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Disappearance of the Self-Interstitial during Diffusion of the Phosphorus-Self-Interstitial Pair in Silicon on the Basis of One-Bond-Type Migration

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Abstract

In the interstitialcy mechanism of diffusion of phosphorus-self-interstitial pairs on the basis of one-bond-type migration, the split-＜100＞ configuration and the bond-centered configuration are repeated. This is studied theoretically using three dimensional schemata. It is found that the self-interstitial disappears in the bond-centered configuration. This finding contrasts with that of Fahey, Griffin, and Plummer, who reported that, probably on the basis of two-bond-type migration, the interstitialcy mechanism will operate only if the diffusing defect, the phosphorus-self-interstitial pair, does not dissociate.

Keywords: *interstitialcy mechanism, one-bond-type migration, disappearance of self-interstitial*

1. Introduction

Watkins and Corbett[1] experimentally studied the reorientation of the phosphorus-vacancy pair, that is, the diffusion of the pair. They proposed that, in the reorientation, a vacancy located at the normal nearest neighbor site of phosphorus atom makes four consecutive jumps, two away from the phosphorus atom and then two back. Note that the phosphorus-vacancy pair must partially dissociate through these jumps. The largest separation between the phosphorus atom and the vacancy during dissociation occurs at the third nearest neighbor site.

Fahey *et al.*[2] theoretically studied the interstitialcy mechanism of impurity diffusion, using two dimensional schemata, and reported the following: “An important difference exists between the interstitialcy diffusion mechanism and the vacancy diffusion mechanism. Whereas migration of a dopant atom (A) by the vacancy mechanism requires that the diffusing defect (AV pair) must at least partially dissociate, the interstitialcy mechanism will operate only if the diffusing defect (AI pair) does not dissociate.”

Yoshida *et al.*[3,4] theoretically studied the interstitialcy mechanism of diffusion of the phosphorus-self-interstitial pairs on the basis of one-bond-type migration, using three dimensional schemata. The purpose of the present work is to comment on the work of Fahey *et al.*[2] based on Yoshida *et al.*[4] In the present work, migration and diffusion have the same physical meaning.

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2. Interstitialcy mechanism

Group-V impurities in silicon are located at substitutional sites.[5] Therefore their diffusion is assisted by vacancies and self-interstitials located at the impurities’ nearest neighbor sites. These types of diffusion are called the vacancy mechanism[6] and the interstitialcy mechanism,[7,8] respectively.

Following Seeger and Chik[8] the interstitialcy mechanism is explained by using Fig. 1.

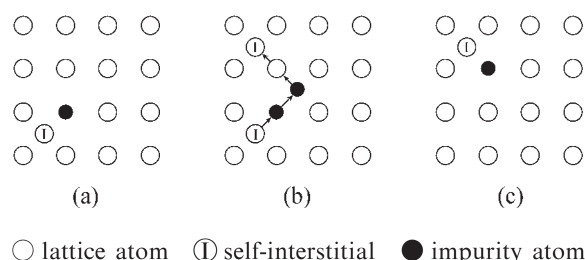

Fig. 1. Interstitialcy mechanism of impurity diffusion. (a) just before diffusion (b) diffusion (c) just after diffusion

Fig. 1 (a): Just before diffusion, a self-interstitial is located at an interstitial site next to a substitutional impurity atom.

Fig. 1 (b): The self-interstitial next to the substitutional impurity atom displaces the impurity atom into an inter-

stitial site, occupying itself the lattice site. The impurity atom subsequently displaces a silicon atom on a neighboring lattice site into an interstitial site. The impurity atom takes up its original nearest neighbor site.

Fig. 1 (c): As a result, the impurity atom has moved by one interatomic distance.

3 . Disappearance of self-interstitial

For the explanation of disappearance of self-interstitial in Fig. 1 (b), Fig. 1 (b) is divided into three parts and is shown in Fig. 2.

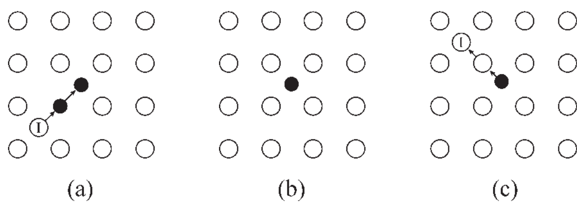

Fig. 2 . Division of Fig. 1 (b) into three parts for the explanationof disappearance of self-interstitial.

Fig. 2 (a): The self-interstitial next to the substitutional impurity atom displaces the impurity atom into an interstitial site, occupying itself the lattice site.

Fig. 2 (b): As a result of Fig. 2 (a), the self-interstitial disappears and the impurity atom moves into an interstitial site. The explanation of Fig. 2 (b) "the self-interstitial disappears" will be presented again in the final part of the present work.

Fig. 2 (c): The impurity atom, which is located at the interstitial site in Fig. 2 (b), subsequently displaces a silicon atom on a neighboring lattice site into an interstitial site. The impurity atom takes up its original nearest neighbor site.

Watkins *et al.*[9] theoretically studied four different self-interstitial configurations of carbon in diamond and concluded that the split-<100> and bond-centered configurations have nearly the same energies and are more stable than the tetrahedral and hexagonal configurations. Although Car *et al.*[10] proposed that the split interstitial configuration lies somewhat higher in energy, the idea of Watkins *et al.*[9] mentioned above is adopted in the present work. The split-<100> and bond-centered configurations are called the "interstitialcy" configuration.[9]

Yoshida *et al.*[3] proposed two types of migration that occur in the interstitialcy configuration, that is, one-bond-type migration and two-bond-type migration. In one-bond-type migration, one bond is first broken and then another new bond is formed. In two-bond-type migration, two bonds are broken simultaneously and then two new bonds are formed simultaneously. It was concluded[3] that one-bond-type migration is more likely to occur, because in two-bond-type migration two bonds have to be broken and formed simultaneously. One-bond-type migration is the repetition of the split-<100> (SP) and bond-centered (BC) configurations. Two-bond-type migration is the repetition of only the split-<100> configuration or only the bond-centered configuration.

Prior to Fahey *et al.*[2] Mathiot[11] schematically showed the interstitialcy mechanism for impurity diffusion in two dimensions. They[2,11] showed the migration of the split configuration without showing the migration of the bond-centered configuration. Therefore their result was most likely caused by two-bond-type migration.

Yoshida *et al.*[4] studied one-bond-type migration of phosphorus-self-interstitial pairs in silicon. Because the first half of Fig. 1 of Yoshida *et al.*[4] shows the shortest migration process for substitutional P to migrate by one interatomic distance, this is shown in Fig. 3. The types of defects shown in Fig. 3 are listed in Table I, where the self-interstitial is denoted by I.

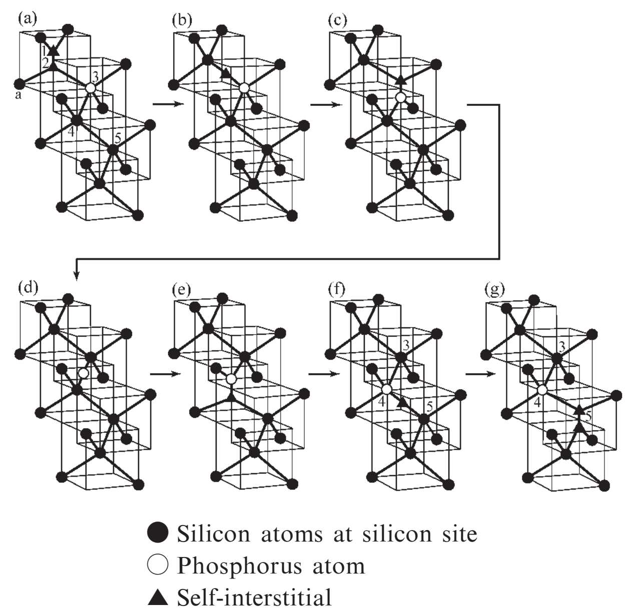

Fig. 3 . One-bond-type migration of the phosphorus-self-interstitial pair. (After Yoshida *et al.*[4])

Figure 3 (a) shows the arrangement of the SP configuration of two self-interstitials (I) and the substitutional P (sub P) before the diffusion of the phosphorus-self-interstitial pair. This is marked in Table I as "SP of 2I" and "sub P". In Fig. 3 (a), "SP of 2I" is located one interatomic distance

away from "sub P" in the opposite direction of the diffusion.

Figure 3 (b) shows the arrangement of the atoms just before the diffusion of the pair. By breaking the a-2 bond and forming a new bond, a-1, in Fig. 3 (a), or by one-bond-type migration, we have Fig. 3 (b), where the BC configuration of I is located 1/2 of an interatomic distance away from "sub P" in the direction opposite to the diffusion. This is marked in Table I as "BC of I" and "sub P".

In Fig. 3 (c) we have a SP configuration that consists of I and P. The distance between them is less than 1/2 of an interatomic distance.

Note that in Fig. 3 (d) only the "BC configuration of P" exists. There is no I in the migration of the phosphorus-self-interstitial pair.

In this way, SP and BC configurations repeat. This is a feature of one-bond-type migration. Through the repetition of one-bond-type migration from Fig. 3 (a) to Fig. 3 (g), the substitutional P migrates by one interatomic distance.

In the present work, the interstitialcy mechanism of diffusion of phosphorus-self-interstitial pairs on the basis of one-bond-type migration, that is, the repetition of SP and BC configurations, was studied theoretically using three dimensional schemata.

Table I. Types of defects shown in Fig. 3.
(Unit of distance between I and P: interatomic distance)

Number of Figure	Type of Defects	Distance between I and P
3 (a)	"SP of 2I" and "sub P"	1
3 (b)	"BC of I" and "sub P"	1/2
3 (c)	"SP of I and P"	$<1/2$
3 (d)	"BC of P"	only P, no I
3 (e)	"SP of P and I"	$<1/2$
3 (f)	"sub P" and "BC of I"	1/2
3 (g)	"sub P" and "SP of 2I"	1

As described already, Fahey *et al*.[2] reported, using two dimensional schemata, that the interstitialcy mechanism will operate only if the diffusing defect (AI pair) does not dissociate. Their report was most probably based on a study using two-bond-type migration, because BC configuration was not shown in their report.

We emphasize that, in the theoretical study of diffusion of phosphorus-self-interstitial pairs on the basis of one-bond-type migration using three dimensional schemata, we find only the "BC configuration of P" and no I as shown in Fig. 3 (d). This finding contrasts with that of Fahey *et al*.[2] and corresponds to "the self-interstitial (I) disappears" in the final part of the description in Fig. 2 (b). These are the comment on the work of Fahey *et al*.[2] based on Yoshida *et al*.[4]

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