Deep-level transient spectroscopy and photoluminescence measurements of dissociation energy of the 1.014-eV copper center in copper-diffused silicon crystal

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Dissociation of the 1.014-eV copper center by annealing in a silicon crystal diffused with dilute copper was measured by deep-level transient spectroscopy (DLTS) and photoluminescence (PL) methods. Clearly different dissociation energies were obtained from the dissociation lifetimes of the center measured by the two methods: 1.01 eV by DLTS and 0.60 eV by PL. On the basis of the previously reported analysis that the precipitation of interstitial copper (Cu_i) at the surface and the subsequent out-diffusion of Cu_i in the bulk are the underlying processes to dissociate the center by annealing, we assumed that the difference in the aforementioned dissociation energies originates from the difference in the influence of the underlying processes at different depths in addition to the difference in the detection depths of both methods (PL: ≥ 30 μm and DLTS: ≈ 3 μm). Using the dissociation energies obtained in this study, together with the reported diffusion barrier of Cu_i, we estimated the binding energy of the center as lower than 0.42 eV and the precipitation barrier of Cu_i as higher than 0.41 eV. This binding energy is low enough to support the presence of weak bonding in the copper center reported in previous researches. © *2012 American Institute of Physics.* [http://dx.doi.org/10.1063/1.3699366]

I. INTRODUCTION

Because of the detrimental effect of copper contamination on silicon devices,[1–3] the behavior of copper in silicon crystals has long been investigated. Measurements using sensitive and species-discriminating probes, such as deep-level transient spectroscopy (DLTS) and photoluminescence (PL), are indispensable for assessing copper contamination. In p-type silicon crystals diffused with copper at various temperatures, two well-known copper centers have been generally observed by DLTS measurements:[4,5] one characterized by an energy level of $E_v + 0.07$ eV (E_v: top energy of the valence band) and another characterized by two energy levels of $E_v + 0.21$ and $E_v + 0.42$ eV. Hereafter, in accordance with the classification by Brotherton *et al.*,[5] the former center is tentatively denoted as the Cu_{DLB} *center* and the latter as the Cu_{DLA} *center*. It has been determined that the Cu_{DLB} center is the same species as the 1.014-eV PL center[6,7] (Cu_{PL} center) and that it contains four copper atoms.[8] It has recently been shown that the Cu_{DLA} center is the dissociation product of the Cu_{DLB} center.[9] However, there is little consensus as to the structures[10,11] or bonding properties of both centers. The argument presented by Istratov *et al.*[12] that the Cu_{DLB} center has strong bonding on the basis of the dissociation energy of the center (1.02 eV measured by DLTS), is inconsistent with the presence of weak bonding in the center observed by Weber *et al.* using PL.[13] On the other hand, there is another inconsistency in the dissociation energy of the Cu_{DLB} center measured by several authors, that is, Minaev *et al.* reported 0.6 eV (observed by PL, Ref. 14), Nakamura and Iwasaki

reported 0.63 eV (observed by PL, Ref. 15), and Ramappa reported 0.42 eV (observed by surface-photovoltage (SPV) measurement[16]). Lemke and Irmscher estimated the binding energy of the center to be 1.15 eV from an analysis of the Cu_{DLA} center formation by DLTS.[17] The above-mentioned dissociation energies or binding energy determined by an electrical method (i.e., DLTS) seem to be significantly larger than those determined by optical methods (i.e., PL and SPV). However, since the above-mentioned dissociation energies were measured by different authors using different samples, it is questionable whether the values obtained by either method are appropriate for the dissociation energy. In other words, to clarify the bonding property of the center, it is necessary to measure the dissociation energy of the Cu_{DLB} center by using the same sample with different methods.

In this study, both the DLTS and PL methods were used to measure the dissociation energy of the Cu_{DLB} center. Clearly different dissociation energies of the center were obtained by the two methods. Assuming that this difference originates from the combination of the difference in the influence of the underlying processes to dissociate the center at different depths with the different detection depths of the measurement methods, we estimated a low value (< 0.42 eV) for the binding energy of the Cu_{DLB} center, which is consistent with the presence of the weak bonding in the center.

II. EXPERIMENT

The preparation method of the samples was identical to that described previously.[9,11] The original samples were 100-mm-diameter, 1.0-mm-thick (100) float-zone-grown silicon wafers doped with $8.5 \pm 1.0 \times 10^{14}$ cm^{-3} of boron (p-type) and mirror-polished on both sides. The wafers were contaminated

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with copper by immersing them in an aqueous solution containing 1 ppm by weight of copper. The contamination level of copper was estimated to be about 6×10^{13} cm^{-2}.[18] The copper-contaminated wafers were diffused at 700 °C for 30 min in a quartz furnace under flowing clean, dry nitrogen gas. Then they were rapidly cooled to room temperature by dropping them into a bath of clean pumping oil located under the furnace. After rinsing the wafers with organic solvent and de-ionized water, they were cut into many small plates (8×20 mm^2). The selected samples (i.e., plates) were annealed at temperatures from 175 to 300 °C for periods from 2 min to 4 h (8 h for special samples) in a quartz furnace under flowing clean, dry nitrogen gas. Then they were rapidly cooled to room temperature by dropping them into a bath of clean water located under the furnace.

First, PL measurements on all the selected samples were carried out using a standard luminescence setup, in which the samples were kept at a constant temperature (4.2 K) in a liquid-helium-cooled cryostat. The luminescence was detected using a liquid-nitrogen-cooled Ge photodiode, and a conventional lock-in amplifier processed the signal. After rinsing the samples with 0.5% HF aqueous solution, 1-mm-diameter, 100-nm-thick Ti Schottky barrier electrodes were formed for DLTS measurements by evaporation on the same samples as used for the PL measurement. A 1-μm-thick Al metal layer was deposited on each Ti electrode by evaporation. An ohmic contact was obtained by rubbing Ga-In alloy on the reverse side of the electrode surface of the sample. Before performing DLTS measurements, capacitance-voltage (C-V) measurements were always carried out. The DLTS measurements were performed using a commercially available spectrometer. Lock-in frequency and pulse width were 244 Hz and 20 μs, respectively, as described previously.[9,11] The bias voltage was -5.0 V, and the pulse voltage determined from the bias voltage was $+ 4.0$ V. The concentrations of the centers measured by DLTS were always calibrated with the dopant concentrations measured by the C-V method.

III. RESULTS

A. Change in DLTS and PL intensities with annealing time

The dopant (hole) concentrations in the copper-diffused samples measured by the C-V method were within the scatterings of those of the original (uncontaminated) samples; no appreciable change of the concentration (or resistivity) was observed by the diffusion of Cu. Changes in a typical DLTS spectrum with annealing time for the samples annealed at 200 °C are shown in Fig. 1. Before annealing [Fig. 1(a)], a dominant peak attributed to the Cu$_{DLB}$ center is observed at 50 K [labeled H(50) in the figure]. The average concentration of the Cu$_{DLB}$ center calibrated with the dopant concentrations in the samples before annealing was 1.2×10^{13} cm^{-3}. The two small peaks observed at 125 and 260 K were probably hydrogen-related.[19] After annealing for a considerable time [Fig. 1(c)], new peaks attributed to the Cu$_{DLA}$ center appeared at 110 [H(110)] and 245 K [H(245)] at the cost of the intensity of H(50). With increasing annealing time, the Cu$_{DLB}$-center peak further decreased, and the Cu$_{DLA}$-center peaks gradually
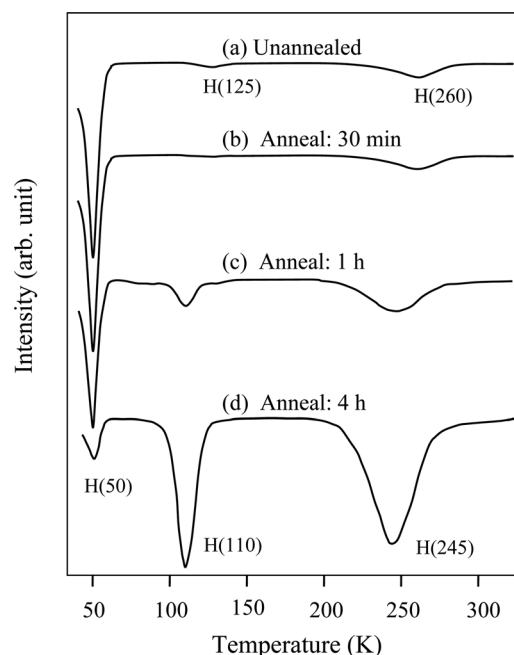

FIG. 1. Change in DLTS spectrum with annealing time for samples annealed at 200 °C. Times indicated are annealing times.

increased. These trends were fundamentally the same for all the samples annealed at temperatures higher than 200 °C. When the annealing temperature was 175 °C, the Cu$_{DLA}$ center did not appear by annealing the sample up to 8 h.

Changes in the concentration ratios of the Cu$_{DLB}$ and Cu$_{DLA}$ centers, normalized by the concentration of the Cu$_{DLB}$ center of the unannealed sample [Fig. 1(a)], with annealing time for the samples annealed at 200 °C are shown in Fig. 2(a). The concentration of the peak H(110) is used as the candidate concentration of the Cu$_{DLA}$ center. The annealing-time dependence of the PL intensity ratio of the 1.014-eV peak of the Cu$_{PL}$ center (i.e., the Cu$_{DLB}$ center), normalized by the initial value before annealing, for the same samples used for the DLTS measurements [Fig. 2(a)] is shown in Fig. 2(b). The annealing-time profile of the concentration ratio
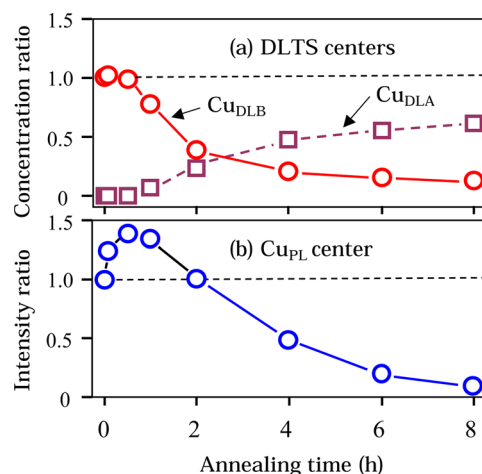

FIG. 2. (a) Changes in concentration ratios of the Cu$_{DLB}$ and Cu$_{DLA}$ centers with annealing time, and (b) change in PL intensity ratio of the Cu$_{PL}$ center with annealing time.

of the Cu_{DLB} center [Fig. 2(a)] is rather different from that of the PL intensity ratio of the Cu_{PL} center [Fig. 2(b)].

The dependencies of the PL intensity ratios on the annealing-time of the Cu_{PL} center, normalized by the average intensity of the respective samples before annealing, at four annealing temperatures are shown in Fig. 3. It is confirmed that these annealing-time dependencies of the intensity are fundamentally the same as those shown in Ref. 15. The annealing-time dependencies of the concentration ratios of the same center measured by DLTS are shown in Fig. 4. A comparison of Figs. 3 and 4 shows that the annealing-time profiles of each ratio at each temperature are rather different. However, we can see that each profile of the DLTS concentration ratio in the short-time region is composed of two components namely, an increasing component and a decreasing component as well as the PL intensity ratio.[15] Under the assumption that the increasing component arises from the transformation of the preceding species (Cu_{PRE}: the intermediate species between the Cu_{DLA} and Cu_{DLB} centers[9,11]) with time constant τ_1 and that the decreasing component arises from the dissociation of the Cu_{DLB} center with time constant τ_2, these time constants can be obtained by fitting the concentration curves shown in Figs. 3 and 4 in the same manner as the analysis of the previous PL data.[15] The change of the concentration of the Cu_{DLB} center with annealing time t is given as[15]

$$
\begin{aligned}
[Cu_{DLB}] =& \{[Cu_{DLB}]_{t=0} + [Cu_{PRE}]_{t=0} \\
& \times \tau_2/(\tau_2 - \tau_1)\}\exp(-t/\tau_2) \\
& - \{[Cu_{PRE}]_{t=0} \times \tau_2/(\tau_2 - \tau_1)\}\exp(-t/\tau_1),
\end{aligned} \tag{1}
$$

in which square brackets denote concentrations. Both τ_1 and τ_2 were estimated by fitting each curve within a short annealing time, as shown by the dashed lines in Figs. 3 and 4. While the PL data for a long annealing time are closely fitted, the fitting curves of the DLTS data considerably deviate after a long annealing time. The reason of this deviation will be discussed in Sec. IV C.
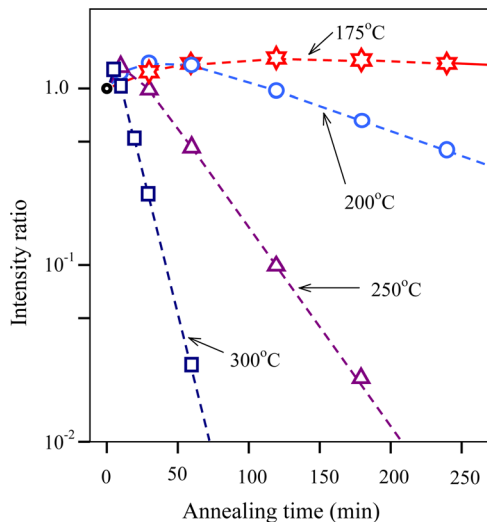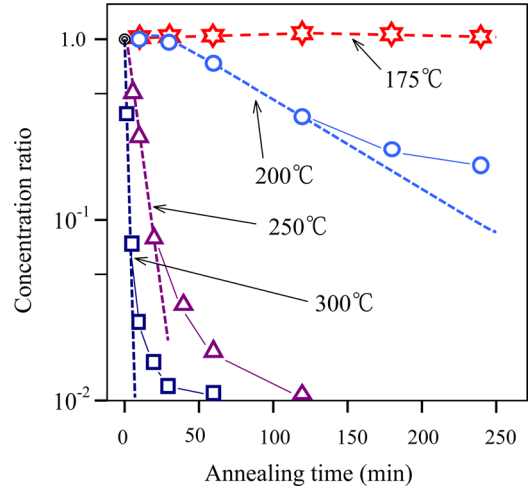

FIG. 4. Change in concentration ratio of the Cu_{DLB} center with annealing time. Temperatures indicated are annealing temperatures. Dashed lines show the best-fit curves of Eq. (1).

B. Dissociation energies of the copper center

Arrhenius plots of the best-fit values of τ_2 obtained from the PL and DLTS measurements are shown in Fig. 5. For the sake of simplicity, τ_1 values are not plotted. The τ_2 values reported by Istratov et al.[12] are plotted by a dotted line. The dissociation energy obtained from the PL data is 0.60 ± 0.03 eV, which is consistent with the energy range ($0.42-0.63$ eV) previously obtained by the optical methods.[14–16] The dissociation energy obtained from our DLTS data, shown by the broken line between 200 and 300 °C, is 1.01 ± 0.03 eV. This dissociation energy agrees well with the value reported by Istratov et al. (1.02 eV, Ref. 12), although the reaction temperatures are rather different. The extrapolated values of τ_2 of our data are two orders higher than theirs at respective temperatures. It is noted that the τ_2 values reported by Istratov et al.[12] were obtained by successive annealing of the samples attached with Schottky electrodes formed before annealing. The high-speed dissociation of the center at low temperatures shown by their data suggests the occurrence of a special action (or actions) of

FIG. 3. Change in PL intensity ratio of the 1.014-eV peak of the Cu_{PL} center with annealing time. Temperatures indicated are annealing temperatures. Dashed lines show the best-fit curves of Eq. (1).
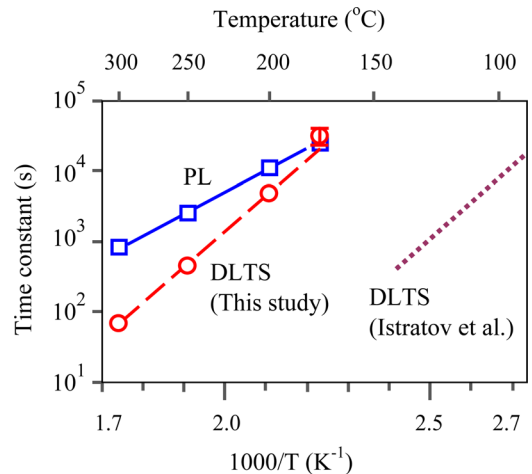

FIG. 5. Arrhenius plots of τ_2 values obtained from DLTS and PL data with annealing temperature. Dotted line shows τ_2 values reported by Istratov et al. (Ref. 12).

constituent ions in the space-charge layer produced by the Schottky electrode. A detailed examination of the transformation reactions of copper centers in the space-charge layer is under way. In summary, clearly different dissociation energies of the Cu_{DLB} center were obtained by PL and DLTS data measured using the same samples. This difference in the dissociation energies is considered to originate from the combination of the difference in the dissociation progressions of the center at different depths observed previously[20] with the different detection depths in the measurement methods discussed in the following section (Sec. IV A).

IV. DISCUSSION

A. Detection depths in DLTS and PL measurements

It is important to discuss the detection depths in DLTS and PL measurements to explain the difference in the dissociation energies obtained in this study. Since we always observe the concentrations of centers in the space-charge layer of the Schottky diode in the DLTS measurement, the detection depth in the DLTS measurement is defined as the width of the space-charge layer,[21]

$$W = [2\varepsilon_s/qN_A(V_{bi} - V - k_BT/q)]^{1/2}, \qquad (2)$$

in which ε_s is the dielectric constant of silicon, q is the electron charge, N_A is an acceptor concentration in silicon, V_{bi} is the built-in voltage formed by the Schottky electrode, V is an applied bias voltage, k_B is the Boltzmann constant, and T is absolute temperature. Since the built-in voltages were located between 0.5 and 0.8 V observed by the C-V method, and the boron concentration is $8.5 \pm 1.0 \times 10^{14}$ cm^{-3} employed in this study, the widths of the space-charge layer at the bias voltage of -5.0 V are estimated to be confined between 2.7 and 3.2 μm. Accordingly, the average detection depth in the DLTS measurement in this study is defined as 3.0 μm.

It is useful to show the relationship between the PL intensity from a doped PL source and the doping depth of the source to evaluate the detection depth in the PL measurement. When a PL source is homogeneously doped to a certain depth from the surface in a thick crystal, the observed PL intensity is roughly given by the function of the doping depth and concentration of the source, as reported previously.[22] We calculated the PL intensity from the sample doped with boron and cooled at 4.2 K, using the same constants (capture cross section, diffusion constant and thermal velocity of free exciton) as reported in Ref. 22. The change of PL intensity of the transverse optical phonon replica of boron-bound-exciton recombination (B_{TO}) (Ref. 22) with doping depth of boron is shown in Fig. 6 in the case when boron concentration is 8.5×10^{14} cm^{-3}, in which the intensity is normalized by that of an infinite crystal homogeneously doped with the same concentration of boron. It is seen from Fig. 6 that only about 20% of the PL intensity is emitted from the region shallower than 3 μm, however, almost 100% of the intensity is emitted from the region within the depth about 100 μm. Allowing the margin of 10% in the estimation of the PL intensity, the least detection depth is
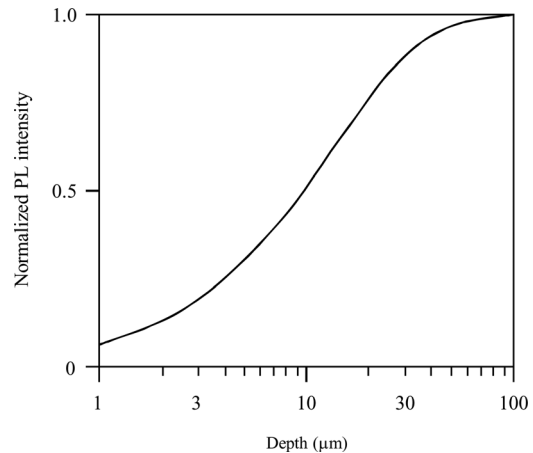

FIG. 6. Change in normalized PL intensity due to boron-bound-exciton recombination with doping depth of boron.

defined as the minimum depth which gives more than 90% of the normalized PL intensity shown in Fig. 6, that is, the detection depth in the PL measurement in the present study is estimated to be larger than 30 μm. Since the concentration of the Cu_{PL} center is more than one order lower than that of boron (see Sec. III A), the depth variation of the intensity from the center is considered to show the same relationship as that shown in Fig. 6, when the concentration of the center is homogeneously distributed through the depth. In the summary of this section, it is concluded that the detection depth of PL is far larger than that of DLTS.

B. Analysis of dissociation energies of the Cu_{DLB} center

It was previously demonstrated that the Cu_{DLB} center dissociates to the Cu_{DLA} center by releasing three interstitial copper (Cu_i) atoms as

$$Cu_{DLB} \rightarrow Cu_{DLA} + 3Cu_i, \qquad (3)$$

in which the Cu_{DLA} center is a single copper atom bonded at a special site, probably the center of the Si-Si bond (BC site).[9,11] It is clear that the dissociation of the center is promoted by the removal of Cu_i around the Cu_{DLB} center. It was observed in a previous study that the dissociation reaction of the Cu_{DLB} center starts at the surface and progresses into the bulk of the sample.[20] From this observation it was analyzed that the precipitation of Cu_i at the surface and the subsequent out-diffusion of Cu_i in the bulk are the underlying processes that dissociate the center by annealing. The energy diagram of Cu_i concerning the present system is shown in Fig. 7. The dissociation energy of the center is, in principle, expressed in terms of the binding energy of the center (E_b), the diffusion barrier of Cu_i (E_d), and the precipitation barrier of Cu_i (E_p). Although the dissociation of all the centers is initiated by the precipitation of Cu_i at the surface, the influence of the precipitation on the dissociation becomes weaker with increasing depth from the surface. Under the assumption that the Cu_{DLB} center residing far remote from the surface in the bulk dissociates by the assistance of the diffusion of Cu_i, the dissociation lifetime of the center is expressed like that
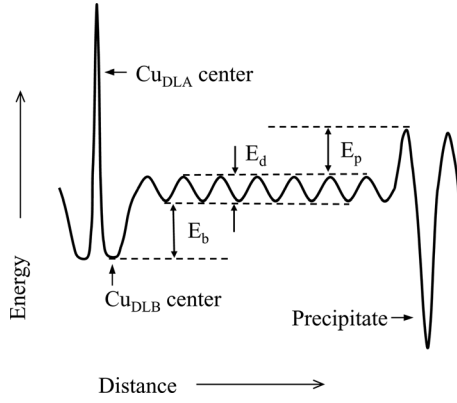
FIG. 7. Energy diagram of Cu_i. E_b, E_d, and E_p indicate the binding energy of the Cu_{DLB} center, the diffusion barrier of Cu_i, and the precipitation barrier of Cu_i, respectively.

of an ion pair of dopants[23] or a hydrogen-dopant complex[24] in the bulk of silicon. The dissociation lifetime (τ_d) of the hydrogen-dopant complex reported by Zhu et al.[25] is

$$\tau_d = (\Omega_0 f/4\pi DR_C)\exp(E_b/k_BT), \qquad (4)$$

where Ω_0 is the primitive-cell volume (two silicon atoms), f is a quantity of order unity involving the number of sites per primitive cell for the related species (hydrogen, dopant, and their complex) and the associated vibrational partition functions,[24] D is the diffusion coefficient of hydrogen, R_C is the capture radius, E_b is the binding energy of the complex, k_B is the Boltzmann constant, and T is absolute temperature. The actual value of R_C in the hydrogen-dopant case is estimated to be in the range of 4–5 nm.[26] When the hydrogen, dopant, and hydrogen-dopant complex are replaced by Cu_i, the Cu_{DLA} center, and the Cu_{DLB} center, respectively, and the factors $\Omega_0 f/4\pi$, D, and R_C are modified to suit the present system, the dissociation lifetime $\tau_{2,b}$ of the Cu_{DLB} center residing far remote from the surface in the bulk is expressed as

$$\tau_{2,b} = (A/D_{Cu}R_D)\exp(E_b/k_BT), \qquad (5)$$

in which A, D_{Cu}, and R_D are the quantity $\Omega_0 f/4\pi$ of the present system, the diffusion coefficient of Cu_i, and the capture radius of the Cu_{DLB} center, respectively. Since the diffusion coefficient can be described as $D_{Cu} = D_{Cu,0} \exp(-E_d/k_BT)$ [$D_{Cu,0}$: constant pre-exponential factor], Eq. (5) is expressed as

$$\tau_{2,b} = (A/D_{Cu,0}R_D)\exp[(E_b + E_d)/k_BT]. \qquad (6)$$

When R_D is assumed to be independent of temperature, the dissociation energy of the center residing far remote from the surface is given by $E_b + E_d$.

When the Cu_{DLB} center resides strictly under the surface, the dissociation lifetime $\tau_{2,s}$ of the center is formally expressed, including the influence of the precipitation of Cu_i, as

$$\tau_{2,s} = (A/D_{Cu,0}R_D')\exp[(E_b + E_d + E_p)/k_BT], \qquad (7)$$

in which R_D' indicates the effective capture radius. When R_D' is assumed to be independent of temperature, the dissociation energy of the center residing strictly under the surface

is given by $E_b + E_d + E_p$. The dissociation lifetime of the center residing in an intermediate region may be, in principle, given by an intermediate formula between Eqs. (6) and (7), however, an explicit formalism is beyond the scope of this study.

Although the theoretical expressions of the dissociation lifetimes observed by PL and DLTS are difficult, the dissociation energies obtained by PL ($E_{dis:PL}$) and DLTS ($E_{dis:DLTS}$) measurements are clearly confined between the dissociation energies $E_b + E_d$ and $E_b + E_d + E_p$. The relationships between these energies can be expressed on the basis of Eq. (6) as

$$E_{dis:PL} = E_d + E_b + \alpha \qquad (8)$$

and

$$E_{dis:DLTS} = E_d + E_b + \beta, \qquad (9)$$

in which α and β indicate the positive energies supplementing the contributions of the energy term included in Eq. (7) ($0 < \alpha, \beta < E_p$). Because the detection depth of PL is larger than that of DLTS, α is smaller than β.

Although the explicit values of E_b and E_p are not obtained, the ranges of these values can be estimated from Eqs. (8) and (9) with the help of the reported value of E_d. When the experimental values of 0.18 eV (reported in Ref. 27) for E_d and 0.60 eV for $E_{dis:PL}$ obtained in this study are used, the value of E_b is estimated from Eq. (8) to be lower than 0.42 eV. This value is low enough to support the presence of weak bonding in the Cu_{DLB} center observed by Weber et al.[13] and to support our center model[9,11] that the Cu_{DLB} center is weakly bonded by joining three Cu_i atoms around the Cu_{DLA} center below 100 °C. Since E_p is larger than β (= $E_{dis:DLTS}$ - $E_{dis:PL}$ + α), the value of E_p is estimated to be larger than 0.41 eV from the experimental values obtained in this study.

C. Deviation of fitting curves from DLTS data

The reason for the considerable deviation of the fitting curves from the DLTS data in a long annealing time region (Fig. 4) is considered as follows. In the analysis of the DLTS data as well as the PL data, we did not take into consideration the effect of the reformation of the Cu_{DLB} center near the surface due to the accumulation of Cu_i out-diffused from deep region. We consider that the deviation of the DLTS data from the fitting curves after a long annealing time is brought about by this reformation effect. Since the detection depth of DLTS is far shallower than that of PL as discussed in Sec. IV A, it is reasonable that the reformation effect of the center gives a much larger contribution to the DLTS data than to the PL data.

In summary, the same samples were used in the measurements of the dissociation of the Cu_{DLB} center by DLTS and PL methods. Different dissociation energies were obtained by the two methods: 1.01 eV by DLTS and 0.60 eV by PL. This difference was assumed to originate from the combination of the difference in the influence of the underlying processes (precipitation and diffusion of Cu_i) to dissociate the center at different

depths with the difference in the detection depths of both methods. From the dissociation energies of the Cu_{DLB} center obtained in this study together with the reported diffusion barrier of Cu_i, the binding energy of the center is estimated to be lower than 0.42 eV and the precipitation barrier of Cu_i higher than 0.41 eV. This binding energy is consistent with the presence of weak bonding of the center reported by others[13] and the structural model of the center proposed by us.[9,11]

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