \exp\left\{-\frac{Q}{k_B T}\right\}, \quad (3)$$

with Q is the activation energy, and the pre-exponential factor D_0 is given by

$$D_0 = n_1 f \frac{\omega}{2\pi} r_1^2, \quad (4)$$

where n_1 denotes the number of the first nearest neighbour; f is the correlation factor; ω denotes the atomic vibrational frequency of impurity atom in silicon crystal and r_1 is the jump distance at temperature T .

The activation volume, V^* , is the sum of the formation volume, V^f , and the migration volume, V^m , [6]

$$V^* = V^f + V^m, \quad (5)$$

These volume changes are shown schematically in Fig. 1.

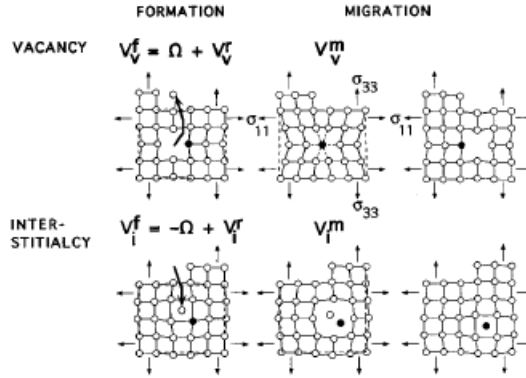


Fig.1. Schematic volume changes (see dashed lines) upon point defect formation and migration for simple vacancy and interstitialcy mechanisms.

The formation volume, V^f , is the volume change in the system upon the formation of a defect from the free surface in its standard state, it is given by Aziz [6]

$$V^f = \pm\Omega + V^r, \quad (6)$$

where Ω is the atomic volume at temperature T , and the plus sign is for vacancy formation, and the minus sign is for interstitial formation throughout this paper. The relaxation volume, V^r , is the amount of outward relaxation of the sample surfaces (if the relaxation is inward, is negative) due to the newly-created point defect.

M.Tang and *L.Colombo* [11] calculated relaxation volumes for self-diffusion via interstitialcy and vacancy mechanisms by

$$V_{I,V}^r = \frac{l_{I,V}^3 - l_{eq}^3}{l_{eq}^3/N}, \quad (7)$$

where $l_{I,V}$ is the box length for interstitial (I) and vacancy (V) defects, respectively; l_{eq} is the original box length (no defect); N is the sum atoms in the box.

The migration volume, V^m , is the additional volume change when the defect reaches the saddle point in its migration path. In interpreting atomistic calculations and experiments in the past, the assumption has been made almost universally that, V^m , is negligible [10]. In the present study, we also assumed that the migration volume was negligible for the calculation of the activation volume of silicon .

With the aid of Eqs. (3) and (4) permits us to determine the diffusion coefficient, $D_{(0,T)}$, at a zero pressure and temperature, T ,. Using Eqs. (5)-(7) we can calculate the values of the activation volume, V^* , at temperature, T , therefore, from Eq. (2) the pressure dependence of the diffusion coefficient, $D_{(p,T)}$, is determined.

III. NUMERICAL RESULTS AND DISCUSSIONS

We now perform the statistical moment method (SMM) to calculate diffusion coefficient of B and P atoms in silicon via an interstitialcy mechanism at various pressure p . Using the empirical many-body potentials was developed for silicon [12]

$$\varphi = \sum_{i<j} U_{ij} + \sum_{i<j<k} W_{ijk}, \quad (8)$$

$$U_{ij} = \varepsilon \left[\left(\frac{r_0}{r_{ij}} \right)^{12} - 2 \left(\frac{r_0}{r_{ij}} \right)^6 \right], \quad (9)$$

$$W_{ijk} = Z \frac{(1 + 3 \cos \theta_i \cos \theta_j \cos \theta_k)}{(r_{ij} r_{jk} r_{ki})^3}, \quad (10)$$

where r_{ij} is the distance between the i -th atom and j -th atom in crystal; $\theta_i, \theta_j, \theta_k$ are the inside angles of a triangle to created from three atoms i, j, k ; ε, r_0, Z are the potential parameters are taken from ref.12; These parameters are determined so as to fit the experimental lattice constants and cohesive properties.

Table 1: Potential parameters of the empirical many- body potential for Silicon[12]

ε (eV)	r_0 (Å)	Z (eV.Å ⁹)
2.817	2.295	3484

With the impurity atoms, using the Pak-Doyam pair potential was developed for boron and phosphorus [13]

$$\varphi_{ij} = \begin{cases} a(r_{ij} + b)^4 + c(r_{ij} + d)^2 + e, & r_{ij} < r_0 \\ 0, & r_{ij} \geq r_0 \end{cases} \quad (11)$$

The parameters(a, b, c, d, e, r_0) for these potentials are presented in Table 2.

Table 2: Potential parameters of the Pak-Doyam pair potential for B and P [13]

	a	b	c	d	e	r_0 (Å)
φ_{BB} (eV)	-0.08772	-2.17709	0.79028	-2.85849	-0.09208	3.79
φ_{PP} (eV)	-0.07435	-2.60709	0.64791	-3.27885	-0.07531	4.21

Using the potential parameters for Si and impurities B and P (Tables 1 and 2), and our theory in Section II, we obtain the values of the activation volume, V^* , and the diffusion coefficient, D , of B and P atoms in silicon via an interstitialcy mechanism. The SMM results are summarized in Tables 3 and 4. The SMM calculated results of the activation volume are in good agreement with the experimental data, and better than other theoretical methods.

Table 3: Comparison of the SMM calculated results of the activation volume, V^* , of B and P in silicon with experiments and other calculations.

Atoms	Expt. and calculations	V^*/Ω	T(K)
B	Expt.[8]	-0.16±0.05	1083
	Expt.[14]	-0.17±0.01	1083
	Expt.[5]	-0.125±0.02	1123
	SMM	-0.17	1083
	GGA (Laudon)[16]	-0.26	0
	GGA (Sadigh)[15]	-0.15	0
	LDA (Sadigh)[15]	-0.11	0
P	Expt.[7]	0.09±0.11	1113
	SMM	0.04	1113

Table 4: The pressure dependence of diffusion coefficient of B and P in silicon.

Atoms	T(K)	p(GPa)	$D(p, T)(cm^2/s)$ [SMM]	$\log D(cm^2/s)$ [SMM]	$\log D(cm^2/s)$ [Expt.]
B	1083	0	$2.9622 * 10^{-17}$	-16.5284	-16.3872 [8]
		1	$3.7662 * 10^{-17}$	-16.4241	-16.2676 [8]
		2	$4.7885 * 10^{-17}$	-16.3198	-16.1487 [8]
		3	$6.0882 * 10^{-17}$	-16.2155	-16.0269 [8]
P	1113	0	$3.9324 * 10^{-16}$	-15.4053	-16.6073 [7]
		1	$3.7255 * 10^{-16}$	-15.4288	-16.6478 [7]
		2	$3.5296 * 10^{-16}$	-15.4523	-16.6883 [7]

In Figs.2 and 3 we show the pressure dependence of diffusion coefficient, $D_{(p,T)}$, of B and P in Si crystal at the temperatures 1083K (for B) and 1113K (for P). It can be seen in these figures that the diffusion coefficient, $D_{(p,T)}$, of B increases with pressure, while of P decreases with pressure and almost independent of pressure. These results are agreement with conclusions by Aziz [8] and Zhao [7].

IV. CONCLUSIONS

In this paper we have performed the statistical moment method (SMM) to study pressure dependence of diffusion coefficient, $D_{(p,T)}$, of B and P in silicon obey an interstitialcy mechanism. The SMM calculated results for the activation volume, V^* , and diffusion coefficient, $D_{(p,T)}$, are in good agreement with the experimental data.

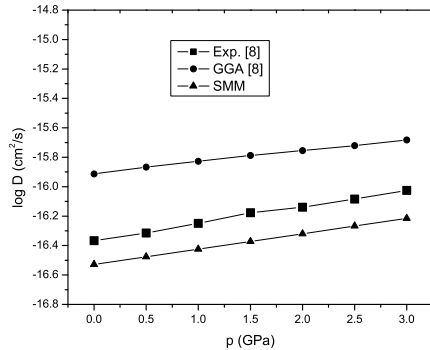


Fig.2. pressure dependence of B diffusion in Si.

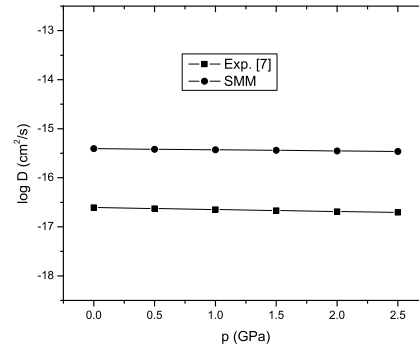


Fig.3. pressure dependence of P diffusion in Si.

REFERENCES

- [1] W. Windl, M. M. Bunea, R. Stumpf, S. T. Dunham, M. P. Masquelier, *Phys. Rev. Lett.* **83** (1999) 4345.
- [2] Jianjun Xie, S. P. Chen, *J. Phys. D: Appl. Phys.* **32** (1999) 1252.
- [3] J. S. Christensen, H. H. Radamson, A. Yu. Kuznetsov, B. G. Svensson, *Appl. Phys. Lett.* **82** (2003) 2254.
- [4] Xiang-Yang Liu, Wolfgang Windl, K. M. Beardmore, M. P. Masquelier, *Appl. Phys. Lett.* **82** (2003) 1839.
- [5] Y. Zhao, M. J. Aziz, S. Mitha, D. Schiferl, *Mat. Res. Soc. Symp. Proc.* **442** (1997) 305.
- [6] M. J. Aziz, Special issue on *Ten Years of Diffusion in Silico* (1998).
- [7] Y. Zhao, M. J. Aziz, *Appl. Phys. Lett.* **86** (2005) 141902.
- [8] M. J. Aziz, Y. Zhao, *Phys. Rev. B* **73** (2006) 054101.
- [9] Vu Van Hung, Phan Thi Thanh Hong, Bui Van Khue, *Proc. Natl. Conf. Theor. Phys.* **35** (2010) 73-79.
- [10] M. J. Aziz, *Appl. Phys. Lett.* **70** (1997) 2810.
- [11] M. Tang, L. Colombo, J. Zhu, T. Diaz de la Rubia, *Phys. Rev. B* **55** (1997) 14279.
- [12] S. Erkoc, *Phys. Reports* **278** (1997) 81-88.
- [13] Vo Van Hoang, *Physica B* **348** (2004) 347-352.
- [14] Y. Zhao, M. J. Aziz, H. J. Gossman, S. Mitha, D. Schiferl, *Appl. Phys. Lett.* **74** (1999) 31.
- [15] B. Sadigh, T. J. Lenosky, S. K. Theiss, M. J. Caturla, T. Diaz de la Rubia, M. A. Foad, *Phys. Rev. Lett.* **83** (1999) 4341.
- [16] M. Laudon, N. N. Carlson, M. P. Masquelier, M. S. Daw, W. Windl, *Appl. Phys. Lett.* **78** (2001) 201.

Received 30-9-2011.