**Ab initio** molecular dynamics simulation of the effects of stacking faults on the radiation response of 3C-SiC

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In this study, an **ab initio** molecular dynamics method is employed to investigate how the existence of stacking faults (SFs) influences the response of SiC to low energy irradiation. It reveals that the C and Si atoms around the SFs are generally more difficult to be displaced than those in unfaulted SiC, and the corresponding threshold displacement energies for them are generally larger, indicative of enhanced radiation tolerance caused by the introduction of SFs, which agrees well with the recent experiment. As compared with the unfaulted state, more localized point defects are generated in faulted SiC. Also, the efficiency of damage production for Si recoils is generally higher than that of C recoils. The calculated potential energy increases for defect generation in SiC with intrinsic and extrinsic SFs are found to be higher than those in unfaulted SiC, due to the stronger screen-Coulomb interaction between the PKA and its neighbors. The presented results provide a fundamental insight into the underlying mechanism of displacement events in faulted SiC and will help to advance the understanding of the radiation response of SiC with and without SFs.

Cubic silicon carbide (3C-SiC) exhibits lots of superior electronic and physical properties such as high electron mobility, saturated electron drift velocity, high corrosion resistance, favorable chemical inertness and small neutron absorption cross-section¹–⁵. It is thus desirable for power switching device applications and is often utilized under harsh environment such as high temperature and high pressure. Due to the superior physical properties of 3C-SiC, it has been considered as a vital component in nuclear applications. For example, 3C-SiC has been considered as an inert-matrix material for water-cooled reactors to burn minor actinides or Pu⁶, a structural material for fusion power reactors⁷, a cladding material for nuclear fuel, and a structural material for the reactor core in high temperature gas-cooled reactors⁸. It is therefore of critical importance to understand the phase stability of 3C-SiC under irradiation and explore the way to enhance its radiation tolerance.

In the past decades, a great number of experimental and theoretical studies have been carried out to investigate the radiation damage effects of SiC⁹–¹². Inui et al. have found that crystalline-to-amorphous transition in single crystalline silicon carbide (sc-SiC) can be induced by electron irradiation at temperatures around 300 K¹³,¹⁴. Several ion irradiation studies on nano-crystalline silicon carbide (nc-SiC) have also been reported and it has been suggested that reducing the grain size may improve the mechanical properties of sc-SiC¹⁵,¹⁶. Recently, Zhang et al. compared the radiation tolerance of sc-SiC and nc-SiC by employing 550 keV Si⁺ ion irradiation, who found that the sc-SiC readily undergoes irradiation-induced structural amorphization, whereas the nc-SiC with a high-density of stacking faults (SFs) exhibits more than an order of magnitude increase in radiation resistance¹⁷. Jamison et al. studied the crystalline-to-amorphous transition in nc-SiC using 1.25 MeV electron irradiation, and found that the nc-SiC has an increased dose to amorphization, as compared with the sc-SiC. They proposed that the addition of a high density of grain boundaries, grain texture, and the presence of SFs may all contribute to the enhanced radiation tolerance¹⁸. Theoretically, the density functional theory (DFT) method has been employed...
Results and Discussion

Ground-state properties for bulk SiC and stacking fault formation energy. To test the pseudopotentials of Si and C, the lattice constant and cohesive energy for bulk SiC are first calculated and compared with experimental and other theoretical values in Table 1. It is shown that our results are in excellent agreement with experiments and are comparable with other theoretical values. The defect formation energy, which is defined by $E_{\text{def}} = E_{\text{def}} - E_{\text{undef}} + \sum \Delta n_i \mu_i$, is calculated for ISFs and ESFs. Here, $E_{\text{def}}$ is the energy of the faulted supercell, $E_{\text{undef}}$ is the energy of the unfaulted supercell, $\Delta n_i$ is the change in the number of species $i$ (Si or C) and $\mu_i$ is the chemical potential of species $i$. The chemical potentials of silicon ($\mu_{\text{Si}}$) and carbon ($\mu_{\text{C}}$) obey the following criteria: $\mu_{\text{Si}} \leq \mu_{\text{Si}}$ (bulk), $\mu_{\text{C}} \leq \mu_{\text{C}}$ (bulk) and $\mu_{\text{Si}} + \mu_{\text{C}} = \mu_{\text{Si}}$ (bulk), where $\mu_{\text{Si}}$ (bulk) and $\mu_{\text{C}}$ (bulk) are the chemical potentials of bulk Si and diamond, respectively, and $\mu_{\text{Si}}$ (bulk) is the total energy of bulk SiC. The SF formation energy is calculated under both carbon-rich ($\mu_{\text{Si}} = \mu_{\text{Si}}$ (bulk) and $\mu_{\text{C}} = \mu_{\text{C}}$ (bulk) condition) and silicon-rich ($\mu_{\text{Si}} = \mu_{\text{Si}}$ (bulk) and $\mu_{\text{C}} = \mu_{\text{C}}$ (bulk) condition) condition. For the three types of ISFs, the calculated formation energies under both conditions are found to be nearly identical to each other, i.e., $\sim 7.8$ mJ/m$^2$, which agrees well with the value of $\sim 3.4$ mJ/m$^2$ reported by Käckell et al. Comparing our results with the classical MD simulation, we find that our calculated value of $\sim 7.8$ mJ/m$^2$ is in good agreement with experiments.

Threshold displacement energies for C and Si recoils in unfauluted and faulted SiC. The critical physical parameter for estimating damage production rates under electron, neutron, and ion irradiation and predicting the defect profile is the threshold displacement energy ($E_d$), which can be defined as the minimum transferred kinetic energy for the primary knock-on atom (PKA) to be permanently displaced from its lattice site and form stable defects. In the past several years, the $E_d$ values in a number of semiconductors and ceramic materials have been investigated employing the AIMD method. In order to explore how the existence of SFs affects the radiation response of SiC, we first calculate the $E_d$s for C and Si recoils in unfaulted SiC along the [001] and [010] directions, which are perpendicular to the SiC(111) plane and correspond to the [111] and [110] directions in bulk SiC, respectively. A comparison of our results with other theoretical values is provided in Table 2. The $E_d$s for C[001] and C[010] are determined to be 19 and 47.5 eV, respectively. For Si recoils, the $E_d$ values are calculated to be 95 eV for the [001] direction and 63 eV for the [010] direction. It is shown that our results are in good agreement with the results reported by Gao et al. Comparing our results with the classical MD simulation carried out by Devanathan and Weber, we find that the $E_d$s obtained by the AIMD method are generally much smaller, except for the case of Si[001]. This may be due to the fact that charge transfer that occurs during the recoil events is taken into account by the AIMD method while not considered in the classical MD simulations.

| Lattice constant (Å) | Cohesive energy (eV/atom) |
|---------------------|--------------------------|
| Our calc. 4.37       | 6.40                     |
| Other calc. 4.361, 4.45 | 6.66*                    |
| Exp. 4.36*           | 6.34*                    |

Table 1. Calculated lattice constant and cohesive energy for bulk SiC. *ref. 27. **ref. 26.
The calculated Eds for C and Si PKAs in SiC with ISFs and ESFs (see Figs 1 and 2) are summarized in Table 3.

As for C recoils around the ISFs, it is found that along both the [001] and [001] directions the Ed values for C3 PKAs are generally larger than those for C1 and C2 PKAs. In the case of C recoils around the ESFs, the Ed values for C1 PKAs are the highest for both [001] and [001] directions. Obviously, the three types of C PKAs that have different interlayer spacing from the SFs exhibit different tolerance to irradiation. Similar phenomenon is also observed for Si recoils, for which the Eds in several cases are larger than 150 eV, i.e., the PKA is not permanently displaced at energy up to 150 eV. It is found that the three types of Si recoils around the SFs are affected remarkably and exhibit different Ed values. Comparing the Eds for C and Si PKAs, we find that generally considerably higher energies are needed for displacing the Si PKAs than those for displacing the C PKAs, similar to the cases in bulk SiC. These results show that the radiation susceptibility of the C and Si atoms around the SFs is affected significantly by the existence of SFs.

In this study, the weighted average Ed values are calculated to be 52.1 eV for C[001], 59.5 eV for C[001], >99.6 eV for Si[001] and >122.1 eV for Si[001] in SiC containing ISFs. As for the PKAs in SiC with ESFs, the average Ed values are calculated to be 37.8, 71.6, >128.4 and >88.1 eV for C[001], C[001], Si[001] and Si[001], respectively. Comparing these results with the values of 19, 47.5, 95 and 63 eV for C[001], C[001], Si[001] and Si[001] in unfaulted SiC, respectively, we find that the Ed values in faulted SiC are generally larger. The maximum energy transferred to an atom can be expressed as $T = \frac{2E_d(E_d + 2m_e c^2) / Me^2$ under electron irradiation, where

| Ed (eV) | Defect type |
|---------|-------------|
| 19      | C_{vac} + C_{int} |
| 20.5, 30.0 | C_{vac} + C_{int} |
| 47.5    | C_{vac} + C_{int} |
| 47.5, 71.0 | C_{vac} + C_{int} |
| 95      | 2Si_vac + 2C_{int} + C_{vac} + C_{int} |
| 105, 108 | Si_{vac} + Si_{int} |
| 63      | Si_{vac} + Si_{int} |
| 62, 38  | Si_{vac} + Si_{int} |

Table 2. Calculated threshold displacement energies (Eds) and the associated defect types for C and Si recoil events along the direction normal to the SiC(111) surface. C_{vac}: C vacancy; C_{int}: C interstitial; Si_{vac}: Si vacancy; Si_{int}: Si interstitial; C_{Si}: C occupying the lattice Si site; Si_{C}: Si occupying the lattice C site. a ref. 12. b ref. 31.

Figure 1. Illustration of schematic view of SiC containing intrinsic SFs with (a) (ABC)(AC)(ABC); (b) (ABC)(AB)(ABC); (c) (ABC)(BC)(ABC) stacking sequences.

The calculated Eds for C and Si PKAs in SiC with ISFs and ESFs (see Figs 1 and 2) are summarized in Table 3. As for C recoils along the ISFs, it is found that along both the [001] and [001] directions the Ed values for C1 PKAs are generally larger than those for C1 and C2 PKAs. In the case of C recoils around the ESFs, the Ed values for C1 PKAs are the highest for both [001] and [001] directions. Obviously, the three types of C PKAs that have different interlayer spacing from the SFs exhibit different tolerance to irradiation. Similar phenomenon is also observed for Si recoils, for which the Eds in several cases are larger than 150 eV, i.e., the PKA is not permanently displaced at energy up to 150 eV. It is found that the three types of Si recoils around the SFs are affected remarkably and exhibit different Ed values. Comparing the Eds for C and Si PKAs, we find that generally considerably higher energies are needed for displacing the Si PKAs than those for displacing the C PKAs, similar to the cases in bulk SiC. These results show that the radiation susceptibility of the C and Si atoms around the SFs is affected significantly by the existence of SFs.
is the incident energy, \(m_e\) is the electronic mass, \(M\) is the atomic mass and \(c\) is the velocity of light\(^3\). Assuming 300 keV electrons incident on SiC, the maximum energy transferred to Si and C atom are 59.5 and 71 eV, respectively. Our finding that the \(E_d\) values of C and Si recoils are increased by the existence of SFs, therefore, suggests that SiC with SFs is less susceptible to low energy irradiation. This is consistent with the experiments carried out by Zhang et al.\(^{17}\) and Jamison et al.\(^{18}\). Employing 550 keV Si\(^+\) ion irradiation, Zhang et al. investigated the radiation tolerance of SiC with and without SFs, and found that the SiC with a high-density of SFs exhibits more than an order of magnitude increase in radiation resistance\(^{17}\). Jamison et al. studied the crystalline-to-amorphous transition in SiC using 1.25 MeV electron irradiation, and also found that SiC with ISFs or ESFs behaves more robustly under irradiation environment\(^{18}\).

Defect distribution in unfaulted and faulted SiC.

The defects created by C and Si PKAs in recoil events are summarized in Tables 4 and 5, respectively. In the case of C PKAs, the defects created in unfaulted SiC mainly consist of the carbon vacancy (\(C_{\text{vac}}\)) and carbon interstitial (\(C_{\text{int}}\)), as shown in Table 2, which agrees well with the results reported by Gao et al.\(^{12}\). Comparing the damage end states created by different carbon recoils in SiC with

| Stacking sequence | Direction | \(E_d\) (eV) |
|-------------------|-----------|-------------|
| (ABC)(AC) (ABC)   | [001]     | 64 40 68.5 69 131 80.5 |
| (ABC)(AB) (ABC)   | [001]     | 57 58 63 >150 65 >150 |
| (ABC)(BC) (ABC)   | [001]     | 54 58 66.5 >150 66 >150 |
| (ABC)(BABC) (ABC) | [001]     | 64 19.5 62 68.5 130 70.5 |
| (ABC)(ABAC) (ABC) | [001]     | 56 57.5 65 >150 68 >150 |
| (ABC)(ACBC) (ABC) | [001]     | 67 19.5 19.5 >150 >150 87.5 |
| (ABC)(BABC) (ABC) | [001]     | 112.5 46.5 50.5 >150 49 65 |
| (ABC)(ABAC) (ABC) | [001]     | 66.5 19 19.5 >150 >150 88.5 |
| (ABC)(ACBC) (ABC) | [001]     | 120.5 50 48.5 >150 49 64 |
| (ABC)(ACBC) (ABC) | [001]     | 67 19.5 42.5 >150 141 88.5 |
| (ABC)(ACBC) (ABC) | [001]     | 115.5 49 51 >150 49 67 |

Table 3. Calculated threshold displacement energies (\(E_d\)) for C and Si in SiC with intrinsic stacking faults (ISFs) and extrinsic stacking faults (ESFs). The maximum \(E_d\) values for C and Si PKAs in each SiC with SFs are indicated in bold.
As a result, the final defect structure consists of a C FP, a SiC antisite defect and a CSi antisite defect. Our calculations show that the total defect number generated by C PKAs in faulted SiC is generally not less than that in unfaulted SiC.
In unfaulted SiC, the defects created by Si PKAs under low energy irradiation are one C FP, two SiC, and two C_{int} antisite defects for Si[001], and one Si FP for Si[00\bar{1}]. Comparing the damage end states created by different Si recoils in SiC with ISFs, we find that Si[001] show similar defect distribution to unfaulted SiC, whereas Si[00\bar{1}], Si[\bar{1}00] and Si[00\bar{1}] recoil events exhibit different character. For Si[001], the damage end states consist of three Si_{vac}, two C_{int}, one Si vacancy and one C interstitial. In the case of Si[00\bar{1}], only two antisite defects (and one C FP for SiC with (ABC)/(AB) stacking sequence) are generated. Regarding Si[\bar{1}00], the created defects are one Si_{vac}, one Si_{int} and one C_{int} for SiC with (ABC)/(AC)/(ABC) and (ABC)/(AB)/(ABC) stacking sequences, and one Si FP for SiC with (ABC)/(BC)/(ABC) stacking sequence.

As for Si PKAs in SiC with ESFs, only one Si FP is generated by Si, along the [00\bar{1}] direction and a two antisite defects are generated by Si along the [00\bar{1}] direction in SiC with (ABC)/(AC)/(ABC) stacking sequence. For the Si[\bar{1}00], the damage end states in SiC with (ABC)/(BABC)/(ABC) and (ABC)/(ACB)/(ABC) arrangements are similar to those in unfaulted SiC, whereas the recoil events in SiC with (ABC)/(ABC)/(ABC) stacking sequence show different end states, i.e., two Si_{vac}, one C_{int}, one Si vacancy and one C interstitial. In the case of Si PKAs along the [00\bar{1}] direction, the defect generation are relatively similar, as indicated by C_{int} + Si_{vac} for (ABC)/(BABC)/(ABC), Si FP for (ABC)/(BABC)/(ABC), and Si_{vac} + Si_{int} for (ABC)/(ACB)/(ABC) stacking sequences.

The total defect number created by C and Si PKAs in faulted SiC is illustrated in Fig. 3. It is found that the Si PKAs are generally more efficient in damage production than C PKAs, which is consistent with our results that generally considerably larger, i.e., the PKAs in faulted SiC are more difficult to be displaced, which may enhance the radiation tolerance of sc-SiC, agreeing well with the recent experiments. In the meantime, the distribution of created defects in faulted SiC is shown to be very localized. These results agree well with the study of radiation tolerance of sc-SiC and SiC with SFs performed by Zhang et al., in which it was found that the existence of SFs leads to more localized point defect production. Comparing the different defect configurations for unfaulted and faulted SiC, we find that antisite defects are the most common defects in faulted SiC, whereas in unfaulted SiC the FPs are dominant. The defect generation in sc-SiC and nc-SiC with a grain size smaller than 12 nm have been investigated by Gao et al. using the MD method, in which the kinetic energies of 10 keV for PKA were simulated. They also found that in nc-SiC the antisite defects are more than other defects, in contrast to those produced in sc-SiC, where the dominant defects are FPs.

Origin of the difference in the radiation response between unfaulted and faulted SiC. Jamison et al. studied the energetics of point defects near the SFs and found that the critical migration and reaction energies are reduced significantly enough to enhance the amorphization resistance by increasing the probability of point defect recombination and annihilation. To explore the origin of the difference in the radiation response behavior of unfaulted and faulted SiC, we further analyze the potential energy increase for stable defect formation in the recoil events of C[001] at 70 eV, C[00\bar{1}] at 70 eV, Si[001] at 141 eV and Si[00\bar{1}] at 152.5 eV. As illustrated in Fig. 4(a), the maximum potential energy increases for C[001] are 25.3, 19.2 and 17.2 eV for SiC with (ABC)/(AC)/(ABC) arrangement, SiC with (ABC)/(ABC)/(ABC) arrangement and unfaulted SiC, respectively. In the case of C[00\bar{1}], the maximum potential energy increases are 20.8, 17.2 and 12.2 eV, corresponding to SiC with (ABC)/(AC)/(ABC), (ABC)/(ABC)/(ABC) and SiC, respectively. The situation in Si[001] at 141 eV and Si[00\bar{1}] at 152.5 eV are very similar to those in C recoil events, i.e., the maximum potential energy increases for SiC with SFs are always larger than those for unfaulted SiC. The maximum potential energy increases represent the maximum in screen-Coulomb interactions between PKAs and one or more atomic nuclei on lattice. As for SiC containing ESFs, the average E_{d} values are 37.8, 71.6, > 128.4 and > 88.1 eV for C[001], C[00\bar{1}], Si[001] and Si[00\bar{1}], respectively. As compared with the E_{d} values in unfaulted SiC, the E_{d} values in faulted SiC are generally larger, i.e., the PKAs in faulted SiC are more difficult to be displaced, which may enhance the radiation tolerance of SiC, agreeing well with the recent experiments. In the meantime, the defect generation mechanism for C and Si PKAs in faulted SiC is generally more complex and the defect contribution is very localized. The most common defect configurations in faulted SiC are antisite defects, whereas the Frenkel pairs are dominant in unfaulted SiC.

Conclusions
In summary, low-energy recoil events in unfaulted and faulted SiC have been investigated by ab initio molecular dynamics method based on density functional theory. The threshold displacement energies are shown to be dependent on the interlayer spacing between the PKA and the SFs. The threshold displacement energies are calculated to be 52.1 eV for C[001], 59.5 eV for C[00\bar{1}], > 99.6 eV for Si[001] and > 122.1 eV for Si[00\bar{1}] in SiC with ISFs. As for SiC containing ESFs, the average E_{d} values are 37.8, 71.6, > 128.4 and > 88.1 eV for C[001], C[00\bar{1}], Si[001] and Si[00\bar{1}], respectively. As compared with the E_{d} values in unfaulted SiC, the E_{d} values in faulted SiC are generally larger, i.e., the PKAs in faulted SiC are more difficult to be displaced, which may enhance the radiation tolerance of SiC, agreeing well with the recent experiments. In the meantime, the defect generation mechanism for C and Si PKAs in faulted SiC is generally more complex and the defect contribution is very localized. The most common defect configurations in faulted SiC are antisite defects, whereas the Frenkel pairs are dominant in unfaulted SiC.
Figure 3. Total defect number created by (a) C PKAs in SiC with intrinsic SFs; (b) C PKAs in SiC with extrinsic SFs; (c) Si PKAs in SiC with intrinsic SFs; and (d) Si PKAs in SiC with extrinsic SFs. Here, the SF_{int1}, SF_{int2} and SF_{int3} represent intrinsic SFs with (ABC)(AC)(ABC), (ABC)(AB)(ABC) and (ABC)(BC)(ABC) atomic arrangements, respectively, and the SF_{ext1}, SF_{ext2} and SF_{ext3} represent extrinsic SFs with (ABC)(BABC)(ABC), (ABC)(ABAC)(ABC) and (ABC)(ACBC)(ABC) atomic arrangements, respectively.

Figure 4. The calculated potential energy increase for (a) C_3[001] at 70 eV; (b) C_3[001] at 70 eV; (c) Si_2[001] at 141 eV; and (d) Si_3[001] at 152.5 eV.
Potential energy increase analysis shows that the existence of SFs increases the energy barrier for defect generation, i.e., the C and Si primary knock-on atoms in faulted SiC need to overcome higher energy barrier than those in unfaulted SiC to generate defects.

Methods

All the calculations are carried out using the Spanish Initiative for Electronic Simulations with Thousands of Atoms (SIESTA) code. The norm-conserving Troullier-Martins pseudopotential are employed to determine the interaction between ions and electrons and the exchange-correlation potential is described by the generalized gradient approximation parameterized by Perdew, Burke and Ernzerhof. The valence wave functions are expanded by a basis set of localized atomic orbitals and single-ζ orbitals. The norm-conserving Troullier-Martins pseudopotential have reported that the SFs lie in the (111) plane of SiC. Hence, both the ISFs and ESFs investigated in this study are created based on the 3C-SiC(111) plane. For SiC with ISFs and ESFs, the supercell consists of 256 and 320 atoms, respectively. Three types of ISFs, i.e., (ABC)(AC)(ABC), (ABC)(AB)(ABC) and (ABC)(BC)(ABC) and three types of ESFs, i.e., (ABC)(ABAC)(ABC), (ABC)(ABAC)(ABC) and (ABC)(ACBC)(ABC), as shown in Figs 1 and 2, have been considered. To simulate the low energy recoil events, three types of Si or C on the boundary of the SFs, as denoted in Figs 1 and 2, are selected as PKA and a certain amount of kinetic energy is provided along the direction perpendicular to the SiC(111) surface, i.e., [001] and [001]. The simulations are conducted with a NVE ensemble and a variable time step scheme is employed to avoid the instability of the system.

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Author Contributions
Z.L. and X.Z. designed the calculations. M.J. conducted the calculations and wrote the manuscript. S.P., H.Z., C.X., H.X. and F. Z. contributed to the discussion and interpretation of the results. All authors discussed the results and reviewed the manuscript.

Additional Information
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