Recombination-enhanced Fe atom jump between the first and the second neighbor site of Fe–acceptor pair in Si

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We studied the recombination-enhanced Fe atom jump between the first (1st) and second (2nd) neighbor sites of Fe–Al and Fe–B pairs in Si. We first annealed specimens at 80 °C to generate Fe–acceptor pairs after doping of Fe. Concentrations of the 1st and 2nd neighbor Fe–acceptor pairs were determined by electron-spin-resonance (ESR) measurement after annealing at around 150 K under optical excitation. The concentration of the 1st neighbor pair was decreased and that of the 2nd neighbor pair was increased by the above annealing. Activation energy for the above changes was about 0.11 eV in the case of the Fe–Al pair. This is much smaller than that (0.8 eV) of thermal annealing alone. In the case of the Fe–B pair, the ESR signal of the 2nd neighbor pair could be detected due to annealing at around 160 K under optical excitation. © *1996 American Institute of Physics.* [S0021-8979(96)04023-6]

I. INTRODUCTION

In this article we report a study of the recombination-enhanced Fe atom jump between the first (1st) and the second (2nd) neighbor sites of Fe–acceptor pairs in Si from the measurement of electron spin resonance (ESR), together with the activation energy of the process.

First, we briefly review the history of research on Fe–acceptor pairs in Si. Since Shepherd and Turner's work[1] on Fe and B atoms pairing, properties of Fe–acceptor pairs in Si have long been studied with various experimental techniques. Energy levels of Fe–acceptor pairs, for example, were determined by the deep level transient spectroscopy (DLTS) method.[2–7] Chantre and Bois[8] found two kinds of donor levels associated with Fe–Al pairs and clearly showed that they corresponded to the stable and metastable configurations of pairs. Kimerling and Benton[9] first showed that Fe in Fe–B pairs in Si showed recombination-enhanced dissociation below room temperature. According to them, Fe–B pairs were dissociated due to minority-carrier injection at temperatures low enough to prevent their thermal dissociation. Nakashima, Sadoh, and Tsurushima[10] studied the above process in a more detailed manner after illumination or injection of minority carriers; their measurement of thermally stimulated capacitance (TSCAP) indicated some new energy levels. They proposed that those energy levels corresponded to the 2nd and more distant neighbor pairs of Fe–B. No one, however, has found ESR signals of the 2nd and more distant neighbor Fe–B pairs in Si. The kinds of neighbors cannot be discriminated based on TSCAP alone.

In general, we can discriminate kinds of pairs and complexes from the measurement of their ESR spectra since we can determine their symmetries from these spectra. The ESR spectra of Fe–acceptor pairs have been extensively studied since Ludwig and Woodbury's pioneering work.[11] One of the important results in relation to our study is that two kinds of ESR signals were detected for each, with the exception of the Fe–B pairs. They were identified as corresponding to the 1st and 2nd neighbor Fe-acceptor pairs since they had trigonal and orthorhombic symmetry.[12] Gehlhoff, Irmscher, and Rehse[13] determined the relation between the two states and the symmetry of Fe–Al pairs from measurements of DLTS and ESR. Takahashi, Suezawa, and Sumino[14] determined the energy difference between the 1st and 2nd neighbor pairs of Fe–acceptor pairs, with the exception of the Fe–B pairs, from the measurement of ESR spectra and established the relation between the stable and metastable states found by the DLTS method and the symmetry of pairs found by the ESR method. Gehlhoff and co-workers[13] also measured the effect of illumination at low temperature and detected an increase of the ESR intensity of 2nd neighbor Fe–Al pairs. Theirs was probably the first study of the recombination-enhanced transformation of pairs by ESR measurement. Their study, however, seems insufficient to understand the recombination-enhanced process since they did not determine quantities which are characteristic of the above process, for example, the threshold energy of the process. (This point is discussed later in Sec. IV).

In what follows we describe our studies of the recombination-enhanced Fe atom jump from the 1st to 2nd neighbor of the acceptor atoms with the measurement of ESR which makes it possible to discriminate the kinds of neighbors. First, we describe the effect of optical excitation on the populations of the 1st and 2nd neighbor Fe–Al pairs since ESR signals of these pairs have previously been identified.[11–13] We then report studies of the Fe–B pair, where we observe for the first time the ESR signals of the 2nd neighbor pair.

II. EXPERIMENT

The crystals used in this experiment were grown by the floating-zone method. The concentration of B and Al was 2×10^{15} cm^{-3}. We cut out specimens from the above crystals in parallepiped shape, $3.5 \times 3.2 \times 3.2$ mm, the longest side of which was parallel to the [110] direction. We polished them
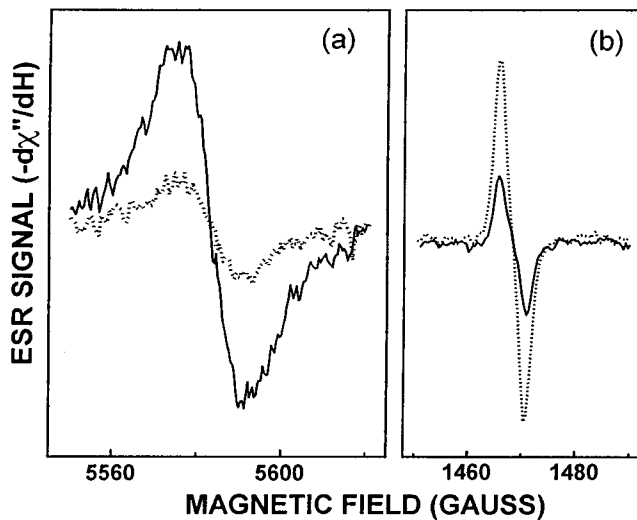
FIG. 1. ESR spectra of the (a) 1st and (b) 2nd neighbor pairs of Fe–Al before (solid lines) and after illumination (dashed lines) of 1.2 eV photons at 150 K. Static magnetic field was applied along the [110] direction. Spectra were measured at 10 K.

mechanically by carborundum and chemically by mixed acid, HNO_3:HF=5:1, at room temperature. We doped specimens with Fe with the vapor method; namely, we sealed specimens in evacuated quartz capsules together with pieces of high-purity Fe wire, annealed them at 1050 °C for 2 h, and then quenched them in iced water. We kept specimens in liquid nitrogen until measurement since Fe in Si is known to diffuse at room temperature. Fe–acceptor pairs were not detected just after quenching since such pairs could not be generated during quenching because of the too high cooling rate. We annealed specimens at 80 °C for 50 min to generate Fe–acceptor pairs. In the case of Fe–Al, we detected ESR signals of both the 1st and 2nd neighbor pairs after the above annealing. On the contrary, we detected only that of the 1st neighbor Fe–B pair after the above annealing. Both findings are in accordance with those of previous studies.[11,15] Annealing conditions were determined based on those of previous studies.[14,16]

We illuminated specimens at around 150 K in a continuous-flow-type liquid-helium cryostat. Thermal diffusion of the Fe atom is almost impossible at around 150 K without optical excitation. Lenses, a halogen lamp, and a grating monochromator were used for monochromatic light illumination. Spectral resolution was about 6 meV at 1.16 eV. We measured ESR in an X-band spectrometer at 10 K to determine concentrations of Fe–acceptor pairs at various neighbors with the use of the above cryostat.

III. RESULTS

A. Fe–Al pair

Figure 1 shows the ESR spectra of the 1st neighbor [Fig. 1(a)] and the 2nd neighbor [Fig. 1(b)] Fe–Al pairs before (solid line) and after (dotted line) illumination with 1.2 eV photons at 150 K for 30 min. As is clearly shown, the intensity of the 1st neighbor pair decreases and that of the 2nd neighbor pair simultaneously increases due to the illumina-
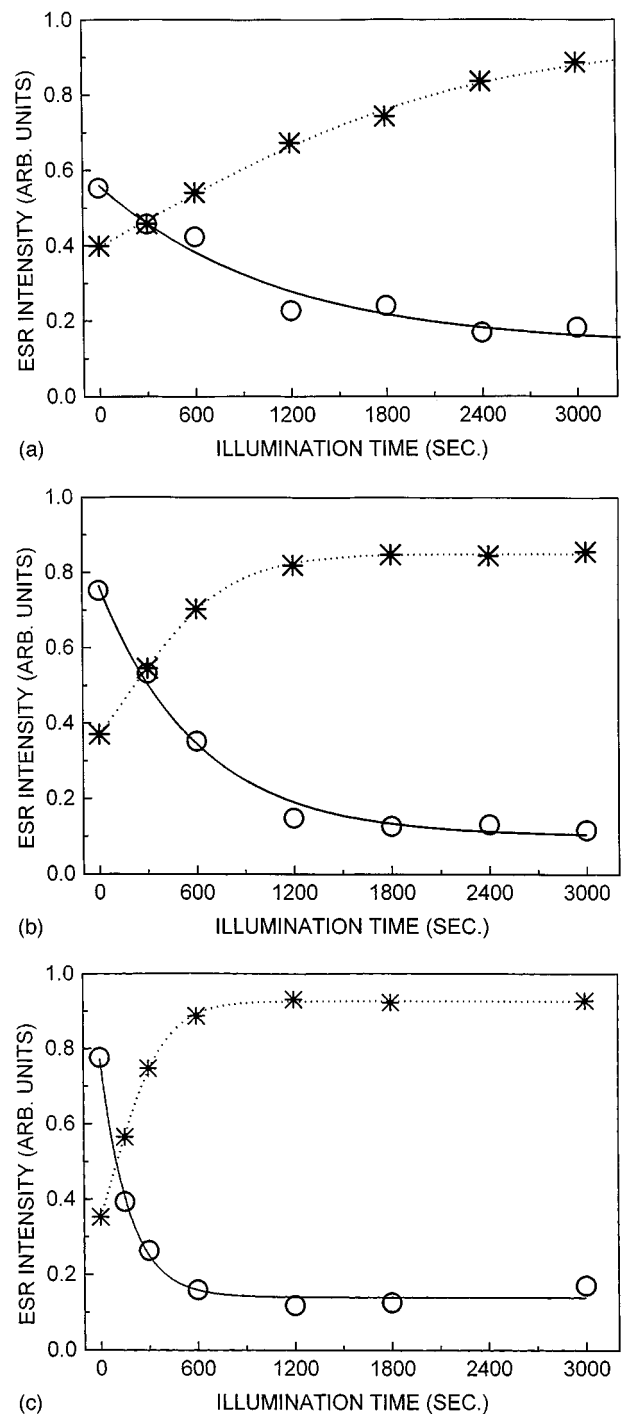

FIG. 2. The dependence of ESR intensities of the 1st and 2nd neighbor Fe–Al pairs on the illumination time at (a) 120 K, (b) 135 K, and (c) 150 K. The solid and dotted lines were the fitting curves with Eqs. (4) and (5), respectively.

tion of light. There may be a possibility that some preexisting 2nd neighbor Fe–Al pairs change to an ESR-active charge state due to illumination. The above changes were not observed when we illuminated specimens at 10 K. This means that the above changes are really caused by the change of site of Fe from the 1st to the 2nd neighbor site of Al since the electronic transition itself occurs even at low temperature. Gehlhoff and co-workers[13] studied the effect of
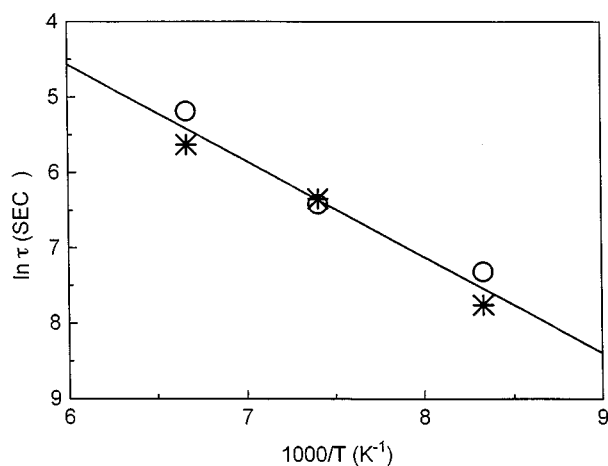
FIG. 3. Arrhenius plot of the rate constants for the forward (circle) and the backward (asterisk) reactions. The activation energy was determined to be about 0.11 eV.

FIG. 5. ESR spectra of the (1) 1st and the (2) 2nd neighbor pairs of Fe–B before (dotted line) and after illumination (solid line) of 1.2 eV photons at 160 K. Static magnetic field was applied along the [112] direction. Spectra were measured at 10 K.

illumination on the intensity of orthorhombic Fe–Al pairs. According to them, they observed an increase of ESR intensity of orthorhombic Fe–Al pairs due to illumination at 20 K. This was interpreted by them as due to the change of charge state of the above pair, not to the increase of concentration itself. However, they observed an increase of the above intensity which was twice that caused by illumination at 20 K when they cooled the specimens under illumination. Based on our experimental results, we interpreted their results that half of this effect was probably due to the increase of the concentration of orthorhombic Fe–Al pairs due to recombination enhanced motion of the Fe atom from the 1st to the 2nd neighbor site of Al.

Our result also suggests that the transformation from the 1st to the 2nd neighbor Fe–Al pair was thermally activated since we observed no such transformation at 10 K. In contrast with our results, Gehlhoff and co-workers[13] reported athermal recombination-enhanced conversion of pairs from the measurement of the effect of illumination on DLTS. Fig-

ure 2 shows the dependence of the effect of illumination on temperature. This saturates faster at higher temperatures. The solid and dotted lines are fitting curves deduced under the assumption that the decrease and the increase of the 1st and the 2nd neighbor pair, respectively, occurred with first-order reaction kinetics. From these fittings, we can determine the time constant for the decrease and increase of Fe–Al pairs.

Figure 3 shows the dependence of the time constant on temperature. The activation energy was determined to be about 0.11 eV.

We obtained the above results when we illuminated specimens with 1.2 eV light. In order to determine the threshold energy for the above phenomenon, we measured the dependence of intensity of 2nd neighbor pairs on the excitation energy. Figure 4 shows the result. The specimen was illuminated for 1 h at 150 K. As shown in Fig. 2(c), the effect of illumination was almost saturated after illumination for 1 h when the photon energy was larger than about 1.13 eV. It was approximately proportional to the illumination time when the photon energy was smaller than about 1.12 eV. Hence, the ESR intensity above 1.13 eV is not proportional to the optical cross section for the excitation. The threshold energy seems to be around 1.1 eV. Detailed analysis is shown in the following section.

B. Fe–B pair

We measured similar properties of Fe–B pairs. As shown in Sec. I, no one to date has reported an ESR signal of the 2nd neighbor Fe–B pair. Figure 5 shows the ESR spectra before (dotted line) and after (solid line) illumination of the specimen with 1.2 eV photons at 160 K for 1 h. The signal intensity of the 1st neighbor Fe–B pair decreased and new ESR signals appeared due to illumination. These signals are different from those observed after illumination by Gehlhoff and Rehse[17] and attributed to the negatively charged 1st neighbor Fe–B pair. We illuminated the specimen at 10 K with 1.2 eV photons, but did not detect these ESR signals. We therefore concluded that they were probably due to the 2nd neighbor Fe–B pair, not the negatively charged 1st neighbor pair. We determined the g tensor of the new ESR
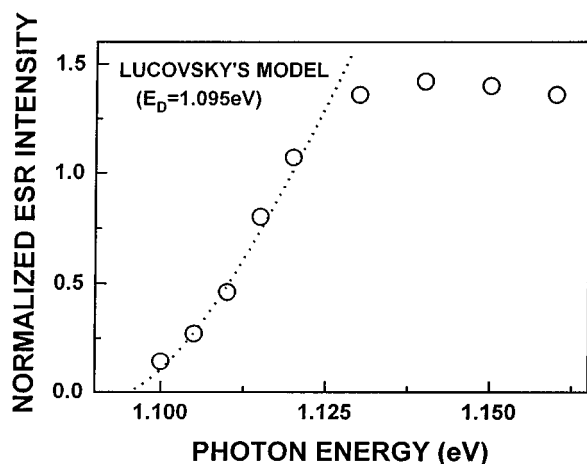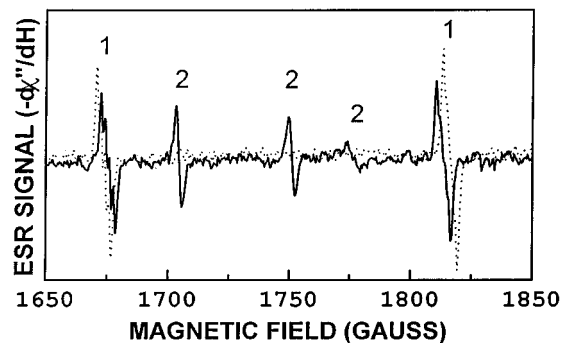

FIG. 4. Excitation energy dependence of the ESR intensity of the 2nd neighbor Fe–Al pairs. The specimen was illuminated by each photon energy for 1 h at 150 K. The dotted line is a fitting curve due to Lucovsky's model.

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TABLE I. Principal values (g_1 through g_3) of g tensors of Fe–acceptor pairs of orthorhombic symmetry. [The g values are those of orthorhombic I in the cases of Fe–Al, Fe–Ga, and Fe–In pairs (Ref. 11).]

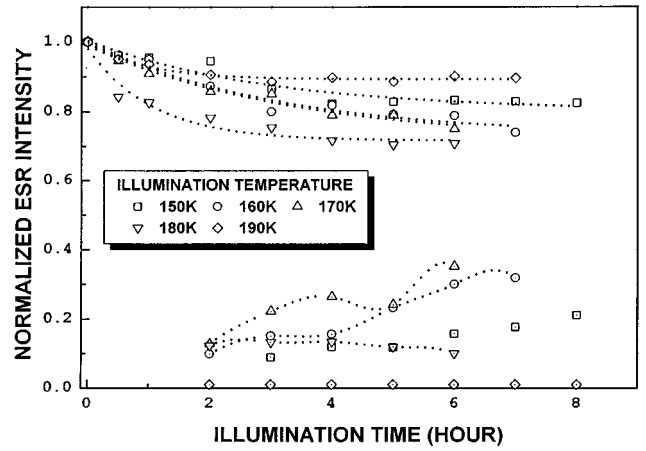|	g_1	g_2	g_3
Fe–B	4.448	2.094	2.232
Fe–Al	5.585	1.236	1.612
Fe–Ga	6.19	0.59	0.69
Fe–In	6.26	0.35	0.36

FIG. 6. The dependence of ESR intensities of the 1st and the 2nd neighbor Fe–B pairs on the illumination time at various temperatures. The ordinate was normalized with respect to the initial ESR intensity of the 1st neighbor Fe–B pairs.

signals. The g tensor had orthorhombic symmetry, confirming the above conclusion (details to be shown in a separate article). The g values are shown in Table I.

Figure 6 shows the dependence of the ESR signal intensity for each pair on the illumination time at various temperatures. Comparing Fig. 6 with Fig. 2, it was noticed that the magnitudes of change of the 1st and 2nd neighbor Fe–B pairs were much smaller than those of the Fe–Al pair.

IV. DISCUSSION

A. Fe–Al pair

The solid and dotted lines in Fig. 2 were deduced under the assumption that transformation between the 1st and 2nd neighbor pairs alone occurred under illumination at low temperature. This assumption is based on the experimental results that we did not observe any other kinds of ESR signals due to, for example, isolated Fe atoms, after illumination at around 120 K. Under this assumption, the following relation holds.

$$P_1 \overset{K_{-1}}{\underset{K_1}{\Leftrightarrow}} P_2. \tag{1}$$

Here P_1 and P_2 mean the 1st and 2nd neighbor pairs. Then we can deduce the following equations for the time dependence of their concentrations:

$$\frac{d[P_1]}{dt} = K_1[P_2] - K_{-1}[P_1], \tag{2}$$

$$\frac{d[P_2]}{dt} = -K_1[P_2] + K_{-1}[P_1]. \tag{3}$$

Here $[P_1]$ and $[P_2]$ are the concentrations of the 1st and the 2nd neighbor pairs. These equations can be solved analytically as follows:

$$[P_1] = \frac{K_1}{K_1 + K_{-1}}\{[P_1(0)] + [P_2(0)]\}$$
$$- \frac{K_1[P_2(0)] - K_{-1}[P_1(0)]}{K_1 + K_{-1}} \exp[-(K_1 + K_{-1})t], \tag{4}$$

$$[P_2] = \frac{K_{-1}}{K_1 + K_{-1}}\{[P_1(0)] + [P_2(0)]\}$$
$$+ \frac{K_1[P_2(0)] - K_{-1}[P_1(0)]}{K_1 + K_{-1}} \exp[-(K_1 + K_{-1})t]. \tag{5}$$

The ratio $[P1]/[P2]$ at $t = \infty$ is equal to K_1/K_{-1}. This ratio is almost independent of temperature in our experiment as can be seen from Fig. 2. Hence we can consider the same activation energy to exist for K_1 and K_{-1}. The activation energy determined by Fig. 3 is, therefore, the activation energy for the jump of Fe between the 1st and 2nd neighbor sites under illumination. This activation energy (0.11 eV) is much smaller compared with those (0.82 and 0.75 eV for the jump from the 1st to 2nd neighbors and the reverse,[14] respectively) without illumination. We conclude that the recombination-enhanced transformation between the 1st and 2nd neighbor Fe–Al pairs occurred, namely, energy (0.71 and 0.64 eV) was supplied from the released energy associated with recombination of an electron and a hole at Fe–Al pairs. The difference of released energy for the 1st and 2nd neighbor pairs is probably due to the difference of energy levels of these pairs as is discussed later.

From simple geometrical considerations, we would expect the probability for a jump of the Fe atom from the 1st to the fourth (4th) neighbor of Al to be 1/3 that of the jump from the 1st to the 2nd neighbor; however we did not detect a strong ESR signal, namely, 1/3 that of the 2nd neighbor, which might correspond to the 4th neighbor Fe–Al pair. We do not know the reason for the above result, namely, whether it was due to the ESR-inactive nature of the 4th neighbor Fe–Al pair or to inapplicability of simple geometrical considerations. Another geometrical consideration gives the ratio of the pre-exponential factor of K_1 and K_{-1} to be 1/4 ($= K_1/K_{-1}$). It was about 1/7 in our experiment. We have not succeeded in explaining the origin of this discrepancy.

To determine the defect level responsible for the recombination, we consider the optical excitation process. Figure 4 shows no sharp peaks. This suggests that the optical transition responsible for the enhanced jump of the Fe atoms is between a band and a localized level. Hence, we analyzed the result of Fig. 4 with the use of the Lucovsky's model[18] which is a simple model applicable to the optical transition

between a localized state and a band. According to this model, the optical cross section for the transition is given as follows:

$$\sigma = \sigma_0 \left(\frac{4E_D(h\nu - E_D)}{(h\nu)^2} \right)^{\frac{3}{2}}. \quad (6)$$

Here σ is the optical cross section, σ_0 the maximum of the cross section, E_D the threshold energy which corresponds to the difference between a localized level and the band edge, and $h\nu$ the photon energy. Fitting this equation to Fig. 4 (dashed line), we obtained $E_D = 1.095$ eV. There is a discrepancy between the experimental results and the fitting curve at high energy in Fig. 4. This is probably due to the saturation of illumination effect at near band-gap energy as shown in Fig. 2(c). We interpret this threshold energy to be the difference between the Al level and the edge of the conduction band. Al is ionized at around 150 K. Electrons captured at these energy levels are excited by the incident photons. Then electrons excited in the conduction band are captured by the acceptor level of the 1st neighbor and the 2nd neighbor Fe–Al pairs, energy levels of which are about $E_c - 0.29$ eV and $E_c - 0.43$ eV, respectively, where E_c is the edge of the conduction band.[10] Finally, holes in the valence band recombine with electrons captured at the above acceptor levels. The greatest part of the recombination energy is probably emitted as multiphonon energy, nonradiative energy, and is consumed for the jump of Fe atoms.

B. Fe–B pair

In the case of Fe–B pairs, we found ESR signals due to the 2nd neighbor pair. We identified them to be due to the 2nd neighbor pair from the determination of the g tensor. The principal values of the g tensor of the Fe–B pairs together with those of other Fe–acceptor pairs are shown in Table I. As the atomic number of acceptor atom increases, the anisotropy of the g tensor [this g tensor corresponds to the g' tensor determined from the assumption that spin is 1/2 (Ref. 19)] also increases. The anisotropy of the g tensor is mainly due to the ratio of orthorhombic and axial fine structure parameters according to Gehlhoff et al.[19] We, however, cannot explain the dependencies of those parameters on the species of acceptors in an intuitive manner.

We cannot determine the activation energy for the transformation from the 1st to 2nd neighbor Fe–B pairs because of large data scatter, i.e., small change, and also because of nonmonotonic temperature dependence, namely, the illumination effect at 190 K is smaller than that at 180 K. The activation energy is apparently almost zero, but it should be positive since we did not observe such behavior in Fig. 6 when we illuminated specimens at 10 K. This means that no recombination-enhanced motion of Fe atoms occurred at 10 K.

C. Comparison of Fe–Al pairs and Fe–B pairs

In comparing Fig. 6 with Fig. 2, we notice that changes of the intensities of the 1st and 2nd neighbor Fe–B pairs are much smaller than those of the Fe–Al pairs. There seem to be two ways to interpret this difference. One is the difference

of optical cross sections for the Fe–Al and Fe–B pairs, and the other is the difference of the stability of the 2nd neighbor pairs relative to the 1st neighbor pairs of Fe–Al and Fe–B. We first discuss the former case. As already shown, we interpreted the optical excitation as that of an electron from the Al level to the conduction band. This is probably the case with B, too. Since the energy levels of B (45 meV) and Al (57 meV) are similar, the extensions of wave functions of electrons trapped by Al and B are also similar; hence, we expect similar optical cross sections for Al and B. We therefore conclude that the former is not the case.

Next, we discuss the latter case. According to Eqs. (4) and (5), $[P_1]/[P_2]$ at $t = \infty$ is proportional to K_1/K_{-1}. Hence, the above experimental results suggest that the magnitude of K_1/K_{-1} of the Fe–B pairs is much larger than that of the Fe–Al pairs. If we assume only the recombination-enhanced jump of the Fe atom from the 1st neighbor pair to the 2nd neighbor pair and vice versa, the ratio K_1/K_{-1} of the Fe–B pair is probably similar to that of the Fe–Al pair. One way to interpret the above result is as follows, under the assumption that the energy barrier from the 2nd to the 1st neighbor jump of the Fe atom in the Fe–B pair is very small even without illumination, an assumption discussed later. From this assumption, K_1 has two components, one from the recombination-enhanced term and the other from the thermal term, the latter being independent of the excitation. Hence, the total K_1 becomes larger than that of the recombination-enhanced term alone. One fact supporting this explanation is that the effect of illumination is smaller at 190 K than at 180 K in the case of Fe–B pairs. Such a phenomenon is expected to occur if the activation energy for the 2nd to 1st neighbor jump due to thermal motion alone is slightly greater than that of the recombination-enhanced jump. Under the above assumption, we consider that the above phenomenon can be explained since the magnitude of the pre-exponential factor for thermal motion alone is usually much larger than that of the recombination-enhanced one, as shown by Kimerling and Benton.[9]

Next, we discuss the difference in relative stability of the 2nd neighbor pair between Fe–Al and Fe–B pairs. As pointed out above, the barrier for the transformation of the Fe–B pair from the 2nd to 1st neighbor seems to be smaller than that of the Fe–Al pair. As described in Sec. I, no one has reported an ESR signal due to the 2nd neighbor Fe–B pair. This suggests that energies of the 1st and 2nd neighbor pairs are different from Fe–Al and Fe–B pairs. One support for this is shown in Fig. 7. The vertical axis of Fig. 7 is the energy difference between the 1st and 2nd neighbor configurations determined by Takahashi and co-workers[14] by the ESR method. These values are similar to those reported by Chantre and Bois[8] who determined them by the DLTS method assuming the 1st and 2nd neighbor configurations. The abscissa is the covalent radius.[20] Extrapolation from the relation of reported values to boron yields energy of about 0.5 eV, which is a much larger difference compared with those of the other pairs. There are two ways to interpret this result. One is that the binding energy of the 1st neighbor Fe–B pair is much larger than those of other Fe-acceptor pairs but with similar binding energy for the 2nd neighbor
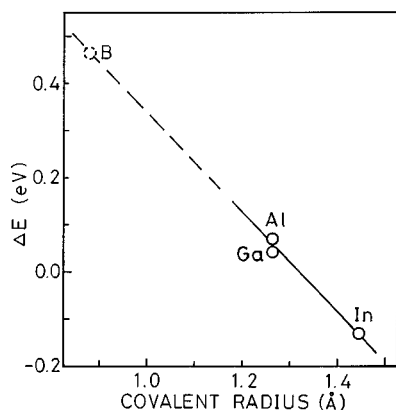
FIG. 7. The dependence of the binding-energy difference (ΔE) of the 1st and 2nd neighbor Fe–acceptor pairs on the covalent radius of acceptor atoms.

<mark>pair. Hence, the population of the 2nd neighbor Fe–B pair is always very small. Another is that the binding energy of the 2nd neighbor Fe–B pair is much smaller than those of other Fe–acceptor pairs but similar to that for the 1st neighbor pair.</mark> The first case is supported by Chantre and Bois[8] and Nakashima and co-workers.[10] Their results show a similar energy barrier from the 2nd to the 1st neighbor pairs for Fe–Al and Fe–B. Both were measured with the capacitance method. On the other hand, the temperature ranges for the dissociation of all Fe group-III acceptors are very similar to each other, namely, the binding energies of the 1st neighbor pair seem to be similar when pair dissociations are studied with the measurement of ESR for the determination of pair concentration.[14,16] In conclusion we have not yet succeeded in explaining the difference between Fe–Al and Fe–B pairs.

V. CONCLUSION

We have studied the recombination-enhanced Fe atom jump associated with Fe–Al and Fe–B pairs under optical excitation based on the measurement of their ESR signals. In the case of the Fe–Al pair, both the jumps from the 1st to 2nd neighbor and vice versa are enhanced by recombination.

The thermal activation energy is about 0.11 eV for both jumps which is much smaller than those (0.82 and 0.75 eV) without optical excitation. We have interpreted the optical excitation as arising from ionized Al to the conduction band. We have proposed that the recombination of electrons at Fe–Al pairs and holes in the valence band induce a recombination-enhanced jump of the Fe atom.

In the case of the Fe–B pair, we have found the ESR signal of the 2nd neighbor pair. It has orthorhombic symmetry. The changes of populations of the 1st and 2nd neighbor Fe–B pairs are smaller than those of Fe–Al pairs under optical excitation. We have not been able to determine the thermal activation energy under optical excitation for the Fe–B pair since the temperature dependence was nonmonotonical.

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