

# Field-Effect Passivation of Undiffused Black Silicon Surfaces

Shaoyou Wang<sup>ID</sup>, Xinyuan Wu, Fa-Jun Ma, David Payne, Malcolm Abbott, and Bram Hoex<sup>ID</sup>

**Abstract**—Black silicon (b-Si) surfaces typically have a high density of extreme nanofeatures and a significantly large surface area. This makes high-quality surface passivation even more critical for devices such as solar cells with b-Si surfaces. It has been hypothesized that conformal dielectrics with a high fixed charge density ( $Q_f$ ) are preferred as the nanoscale features of b-Si result in a significant enhancement of field-effect passivation. This article uses 1-D, 2-D, and 3-D numerical simulations to study surface passivation of b-Si, where we particularly focus on the charge carrier control by  $|Q_f|$  up to  $1 \times 10^{13} \text{ cm}^{-2}$  under accumulation conditions. We will show that there is a significant space charge region compression in b-Si nanofeatures, which affects the charge carrier population control for moderate  $|Q_f|$  up to  $\approx 1 \times 10^{12} \text{ cm}^{-2}$ . The average surface minority charge carrier density can be reduced by 70% in some cases, resulting in an equivalent reduction in area-normalized surface recombination losses if the effective surface recombination velocity ( $S_{\text{eff}}$ ) is limited by minority carriers. This provides a possible solution for the empirical  $S_{\text{eff}} \propto 1/Q_f^4$  reported previously. We will also show that the situation is more complicated for surface passivation films where the ratio between the electron and hole capture cross section ( $\sigma_n/\sigma_p$ ) is higher than 10 for  $p$ -type surfaces. For commonly used surface passivation films with a  $|Q_f|$  larger than  $\approx 1 \times 10^{12} \text{ cm}^{-2}$ , there is little space charge compression for b-Si. Consequently,  $S_{\text{eff}}$  simply scales with the surface area, i.e., there is no enhanced reduction of surface recombination by field-effect passivation on b-Si.

**Index Terms**—Black silicon (b-Si), charge carrier population control, field-effect passivation, simulation.

## I. INTRODUCTION

**L**IGHT trapping and surface passivation are two important aspects of surface engineering for high-efficiency solar cells. Black silicon (b-Si) is a textured surface with nanoscale high-aspect-ratio features. These nanofeatures contribute to the advanced light trapping, which can potentially realize high-efficiency b-Si solar cells with near-zero reflectance [1], [2]. However, the surface area of b-Si is significantly larger than

that formed by conventional texturing. Thus, a high level of surface passivation is critical for b-Si solar cells [3]. Surface passivation by the industry-standard plasma-enhanced chemical vapor deposited (PECVD) hydrogenated amorphous silicon (a-Si:H) and silicon nitride ( $\text{SiN}_x$ ) could be problematic for b-Si because of the nonconformal deposition resulting from the PECVD process for high-aspect-ratio surface structures [4]. Atomic layer deposition (ALD) is the most promising deposition technique for the surface passivation of the extreme b-Si surfaces since it can achieve a conformal deposition on such structures [5]–[8], and especially ALD  $\text{Al}_2\text{O}_3$  has been widely studied [2], [5], [6], [9]–[12]. Experimental studies have noted that the passivation provided by ALD  $\text{Al}_2\text{O}_3$  layers on b-Si surfaces is often better than what would be expected when taking into account the increased surface area. It has been hypothesized that this improved performance by ALD- $\text{Al}_2\text{O}_3$  on b-Si is attributed to the enhanced repulsion of minority carriers from the entire nanofeature by a strong interface fixed charge ( $Q_f$ ), i.e., the field-effect passivation is enhanced on b-Si [10], [13]. By depositing corona charge on the b-Si surface, von Gastrow *et al.* [6] found that the surface recombination velocity ( $S_{\text{eff}}$ ) on b-Si scaled with the inverse of  $Q_f$  to the power of four in contrast with planar surfaces where  $S_{\text{eff}}$  scales with the inverse of  $Q_f$  to the power of two. However, it should be noted that it is unlikely that the corona charges can be deposited uniformly on a b-Si surface, which might, at least partly, explain this empirical result [14]. Using 2-D numerical simulations, Turkay *et al.* [15] found that the surface nanofeatures would affect the field-effect passivation and that there could be a field-effect passivation enhancement for lightly doped c-Si under low-injection condition when  $Q_f$  magnitude is moderate ( $5 \times 10^8 \text{ cm}^{-2} < |Q_f| < 3 \times 10^{11} \text{ cm}^{-2}$  for accumulation conditions and  $3 \times 10^{10} \text{ cm}^{-2} < |Q_f| < 3 \times 10^{11} \text{ cm}^{-2}$  for inversion conditions). Although these studies have shed some light on the nature of surface passivation of nanofeatures, the detailed mechanism of field-effect passivation on b-Si and its dependence on the nanofeature morphology should be systematically investigated.

From first principles, we know that field-effect passivation relates to  $Q_f$ , space charge, band bending, and carrier densities as described in detail by Grove and Fitzgerald [16] and Aberle *et al.* [17]. More recently, Cuevas *et al.* demonstrated that field-effect passivation more generically can be described as a form of charge carrier population control similar to front surface fields by dopant diffusion or band bending resulting from differences in work function. All these approaches result in a change in the charge carrier density, typically resulting

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in the concentration of one charge carrier (i.e., the minority carrier) to become significantly lower and thus limiting the surface recombination rate [18]. Recently we reported about charge-assisted carrier population control in 1-D simulations. In that work, we revealed that the space charge regions could be compressed, leading to a significant change in the charge carrier control resulting in a further reduction in the minority charge carrier density. The enhancement of field-effect passivation has been found to strongly depend on both  $Q_f$  and the nanofeature diameters [19].

In this work, we will revisit the charge carrier distribution in 1-D and subsequently investigate the charge carrier population control in 2-D and 3-D using Sentaurus TCAD [20]. We will study the surface minority carrier distributions in 2-D and 3-D for  $Q_f$  magnitudes from  $1 \times 10^9 \text{ cm}^{-2}$  to  $1 \times 10^{13} \text{ cm}^{-2}$  and quantify the impact on the surface recombination rate. Subsequently, we present experimental results that confirm the main findings from the 3-D simulations. Finally, we provide guidance for the optimization of b-Si surface passivation for silicon photovoltaics.

## II. SIMULATION AND EXPERIMENTAL DETAILS

### A. Model and Parameter Review

This work aims to determine guiding principles for the optimization of the passivation of b-Si surfaces with a particular focus on field-effect passivation using the classic simulation models. The surface recombination model used is the extended Shockley–Read–Hall (SRH) equation for single-energy-level defects [17]

$$U_S = \frac{p_s n_s - n_{ie}^2}{\frac{p_s + p_1}{S_{n0}} + \frac{n_s + n_1}{S_{p0}}} \quad (1)$$

where  $U_S$  is the surface recombination rate,  $n_{ie}$  is the effective intrinsic carrier density,  $p_s$  and  $n_s$  are the surface carrier densities,  $p_1$  and  $n_1$  are carrier densities by thermal emission of defects, which are sufficiently small and negligible, and  $S_{p0}$  and  $S_{n0}$  are the intrinsic surface recombination velocities. As we mainly focus on moderate- and high-level injection conditions in this work, the surface recombination equation can be simplified for the following analysis. Assuming  $p_s n_s \gg n_{ie}^2$ ,  $p_s \gg p_1$ , and  $n_s \gg n_1$ , which are generally valid [21], (1) can be simplified as

$$U_S = \frac{p_s n_s}{\frac{p_s}{S_{n0}} + \frac{n_s}{S_{p0}}} \quad (2)$$

The level of surface passivation was quantified by the effective surface recombination velocity  $S_{\text{eff}}$  defined as

$$S_{\text{eff}} = \frac{U_S}{\Delta n} \quad (3)$$

where  $\Delta n$  is the excess minority carrier density in the bulk at the edge of the space charge region.

A great diversity of passivation materials and relevant stacks has been studied in recent decades. The electrical properties and the corresponding passivation performance not only depend on

TABLE I  
SUMMARY OF THE  $Q_f$  AND  $\sigma_n/\sigma_p$  VALUES REPORTED FOR VARIOUS SURFACE PASSIVATION MATERIALS

Schemes	$Q_f \text{ (cm}^{-2}\text{)}$	$\sigma_n/\sigma_p$
a-Si:H	$\pm 10^9, \pm 10^{10}, \pm 10^{11}$ [22]–[24]	-
SiO <sub>x</sub>	$+10^{10}, +10^{11}, +10^{12}, +10^{13}$ [17], [25]–[27]	100 – 1000 [17], [28]
SiN <sub>x</sub>	$+10^{11}, +10^{12}, +10^{13}$ [29]–[33]	0.01 – 1* [34]–[36]
SiC <sub>x</sub>	$+10^{10}, \pm 10^{11}, +10^{12}$ [37]–[39]	-
AlO <sub>x</sub>	$-10^{11}, -10^{12}, -10^{13}$ [40]–[43]	10 – 1000 [42], [44], [45]
AlN <sub>x</sub>	$+10^{10}, -10^{11}, \pm 10^{12}$ [46], [47]	-
TiO <sub>x</sub>	$\pm 10^{11}, -10^{12}$ [48], [49]	-
HfO <sub>x</sub>	$\pm 10^{11}, \pm 10^{12}$ [43], [50]–[52]	-
GaO <sub>x</sub>	$\pm 10^{11}, \pm 10^{12}$ [53]–[55]	-
MgO <sub>x</sub>	$\pm 10^{10}, \pm 10^{11}$ [56]	-
PO <sub>x</sub>	$+10^{12}$ [57], [58]	-
TaO <sub>x</sub>	$-10^{12}$ [59], [60]	-
NbO <sub>x</sub>	$-10^{12}$ [61]	-
ZrO <sub>x</sub>	$-10^{10}$ [62]	-

\*Ratio of the dominant defect.

the material itself, but also heavily rely on the scheme structures, process conditions, and postannealing conditions. The basic principle of field-effect passivation is the charge-assisted population control, hence, the magnitude of fixed charge  $Q_f$  at the Si-dielectric interface is our main focus. Table I presents a summary of the typical ranges of  $Q_f$  that are reported for the most widely studied silicon surface passivation films, revealing that the magnitude of  $Q_f$  is typically in the range of  $10^9$ – $10^{13} \text{ cm}^{-2}$ .

However, the extended SRH model (1) governs that the intrinsic recombination velocity ratio of electron and hole ( $S_{n0}/S_{p0}$ ), which relates to the ratio of the electron and hole capture cross section ( $\sigma_n/\sigma_p$ ), is also critical for quantifying the surface recombination rate. The surface recombination rate is highest when  $p_s/n_s \approx \sigma_n/\sigma_p$  [17], and is limited by either the electron concentration (when  $n_s/\sigma_p < p_s/\sigma_n$ ) or hole concentration (when  $n_s/\sigma_p > p_s/\sigma_n$ ). Furthermore, combining with (2) and acknowledging that  $S_{n0} = v_{thn} N_{it} \sigma_n$  and  $S_{p0} = v_{thp} N_{it} \sigma_p$ , (3) can be simplified under  $p$ -type accumulation condition

$$S_{\text{eff}} = \left( \frac{N_{it}}{\Delta n} \right) \frac{p_s n_s}{\frac{p_s}{v_{thn} \sigma_n} + \frac{n_s}{v_{thp} \sigma_p}} \approx \frac{N_{it} v_{thn} \sigma_n n_s}{\Delta n} \quad (4)$$

where  $v_{thn}$  and  $v_{thp}$  are the thermal velocities of electrons and holes, and  $N_{it}$  is the energy-independent interface defect density, which relates to chemical passivation. Equation (4) reveals that the surface recombination only depends on the surface minority carrier concentration when the majority-carrier-related term can be neglected. As the asymmetry of  $v_{thn}$  and  $v_{thp}$  is small ( $v_{thn}/v_{thp} \approx 1.2$ ), this condition will be satisfied only when  $p_s/\sigma_n \gg n_s/\sigma_p$ . Since the asymmetry of surface carrier densities is typically larger than that of the surface capture cross section,  $p_s \gg n_s$  should be satisfied primarily, which is generally realized when  $Q_f$  is effectively high.

TABLE II  
SUMMARY OF WAFER DIAMETERS, PHYSICS MODELS, AND PARAMETERS USED  
IN THE SIMULATIONS

Basic setup	
Silicon bulk thickness	200 $\mu\text{m}$
Dielectric layer thickness	20 nm
Bulk doping	Boron $5 \times 10^{15} \text{ cm}^{-3}$
Temperature	298 K
Injection condition	Quasi-steady-state conditions with a uniform generation
Carrier statistics	Fermi–Dirac statistics and statistic quantum correction by the basic density gradient quantization model [66]
Bulk setup	
Recombination	Richter’s Auger recombination model [67], radiative recombination model, and single-level-defect Shockley–Read–Hall (SRH) recombination model [68]
SRH carrier lifetime	$\tau_{n0} = \tau_{p0} = 2 \times 10^{-3} \text{ s}$
Band gap narrowing	Schenk’s model [69]
Mobility	Philips unified mobility model [70]
Space charge distribution	Poisson’s equation [16]
Surface setup	
Surface recombination rate $U_s$	Extended SRH equation for single-level defects
Interface fixed charge $Q_f$	From $-1 \times 10^9$ to $-1 \times 10^{13} \text{ cm}^{-2}$
Local intrinsic surface recombination velocity $S_0^*$	$S_{n0} = 0.1 \times S_{p0} = 3000 \text{ cm s}^{-1}$ $S_{n0} = 10 \times S_{p0} = 3000 \text{ cm s}^{-1}$ $S_{n0} = 100 \times S_{p0} = 3000 \text{ cm s}^{-1}$

\* Assuming the thermal velocities of electrons and holes are identical ( $v_{thn} = v_{thp}$ ), therefore  $S_{n0}/S_{p0} = \sigma_n/\sigma_p$ .

Since the  $\sigma_n/\sigma_p$  values have not been reported for all surface passivation films, we will predominantly focus on the  $\sigma_n/\sigma_p$  ranges, which are reported in Table I for the most widely studied surface passivation films. The  $\sigma_n/\sigma_p$  range of  $\text{AlO}_x$  is similar to that of  $\text{SiO}_x$ , very likely because of the presence of a thin  $\text{SiO}_x$  at the  $\text{AlO}_x$ –Si interface [44], [63]. It is not unrealistic to assume that the  $\sigma_n/\sigma_p$  of other oxide passivation layers would have a similar thin interfacial  $\text{SiO}_x$  and consequently a similar  $\sigma_n/\sigma_p$  ratio. In this work, we will examine the following three  $\sigma_n/\sigma_p$  ratios.

- 1)  $\sigma_n/\sigma_p = 0.1$ , which represents the condition of  $\sigma_n < \sigma_p$  observed at  $\text{SiN}_x$ –Si interfaces.
- 2)  $\sigma_n/\sigma_p = 10$ , which represents the condition of  $\sigma_n > \sigma_p$  observed at oxide–Si interfaces.
- 3)  $\sigma_n/\sigma_p = 100$ , which represents the condition of  $\sigma_n \gg \sigma_p$  also observed at oxide–Si interfaces.

### B. Simulation Setup

The numerical simulation work was conducted by means of multidimensional models using Sentaurus TCAD [20], [64], [65]. The simulations focused on *p*-type silicon with negative  $Q_f$  values (in  $\text{cm}^{-2}$ ), i.e., we focused on accumulation conditions. The injection level was determined by the excess minority carrier density at the edge of the space charge region. The details of the simulation setup in this work are summarized in Table II, and a simplified determination procedure of surface passivation

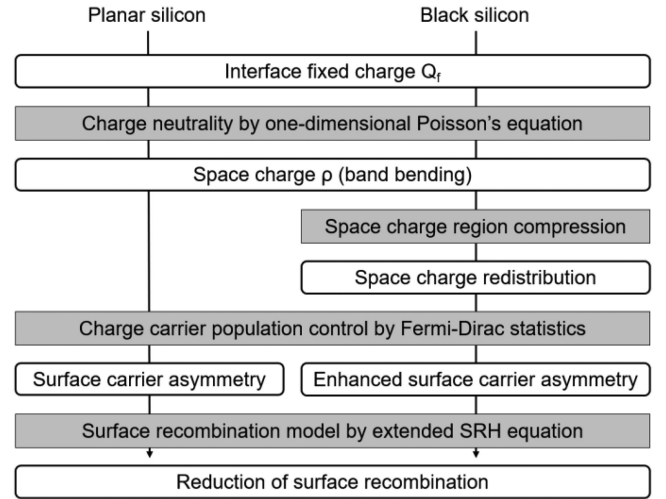


Fig. 1. Simplified schematic diagram of a procedure for the determination of field-effect passivation on planar silicon and b-Si.

performance is shown in Fig. 1. The space charge and minority carrier density in 1-D were determined by a simple two-parallel-surface model. The minority carrier distribution and local surface recombination in the nanofeature were modeled in 2-D, and the b-Si surface recombination was modeled in 3-D numerically for both b-Si wafers and planar wafers. The unit cell representing the b-Si wafer was modeled by using a rotationally symmetric 2-D structure, as shown in Fig. 2, which resulted in a cone-like feature. To unambiguously determine the influence of the nanofeature on the surface passivation compared with a planar surface, we define two factors that associate the absolute effective surface recombination velocities of b-Si ( $S_{\text{eff BS}}$ ) and the reference planar surface ( $S_{\text{eff planar}}$ ): 1) the area factor  $F_{\text{area}}$ , which is the ratio of total surface area and projected area; 2) the  $S_{\text{eff}}$  improvement factor  $F_{\text{SRV}}$ , which is defined as

$$F_{\text{SRV}} = \frac{S_{\text{eff BS}}/F_{\text{area}}}{S_{\text{eff planar}}} \quad (5)$$

where  $S_{\text{eff BS}}/F_{\text{area}}$  is the area-normalized  $S_{\text{eff}}$  of the b-Si surface. An  $F_{\text{SRV}}$  value of 1 means that the surface recombination on b-Si simply scales with the surface area, whereas an  $F_{\text{SRV}}$  lower than 1 implies that the surface recombination is less than you would expect from the increase in surface area.

For a more comprehensive investigation on the characteristics of b-Si surface passivation, a more sophisticated optical simulation method would be required such as finite-difference time domain to quantify the spatially resolved electron-hole pair generation rate. It is shown by Rahman and Boden [71] that the injection levels can be very nonuniform for b-Si surfaces, some parts of which having  $\Delta n \gg 1 \times 10^{15} \text{ cm}^{-3}$ . However, as we wanted to focus on the perturbation of charge-carrier control by b-Si nanofeatures, we decided to assume a uniform optical generation rate in this work as well as a constant bulk injection level of  $\Delta n = 1 \times 10^{15} \text{ cm}^{-3}$ . As this injection level is well below the bulk doping level, it is not expected to change the band bending close to the surface significantly [17].



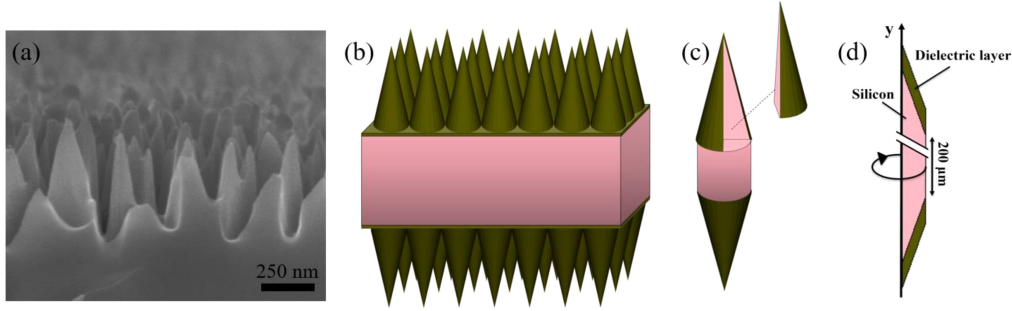


Fig. 2. (a) SEM image of RIE b-Si used in experiments and the schematic of (b) the ideal b-Si wafer model, (c) the unit cell of the ideal b-Si wafer model, and (d) the 2D-to-3D structure of the unit cell by cylindrical coordinate for the numerical simulation. The dielectric layer thickness was 20 nm and the unit cell bulk thickness was 200  $\mu\text{m}$ .

### C. Experimental Details

The experiments were performed on double-side polished, 500  $\mu\text{m}$  thick, boron-doped Czochralski silicon wafers with  $\langle 100 \rangle$  crystal orientation and a resistivity of 5–6  $\Omega\cdot\text{cm}$ . A b-Si surface texture with an average height of  $\approx 300$  nm and an average diameter of  $\approx 150$  nm was formed on a single side of these polished samples using reactive ion etching (RIE) with an STS DRIE Pegasus tool. The samples were etched in an  $\text{SF}_6$  (70 sccm) and  $\text{O}_2$  (100 sccm) plasma for 6 min at a coil power of 3 kW. Before the dielectric layer deposition, the b-Si samples and reference planar samples received a standard Radio Corporation of America cleaning process. A  $\approx 22$  nm ALD  $\text{Al}_2\text{O}_3$  dielectric layer was deposited on both sides of the samples using a CNT Savannah S200 tool with trimethyl aluminum as the precursor and  $\text{H}_2\text{O}$  as the oxidant at a substrate temperature of 200  $^\circ\text{C}$ . The surface passivation provided by the dielectric layers was activated by rapid thermal annealing using a Semco RTP-Jetfirst 200 tool with two different recipes: 400  $^\circ\text{C}$  for 10 min (Group 1) and 350  $^\circ\text{C}$  for 1 min (Group 2) in order to achieve different  $Q_f$  values in the films [72]. Topographical characterization in this work was performed by a field-emission scanning electron microscope (SEM) using an FEI Nova NanoSEM 450 system. The  $\tau_{\text{eff}}$  was measured by quasi-steady-state photoconductance decay method using a Sinton WCT-120 tool with the polished side facing up in order to ensure an equal generation rate in both samples. The  $\text{Al}_2\text{O}_3$ -Si interface total charge density  $Q_{\text{tot}}$  and defect density  $D_{\text{it}}$  of the polished surfaces were determined by corona oxide characterization of semiconductors [73] using a Semilab SDI PV2000 tool.

## III. RESULTS AND DISCUSSION

### A. Minority Carrier Distribution in 1-D Simulations

In this section, we will discuss the main findings from our earlier work about the charge carrier population control resulting from space charge compression in 1-D, which is relevant for understanding the results in 2-D and 3-D. Space charge  $\rho$  induced in the near-surface region is the mirrored charge of  $Q_f$  because of the nature of charge neutrality. We define the effective relative charge  $\omega$  to evaluate the proportion of nonmirrored charge at a

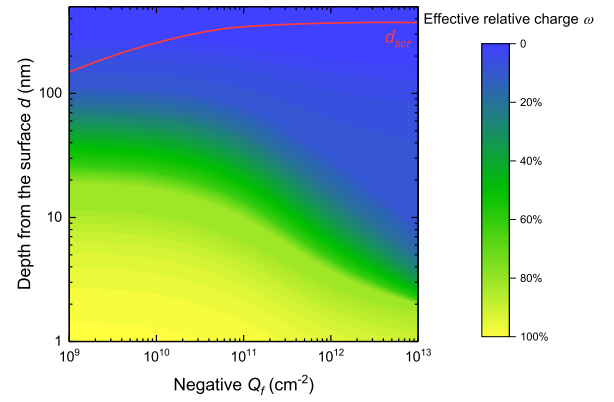


Fig. 3. Effective relative charge  $\omega$  as a function of negative  $Q_f$  and depth from the surface  $d$  of the planar silicon under an injection level of  $1 \times 10^{15} \text{ cm}^{-3}$ .  $\omega$  indicates the fraction of nonmirrored  $Q_f$  at a certain depth  $d$ . Since the space charge  $\rho$  has an opposite polarity to  $Q_f$ ,  $\omega$  is 100% at the surface and reduced as  $d$  increases, and will be  $\approx 0$  at the edge of space charge region  $d_{\text{scr}}$ . The red line shows  $d_{\text{scr}}$  as a function of negative  $Q_f$ .  $d_{\text{scr}}$  is defined at the depth where  $\rho = 1 \times 10^{13} \text{ cm}^{-3}$  ( $\rho \ll N_A + \Delta n$ ). The result is reproduced from [19].

certain depth for an infinite-thick substrate. It is defined as

$$\omega = \frac{Q_f + \int_0^d \rho(x) dx}{Q_f} \quad (6)$$

where  $d$  is the investigated depth and  $\rho(x)$  is the space charge density at depth  $x$ . When  $d = 0$ ,  $\omega = 100\%$ . When  $d$  is equal to the depth of the space charge region,  $\omega = 0$ . Fig. 3 shows the relative distribution of  $\rho$  resulting from  $Q_f$  at the surface. When  $|Q_f| < 1 \times 10^{11} \text{ cm}^{-2}$ ,  $\rho$  extends very deep into the wafer and  $\omega \approx 80\%$  at 10 nm, meaning that 80% of charge is nonmirrored at this depth. However, when  $Q_f$  is relatively large ( $|Q_f| > 1 \times 10^{12} \text{ cm}^{-2}$ ),  $\rho$  is mainly concentrated in the near-surface region.  $> 80\%$  of  $\rho$  is already mirrored in the first 10 nm ( $\omega < 20\%$ ) and there is  $\approx 50\%$  of  $\rho$  already mirrored in the first 3 nm ( $\omega = 50\%$ ) for a  $Q_f = -1 \times 10^{13} \text{ cm}^{-2}$ . Therefore, the first finding is that  $Q_f$  is almost fully mirrored at 100 nm from the surface for all relevant  $Q_f$  values and is mirrored increasingly closer to the surface for higher  $Q_f$  values. In Fig. 4, we demonstrate the impact on the  $\rho$  distribution when the wafer thickness is smaller than the depth of the space charge region. We simulate the impact by the addition of second surface

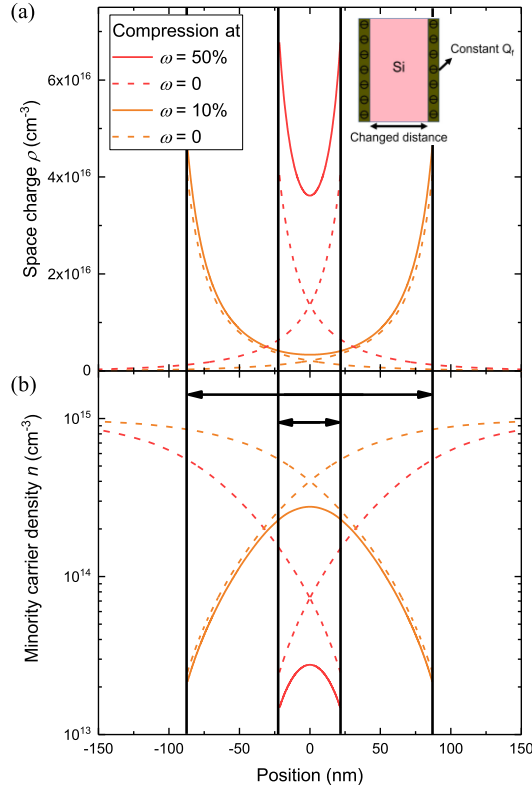


Fig. 4. (a) Space charge density  $\rho$  and (b) minority carrier density as a function of the position in two symmetrically lifetime structures. The position is shown relative to the middle of the sample for easy comparison. The thickness of the two lifetime structures (indicated by the black arrows) was chosen such that 50% (red) or 90% (yellow) or the charge was already mirrored at the depth of the second surface. The solid lines show the values for the symmetrical structures, whereas the dashed lines show the values for each surface without the effect of the second surface. The results clearly show compression of the space charge and corresponding reduction in the minority carrier density at the surface. The result is reproduced from [19].

with an identical  $Q_f$  in a similar way as would happen for a typical symmetrically coated minority charge carrier lifetime sample that is used for experimentally determining  $S_{\text{eff}}$ . We reduce the distances of opposite surfaces of wafers to two conditions: 1) 43 nm opposite-surface distance where 50% of  $\rho$  is redistributed; 2) 174 nm opposite-surface distance where 10% of  $\rho$  is redistributed. We show that this results in space charge region compression and a corresponding change in the minority carrier density. As the model is symmetric and the net electric field is zero at the center, the compressed space charge region depth is half of the opposite-surface distance. The impact strongly depends on the original  $\omega$  at that position. When there is 50% of  $\rho$  redistributed (compression starts at the position where  $\omega = 50\%$  originally), we see a remarkable difference in  $\rho$  and the resulting minority carrier charge density. When there is only 10% of  $\rho$  redistributed, the impact on  $\rho$  is relatively small and, consequently, the minority carrier concentration at the surface is barely affected [19].

Consequently, we can conclude that space charge region compression is determined by the original  $\omega$  value at the center of opposite surfaces. There will be a significant  $\rho$  increase when  $\omega$  is relatively high, whereas for small  $\omega$  values, there will be no impact. As we are focussing on accumulation conditions, space

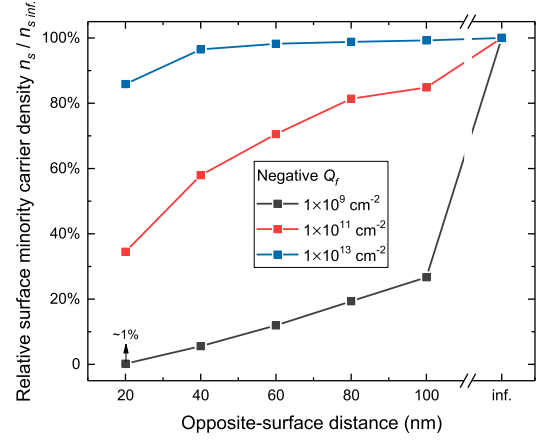


Fig. 5. Effects of opposite-surface distance on the surface minority carrier densities for different  $Q_f$  in 1-D simulations. The surface minority carrier densities are compared with the densities in the substrate with an infinite thickness to evaluate the effectiveness (relative surface minority carrier density in percentage).

charge region compression will always result in a reduction of the minority carrier density at the surface. In Fig. 5, we show the relative surface minority carrier density as a function of the distance between the opposite surfaces for three  $Q_f$  values. When the  $Q_f$  value is high, we can only see a marginal impact on the relative surface minority carrier density with only a  $\approx 15\%$  reduction for a distance of 20 nm, which can be attributed to the fact the  $\rho$  is mainly concentrated at the first 5 nm from the surface. For moderate  $Q_f$  value of  $-1 \times 10^{11} \text{ cm}^{-2}$ , the relative surface minority carrier density is decreased from  $\approx 83\%$  with a 100 nm distance, to  $\approx 35\%$  with a 20 nm distance. Under the low  $Q_f$  value of  $-1 \times 10^9 \text{ cm}^{-2}$ , the effects of the decreasing opposite-surface distance are the most remarkable. There is  $\approx 75\%$  reduction of the relative surface minority carrier density with a 100 nm distance, and the reduction can be even up to  $\approx 99\%$  when the opposite surfaces are only 20 nm apart.

### B. Minority Carrier Distribution in 2-D Simulations

Next, we will investigate the minority carrier distribution in 2-D nanofeatures and compare them to planar surfaces.

Fig. 6(a)–(c) shows the minority carrier distribution in the 2-D nanofeatures with a width of 100 nm and a height of 500 nm relative to planar surfaces. When  $Q_f$  is low, the nanofeature can enhance the carrier asymmetry and reduce the minority carrier density  $n$ , as illustrated in Fig. 6(a). For a moderate  $Q_f = -1 \times 10^{11} \text{ cm}^{-2}$  shown in Fig. 6(b), it can be seen that there is a reduction of  $n$  up to 90% in the nanofeature compared with the planar surface, especially near the nanofeature peak. In Fig. 6(c), there is almost no difference for  $n$  of the nanofeature compared with the planar surface. This means that the nanofeature will hardly affect the charge carrier population control when  $Q_f$  is high. Fig. 6(d) shows the relative surface minority carrier density of nanofeatures ( $n_s \text{ BS} / n_s \text{ planar}$ ). It indicates that the nanofeature leads to a relatively uniform  $\approx 35\%$  to  $\approx 45\%$  reduction of  $n_s$  for a low  $Q_f$  ( $-1 \times 10^9 \text{ cm}^{-2}$ ). When the  $Q_f$  value is moderate at  $-1 \times 10^{11} \text{ cm}^{-2}$ , the  $n_s$  is decreased to  $< 40\%$  except for the region near the bottom of nanofeature, whereas

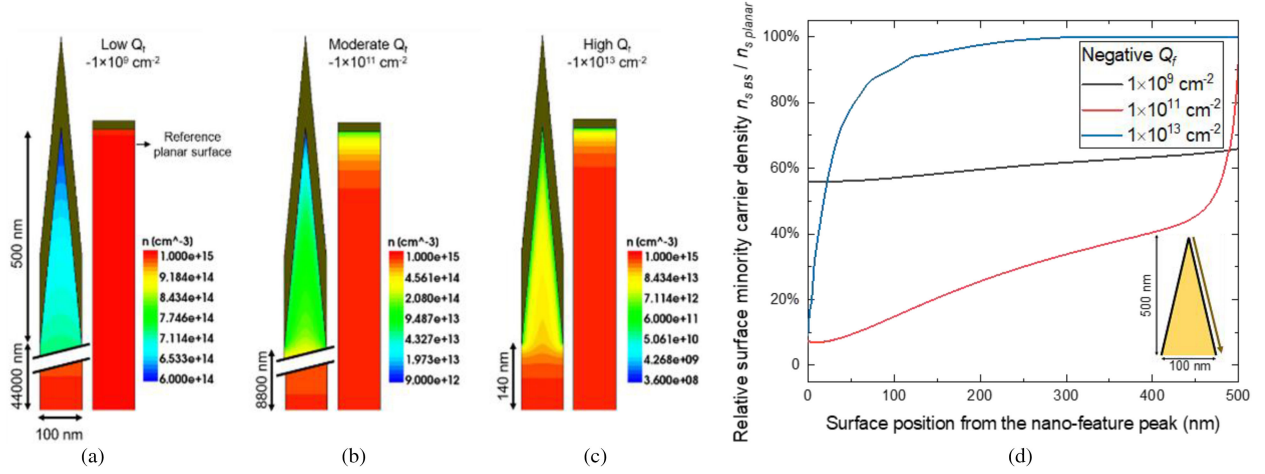


Fig. 6. Minority carrier distributions under (a) low, (b) moderate, and (c) high  $Q_f$  conditions with  $1 \times 10^{15} \text{ cm}^{-3}$  injection in the nanofeatures compared with a planar surface, and (d) the relative surface minority carrier density at the nanofeature surfaces from the peak to the bottom. The simulation setup is shown in Table II. The simulated feature had a width of 100 nm and a height of 500 nm.

the significant reduction in  $n_s$  is concentrated in the peak of nanofeature for the high  $Q_f$  value at  $-1 \times 10^{13} \text{ cm}^{-2}$ . In general, we can see some consistency as well as inconsistency between the 1-D results in Fig. 5 and 2-D results in Fig. 6. Both results of high  $Q_f$  show a near 100% of relative surface minority carrier density, except when the opposite-surface distance is extremely small. However, when comparing the low and moderate  $Q_f$  conditions, the relative surface minority carrier density of low  $Q_f$  is lower in 1-D, whereas its 2-D result is higher. This can be explained by the effect of dimension expansion where the minority carriers will be repelled into a deep region in 2-D. It should be noted that the carrier concentration is affected up to depths of 44 and 8.8  $\mu\text{m}$ , respectively, for low and moderate  $Q_f$ . This is not the results of space charge compression but from a relatively high surface recombination rate. For example, the surface recombination current for a 500 nm height nanofeature with  $Q_f = -1 \times 10^9 \text{ cm}^{-2}$  is  $3598 \text{ fA cm}^{-2}$ , extremely large compared with the bulk recombination current of only  $20 \text{ fA cm}^{-2}$ . As we are simulating steady-state conditions, the cumulative recombination rate has to equal the cumulative generation rate. The high surface recombination current results in a high minority carrier diffusion current to the surface, and the magnitude of the diffusion current depends on the nanofeature size (as the area factor  $F_{\text{area}}$  increases as a function of the nanofeature size), i.e., the minority carrier profile in the sample is the result of a diffusion current and not the result of charge carrier population control from the surface  $Q_f$ . This work predominantly focuses on the minority carrier density at the surface, which is, in most cases, not materially affected by the diffusion current.

### C. Surface Minority Carrier Density in 3-D Simulations

In the previous sections, we revealed the mirror  $\rho$  distribution characteristics and examined the minority carrier distribution in nanofeatures by 1-D and 2-D simulations, especially the surface minority carrier. In this section, we will still focus on the surface minority carrier and expand the simulations to 3-D.

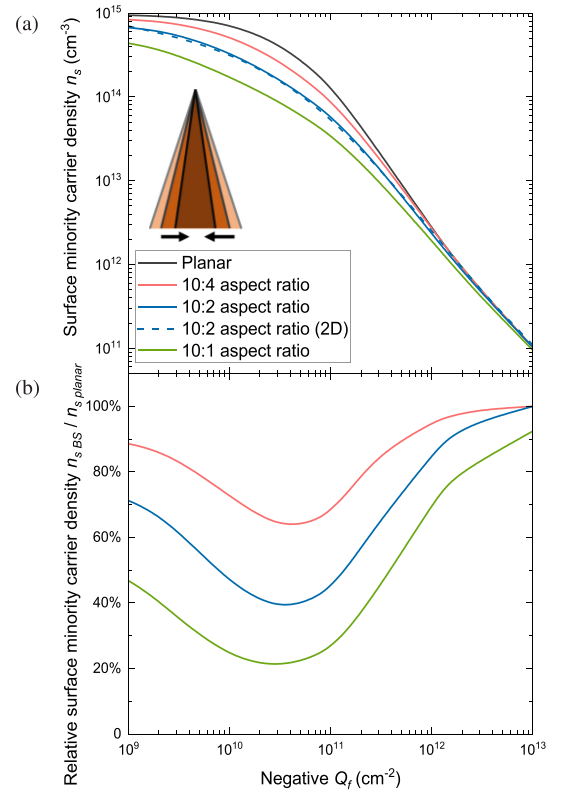


Fig. 7. 3-D comparison of (a) the average surface minority carrier density of planar and b-Si surfaces and (b) the corresponding relative surface minority carrier density with 500 nm height and different aspect ratios under  $1 \times 10^{15} \text{ cm}^{-3}$  injection condition. The simulation setup is shown in Table II.

Fig. 7(a) presents the effects of the nanofeature aspect ratio on surface minority carrier density  $n_s$  under different  $Q_f$  conditions. For a 10:2 aspect ratio, the 2-D and 3-D results are compared and show a nonsignificant difference. This means the findings by 2-D simulations can be extrapolated for 3-D. In Fig. 7(b), the 3-D results demonstrate that the relative surface

minority carrier density is effectively reduced in the moderate  $Q_f$  range and the reduction is enlarged as the nanofeature aspect ratio increases, because of the reduction mainly depending on the distance between the surfaces. In the investigated highest aspect ratio, the surface minority carrier density can be reduced to 20%, and it can be expected that the reduction can be  $> 80\%$  when the aspect ratio is larger than 10:1. However, as a result of a deeper influenced region, the nanofeature with low  $Q_f$  values has a higher relative surface minority carrier density. In addition, the surface minority carriers of nanofeature with high  $Q_f$  values are hardly affected, and this can be explained by the fact that the charge carrier population, in this case, is not significantly affected by nanofeature diameters  $> 10$  nm.

#### D. Effects of $\sigma_n/\sigma_p$ and Injection Levels on Surface Passivation

We have investigated the relative surface minority carrier densities of nanofeatures by 1-D, 2-D, and 3-D simulations. However, the relative surface minority carrier can be used to evaluate the surface passivation performance only when  $n_s/\sigma_p \ll p_s/\sigma_n$  as discussed in Section II-A. Here, we will go further to determine the effects of  $\sigma_n/\sigma_p$  and injection levels on the surface passivation of a nanofeature by 2-D simulations. The surface passivation performance is evaluated by the  $S_{\text{eff}}$  improvement factor  $F_{\text{SRV}}$  calculated by (5).

Fig. 8 presents the corresponding surface passivation performances of cases in Fig. 6 for three different  $\sigma_n/\sigma_p$  and two injection levels for a nanofeature with a width of 100 nm and a height of 500 nm. For the moderate ( $-1 \times 10^{11} \text{ cm}^{-2}$ ) and high ( $-1 \times 10^{13} \text{ cm}^{-2}$ )  $Q_f$ , the graphs are mostly identical to the relative minority carrier density graphs shown in Fig. 6(d) for an identical nanofeature, in particular for all conditions shown with  $\sigma_n/\sigma_p = 0.1$ . This is because of the fact that surface recombination is limited by the supply of minority carriers and can be described by (4). For low  $Q_f$  ( $-1 \times 10^9 \text{ cm}^{-2}$ ), the value of  $F_{\text{SRV}}$  is higher than that of relative minority carrier density as surface recombination in this case also is determined by the majority carrier density. The situation gets a bit more complicated when the  $\sigma_n/\sigma_p$  is 10 or 100. For low injection levels, surface recombination is still mainly limited by the surface minority carrier density. For an injection level of  $1 \times 10^{15} \text{ cm}^{-3}$ , however, surface recombination has a strong dependence on the supply of both electrons and holes and field-effect passivation can, in some cases, even increase surface recombination losses. This phenomenon has been well discussed in the work of Aberle *et al.* [17], where it was presented that there is a maximum  $S_{\text{eff}}$  when  $p_s/n_s \approx \sigma_n/\sigma_p$ , which is valid for both of accumulation and inversion conditions. This maximum  $S_{\text{eff}}$  was also observed in previous work [18], [42], [74]. Here, assuming  $\sigma_n/\sigma_p = S_{n0}/S_{p0} = 100$  under  $1 \times 10^{15} \text{ cm}^{-3}$  injection, we find that the maximum  $S_{\text{eff}}$  at  $Q_f \approx 5 \times 10^{10} \text{ cm}^{-2}$  in 1-D planar condition. When  $Q_f = 1 \times 10^9 \text{ cm}^{-2}$  on the nanofeature surface, compared with the planar surface, the equivalent surface carrier densities will be approaching the condition where  $Q_f \approx 5 \times 10^{10} \text{ cm}^{-2}$  on the planar surface. This phenomenon is not only of academic interest as a  $1 \times 10^{15} \text{ cm}^{-3}$  injection level is quite typical for solar cell operations. Consequently, enhanced

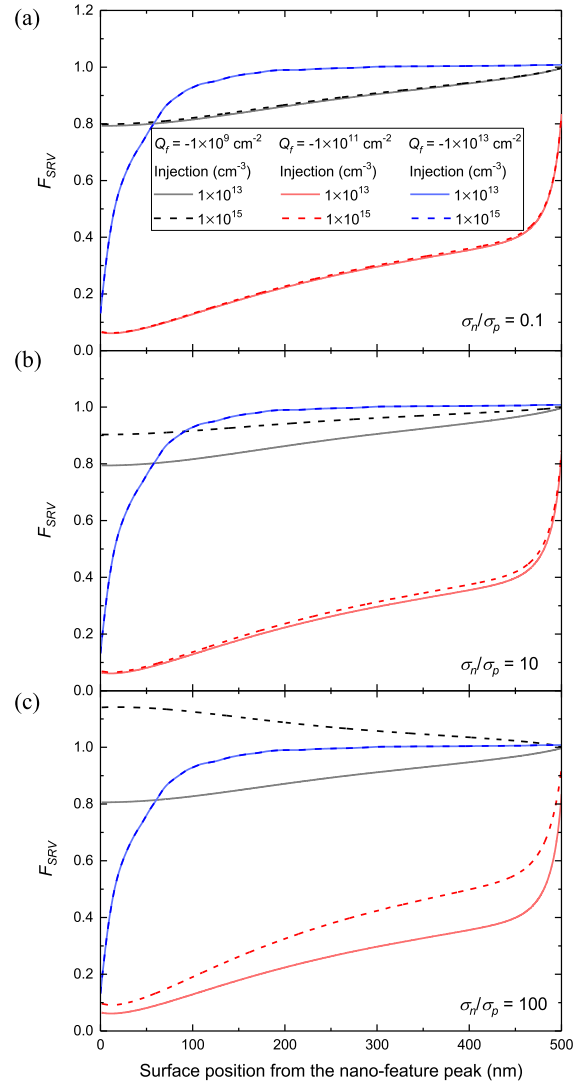


Fig. 8. Effects of  $\sigma_n/\sigma_p$ ,  $Q_f$ , and injection levels on the surface passivation performance for a nanofeature with a width of 100 nm and a height of 500 nm (identical case in Fig. 6). Three  $\sigma_n/\sigma_p$  ratios are shown: (a) 0.1, (b) 10, and (c) 100. For each  $\sigma_n/\sigma_p$  ratio, three different  $Q_f$  and two different injection levels are applied. The change of surface passivation performance is evaluated by  $F_{\text{SRV}}$ . A lower  $F_{\text{SRV}}$  means a better surface passivation compared with a planar surface.

charge carrier population control will not always contribute to the reduction of surface recombination losses. An improvement in surface passivation performance can always be achieved only when  $\sigma_n$  is not much larger than  $\sigma_p$  for  $p$ -type accumulation conditions, and vice versa for  $n$ -type accumulation conditions.

#### E. Surface Passivation Under a High $\sigma_n/\sigma_p$ Condition in 3-D Simulations and Experiments

In this section, we will focus on the improvement of surface passivation performance under a  $1 \times 10^{15} \text{ cm}^{-3}$  injection with a high  $\sigma_n/\sigma_p = 100$  (i.e.,  $S_{n0}/S_{p0} = 100$ ), which is widely observed in oxide surface passivation films. This section includes defining  $Q_f$  ranges based on  $F_{\text{SRV}}$  and investigating the effects of the b-Si nanofeature diameter, size, and height on the



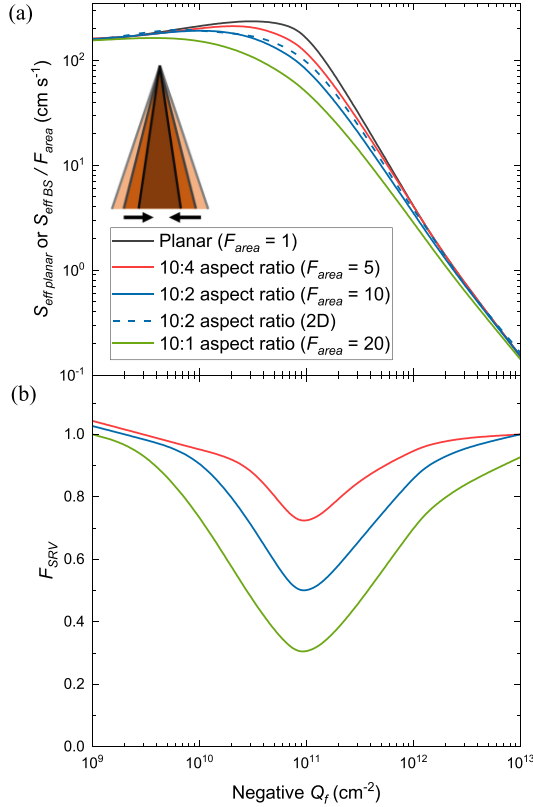


Fig. 9. Corresponding (a) effective surface recombination velocities of reference planar surface and area-normalized b-Si and (b)  $F_{SRV}$  of cases in Fig. 7 under  $S_{n0} = 100 \times S_{p0} = 3000$  cm s<sup>-1</sup> ( $\sigma_n/\sigma_p = 100$ ) and  $1 \times 10^{15}$  cm<sup>-3</sup> injection condition. The absolute  $S_{eff, BS}$  can be determined accordingly.

field-effect passivation under different  $Q_f$  conditions. Finally, the findings will be validated by experiment results.

Fig. 9 shows the corresponding area-normalized  $S_{eff}$  and  $F_{SRV}$  of Fig. 7 to quantify the change of surface passivation performance. We can see a very similar trend of the relative surface minority carrier densities in Fig. 7(b) and  $F_{SRV}$  in Fig. 9(b) when  $|Q_f| > 1 \times 10^{11}$  cm<sup>-2</sup>. This is attributed to the fact that the surface recombination is only decided by the surface minority carrier density when  $Q_f$  is moderate or high. Hence, the reduction of surface minority carrier density will contribute to the reduction of  $F_{SRV}$  directly. However, when  $|Q_f| < 1 \times 10^{11}$  cm<sup>-2</sup>, the surface passivation will also be limited by the supply of majority carriers, and there is even inferior surface passivation under low  $Q_f$  conditions as discussed in Section III-D. According to Fig. 9(b), we can define the  $Q_f$  range by low ( $|Q_f| < 1 \times 10^{10}$  cm<sup>-2</sup>), moderate ( $1 \times 10^{10}$  cm<sup>-2</sup>  $< |Q_f| < 1 \times 10^{12}$  cm<sup>-2</sup>), and high ( $|Q_f| > 1 \times 10^{12}$  cm<sup>-2</sup>).

The effects of the b-Si nanofeature sizes and heights are investigated by three surface passivation schemes with widely observed  $Q_f$  ( $-1 \times 10^{11}$  cm<sup>-2</sup>,  $-1 \times 10^{12}$  cm<sup>-2</sup>, and  $-3 \times 10^{12}$  cm<sup>-2</sup>) and constants  $S_{n0}$  and  $S_{p0}$ , as shown in Figs. 10 and 11. The simulations investigate the b-Si with diameters from 60 to 180 nm, and heights from 100 to 500 nm ( $F_{area} = 2 - 10$ ), which are practical for most RIE fabricated b-Si surfaces [3]. Fig. 10 shows that increasing the nanofeature size will lead to the enlargement of  $F_{SRV}$ . Specifically, the area-normalized  $S_{eff}$

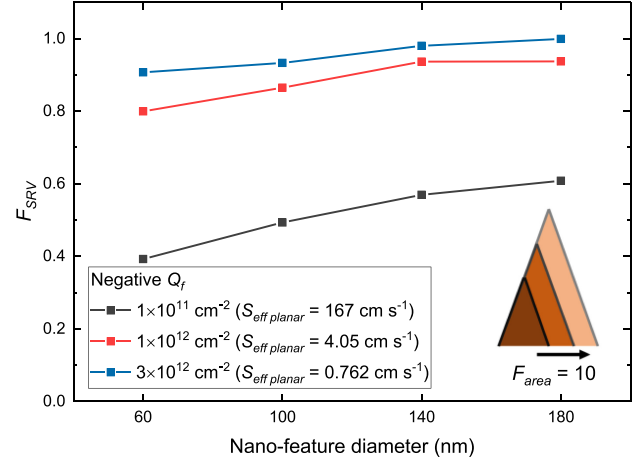


Fig. 10. Effects of nanofeature sizes on  $F_{SRV}$  with the constant aspect ratio 10:2 (area factor  $F_{area} = 10$ ). Three different  $Q_f$  are investigated under  $S_{n0} = 100 \times S_{p0} = 3000$  cm s<sup>-1</sup> and  $1 \times 10^{15}$  cm<sup>-3</sup> injection condition. The absolute  $S_{eff, BS}$  can be determined by (5).

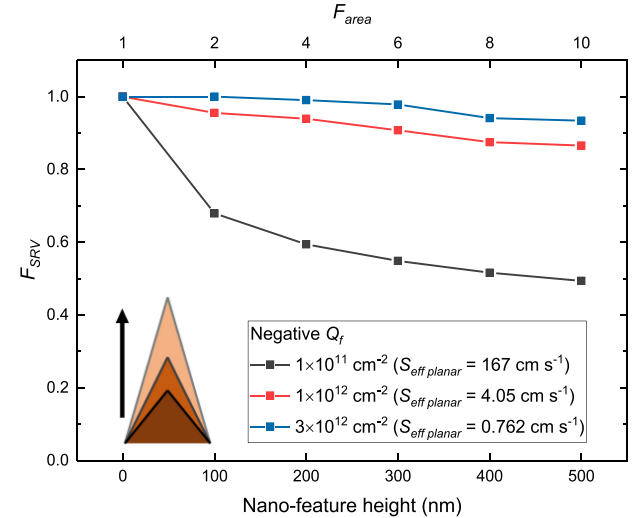


Fig. 11. Effects of nanofeature heights on  $F_{SRV}$  by the constant feature diameter 100 nm. Three different  $Q_f$  are investigated under  $S_{n0} = 100 \times S_{p0} = 3000$  cm s<sup>-1</sup> and  $1 \times 10^{15}$  cm<sup>-3</sup> injection condition. The absolute  $S_{eff, BS}$  can be determined by (5).

reduction is relatively significant under moderate  $Q_f$  conditions ( $-1 \times 10^{11}$  cm<sup>-2</sup>) and its  $F_{SRV}$  value is in the range of 0.4 – 0.6. Nevertheless, for high  $Q_f$  values, the area-normalized  $S_{eff}$  reduction is relatively modest ( $F_{SRV} > 0.8$ ), which is consistent with the previous conclusions. Fig. 11 indicates that increasing the nanofeature height will contribute to the reduction of  $F_{SRV}$ . The nanofeature with moderate  $Q_f$  has a  $F_{SRV} = 0.5 - 0.7$ , whereas the high  $Q_f$  will only lead to  $F_{SRV} > 0.9$ . It should be noted that there is a significant area-normalized  $S_{eff}$  reduction from the planar surface to the short nanofeature (from 0 to 100 nm height) with  $F_{SRV} \approx 0.7$  for  $Q_f = -1 \times 10^{11}$  cm<sup>-2</sup>. This means even a slight b-Si texturing can cause a remarkable reduction of surface recombination losses for moderate  $Q_f$ .

The results of Figs. 10 and 11 can be understood by the findings from Sections III-A and III-B. For high negative  $Q_f$



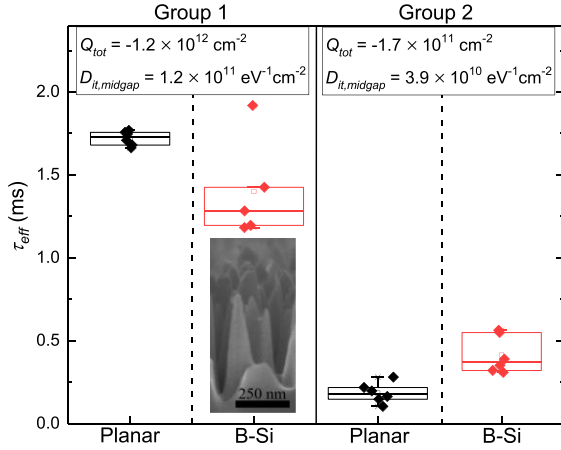


Fig. 12. Measured  $\tau_{\text{eff}}$  of Groups 1 and 2 at injection  $3 \times 10^{15} \text{ cm}^{-3}$ . The interface properties shown were determined on planar samples.

of  $-3 \times 10^{12} \text{ cm}^{-2}$ , the space charge is mirrored close to the surface and consequently there is no improvement in field-effect passivation by space charge compression with a  $F_{\text{SRV}}$  value of 1 irrespective of the shape of the nanofeature. For lower negative  $Q_f$ , the  $F_{\text{SRV}}$  is lower than 1 indicating a relative improvement in surface passivation and the value reduces for smaller features because of space charge compression. In addition, Figs. 10 and 11 compare three  $Q_f$  cases where there is either moderate or strong field-effect passivation with constant chemical passivation, which leads to large differences in  $S_{\text{eff planar}}$ . The main focus of this work is on the relative surface recombination compared with the projected area as expressed by  $F_{\text{SRV}}$ . The absolute  $S_{\text{eff BS}}$  can easily be calculated from (5).

We empirically validate the findings by comparing the change of surface passivation performance for a moderate  $Q_f$  case and a high  $Q_f$  case. We propose reasonable assumptions for the experimental results shown in Fig. 12, to focus on the effects of b-Si nanofeatures on the surface carrier densities within the scope of this work. The  $D_{it}$  and  $Q_{\text{tot}}$  of each group were only measured on planar samples. It is assumed that the measured lowest  $D_{it}$  is  $D_{it,\text{midgap}}$ ;  $Q_{\text{tot}} = Q_f$  as  $D_{it,\text{midgap}}$  is relatively small; the effects of surface damage and crystal orientations on b-Si surfaces are negligible; the surface passivation layers on b-Si surfaces are conformal and identical to those on planar surfaces; the sole factor that causes the variation of  $\tau_{\text{eff}}$  is the surface passivation. The experimental results validate that there is a beneficial surface carrier population control enhancement (field-effect passivation enhancement) when  $Q_f$  is moderate. Since  $Q_f$  was high in Group 1, the surface passivation on the b-Si samples was inferior compared with the reference planar samples because of the larger surface area and the modest field-effect passivation enhancement. However, when  $Q_f$  was moderate as resulted in Group 2, the surface recombination losses on the b-Si samples had a clear reduction caused by the field-effect enhancement, which even compensated for the increase in surface area as the b-Si  $\tau_{\text{eff}}$  was higher than the planar  $\tau_{\text{eff}}$ . Therefore, instead of the field-effect passivation enhancement, which was proposed in the literature, the excellent

surface passivation of the high- $Q_f$  ALD- $\text{Al}_2\text{O}_3$  layers on b-Si surfaces can be attributed to the extremely low  $S_{\text{eff}}$  [40], [67], [75], [76], and consequently, the total recombination in the solar cell is not dominated by surface recombination despite the larger surface area.

#### F. Suggestions for Black Silicon Surface Passivation Optimization

Table I suggests that most surface passivation schemes will show a moderate or high  $Q_f$ , except a-Si:H and some less common novel passivation schemes. This means there is no universal solution to the b-Si surface passivation optimization for a given passivation material. According to the conclusions of Sections III-D and III-E, assuming the passivation layer coverage is conformal on the b-Si surface, decreasing the b-Si surface area will reduce surface recombination losses as the number of surface defects scales with the surface area. For passivation films with a low  $Q_f$  at an injection level of  $1 \times 10^{15} \text{ cm}^{-3}$ , the effects of nanofeatures on the surface passivation depend on  $\sigma_n/\sigma_p$ , which is determined by the passivation film. For films with a  $\sigma_n/\sigma_p$  above 10, we can see an increase in surface recombination losses when using surface passivation films with a low  $Q_f$ . For surface passivation films with a moderate  $Q_f$ , balancing the surface area and the nanofeature structure is important, since both increasing the aspect ratio and decreasing the size can enhance the field-effect passivation effectively but also change the surface area. According to Section III-E, the typical RIE fabricated b-Si surfaces with moderate  $Q_f$  will show a  $F_{\text{SRV}} = 0.3\text{--}0.7$ . This means the issue of increased surface areas with  $F_{\text{area}} = 1.4\text{--}3.3$  for such b-Si surfaces could be eliminated by moderate  $Q_f$  because of the compensation of enhanced field-effect passivation. Finally, although there is no additional reduction in surface recombination for b-Si surfaces compared with planar surfaces when using passivation films with a high  $Q_f$ , obviously these films still provide the best surface passivation on these surfaces.

In this work, we only focused on accumulation conditions, but the conclusions also guide the surface passivation under inversion conditions. For optimal surface passivation, a relatively high  $Q_f$  is required to invert the surface. However, because of the effects of enhanced charge carrier population control in the nanofeatures, the required magnitude of  $Q_f$  will be lower on b-Si compared with planar surfaces. One representative case is thermally grown  $\text{SiO}_2$  on *p*-type substrates. Khandelwal *et al.* [77] found that the surface passivation of the undiffused *p*-type b-Si surface by thermally grown  $\text{SiO}_2$  is better than that of the reference random-pyramid surface, whereas the b-Si area was beyond twice of the random-pyramid area. Thermally grown  $\text{SiO}_2$  typically shows a moderate positive  $Q_f$  [17], which may not be able to cause a beneficial inversion depending on the surface doping. However, in this case, it is possible that the inversion is beneficial and the improved field-effect passivation of the b-Si sample overcomes the drawback of its larger surface area.

## IV. CONCLUSION

The characteristics of field-effect passivation on undiffused b-Si surfaces under accumulation conditions have been investigated through 1-D/2-D/3-D wafer modeling using Sentaurus TCAD. The effects of b-Si nanofeatures on the charge carrier population control for the surface passivation have been studied. It is shown that the minority charge carrier concentration can be significantly lower on b-Si compared with a planar surface. This possibly explains why a  $1/Q_f^4$  dependence was reported in [6]. By examining the surface carrier population control of the b-Si nanofeatures and extracting the corresponding area-normalized  $S_{\text{eff}}$ , we find low  $Q_f$  conditions ( $|Q_f| < 1 \times 10^{10} \text{ cm}^{-2}$ ) will lead to an improved or inferior field-effect passivation depending on  $\sigma_n/\sigma_p$  and injection levels. When  $Q_f$  is in the moderate range ( $1 \times 10^{10} \text{ cm}^{-2} < |Q_f| < 1 \times 10^{12} \text{ cm}^{-2}$ ), there is a remarkable reduction of the area-normalized  $S_{\text{eff}}$  by up to  $\approx 70\%$ . Moreover, the results show that field-effect passivation on b-Si surfaces works identically to that on planar surfaces when  $Q_f$  conditions are high ( $|Q_f| > 1 \times 10^{12} \text{ cm}^{-2}$ ), this contradicts the previous hypothesis that a high  $Q_f$  will contribute to the minority carrier depletion in b-Si nanofeatures and lead to a boost in surface passivation. Finally, we used the findings of this work to guide how to select the appropriate surface passivation film for b-Si surfaces. For  $p$ -type accumulation conditions, a low- $Q_f$  scheme results in a relative improvement when  $\sigma_n/\sigma_p < 10$ . A moderate- $Q_f$  scheme can result in a significant improvement in surface passivation for high-aspect-ratio b-Si surfaces. A high- $Q_f$  scheme will not show a relative improvement in surface passivation compared with a planar surface; however, these schemes are obviously still preferred as the absolute surface recombination velocities will be the lowest.

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