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First-Principles Study of Radiation-Induced Defects in Silicon Solar Cells Using Density-Functional Theory Simulation

O. Perevozchikov[1], V. Perevoztchikov[1], A. Khan[2], and A. Fedoseyev[3,*]

[1]PLab Inc, USA
[2]University of South Alabama, USA,
[3]Solestial Inc, USA
*Correspondence: Alex Fedoseyev, af@solestial.com

Abstract. Displacement damage from high-energy electron and proton irradiation is a critical degradation mechanism in space solar cells, particularly within the Van Allen radiation belts. These energetic particles induce atomic displacements in semiconductor materials, generating lattice defects such as vacancies, di-vacancies, and impurity-related complexes (e.g., B_iO_i, B_iC_s and B_iH_i) that significantly impact the electronic structure of silicon, reducing solar cell efficiency and power output. A fundamental understanding of these defects is critical for designing radiation-resistant photovoltaics. To address this challenge, we employ first-principles Density Functional Theory(DFT) using the SIESTA code with localized orbital basis sets to model the electronic structure of silicon systems with induced defects and impurities. Our study focuses on boron-related defect complexes, including interstitial boron (Bi) and its interactions with oxygen (O) and hydrogen (H), with validation against experimental data and comparative calculations using QUANTUM-ESPRESSO to assess computational robustness. Our simulation identifies key defect energy levels, including B_iO_i at $E_c - 0.23$ eV and B_iC_s at $E_v + 0.31$ eV, which exhibit strong agreement with experimental data, reinforcing the reliability of our approach. We further analyze the passivating role of interstitial hydrogen (H_i) and its influence on defect neutralization. These findings provide critical insights for defect engineering strategies, enabling optimized doping and thermal processing to mitigate radiation-induced degradation. This research advances the development of next-generation, radiation-tolerant photovoltaics for prolonged space missions by identifying dominant defect configurations and their electronic structure.

Keywords: Silicon Solar Cells, Space Radiation, Displacement Damage, Lattice Defects, Crystalline Structure, DFT Simulation

1. Introduction

Specific defect energy calculations relevant to Technology Computer-Aided Design (TCAD) are performe<d using first-principles Density Functional Theory (DFT). These calculations are implemented in the SIESTA code, which uses local orbital pseudopotentials for electronic structure calculations, to compare the results with experimental data and identify the dominant defects.

Meticulous determination of the defect and impurity signatures (apparent activation energy, capture cross-section for holes and electrons as well as their concentration) can considerably facilitate the defect engineering strategies for doping and thermal processing to achieve the desired materials properties. That can be done with the Density-Functional Theory (DFT) powerful tool for atomic-scale computational material science, which is widely used to study defects in semiconductors, predict their structural and electronic properties, vibrational and diffusional dynamics as observed by the various experiments. Experimental results are required as an important input for such defects that affect the device performance. These results can be obtained through the material database NERSC.

Precise characterization of defect signatures including activation energies, capture cross-sections for holes and electrons, and defect concentrations enables advanced defect engineering strategies for optimizing doping and thermal processes to achieve the desired materials properties for space solar cell applications.

DFT has proven to be a powerful tool for predicting defects' structural, electronic, vibrational, and diffusional properties, validated through published experimental data.

Previous studies have demonstrated the high accuracy of DFT in predicting defect energy levels, particularly those responsible for the degradation of boron-doped Czochralski silicon (CZ-Si) solar cells. The optical and electrical activity of boron interstitial defects in silicon have been systematically investigated using the AIMPRO DFT code [1], providing critical insights into defect-induced electronic states. Furthermore, the formation and stability of key defect complexes, including BiOi, BiCs, and BiBsHi, in electron-irradiated or ion-implanted boron-doped silicon have been extensively analyzed [2]. Additionally, the identification and characterization of boron clusters and boron-interstitial aggregates in silicon have been reported in [3], further substantiating the role of boron-related defects in solar cell degradation. These findings reaffirm the capability of DFT-based approaches in predicting defect properties and guiding material optimization for high-performance photovoltaic devices.

2. DFT simulation software

We have access to several sources for DFT codes, including:

(1) SIESTA code – open-access and open-source DFT code developed as a part of Spanish Initiative for Electronic Simulations with Thousands of Atoms; A very important feature of the code is that its accuracy and cost can be tuned in a wide range, from quick exploratory calculations to highly accurate simulations matching the quality of other approaches, such as plane-wave methods.

(2) Quantum ESPRESSO – another open-access and open source DFT code.

(3) SeqQuest (Sandia National Laboratories) - a versatile electronic structure code developed to compute energies and forces for periodic surfaces (slabs), solids, or finite molecules.

Typically, computation with DFT code consists of (a) choosing the appropriate pseudopotential, generating a basis set, specifying cut-off radii, providing the atomic structure as an input, performing calculation, analysis, and then structural optimization of the atomic coordinates.

3. Simulation of silicon crystal with specific displacement damages

The SIESTA package code is used to provide the calculation of the atomic systems. The 64 silicon atoms system was tested with the emphasis on the bands structure specifically of the energy levels corresponding to the valence and conduction bands. The results of this simulation are used as a reference point for the simulation of the silicon system with impurities. The 64 atoms system was constructed as a silicon crystal and the SIESTA code calculations were performed in order to obtain valence band maximum and conducting band minima to observe the indirect energy gap. The Hamann – Schluter - Chiang pseudo-potential for Si was used as an input for SIESTA. The band structure of the 64 atoms silicon crystal is shown in Fig. 1. The

E_v corresponds to the -0.73 eV and the E_c corresponds to the 0.26 eV with the E_{gap} of 0.99 eV. The Fermi level is at 0. This result was used as the reference for calculations of silicon systems with impurities. Calculations were also made for Troullier-Martin's pseudopotential. We were using double and triple atoms defect in 64 Si atoms system. Simulations were performed for H, B, C, and O atoms as interstitials and substitutional atoms. Using the molecular dynamic option the atomic system was fully relaxed. Electronic structures of the silicon systems with impurities boron interstitial(B_i), boron interstitial + carbon substitutional(B_iC_i), boron interstitial + oxygen interstitial(B_iO_i) and boron interstitial + hydrogen interstitial(B_iH_i) are shown in Fig.2.

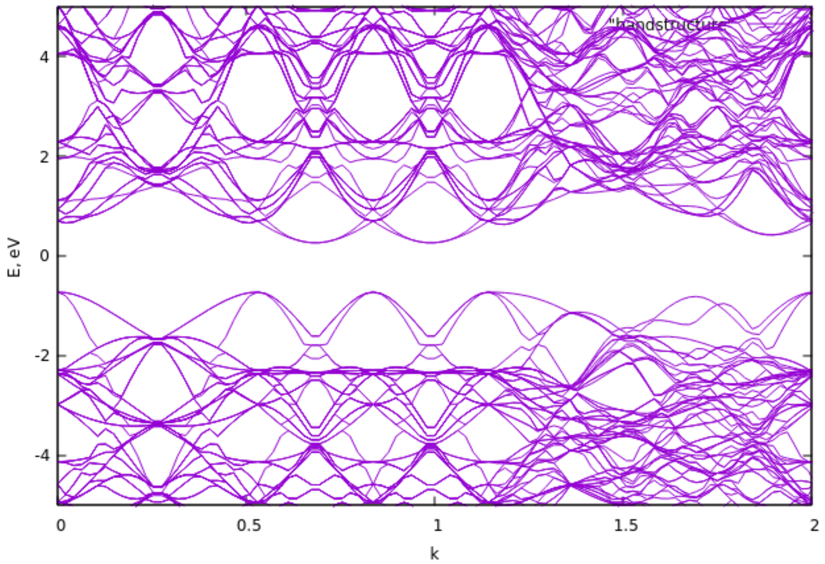

Figure 1. *Bands structure for the 64 atoms silicon crystal*

4. Results and Discussion

Electrical Activity of Boron-Related Defect Complexes. Interstitial boron B_i, is a highly reactive defect in silicon, readily forming complexes with common impurities such as oxygen (O) and hydrogen (H). We performed first-principles calculations to assess their impact on electronic properties and compared our findings with available experimental data.

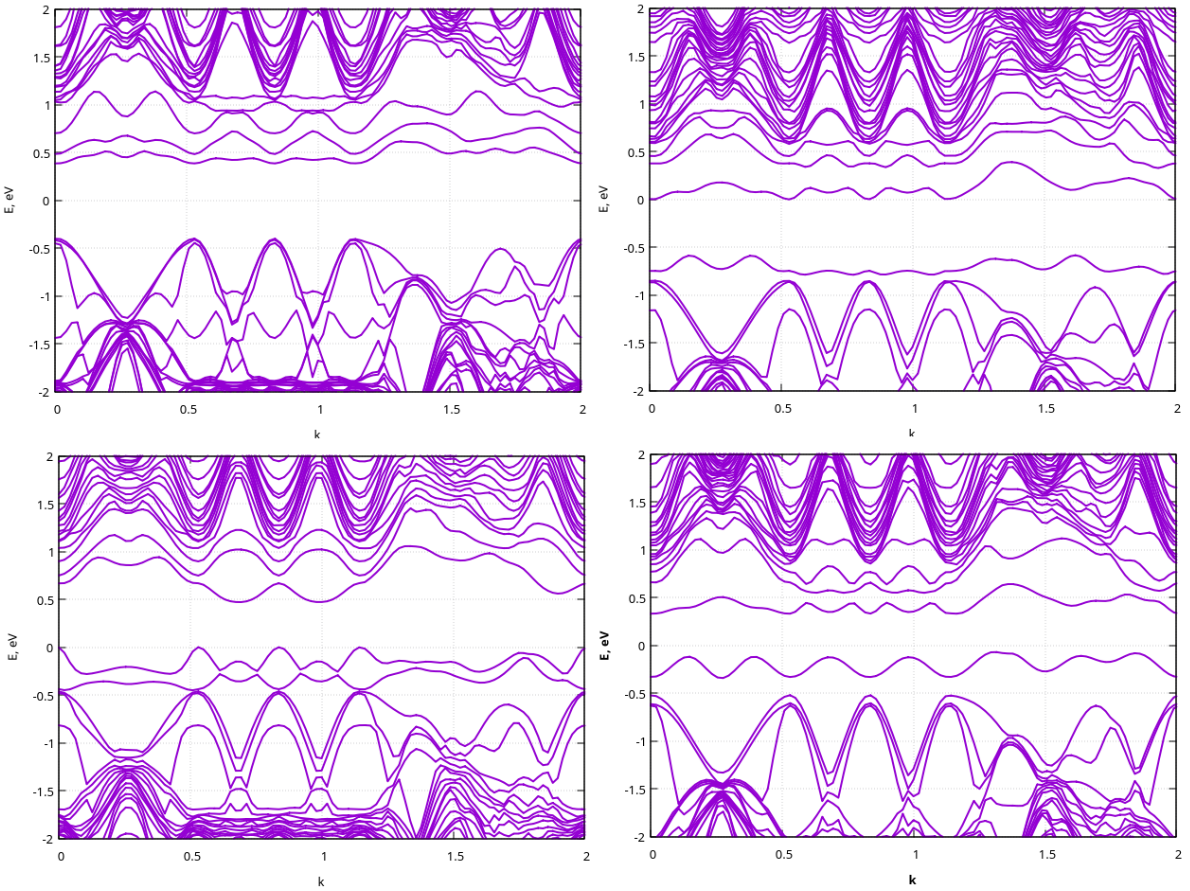

Figure 2. *Electronic structure of the silicon system with impurities:* B_i*(top left),* B_iO_i*(top right),* B_iC_s*(bottom left) and* B_iH_i*(bottom right)*

B_iO_i Complex. Our first-principles calculations indicate that the energy band level of the B_iO_i complex is positioned near E_C - 0.23 eV [4], aligning well with previous theoretical results. Additionally, we identify two new defect states near the valence band edge at E_V + 0.17 eV and E_V + 0.12 eV with different pseudopotentials, suggesting possible variations in defect configurations or computational methodology.

B_iC_S Complex. For the B_iC_S defect, our structural analysis reveals a ground-state configuration closely resembling that of the previously studied B_iB_S defect [5-7]. Our results indicate a defect level at E_V + 0.31 eV, demonstrating excellent consistency with experimental results, further supporting the reliability of our approach.

Role of Hydrogen in Defect Passivation. Interstitial Hydrogen (H_i) plays a critical role in silicon processing due to its high diffusivity and ability to passivate electrically active defects. While no direct experimental data on B_iH_i defects is available, we analyzed the B_iH_i complex with SIESTA (a localized orbital, linear-scaling code) and compared with results obtained using Quantum ESPRESSO [8] (a plane-wave code) under identical physical conditions, which provides a built-in cross-validation. Both codes showed consistent results for the B_iH_i electronic defect level, giving high confidence in our findings. These results provide valuable insight into the potential impact of hydrogen on B_i-related defects, which warrants further experimental investigation.

The SIESTA simulation results of the calculated energy structure of the silicon systems with impurities are summarized in Table 1.

5. Conclusion

High-energy radiation-induced displacement damage in space solar cells introduces detrimental defects that significantly impact efficiency and power output. Through first-principles Density Functional Theory (DFT) calculations using the SIESTA code, this study comprehensively analyzes defect-induced electronic structures in silicon, including B_iO_i, B_iC_s, and B_iH_i. Our results identify key defect configurations, including interstitial boron (Bi) and its complexes with oxygen and hydrogen, revealing their electrical activity and energy band levels. The computed defect states, such as B_iO_i (E_C- 0.23 eV) and B_iC_s (E_V + 0.31 eV), align well with experimental data, reinforcing the reliability of our computational approach. Furthermore, our analysis highlights the passivating role of hydrogen (Hi) in mitigating electrically active defects, providing key 0insights for defect engineering in radiation-hardened solar cells. These findings validate DFT as a robust predictive tool for providing critical insights into defect engineering strategies, enabling the development of advanced material strategies to enhance radiation resistance in space photovoltaics. By identifying dominant defect configurations and their electronic impact, this work paves the way for optimized silicon-based solar cells with improved longevity and performance in harsh radiation environments.

Table 1. *Energy level within energy gap due to defects in silicon system.*

Defect	HSC pseudopot	TM pseudopot	Experiment	Abdurrazaq [8]
B_i	Ec – 0.26eV Ec – 0.17eV Ec – 0.05eV	Ec – 0.60eV Ec – 0.25eV Ec – 0.10eV	Ec – 0.15eV [9] Ec – 0.45eV [9]	Ec – 0.26eV Ec – 0.33eV
B_iO_i	Ec – 0.25eV Ev + 0.17eV	Ec – 0.48eV Ec – 0.20eV Ec – 0.06eV Ev + 0.12eV	Ec – 0.23eV [4] Ec – 0.27eV [10]	Ec – 0.26eV
C_iO_i	Ev + 0.05eV Ev + 0.40eV	Ev + 0.04eV Ev + 0.41eV Ec – 0.13eV	Ev +0.363eV	
B_iC_s	Ev + 0.32eBV Ev + 0.21eV Ec – 0.21eV	Ev + 0.31eV Ev + 0.17eV Ec – 0.34eV Ec – 0.26eV Ec – 0.09eV	Ev + 0.29eV [11, 12]	Ev + 0.28eV
B_iH_i	Ev + 0.42eV Ec – 0.18eV	Ev + 0.46eV Ec – 0.45eV Ec – 0.13eV Ec – 0.05eV		Ev + 0.37eV Ec – 0.07eV
$B_sB_iH_i$	Ev + 0.50eV Ec – 0.34eV	Ev + 0.70eV Ec – 0.55eV Ec – 0.16eV	Ev + 0.50eV [13]	Ev + 0.50eV

Data availability statement

The data is available upon reasonable request to the authors.

Author contributions

CRediT roles: Conceptualization, A.F.; methodology, A.F.; software installation and simulation, O.P., V.P.; validation, O.P., V.P., A.F. and A.K.; writing – original draft preparation, O.P., V.P.; writing – review and editing, A.K., A.F. and Yana Gurimskaya; supervision, A.F.

Competing interests

The authors declare that they have no competing interests

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References

[1] J. Adey, R. Jones, and P. R. Briddon, “Formation of B_iO_i, B_iC_s, and $B_iB_sH_i$ defects in e-irradiated or ion-implanted silicon containing boron”, Applied Physics Letters 83 (4), 665–667 (2003).
[2] J. Adey, J. P. at al, “Interstitial boron defects in Si”, Physica B: Condensed Matter 340–342, 505–508(2003).
[3] J. Adey, J. P. Goss, R. Jones, and P. R. Briddon, “Identification of boron clusters and boron-interstitial clusters in silicon”, Physical Review B 67, 245325 (2003).
[4] A. Carvalho, R. Jones, J. Coutinho, P. Briddon, “Ab initio calculation of the local vibrational modes of the interstitial boron–interstitial oxygen defect in Si”, J. Phys. Condens. Matter 17 (17) (2005) L155.
[5] E. Tarnow, “Theory of two boron neutral pair defects in silicon”, J. Phys. Condens. Matter 4 (1992) 5405.
[6] J. Zhu, et al., “Ab initio pseudopotential calculations of B diffusion and pairing in Si”, Phys. Rev. B 54 (1996) 4741.
[7] X. Liu, W. Windl, M. Masqueleir, “*Ab initio* modeling of boron clustering in silicon”, Appl. Phys. Lett. 77(2000) 2018
[8] A. Abdurrazaq, Abdulrafiu T. Raji, Walter E. Meyer, “Ab initio study of the effect of hydrogen passivation on boron-oxygen-carbon related defect complexes in silicon” Materials Science in Semiconductor Processing 110 (2020) 104967
[9] J. Troxell, G. Watkins, “Interstitial boron in silicon: A negative – U system”, Phys. Rev. B 22 (2) (1980) 921.
[10] P. Mooney, L. Cheng, M. Süli, J. Gerson, J. Corbett, “Defect energy levels in boron-doped silicon irradiated with 1-MeV electrons”, Phys. Rev. B 15 (8) (1977) 3836.
[11] X. Chen, X. Yu, X. Zhu, P. Chen, D. Yang, “First-Principles Study of Interstitial Boron and Oxygen Dimer Complex in Silicon”, APEX 6 (1) (2013), 041301.
[12] J. Adey, R. Jones, P. Briddon, Appl. “Formation of BiOi, BiCs, and BiBsHi defects in e-irradiated or ion-implanted silicon containing boron”, Phys. Lett. 83 (4) (2003) 665–667.
[13] S. Fatima, C. Jagadish, J. Lalita, B. G. Svensson, A. Hallen, “Hydrogen interaction with implantation induced point defects in *p*-type silicon”, Appl. Phys. 85 (1999) 2562.