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Carrier-induced formation of electrically active boron-interstitial clusters in irradiated boron-doped silicon

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ABSTRACT

Excess minority carriers create boron-related recombination centers that degrade the efficiency of the non-particle-irradiated silicon solar cells. However, the carrier-induced reactions among the radiation-induced defects are poorly understood for devices exposed to particle radiation. This study investigates the structure, electronic properties, formation and annihilation mechanisms, and diffusion dynamics of the carrier-induced defects in particle-irradiated boron-doped silicon using density-functional modeling and junction spectroscopy. By revisiting the ground-state structures of the boron-di-interstitial clusters (BI_2), we find that the calculated acceptor and donor levels of such defects agree well quantitatively with the carrier-induced deep-level transient spectroscopy (DLTS) hole emission signatures at 0.43 and 0.53 eV above the valence band edge (E_v), respectively. We also find that the formation of BI_2 is thermally activated by an energy of 0.50 eV, which we explain theoretically by the reduction of the migration barrier of mono-interstitials to 0.53 eV in the presence of excess minority carriers. Moreover, we discover that the BI_2 are potentially mobile with a migration barrier of 1.18 eV, contrary to the present understanding.

I. INTRODUCTION

Carrier-induced defect formation and transformation have detrimental effects for boron-doped silicon semiconductor devices. A continuous interest has been devoted to such effects occurring in the silicon solar cells for almost 50 years (also known as light-induced degradation, e.g., Ref. 1), where the formation of electrically active boron-oxygen complexes, via either above-bandgap illumination or forward biasing, has been considered to result in a significant drop in the carrier lifetime and, hence, the cell efficiency. While most of the previous works have been focused on such carrier-induced phenomena occurring only in the non-particle-irradiated solar cells, however, the carrier-induced reactions and transformations among the radiation-induced defects remain much more elusive for boron-doped silicon devices exposed to intense particle radiation such as in outer space. Without careful scrutiny of such carrier-induced processes, it is not possible to predict the reliability of the electronics in the radiation environment over their lifespan.

Such issues have been raised more recently regarding the carrier-induced changes of electrical properties of the particle-irradiated devices, such as the effect doping concentration of the bulk devices, the leakage current and the charge collection efficiency of the radiation detectors,[2–5] and the current gain of the bipolar transistors.[6–8] One of the major concerns is the creation of a considerable amount of defect centers at 0.43 and 0.53 eV above the valence band edge (E_v), respectively, by the injection of excess carriers in the B-doped silicon after exposure to particle irradiation; this has been reported to significantly degrade the electrical performance of the silicon bipolar devices.[8–10] However, the knowledge regarding the composition and dynamics of such defect centers is far from clear. These defect centers were initially assigned to carbon-di-interstitial complexes (CI_2),[11] and later by re-examining the concentrations of the impurity atoms, the defect assignment was then revised to boron-di-interstitial clusters (BI_2).[10] In the previously proposed models,[9–11] BI_2 are considered to be formed due to the trapping of a mobile di-interstitial by boron, which are

released by di-interstitial-oxygen complexes (I_2O), and can transform between two configurations via the reversible injection-annealing cycles. However, further experiments[8] challenge these models by showing the increase in the effective doping concentrations upon defect formation, whereas the decrease in the effective dopants is expected according to the models in Refs. 9–11.

In this study, we identify new ground-state structures for BI_2 and confirm the assignment of the E_v+0.43 eV and E_v+0.53 eV defect centers to BI_2 by reproducing the electronic and dynamical properties with *ab initio* calculations. Neither the formation of BI_2 involving I_2O breakup nor the configurational transformations of BI_2 upon carrier injection proposed in the previous models are supported by our further experimental evidence. We instead propose the charge-state-dependent migration behavior of the mono-interstitials (I) to be attributed to the carrier-induced formation of the deep recombination centers BI_2. Such a process of defect formation may also be responsible for the carrier-induced degradation in the non-particle-irradiated silicon. We also indicate that the mobility of BI_2 should be considered contrary to the assumptions of most defect models;[12–17] it can diffuse by a two-step process consisting of translation and reorientation with a barrier of 1.18 eV.

II. METHOD DETAILS

A. Calculation details

Ab initio calculations were carried out with a plane-wave density-functional code, CASTEP.[18] For each system, the generalized gradient approximation (GGA) ultrasoft pseudopotential[19,20] was employed for the search of the ground-state and saddle point structures along the minimum energy paths of atomic mechanisms, and then the hybrid density functional of Heyd–Scuseria–Ernzerhof (HSE06)[21,22] with a norm-conserving pseudopotential was performed for the single-point energy calculations. This two-step method, first calculating a GGA-level structure followed by a single-point energy calculation within HSE06, has been shown to be quite accurate in terms of formation energies and migration barriers.[23,24] 216-atom supercells of silicon were used, in which self-interstitials and boron atoms were inserted to produce defects. The Brillouin zone of GGA- and HSE06-level calculations was sampled at $2 \times 2 \times 2$ and $1 \times 1 \times 1$ k-point meshes, respectively. The nudged elastic band method[25] was adopted to investigate defect migration and transformation. The energy cutoff was 400 eV. Atoms were relaxed until the forces were less than 0.03 eV/Å.

The stability of the defects was calculated through the use of formation energies. The formation energy (E_f^Q) of defects with the charge state Q is evaluated as[26]

$$E_f^Q = (E_D^Q - E_X^0) + Q(\varepsilon_F + \varepsilon_v) - \sum_s n_s\mu_s + E_{\text{corr}}, \tag{1}$$

where E_D^Q is the calculated total energy of the supercell containing the defect D, E_X^0 is the total energy of the corresponding perfect crystal supercell, ε_F is the fermi level, ε_v is the top of the valence band, n_s is the number of atoms of species s, μ_s is the chemical potential corresponding to that species, which is not critical since the quantities of interest (the total-energy differences and the ionization levels of defects) do not depend on the chemical potentials, provided that the defects compared contain the same number of Si and B atoms, and E_{corr} is the correction term accounting for any spurious effects such as the finite-size supercell errors. Unfortunately, E_{corr} is sensitive to the defect species and their respective charge states and is practically hard to obtain.[27] We employed the *marker method* to cancel out the E_{corr} term by introducing appropriate experimental data. This method basically assumes that the offsets of the ionization potentials between the calculated defect and the mark defect that is well established experimentally are essentially identical to that of the calculated defect level and the experimentally observed marker level.[28,29] Although the formation energy method with the supercell-size corrections, e.g., Ref. 30, has become popular in the last 10 years, the empirical marker method has proved to be an efficient way to cancel the systematic errors derived from the non-exact treatment of the electronic exchange-correlation and finite-size effects.[31] The formation energy method and the marker method are reported to be essentially equivalent[32] and agree to within 0.1 eV.[33,34] The application of this method has successfully reproduced many defect levels in semiconductor including silicon,[34–43] diamond,[44] and 2D materials.[45–47]

By comparing the total energy differences between the relaxed, positively (negatively) charged states, and the neutral defects, $\Delta E(Q/Q+1) \equiv E_D^Q - E_D^{Q+1}$, for the defect under scrutiny (subscripted with "d") with that of a marker defect (subscripted with "m"), the calculated defect level $E_d(Q/Q+1)$ is predicted at[28,29]

$$E_d(Q/Q+1) \approx E_m(Q/Q+1) + \Delta E_d(Q/Q+1) - \Delta E_m(Q/Q+1), \tag{2}$$

where $E_m(Q/Q+1)$ is the experimentally observed level of the marker defect. The formation energies of the charged defects relative to their neutral states are, hence, expressed as

$$E_f^{+1} - E_f^0 = \varepsilon_F - [\Delta E_d(Q/Q+1) - \Delta E_m(Q/Q+1) + E_m(Q/Q+1)], \tag{3a}$$

$$E_f^{-1} - E_f^0 = -\varepsilon_F + [\Delta E_d(Q/Q+1) - \Delta E_m(Q/Q+1) + E_m(Q/Q+1)], \tag{3b}$$

where E_X, ε_v, and $\sum_s n_s\mu_s$ in Eq. (1) all cancel out. The error of the marker method is eliminated when the marker defect has ideally similar electronic properties to the defect under scrutiny. We selected the interstitial boron (BI) as the marker with the well-known donor and acceptor levels as listed in Table SI in the supplementary material.

B. Experiment details

The samples studied here were a group of p–n–p silicon bipolar devices made by growing an epitaxial p-type silicon layer that is subsequently phosphorus and boron doped which the doping profiles by secondary-ion-mass spectroscopy (SIMS) have

been previously described in detail elsewhere.[8,48,49] The defects were introduced at room temperature by 14 MeV fusion neutron irradiation (by bombarding the deuterium target with triton beams) to fluences of 10^{13} cm^{-2}. All leads were shorted during both the irradiation and annealing treatments. The minority carriers were injected into the base/collector diode with the emitter shorted to the base. All the injection and annealing treatments were performed in the vacuum chamber of the junction spectroscopy apparatus. The experimental results in the present work were obtained by means of deep-level transient spectroscopy (DLTS) and minority-carrier transient spectroscopy (MCTS). Both majority (DLTS) and minority (MCTS) carrier spectra were recorded with a rate window of 255.8 s^{-1}, filling pulse width of 100 ms, and bias of −9.5 V, while the filling pulse amplitude was set to 9.5 and 10.5 V for the majority and minority-carrier measurements, respectively. The DLTS/MCTS spectra were acquired using the base/collector diode with the emitter shorted to the base.

III. RESULTS

A. Electronic properties

Our calculations identified three BI_2 states labeled BI_2^a, BI_2^b, and BI_2^c as shown in Fig. 1. The BI_2^a has C_{1h} symmetry, which resembles the ground-state structure of di-interstitial (I_2)[50–52] except that a boron atom replaces the central interstitial Si atom. Previous studies have reported this structure.[53–57] The BI_2^b also has C_{1h} symmetry and forms a planar configuration, where the two interstitial silicon atoms and the boron atom all lie in the (110) plane. The BI_2^c has C_{2v} symmetry with the clustered interstitial silicon and boron atoms lying in the (101) plane. As discussed later, the BI_2^b corresponds to one local minimum configuration after rotation in the two-step diffusion pathway, and the BI_2^c corresponds to the other local minimum configuration by a subsequent translation of BI_2^b within the $(1\bar{1}0)$ plane. Previous studies considered BI_2^a as the ground state in p-type silicon (BI_2^+),[53–57] but we found that it to be metastable by 0.20 eV (0.14 eV) in the 1+ charge state with the HSE (PBE) functional (see Table SII in the supplementary material). The ground-state structures depend on the functionals; PBE favors BI_2^b while HSE prefers BI_2^c. However, the energy differences between BI_2^b and BI_2^c are small: 0.03 eV (0.06 eV) with HSE (PBE).

Figure 2 shows the formation energies and the charge-transfer levels of BI_2 calculated by HSE06. The charge-transfer levels $\varepsilon(-/0)$ and $\varepsilon(0/+)$ at $E_v + 0.47$ eV and $E_v + 0.54$ eV, respectively, match well with the single electron emission signatures H(228K) and H(256K) measured by DLTS at $E_v + 0.43$ eV and $E_v + 0.53$ eV, respectively.[8–10] The lower position of $\varepsilon(-/0)$ than $\varepsilon(0/+)$ implies a negative-U behavior for BI_2. We note that transitions measured by optical absorption and luminescence should differ from the levels demonstrated in Fig. 2. A Franck–Condon shift of 0.23 eV (by HSE) is calculated for the photon-excited process of BI_2^+. This Franck–Condon effect is illustrated by the configuration-coordinate total energy diagram in Fig. S1 in the supplementary material. Based on previous theoretical[56] and experimental[8] studies, charge states above 1+ and below 1− are unstable in the bandgap and, thus, are not considered in this paper.

B. Dynamic properties

Figure 3(a) shows the minority-carrier transient spectroscopy (MCTS) measurements of the boron-doped silicon subjected to the same reversible cycles of annealing and injection as in Ref. 8. Despite the agreement on the growth of the H(228 K) and H(256 K) peaks upon minority carrier injection, we note that neither the hole emission signature in the range of 50–70 K (assigned to I_2O[10,11]) nor the electron emission signature in the range of 160–180 K (labeled $ME1$ and assigned to one configuration of BI_2[10]) was observed in our samples. In their previously proposed model,[10,11] BI_2 form when the mobile di-interstitial (I_2) released by the breakup of I_2O is trapped at a substitutional boron, and the configurational transformation of BI_2 is indicated by the correlated changes of H(228 K)/H(256 K) and $ME1$ peaks via injection-annealing cycles. It is noted that H(228 K)/H(256 K) can be formed at a temperature as low as 250 K as shown in Fig. 3(b), which is far lower than the dissociation temperature of I_2O starting

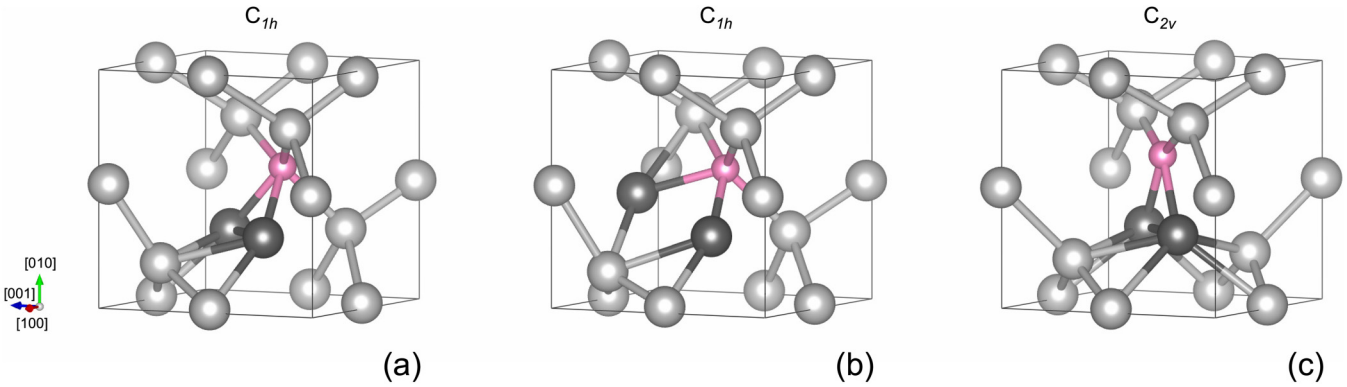

FIG. 1. Calculated atomic structures of BI_2 in three possible configurations. Magenta balls denote boron atoms, and darker gray balls denote interstitial silicon atoms. (a) BI_2^a, (b) BI_2^b, and (c) BI_2^c configuration.

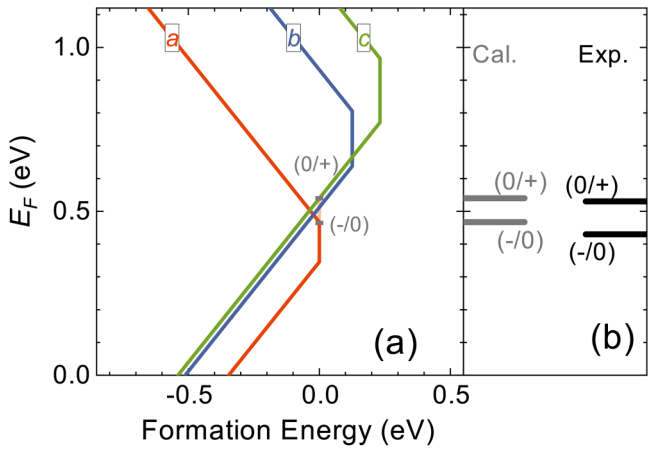

FIG. 2. (a) Formation energies for BI_2 as a function of the Fermi level (E_F) and (b) the corresponding electrical level diagram. The red, blue, and green lines represent the configurations of BI_2^a, BI_2^b, and BI_2^c, respectively. The light-colored lines show the energetically unfavorable charge states. The energies of the charge-neutral BI_2^a configurations are set to zero. The $\varepsilon(-/0)$ and $\varepsilon(0/+)$ levels marked by gray horizontal lines correspond to the $H(228\,K)$ and $H(256\,K)$ traps detected by DLTS.

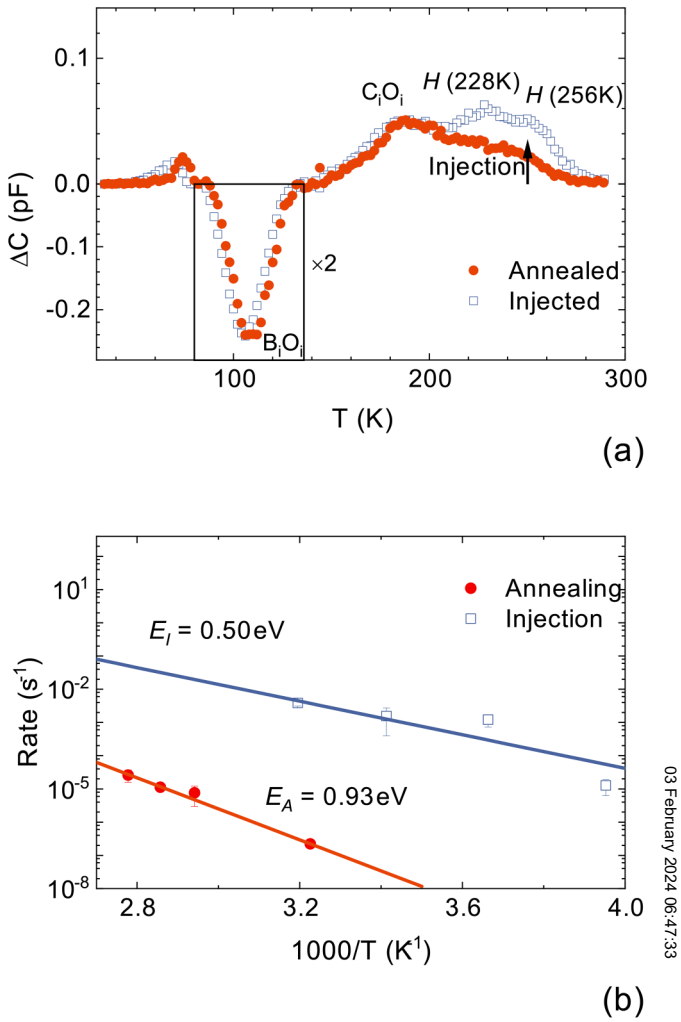

FIG. 3. (a) MCTS spectra of the base-collector diode of fusion neutron damaged *p–n–p* transistors. The open symbols are obtained immediately after annealing for 2 h at 350 K. The solid symbols are obtained subsequently after forward current injection with density of 12.5 A · cm^{-2} at 293 K for 20 min. (b) Arrhenius plot for the formation and annealing rates of the $H(228\,K)$ and $H(256\,K)$ traps obtained by DLTS. The growth of these two traps is measured upon 2.5 A · cm^{-2} forward current injection.

at 330 K.[9,10] Hence, it is concluded that I_2O plays little or no role in the formation of BI_2. By extracting the fitted reaction rate constant, Fig. 3(b) shows the Arrhenius behaviors for both generation and annihilation processes of the defect centers, and the activation energies are determined to be 0.50 and 0.93 eV, respectively. The pre-exponential factor of $\sim 10^5$ determined from carrier injection further reflects a long-range migration character rather than a single jump or reorientation upon defect formation.

Considering the experimental evidence above, we attribute the carrier-induced defect formation of BI_2 to the charge-state-dependent diffusion of the reactant species, the silicon mono-interstitials (I). Although I has a tendency to aggregate to large interstitial clusters $I_n(n > 3)$,[58–60] a larger amount of mono-interstitials are found to survive from clustering in the post-irradiation silicon.[16,17,61] Previous density functional calculations using a GGA functional,[52,56,62,63] a hybrid functional,[64] a *GW* scheme,[65] or an H-terminated cluster method[66,67] have all made an agreement that the +2 charge state (I^{2+}) is predominant when the Fermi level is located at the lower half of the bandgap. For *p*-type silicon, the stable charge state I^{2+} is almost immobile with a migration barrier of 1.49 eV (by HSE). By injecting minority carriers, I^{2+} is able to trap an electron, becoming I^+, and BI_2 can form by capturing two mobile I^+ at a substitutional boron site with the migration barrier greatly reduced from 1.49 to 0.53 eV (by HSE). We plot the configuration-coordinate diagram for both the +2 and the +1 charged I (by PBE) in Fig. S2 in the supplementary material. It is noteworthy that previous studies have reported the overestimation of HSE on the defect migration barrier.[68] However, as listed in Table I, the discrepancies are small between the barriers obtained using HSE and PBE.

The diffusion pathway for BI_2 is demonstrated in Fig. 4. This trajectory consists of a rotation and then a translation step with similarities to I_2 and AsI_2.[69,70] The interstitial silicon atom (2) in the ground-state configuration BI_2^c is initially rotated by 60°*irc* about the $[11\bar{1}]$ axis, with the clustered atoms lying in the (101) plane changing to the $(1\bar{1}0)$ plane in order to reach the BI_2^b configuration. With all the subsequent translational movements constrained in the $(1\bar{1}0)$ plane, the clustered atoms are then translated to the nearby BI_2^c site by kicking out the atom (1) to form the interstitial pair and relaxing the atom (3) back to the lattice site. The rotation from BI_2^c to BI_2^b has a barrier of 0.50 eV, and the translation to the neighboring BI_2^c site has a barrier of 1.18 eV. Such relatively low migration barrier for the BI_2 is against

TABLE I. Migration barriers of I^{2+}, I^{+}, and BI_2^{+}. The results from PBE and HSE06 are compared. All values are reported in eV.

	PBE	HSE06
I^{2+}	0.55	0.53
I^{+}	1.33	1.49
BI_2^{+}	1.24	1.18

the present understanding of processes such as boron transient enhanced diffusion (TED), where this cluster has been considered to be immobile and act as precursors for the growth of larger boron-interstitial clusters.[12,13] Due to its migration barrier of 1.18 eV, BI_2 may diffuse away and interact with other defects far below the TED temperature of ~800 °C. The mobility of BI_2 should be included in the continuum models regarding the defect annealing process.

Dissociation energies for BI_2 were reported in Ref. 15 via the $B_s + I_2$ reaction ranging from 1.10 to 1.77 eV and via the $B_i + I$ reaction ranging from 2.60 to 2.99 eV with the assumption that all defect species are neutral. By considering the $\varepsilon(2+/0)$ level at $E_v + 0.2$ eV for I_2,[52] the $\varepsilon(+/0)$ level at $E_v + 0.53$ eV for BI_2, and the $\varepsilon(0/-)$ level at $E_v + 0.05$ eV for B_s, the dissociation energy for the favored reaction path $B_s + I_2$ is modified to range from 1.02 to 1.69 eV. However, it should be noted that those values may be underestimated since further EPR experiments have indicated a larger value of 0.88 eV for I_2 in *p*-type silicon[71] rather than the significantly smaller value of 0.26 eV adopted in Ref. 15. Therefore, BI_2 are unlikely to dissociate before diffusing away.

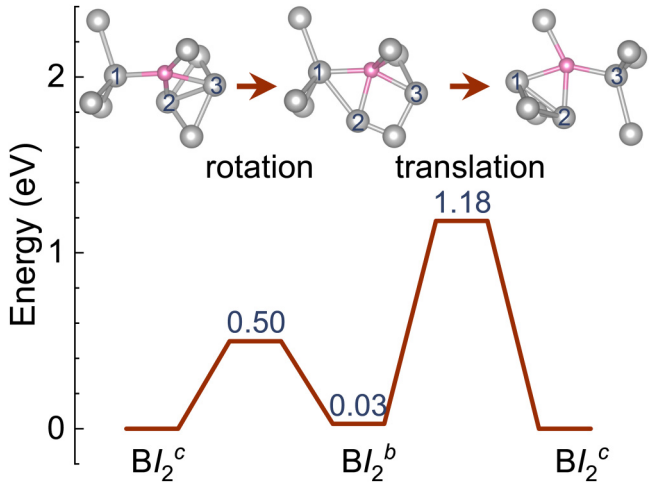

FIG. 4. The diffusion pathway of positively charged BI_2. The path consists of a combination of two steps, rotation and translation. The rotation from BI_2^c to BI_2^b has a barrier of 0.50 eV, and the translation to the neighboring BI_2^c site has a barrier of 1.18 eV. Magenta balls denote boron atoms, and gray balls denote silicon atoms. The moving silicon atoms are marked with numbers. Shown is the $(1\bar{1}0)$ projection of the BI_2.

TABLE II. The energy levels of BI_2 and the activation energies for formation and annealing obtained from DLTS measurements as well as *ab initio* calculations. All values are in eV.

	Exp.	Cal.
$\varepsilon(0/+)$	E_v+0.53	E_v+0.54
$\varepsilon(-/0)$	E_v+0.43	E_v+0.47
E_{form}	0.50	0.53
E_{ann}	0.93	0.95[72]

IV. DISCUSSIONS

Table II lists the electronic levels and reaction dynamics of the carrier-induced centers determined by junction spectroscopy and reproduced by the BI_2 defect models with *ab initio* calculations. A generally very good agreement between experiments and calculations supports the assignment of the DLTS signals to the energy levels of BI_2 and the carrier-induced formation mechanisms proposed by us. Although the experimental activation energy of 0.93 eV for the defect annealing is lower than the calculated migration barrier of 1.18 eV for the BI_2, this discrepancy indicates that faster annihilation channels may exist in the irradiated B-doped silicon before the BI_2 migrate to sinks. For example, BI_2 may capture a mobile BI to form a larger cluster[13] with a migration barrier of 0.95 eV for BI^+ to overcome[72] assumed from the evidence of plenty of boron and interstitial atoms supplied in the samples. Our present model can also explain the experimental findings that acceptors in the lower half of the bandgap are produced upon minority carrier injection,[8] where two minority carriers are consumed by the reaction of cluster formation, i.e., $B^- + 2I^{2+} + 2e^- \rightarrow BI_2^+$. These experimental data can rule out the acceptor removal model of $B_s^- + I_2O \rightarrow BI_2^+ + O_i + 2e^-$ in Refs. 10 and 11 in terms of the changes of the effective doping concentrations.

For non-particle-irradiated boron-doped silicon, it has been proposed that the carrier-induced formation of recombination centers responsible for the solar cell degradation is associated with the charge-state-driven diffusion of the oxygen dimers (O_{2i}).[73–76] However, further experimental data have cast doubt on the B_sO_{2i} formation process due to the lack of evidence for the existence of the doubly positively charged oxygen dimer (O_{2i}^{++}).[77] Due to the similarities of the reversible injection–annealing cycles and the thermal activation energies in both particle-irradiated and non-particle-irradiated boron-doped silicon (the annihilation and recovery activation energies of ~1.0 and ~0.4 eV, respectively, in non-particle-irradiated silicon as summarized in Ref. 78), it is natural to link the role of the mono-interstitials to the formation of recombination centers in non-particle-irradiated solar cells. With a much lower concentration of interstitials in non-particle-irradiated silicon, more precise experiments are needed.

V. CONCLUSION

In summary, we have studied the structure, electronic properties, formation and annihilation mechanisms, and diffusion dynamics of the BI_2^+ clusters in particle-irradiated boron-doped silicon by combining density-functional modeling with the junction

spectroscopy. A BI_2^+ configuration with C_{2v} symmetry is identified as responsible for the carrier-induced formation of recombination centers corresponding to the previously characterized defect levels at 0.43 and 0.53 eV above E_v. Consistent with both experiments and calculations, its formation process is due to trapping by boron of two mono-interstitials with a migration barrier reduced to 0.5 eV when the immobile I^{2+} captures a photogenerated or injected electron. The diffusion barrier for BI_2^+ is calculated to be 1.18 eV, and hence, the mobility of BI_2 should be considered in situations such as TED.

SUPPLEMENTARY MATERIAL

See the supplementary material for calculation details.

ACKNOWLEDGMENTS

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

X. C. Chen: Conceptualization (lead); Data curation (equal); Formal analysis (lead); Investigation (lead); Methodology (lead); Resources (lead); Software (equal); Validation (equal); Visualization (equal); Writing – original draft (lead); Writing – review & editing (lead). **L. Li:** Conceptualization (equal); Data curation (equal); Formal analysis (equal); Funding acquisition (lead); Investigation (equal); Methodology (equal); Project administration (lead); Validation (equal). **M. Y. Wang:** Data curation (lead); Formal analysis (equal); Investigation (equal); Validation (equal); Visualization (equal). **H. Ren:** Investigation (equal); Methodology (equal); Software (lead); Validation (equal). **X. Q. Liu:** Resources (equal); Validation (equal); Visualization (equal). **G. Zeng:** Formal analysis (equal); Writing – original draft (equal). **G. X. Yang:** Funding acquisition (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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