Theoretical insights into the minority carrier lifetime of doped Si—A computational study

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Using density functional theory, we have analyzed the ways and means of improving the minority carrier lifetime (MCL) by calculating the band structure dependent quantities contributing to the MCL. We have computationally modeled silicon doped with different elements like B, C, N, O, P, Ti, Fe, Ga, Ge, As, In, Sn, Sb, and Pt and looked at the effect of doping on MCL. In co-doping, the systems Si-B-Ga, Si-B-Ge, Si-B-2Ge, Si-B-Pt, Si-Ga-Ge, Si-Ga-2Ge, and Si-Ga-Pt are investigated. From our calculation, it is found that by doping and co-doping of Si with suitable elements having "s" and "p" electrons, there is a decrease in the recombination activity. The predicted effective minority carrier lifetime indicates the possibility of significant improvements. Based on the above studies, it is now maybe possible, with suitable choice of dopant and co-dopant material, to arrive at part of a standard production process for solar grade Si material. *Published by AIP Publishing.*
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I. INTRODUCTION

Currently, there is a great demand for silicon solar cells with high efficiency. Photovoltaic manufacturing has surpassed the 10 GW/year production threshold and is expected to reach TW/year manufacturing levels. In spite of its high cost, twice as expensive as conventional generation, installed solar capacity grows by 25% each year. There are different factors contributing to the reduction of solar cell cost. They depend on novel techniques or enhance existing technology. The production of solar grade silicon (SG-Si) contributes significantly to the reduction of cell cost.[1] It is expected that various forms of crystalline silicon will dominate the market for the foreseeable future.[2,3] The electronic grade silicon can have high efficiency, but this will increase the cost of solar cell enormously. The cost can be very much reduced if solar grade silicon can be defect engineered to have low recombination rate (high MCL) leading to improved conversion efficiency of the solar cell. To enhance the MCL, it is essential to go into the theoretical insight of the defect process leading to the recombination.[4] The defect levels acting as traps aid recombination through a two-step process and one has to understand the dynamics of the recombination in relation to the band structure of the system with defects. Lot of research is going on in search of new solar material with improved efficiency. Focus is on the existing solar cells, especially the Si solar cells which are cheap and cost effective. The advantages of silicon are its elemental abundance and decades of investment. It is hard to ignore these factors. The challenge in this field is to improve the efficiency while minimizing the cost.[5]

Mixing mismatched elements can enhance the efficiency of solar cells. In this process, the parent material is doped and co-doped with suitable elements so as to improve the photovoltaic efficiency. In these solar cells, the minority carrier lifetime (MCL) is one of the major deciding factors of the efficiency. There is a direct relation between the minority carrier lifetime and the solar cell efficiency. The higher lifetime of minority carrier results in increased conversion efficiency of silicon solar. The formation of different types of grown-in micro-defects (GMD) is responsible for limiting the MCL by acting as recombination centers. Si solar cell doped with Boron (B) has low MCL and hence low efficiency, whereas gallium (Ga)-doped Si has high MCL. When a third element, say tetravalent Ge, is co-doped in B-doped or Ga-doped Si, interesting properties are observed.[6,7] When tetravalent Ge is co-doped in doped Si, the MCL increases when the co-doped element (Ge) concentration increases in Czochralski silicon (CZ-Si).[6,7] The *Czochralski* process is a method of crystal growth used to obtain single crystals of semiconductors. Moreover, the formation of detectable B–O defects is reduced in the presence of Ge; thus, B and Ge co-doped CZ-Si shows only a small degradation effect. In the Ga and Ge co-doped Si crystal, Ge favors the reaction with free vacancies and O, which results in strain-relaxed Ge-vacancy and Ge-vacancy-O complexes.[6–8]

The above-mentioned facts are based on various experimental observations.[6,7] The properties like formation of GMD and the effect of dopant Ge on GMD and hence on MCL in doped Si are not fully understood. Several theoretical models[6–9] were proposed to explain the GMD effect on minority carrier lifetime; however, the problem has not yet been completely solved. A better understanding of GMD formation in impurity-doped Si and its effect on minority carrier lifetime may lead to better-performing solar cell material.

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Further accurate calculations are needed to estimate MCL and fix the maximum limit of dopant content that is essential for controlling GMD and enhancing the PV characteristics of solar grade silicon (SG-Si).[6] Supportive theoretical investigations are necessary in order to reveal the detailed structure and the formation kinetics of GMD and Ge-vacancy-O complexes (defect compound). The total energy and band structure calculation will reveal the electronic process in the doped and co-doped systems.

A. Recombination rate

The simple term "lifetime" almost always refers to the recombination lifetime of excess minority carriers. If the number of minority carriers is increased above the equilibrium value by some transient external excitation (such as incident sun light), the excess minority carriers will decay back to that equilibrium carrier concentration through the process of recombination. A critical parameter in a solar cell is the rate at which recombination occurs. It is known as the "recombination rate" and it depends on the number of excess minority carriers. If the solar grade silicon can be defect engineered to have low recombination rate or high minority carrier lifetime (MCL), then there is a possibility for getting improved conversion efficiency.[10,11] The defect levels located close to the middle of the band gap act as traps and aid recombination through a two-step process. The electron lifted from the valence band to the conduction band by the solar photon first relaxes to the defect level and then relaxes to the valence band where it recombines with a hole. The arrived electron in the conduction band has to be harvested before it recombines with the hole. To achieve this, the recombination process has to be delayed or the lifetime of the MC has to be increased.

Theoretical studies[12–18] regarding the electronic properties of the defects and recombination centers responsible for the light-induced carrier lifetime degradation will be an added advantage in understanding the current problem. There are not many first principle calculations using Density Functional Theory (DFT) for the above-mentioned doped Si systems. We have computationally modeled silicon ($1s^2\ 2s^2\ 2p^6\ \mathbf{3s^2\ 3p^2}$) doped with the following elements:[19,20]

B—Boron, C—Carbon, N—Nitrogen, O—Oxygen, P—Phosphorus, Ti—Titanium, Fe—Iron, Ga—Gallium, Ge—Germanium, As—Arsenic, In—Indium, Sn—Tin, Sb—Antimony, Pt—Platinum.

In some cases, we have investigated the interstitial doping in addition to the substitutional doping. In a few cases co-doping also tried. We have computed the total energy, the bandstructure, and the density of states for all the above mentioned systems.

II. METHODOLOGY

Density Functional Theory, which describes the ground state properties of many-body systems, with a plane wave basis set as implemented in the Vienna ab-initio simulation package (VASP)[21] is used in our calculation. The projector augmented-wave (PAW) is used to describe the interaction between ions and electrons. The PAW potential has two advantages over ultrasoft pseudo potentials (USPP). It provides all-electron wave functions for valence electrons (with s, p, and d orbitals) and shows a better convergence behavior than USPP. Exchange correlation energy is evaluated with generalized gradient approximation (GGA) developed by Perdew *et al.*[22] Super cell approach is employed to study the system.[23] Non-covalent interaction in the system is described by van der Waals, hydrogen bonding, and ion-pairing interactions. For the structural relaxation, the integration over the Brillouin zone (B.Z.) is performed for the k-points meshes generated by the Monkhorst-Pack scheme with Γ centered grid.[24] For the band structure studies, more number of k-points are chosen along the symmetric directions distributing good number of k-points between two high symmetry points in the B.Z. Suitable convergence criteria are set for ionic iteration, electronic iteration, and forces.

The minority carrier "lifetime" (τ) measures how long a carrier is likely to stay around before recombining. It is one of the most important parameters for the characterization of semiconductor wafers used in the preparation of photovoltaic solar cells.[3] The lifetime is related to the recombination rate by $\tau = \frac{\Delta n}{R}$, where "$\Delta n$" is the excess carrier density, "R"' is the recombination rate, and "τ" is the minority carrier lifetime. In this work, we mainly examined the trap-assisted recombination, also called Shockley-Read-Hall (SRH) recombination process, in minority carrier lifetime. The effective lifetime in multicrystalline silicon is mostly dominated by SRH recombination process at the high injection level of carrier densities.[15]

The recombination rate will depend on the number of defects present in the material. As the defect concentration in the solar cell increases with doping, the rate of SRH recombination will increase. The material quality is strongly related to cell efficiency and to the cost of the solar cell. The defects introduced during the crystal growth process or during the solar cell production will have an impact on the quality of the material.

The rate of recombination of electrons and holes depends on the magnitude of the disturbance and on the recombination process. The recombination and generation processes depend on the capability of a recombination center to capture or emit an electron.

The presence of defects in a semiconductor crystal due to impurities or crystallographic imperfections such as dislocations produces discrete energy levels within the band gap. These defect levels, also known as traps, greatly facilitate recombination through a two-step process where a free electron from the conduction band first relaxes to the defect level and then relaxes to the valence band where it annihilates a hole.

The SRH lifetime can be expressed as[15]

$$\tau_{SRH} = \frac{\tau_{n0}(\mathrm{p_0} + \mathrm{p_1} + \Delta \mathrm{n}) + \tau_{p0}(\mathrm{n_0} + \mathrm{n_1} + \Delta \mathrm{n})}{n_0 + p_0 + \Delta n}, \quad (1)$$

where

τ_{n0} is the minority carrier lifetime of electrons,
τ_{p0} is the minority carrier lifetime of holes,

TABLE I. Band structure and τ_{SRH} data for doped and co-doped Si-Systems.

S.No.	System	E_F (eV)	E_C (eV)	E_V (eV)	E_g (eV)	E_t (eV)	$N_C(E_c)$	N_V (E_v)	τ_{SRH} (s)
1	Si-B	5.7	6.4	5.8	0.6	6.4	17	7	1.7×10^{-6}
2	Si-C	6.0	6.7	5.7	1.0	6.4	20	10	1.8×10^{-5}
3	Si-N	6.1	6.5	5.5	1.0	6.1	13	5	1.7×10^{-6}
4	Si-O	6.0	6.6	5.6	1.0	6.4	16	13	1.1×10^{-3}
5	Si-P	6.4	6.5	5.5	1.0	6.3	13	7	5.6×10^{-4}
6	Si-Ti	5.9	6.2	5.5	0.7	6.2	10	8	1.5×10^{-5}
7	Si-Ti(i)	6.4	6.6	5.5	1.1	5.9	19	10	4.7×10^{-5}
8	Si-Fe	5.8	6.8	5.5	1.3	6.2	18	12	2.3×10^{-5}
9	Si-Fe(i)	6.2	6.8	5.8	1.0	6.2	20	8	2.5×10^{-5}
10	Si-Ga	5.8	6.3	5.8	0.5	6.3	22	8	1.5×10^{-6}
11	Si-Ge	6.0	6.8	5.7	0.8	6.6	18	16	6.2×10^{-2}
12	Si-As	6.4	6.5	5.6	0.9	6.3	17	9	1.7×10^{-5}
13	Si-In	5.9	6.7	5.9	0.8	6.6	17	10	1.8×10^{-5}
14	Si-Sn	6.2	6.7	5.8	0.9	6.6	16	8	6.5×10^{-4}
15	Si-Sb	6.4	6.5	5.6	0.9	6.3	14	12	2.2×10^{-5}
16	Si-Pt	6.2	6.7	5.2	1.5	6.0	19	12	1.0×10^{-3}
17	Si-Pt(i)	6.2	6.9	6.0	0.9	6.2	12	10	3.0×10^{-5}
18	Si-B-Ga	6.1	6.6	5.8	0.8	6.5	14	10	1.8×10^{-5}
19	Si-B-Ge	6.4	6.5	5.7	0.8	6.4	21	9	1.7×10^{-5}
20	Si-BGeGe(i)	6.4	6.6	5.6	1.0	6.5	17	13	5.0×10^{-2}
21	Si-B-Pt	5.9	6.9	5.9	1.0	6.6	18	13	2.4×10^{-5}
22	Si-Ga-Ge	6.5	6.6	5.7	0.9	6.5	22	11	1.1×10^{-4}
23	SiGaGeGe(i)	6.4	6.9	5.8	1.1	6.4	20	10	1.9×10^{-6}
24	Si-Ga-Pt	6.2	6.6	5.8	0.8	6.2	14	10	2.7×10^{-5}

p_1 is the equilibrium concentration of holes,
p_0 is the intrinsic carrier concentration of holes,
n_0 is the intrinsic carrier concentration of electrons,
n_1 is the equilibrium concentration of electrons,
Δ_n is the excess carrier concentration of electrons,

and

$$\tau_{p0} = \frac{1}{\sigma_p \nu_{th} N_t}, \tag{2}$$

$$\tau_{n0} = \frac{1}{\sigma_n \nu_{th} N_t}, \tag{3}$$

$$n_1 = N_C \exp\left\{\frac{(E_t - E_v)}{kT}\right\}, \tag{4}$$

$$p_1 = N_v \exp\left\{\frac{(E_v - E_t)}{kT}\right\}. \tag{5}$$

In the above equations σ_p is the capture cross section of holes, σ_n is the capture cross section of electrons, ν_{th} is the thermal velocity, N_t is the density of defects, and N_c and N_V are the effective density of states at the conduction and valence band edges, respectively. E_c is the minimum energy of the conduction band, E_V is the maximum energy of the valence band, and E_t is the energy level of the defect.

III. CALCULATION AND RESULTS

The computation of MCL (SRH lifetime) precedes by the evaluation of quantities defined in Eqs. (2)–(5). Using our data and the data available for σ_p, σ_n, Δ_n, p_0, and n_0 in the literature,[6,7,15,19,20] we have evaluated all quantities [of Eqs. (2)–(5)] for doped Si including τ_{n0} ($=1.380 \times 10^{-6}$ S) and τ_{p0} ($=2.266 \times 10^{-6}$ S) and used them in calculating SRH lifetime. The calculated bandstructure data and SRH lifetime [τ_{SRH}(s)] for the following systems are given in Table I.

1. Silicon doped with boron substitutionally (Fig. 1).
2. Silicon doped with gallium substitutionally (Fig. 2).
3. Silicon doped with germanium substitutionally (Fig. 3).
4. Silicon doped with platinum substitutionally (Fig. 4).
5. Silicon doped with platinum interstitially.
6. Silicon doped with boron substitutionally and co-doped interstitially with Ga (Fig. 5).
7. Silicon doped with boron substitutionally and co-doped interstitially with Ge.
8. Silicon doped substitutionally with boron and Ge, co-doped interstitially with Ge.
9. Silicon doped substitutionally with boron and co-doped interstitially with Pt.

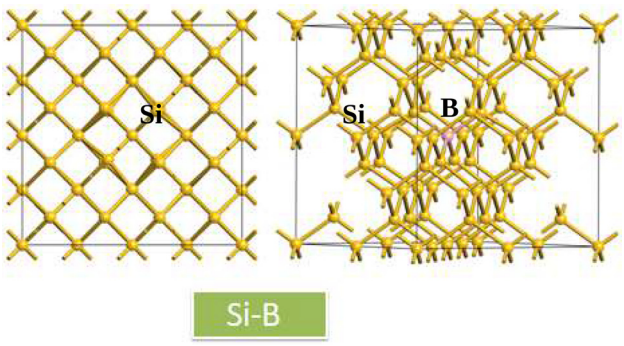

FIG. 1. Computer simulated model of silicon crystal doped with boron substitutionally.

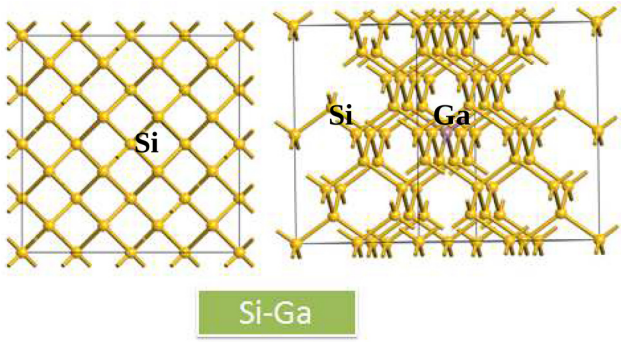

FIG. 2. Computer simulated model of silicon crystal doped with gallium substitutionally.

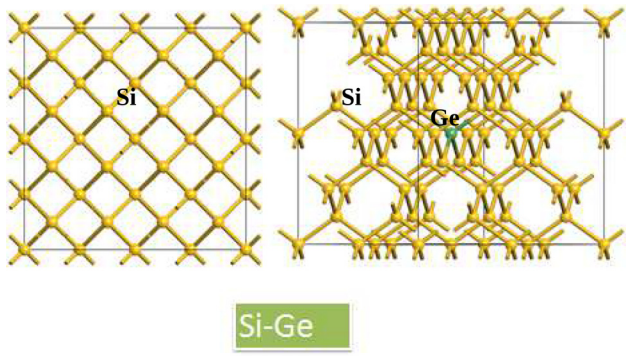

FIG. 3. Computer simulated model of silicon crystal doped with germanium substitutionally.

10. Silicon doped substitutionally with Ga and co-doped interstitially with Ge.
11. Silicon doped substitutionally with Ga and Ge, co-doped interstitially with Ge.
12. Silicon doped substitutionally with Ga and co-doped interstitially with Pt (Fig. 6).

IV. DISCUSSION

A. Effect of bandstructure on MCL

The MCL {SRH lifetime [Eq. (1)]} mainly depends upon n_1 (the equilibrium concentration of electrons) and p_1 (the equilibrium concentration of holes) which in turn depend upon [Eqs. (4) and (5)] the bandstructure data N_C and N_V [the effective density of states (DOS) at the conduction and valence band edge], E_C (minimum energy of the conduction band), and E_t (energy level of the defect). Doping introduces the defect levels near the valence/conduction bands. The presence of these defect levels alters the DOS at the valence/conduction band edges. As a result, the above bandstructure data will have a definite impact on SRH lifetime. Especially the DOS will have a more impact on MCL than the other quantities (E_C and E_t) since n_1 and p_1 are directly proportional to DOS values [Eqs. (4) and (5)].

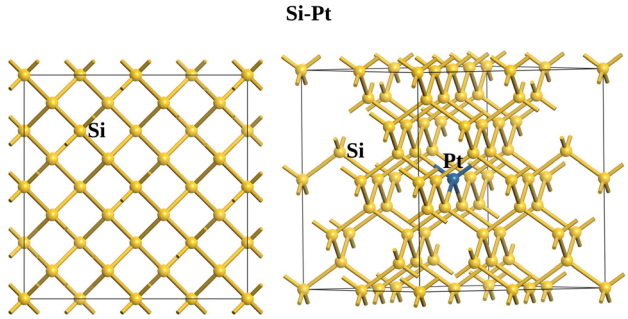

FIG. 4. Computer simulated model of silicon crystal doped with platinum substitutionally.

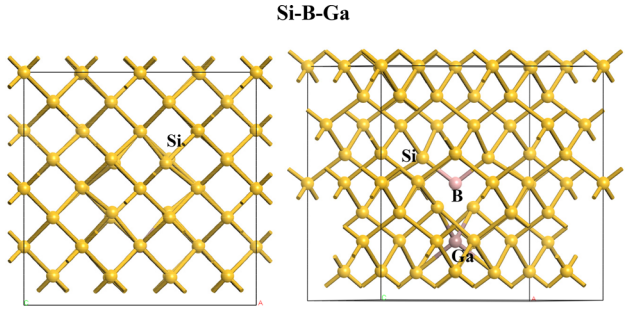

FIG. 5. Computer simulated model for silicon doped substitutionally with boron and co-doped interstitially with Ga.

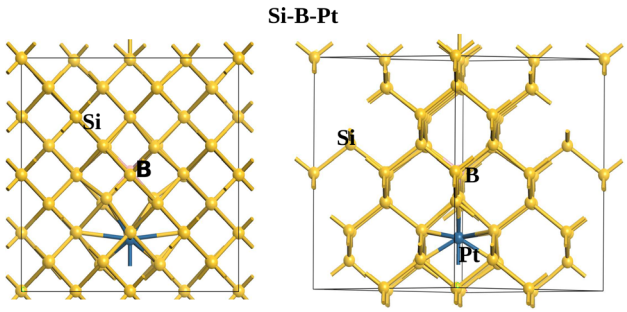

FIG. 6. Computer simulated model for silicon doped substitutionally with boron and co-doped interstitially with Pt.

It is important to incorporate certain processing steps to decrease the recombination activities. Doping and co-doping are some of the processes in this direction. Among the single element doping of Si, doping with O, P, Ge, Sn, and Pt leads to enhanced MCL [SRH lifetime (τ_{SRH})]. These elements, except Pt, have more than one p electrons. The s and p valence electrons of the dopant element play an important role in delaying the recombination process. These defect states appearing in the gap facilitate the extended relaxation of the photo lifted electron from the valence band of Si. The d electrons have strong interaction with the valence band of Si leading to complete modification of the band which is conducive for quick recombination. The doped systems Si-C and Si-O serve as platforms for investigating metal-oxide-semiconductor and oxygen defect processes in silicon.[25–27]

When Si is doped with Pt, apart from the generation of electron hole pair due to photon irradiation, Pt oxidizes Si. As a result, the DOS values at the top of the VB and bottom of CB increase leading to the enhancement of MCL. Even though Pt is costly material (dopant), the cast can be compensated later by recovering (80%) Pt, which is less poisoned compared to other dopants. So presently Pt is preferred over other less efficient cheap dopants.

The co-doping process presents an interesting situation. Out of the seven systems tried, Si-B-2Ge and Si-Ga-Ge turn out to be better systems. In the system Si-B-Ge when the concentration of the co-dopant (Ge) is increased (Si-B-2Ge), the MCL increases. In the system Si-Ga when Ge is co-doped (Si-Ga-Ge), the MCL increases. These results are in agreement with the experimental observation.[6,7] The substituted Ge atom induces local strain in the Si lattice due to the lattice misfit of Ge and Si. From our study[4] of the system Si with vacancies, it is found that with the controlled number of vacancies, the system has an enhanced MCL. As pointed out above, the dopants favor reaction with these vacancies. Also there is a possibility that around the doped site nanostructurization may happen.

This localized nonostructurization may enhance the MCL and hence the photovoltaic (PV) efficiency. In a recent study, it is reported[28] that graded band gap helped to suppress the surface recombination. In doping and co-doping of Si with suitable dopants, it is possible to achieve graded band gap. Also with the modern dopant incorporation mechanism,[29] controlled and selective doping and co-doping can be achieved with required accuracy.

V. SUMMARY

Through a density functional study, we have analyzed the process of improving the MCL through the band structure dependent quantities contributing to the MCL. We have computationally modeled silicon doped with different elements like B, C, N, O, P, Ti, Fe, Ga, Ge, As, In, Sn, Sb, and Pt and looked at the effect of doping on MCL. The band-structure data, $N_C(E_c)$ and $N_V(E_v)$ (the effective density of states at the conduction and valence band edges), E_C (minimum energy of the conduction band), E_v (maximum energy of the valence band), E_t (energy level of the defect), E_g (the band gap), E_F (Fermi energy), and the SRH lifetime (τ_{SHR}), are obtained for the above systems. It is found that Si doped with O, Ge, Pt and co-doped systems Si-B-2Ge and Si-Ga-Ge give enhanced MCL. Materials such as Boron, Gallium, Germanium and Platinum turn out to be the important dopants in the production of cheap solar-grade silicon. We have shown that with atomic-level substitutional doping, the electronic properties of silicon can be tuned significantly.

At this point, we must have in mind the serious weakness of the method used. Since it is well known that DFT calculations on Si grossly underestimate the band gaps, we have not made any comparisons with the experimental band gaps. Even though in the calculation of MCL the band gap is not directly involved, underestimated band gaps will have their bearing on the quantitative estimation of MCL to some extent. But correct qualitative information (selection of suitable dopant and co-dopant) is not lost.

The effect of temperature on the recombination process is not considered here because we have used a simple model of recombination. However, this model predicts the MCLs (SRH lifetime) which are comparable qualitatively with the experimental observations.[6,7,28] In view of the above two facts, we are aware that our calculational method may not give complete "solar-cell production" protocols, but in spite of the simple approach, with the data generated now it may be possible to choose suitable dopant and co-dopant material for the production of solar grade Si material which is part of the protocol for solar-cell production.

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