

Isotopic enrichment of silicon: A molecular dynamics study on ^{28}Si ion implantation at low energies

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High-fluence silicon-28 (^{28}Si) ion implantation has been shown to produce isotopically enriched surface regions within natural silicon (Si) wafers through localized focused ion beam implantation. In this work, molecular dynamics simulations are performed to simulate ^{28}Si ion implantations into a Si sample for insights into the enrichment process dynamics. We conduct a series of simulations to emulate the irradiation process at incident energies, ranging from 0.5 to 2 keV, and fixed angles of incidence of 0° , 7° , and 15° . Our findings elucidate how implantation energy and angle of incidence affect sputter yield and enrichment levels. The outcomes of this study highlight the importance of atomistic simulations in providing a mechanistic understanding of deposition and sputtering for the optimization of the enrichment process. Moreover, comparisons with transmission electron microscopy images of natural silicon wafers enriched using focused ion beam performed by Acharya *et al.* [Commun. Mater. **5**, 57 (2024)], show strong agreement for both postirradiated and postannealed configurations, further validating the simulation approach. This work will support future studies of isotopic enrichment of natural Si and the development of novel methods to fabricate spin-qubit devices for quantum computing architectures.

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I. INTRODUCTION

Quantum computing architectures composed of quantum bits (qubits) may facilitate technological breakthroughs in numerous fields, including encrypted communication, quantum sensing, computing, and imagining [1–3]. Technologies are currently being developed to address the challenges in the manufacture of the foreseen quantum computing architecture, notably focusing on the development of robust qubits that enable high-fidelity operations. Among the proposed qubits, spin-qubits employ the interactions between the donor's (e.g., ^{31}P) nucleus and the orbiting electrons, which demand the careful isolation of these donors from environmental perturbation [4]. Given its lack of nuclear spin and compatibility with existing nanofabrication techniques [5], silicon-28 (^{28}Si) emerges as an ideal isotope for a matrix hosting such qubits, effectively acting as a solid-state vacuum [6,7]. Nonetheless, the nuclear spin ($I = 1/2$) of the silicon-29 (^{29}Si) isotope present in natural silicon (Si) with an abundance of 4.67%, causes magnetic perturbations on its surroundings, [8–10] limiting the spin-qubit coherence [11,12]. Previous studies [9] demonstrated that embedding ^{31}P in isotopically enriched ^{28}Si layers, with Si depleted to 800 ppm, enhanced electron spin coherence times by up to a factor of 5000 in the dephasing

time (T_{2e}^*), and extended coherence to 0.56 s under dynamical decoupling (T_{2e}^{CPMG}).

Several techniques have been proposed to produce enriched ^{28}Si layers, including chemical vapor depositions (CVD) [13] and hyperthermal ion beam depositions [14,15]. Until recent years, the highest quality material in terms of both enrichment and contamination was produced for the Avogadro project [16,17], where centrifugation was employed to isolate $^{28}\text{SiF}_4$ as a source for wafer growth. More recently, localized focused ion beams (FIB) utilizing high-fluence implantations of ^{28}Si ions have shown promising levels of enrichment [18,19]. Nanoscale secondary ion mass spectrometry analysis of the irradiated volumes has shown that FIB can produce isotopically enriched layers with residual ^{29}Si concentrations as low as 2.3 ± 0.7 ppm, while maintaining high elemental purity in the postirradiated substrates, surpassing the levels achieved in the Avogadro project [19]. To guide and analyze the outcomes of experimental studies, researchers have relied on binary collision approximation (BCA) models due to their computational efficiency and ability to provide insights into the deposition process. Simulations using TRIDYN, a binary collision Monte Carlo simulation package [20,21], have been employed to guide the experiments, showing the relationship between sputter yield and ^{28}Si implantation energy. These simulations helped to identify postimplantation surface regimes, e.g., erosion, one-for-one replacement, and accumulation. Notably, the results revealed accumulation regimes at both low (below 3 keV) and high (above 45 keV) implantation energies [18]. However, despite the insights provided, BCA models do not provide a mechanistic understanding of the many-body collisions taking place during the implantation of ^{28}Si ions [22]. BCA models treat the material as an amorphous

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continuum and are unable to investigate dynamic processes at different temperatures. Consequently, a more comprehensive description of the many-body collision mechanisms, required to optimize the process cannot be studied using this methodology [23]. In this context, molecular dynamics (MD), with its all-atom approach and temporal and spatial scale, becomes a suitable technique to predict the implantation dynamics during the irradiation process. Unlike BCA models, MD simulations can self-consistently model many-body collisions, which play a key role when atoms with relatively low kinetic energies collide with other atoms in materials [24]. Furthermore, MD can explore the crystalline structure of atoms in the substrate and subsequent annealing configurations, which have been shown to annihilate damage caused by the ion irradiation process.

Past studies employed MD to emulate FIB and study ion irradiation processes [25,26]. Fu *et al.* [27] analyzed the damage evolution and distribution during the process of (charge neutral) Si ion implantation into bulk diamond. Gennetidis *et al.* [28] bombarded pure Si substrates with Ga to investigate the formation of Si tri-interstitial clusters. Furthermore, MD simulations have been employed to study many parameters that impact the cumulative deposition of impacting projectiles in materials [29–32], including sputtering yield [33–35], as well as the annealing recovery [36]. Additionally, MD simulations have provided insights into using PF₂ ions instead of monoatomic P ions to improve donor implantation for spin-qubit arrays [37]. So far, there is no work to study the enrichment process via ²⁸Si ion implantation with an all-atoms approach that accounts for many-body collisions taking place during the ion bombardment.

In the present work, the isotopic enrichment via ²⁸Si ion implantation is investigated using MD simulations. We model the cumulative depositions of ²⁸Si projectiles into a natural Si substrate to elucidate the enrichment of the sample. We employ implantation energies in the range of 0.5 to 2 keV and angles of incidence of 0°, 7°, and 15°, to examine how the choice of these parameters impacts the sputtering yield and the overall enrichment of the sample. This energy range has previously been reported to result in postimplantation surface accumulation, as predicted by TRIDYN simulations [18]. Moreover, by comparing with experimental outcomes, we aim to validate and enhance the understanding of the ²⁸Si enrichment process. This research will provide a basis for further studies on isotopic enrichment and ion irradiation, supporting the development of novel methods for fabricating Si spin-qubit devices for quantum computing.

II. METHODS

All MD simulations were performed using the LAMMPS code [38]. To describe the Si interactions, we employed the modified Tersoff potential developed by Kumagai *et al.* [39]. This potential reproduces many of the experimentally observed properties of Si, including the melting temperature. Moreover, to describe properly the collisions between atoms, we coupled the two-body component of the modified Tersoff potential ($V_{\text{Tersoff-mod}}$) with the diatomic repulsive Ziegler-Biersack-Littmark (ZBL) (V_{ZBL}) potential [40]. The

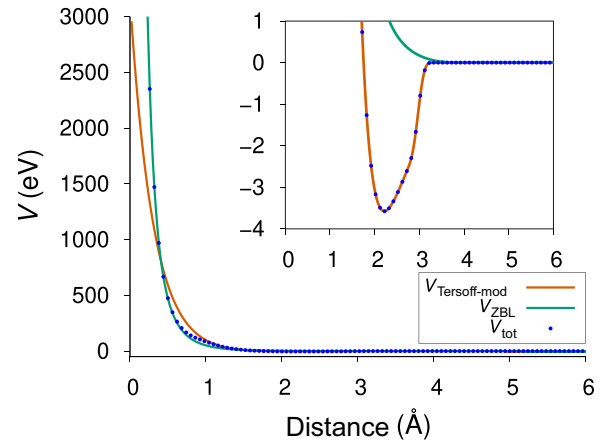


FIG. 1. Si-Si pair potential (V) for the Kumagai ($V_{\text{Tersoff-mod}}$), ZBL (V_{ZBL}), and joined potential through a Fermi-type function (V_{tot}). The inset displays a zoom of the pair potentials between -4 and 1 eV.

two potentials were combined employing a Fermi-type function

$$V_{\text{tot}} = [1 - F(r)]V_{\text{ZBL}} + F(r)V_{\text{Tersoff-mod}}(r), \quad (1)$$

$$F(r) = \frac{1}{1 + \exp[-b_f(r - r_f)]}, \quad (2)$$

where V_{tot} is the total potential, and b_f and r_f are free parameters of the Fermi function $F(r)$. The parameters b_f and r_f were chosen as $8.5 \text{ \AA}^{-1}$ and $0.9 \text{ \AA}$ to make the V_{tot} and its first derivative smoothly transition between V_{ZBL} and $V_{\text{Tersoff-mod}}$. Further, we ensure an accurate description of the two-body interatomic potential at short distances with the repulsive V_{ZBL} , while maintaining the $V_{\text{Tersoff-mod}}$ when atoms are far apart, as depicted in Fig. 1.

To verify that the modified potential used in this study accurately models Si solids, we evaluated the cohesive energy (E_0), lattice parameter (a), elastic constants (C_{11} , C_{12} , C_{44}), melting temperature (T_m), and surface formation energy (γ_s) along the Si (100) surface. The elastic constants were evaluated by employing the method described in Ref. [41]. The melting temperature was evaluated by simulating the coexistence of the two phases (liquid and crystal), as described by Marqués *et al.* [42]. The measured values are summarized in Table I alongside data from the original Kumagai *et al.* [39] and experiments.

In the simulations, the substrate (target) material was represented by Si atoms arranged in the cubic diamond crystalline structure with a lattice parameter of $a = 5.429 \text{ \AA}$ [39]. The supercells were created by taking $10 \times 10 \times 20$ and $20 \times 20 \times 60$ repetitions of the Si diamond unit cell in the x , y , and z axes. Resulting in Si (100) substrates of 16 000 atoms for implantation energies of 0.5 and 1 keV, and 192 000 atoms for energies of 2 keV. The smaller cross section of the system was crucial for limiting the total number of atoms and reducing the cost, as approximately 13 500 simulation runs were required to gather sufficient statistics. To replicate the natural abundances of Si isotopes, i.e., 92.23%, 4.67%, and 3.1% for ²⁸Si, ²⁹Si, and silicon-30 (³⁰Si) [46], the masses of randomly selected atoms were modified. In the present work,

TABLE I. Physical properties of diamond Si calculated with our modified potential compared to values from the original Kumagai *et al.* and to the experimental data.

	Experiments ^a	Kumagai ^b	Modified ^c
E_0 (eV/Atom)	−4.63	−4.630	−4.630
a (Å)	5.429	5.429	5.429
C_{11} (GPa)	167	166.374	166.377
C_{12} (GPa)	65	65.302	65.309
C_{44} (GPa)	81	77.106	77.105
T_m (K)	1687 ^d	1681 (± 5)	1681 (± 5)
γ_s (Jm ^{−2})	1.36 ^e	1.773	1.773

^aReference [39,43] and references therein.

^bReference [39].

^cOur modified potential.

^dReference [44].

^eReference [45].

the interatomic potentials for different Si isotopes were treated as identical.

The supercells were aligned along the z axis of the simulation box, while periodic boundary conditions were applied. The systems were initially equilibrated at 300 K under the NVT ensemble using a time step of 1 fs and the Nosé-Hoover thermostat [47] with a relaxation time of 1 fs for 100 ps. Once equilibrated, the simulation box was extended by 4 nm along the positive z axis, while the periodicity was kept in the x and y axes to model an infinitely large surface. Atoms in the bottom layers (0–0.8 nm) were fixed to prevent drifting during ion irradiation, while atoms in the subsequent layers (0.8–1.8 nm) were coupled to a Berendsen thermostat [48] with a coupling constant of 1 ps. The remaining atoms, located above 1.8 nm, formed the free layer and evolved according to Newton's equations of motion under the NVE ensemble. A representation of one of the MD models used in this study is presented in Fig. 2. This figure shows the initial material, which consists of 16 000 atoms and whose horizontal dimensions and depth are $54 \times 54 \text{ Å}^2$ and 108 Å. In these conditions, the boxes were equilibrated for another 100 ps at 300 K, maintained by the thermalized layer, before performing overlapping depositions of ^{28}Si ions. Here, implantation is modeled by directing ^{28}Si projectiles at the top layers of the free region.

In the present work, we employ a substrate model without impurities because our primary aim is to capture the fundamental response of pure silicon under irradiation, i.e., amorphization, sputtering, and implantation dynamics. Low impurity concentrations are unlikely to significantly alter the deposition yield of implanted ^{28}Si . Nonetheless, it is worth mentioning that, depending on their concentration and whether they are retained or removed by sputtering, impurities could have an effect on the evolution and stability of remnant defects.

To emulate the ion implantation process [18], (charge neutral) ^{28}Si ions were launched into the Si (100) surface one by one. The selected incident energies were chosen because they are in the low-energy accumulation regime and are expected to concentrate the implant profile near the surface of the natural Si substrate, thereby facilitating the rapid formation of an enriched layer. The incident ^{28}Si (projectile) ion charge was

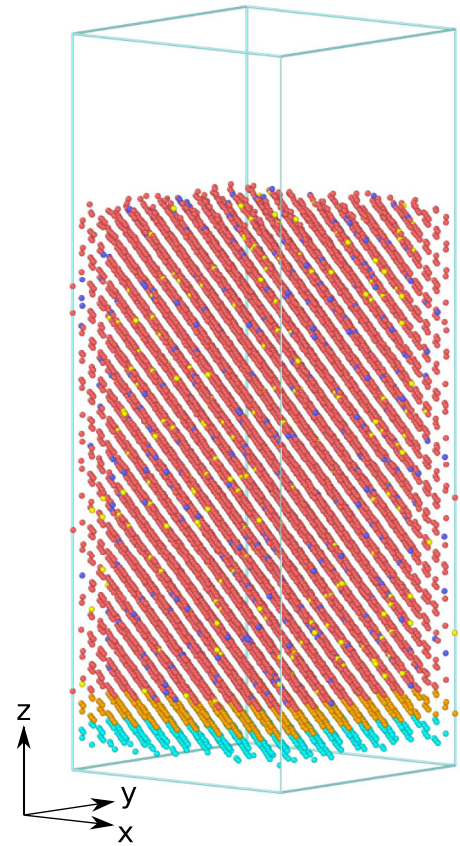


FIG. 2. MD model of the substrate material used for this study for projectiles with an incident energy of 1 keV. The cyan lines represent the size of the simulation box, which has a height of 148 Å to create a free surface. Periodic boundary conditions are applied in the x and y axes. The cyan and orange spheres represent the atoms in the fixed and thermalized layers, while the atoms above compose the free layer. The red, blue, and yellow spheres represent ^{28}Si , ^{29}Si , and ^{30}Si isotopes, respectively.

not considered since the effects of low charge states were assumed negligible in bulk materials [49]. The projectiles entered the system from a randomised position 2 nm above the target surface, with an initial velocity corresponding to the selected incident energy. Projectiles were launched toward the surface at different angles (0° , 7° , and 15°) measured from the surface normal pointing into the sample. The azimuthal angle was $\phi = 0^\circ$, as the irradiation was conducted in the x - z plane. A variable time step was used to describe the atomic motion throughout the deposition of incident ^{28}Si projectiles. The maximum allowed time step was recomputed at each time step and had a value of 1 fs, while the maximum allowed displacement was 0.1 Å. Here, each projectile worked as a primary knock-on atom (PKA) that shocked other atoms and created a collision cascade, which has the ability to sputter surface atoms in the substrates. We considered atoms leaving the simulation box from the top surface sputtered and removed from the system. Since the substrates were thick enough, atoms leaving the simulation box through the bottom boundary were negligible. In the present work, only the nuclear stopping from the ballistic collisions was taken into account. As electronic stopping from inelastic collisions of the Si atoms

with the electrons is considered to have a minor impact within the range of energies employed [50,51]. We launched subsequent ^{28}Si projectiles once each cascade collision ended, dictated by the time it takes for the temperature of atoms in the free layer of the system to return to its reference value (300 K). For implantation energies of 0.5, 1, and 2 keV, we find that the time required for the temperature in the free layer to return to the reference value was 123, 180, and 182 ps, respectively. Consequently, we ran at least 200 ps for each injection cycle to ensure sufficient relaxation time, which exceeds the longest recovery time observed.

To ensure the substrate size realistically represented a Si surface, we performed MD simulations using a supercell created by replicating the Si diamond unit cell $15 \times 15 \times 30$ repetitions along the x , y , and z axes (54 000 atoms). For this larger substrate, we measured a sputtering yield of 0.545 and an implantation depth of 2.9 nm, compared to 0.551 and 2.7 nm for the smaller substrate model. These small differences demonstrate that the smaller substrate geometry used in Fig. 2 is sufficient to capture the relevant sputtering and implantation dynamics.

After the irradiation process systems were annealed at 1273 K (1000°C). To conduct the annealing, the system was heated with a heating rate of 1.2 K/ps to the annealing temperature. Once the target temperature was attained, the system was modeled for 10 ns. Then, the system was quenched at the same rate to 300 K where it was thermalized for 1 ns followed by a 1-ns simulation under the NVE ensemble to distinguish atoms classified within the cubic diamond structure while minimizing any thermostat effects. Here, we employed an extended version of the common neighbor and dislocation analyses, as implemented in Ovito [52], to identify atoms in the cubic diamond structure and to analyze the morphology of the remnant defects.

III. RESULTS

A. Sputter yield

The sputter yield (Y) of surface atoms is defined as the average number of atoms removed from the material per ion impact

$$Y = \frac{N_{\text{sput}}}{N_{\text{in}}}, \quad (3)$$

where N_{sput} and N_{in} are the atoms removed from the material surface and the number of incident projectiles. When Y is less than 1, net deposition occurs, whereas a value greater than 1 represents erosion of the material.

Figure 3 shows Y as a function of fluence for an ion implantation energy of 1 keV where the angles of incidence are tilted by 0° , 7° , and 15° from the surface normal. We modeled 1000 implantation events, representing a fluence of $3.391 \times 10^{15} \text{ cm}^{-2}$. From this figure, we observe that during the initial stages of the Si (100) irradiation, Y decays before reaching a plateau at fluences above $1 \times 10^{15} \text{ cm}^{-2}$ for all angles. As the implanted ions lead to the formation of a noncrystalline material, amorphous Si is anticipated for such fluences [53], demonstrating that the transition from a crystalline flat surface to an amorphous substrate with varying surface roughness influences the sputtering behavior. Following the approach

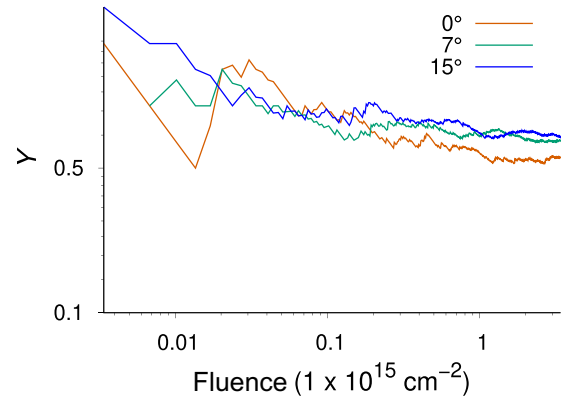


FIG. 3. Evolution of the sputtering yields of surface atoms (Y) as a function of fluence for different angles of incidence. The vermilion, teal, and blue lines represent Y for projectiles with fixed angles of incidence of 0° , 7° , and 15° , respectively. The ion implantation energy is 1 keV.

from Ref. [33], we determine Y in the steady state, i.e., independently of the number of projectiles, by averaging the instantaneous values over a fluence range after convergence. We obtain values of 0.551, 0.699, and 0.729 for incidence angles tilted by 0° , 7° , and 15° from normal. Indicating the net deposition of ^{28}Si atoms, i.e., more atoms are being implanted into the substrate than being sputtered.

To evaluate the role of the incident energy of the projectiles, we model two additional cases with normal incidence, employing incident ion energies of 0.5 and 2 keV. For these cases, we modeled implantation events corresponding to a fluence of $3.391 \times 10^{15} \text{ cm}^{-2}$. Table II presents the average values for Y across different implantation energies, angles of incidence, and fluences. From this table, we observe that Y is less than 1 in all cases, indicating a net deposition of ^{28}Si isotopes. With respect to Y at different energies, our results qualitatively align with previous studies [18,54] that utilized TRIDYN and experimental data, which reported an increase in Y with implantation energy and an accumulation regime within this energy range. However, we find that TRIDYN values of 0.61 and 0.91 at 0.8 keV and 2 keV [54], respectively, are overestimated relative to our MD results. Possible explanations for this difference include the detailed many-body collisions in our MD simulations and the role of the angle of incidence. The MD approach provides a reliable representation of many-body collisions, which play a crucial role when atoms with relatively low kinetic energies collide with

TABLE II. Sputter yield (Y) across different implantation energies (E), angles of incidence (θ), and number of launched projectiles (N_{proj}), at a fluence of $3.391 \times 10^{15} \text{ cm}^{-2}$.

E (keV)	θ (deg)	N_{proj} (count)	Y
1	0	1000	0.551
1	7	1000	0.699
1	15	1000	0.729
0.5	0	1000	0.531
2	0	4000	0.566

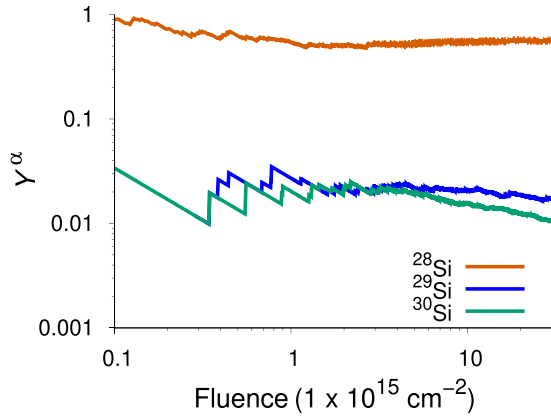


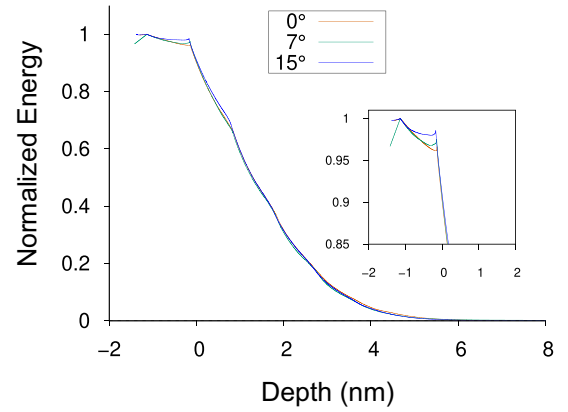
FIG. 4. Evolution of the sputtering yields of surface atoms per species (Y^α) as a function of fluence. The sputtering yields of ^{28}Si , ^{29}Si , and ^{30}Si is represented by the vermilion, blue, and amber lines. Notice the decay of $Y^{29\text{Si}}$ and $Y^{30\text{Si}}$, as a consequence of the depletion of ^{29}Si and ^{30}Si abundances in the surface layers.

other atoms within the material. BCA models account only for binary collisions; consequently, many-body interactions, particularly low-energy collective interactions that lead to small but important atomic displacements, are neglected. The predicted atom redistribution in BCA simulations depends strongly on the specific model implementation, including parameters such as the displacement energy, free-flight path, and maximum impact parameter [55]. These limitations lead to a disproportionate contribution of the erosive component, inaccurate descriptions of surface-pattern formation, and an overestimation of ion penetration depths in non-channelling directions when compared with MD simulations [56].

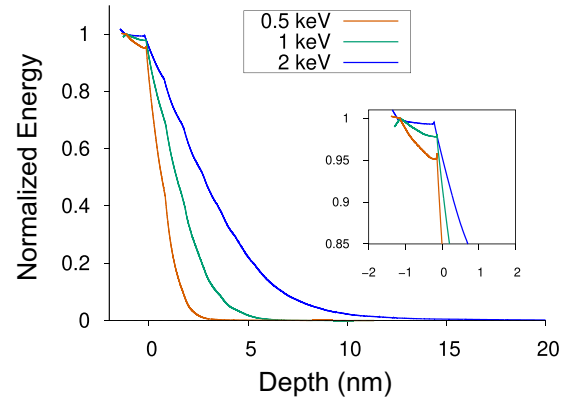
To evaluate the rate at which ^{28}Si , ^{29}Si , and ^{30}Si are sputtered from the material, we calculate the sputter yield of surface atoms of the different species (Y^α), defined as the number of atoms of a determined species removed from the material per ion impact

$$Y^\alpha = \frac{N_{\text{sput}}^\alpha}{N_{\text{in}}}. \quad (4)$$

Here, we model 9000 implantation events, representing a fluence of $3.052 \times 10^{16} \text{ cm}^{-2}$. Figure 4 shows Y^α as a function of fluence for an ion implantation energy of 1 keV and normal incidence. From this figure, we find that as shown in Fig. 3, $Y^{28\text{Si}}$ depicts the overall deposition, and consequently enrichment of ^{28}Si isotopes in the substrate. With respect to $Y^{29\text{Si}}$ and $Y^{30\text{Si}}$, we observe a higher value of $Y^{29\text{Si}}$, indicating that more ^{29}Si atoms are sputtered than ^{30}Si due to the greater abundance of ^{29}Si . Moreover, the transition from a flat crystalline surface to an amorphous substrate with varying surface roughness enhances the deposition of ^{28}Si projectiles, as indicated by the early decrease of $Y^{28\text{Si}}$. As the fluence further increases, $Y^{29\text{Si}}$ and $Y^{30\text{Si}}$ decrease as these isotopes become depleted near the surface. We will perform a more detailed analysis of this high-fluence model in Sec. III C.



(a)



(b)

FIG. 5. Normalized-averaged kinetic energy of the incident projectile as a function of the depth of the target substrate for different (a) angles of incidence and (b) ion implantation energies. The projectiles have an implantation energy of 1 keV in (a) and normal incidence in (b).

B. Implantation depths

Figure 5 shows the normalized-averaged kinetic energy of the projectile as a function of the substrate depth. Here, the normalized-averaged kinetic energy refers to the average kinetic energy normalized (divided) by the corresponding energy given to the projectiles at the start of the implantation events. Note that the energies displayed just above the surface ($\leq 0 \text{ nm}$, where 0 nm defines the substrate surface) are less than 1, indicating they are lower than the initial kinetic energy given to the projectiles at the beginning of the implantation process. This decrease occurs because the average includes reflected projectiles that lose energy during collisions with the substrate. From Fig. 5(a), we observe that *on average* the projectiles lose energy at the same rate regardless of the angle of incidence, explained by the larger sputter yield at higher angles of incidence. Further, Figure 5(b) shows that as implantation energy increases, projectiles penetrate deeper into the substrate, resulting in ion deposition occurring at greater depths.

To perform a more detailed analysis of the final configurations after irradiation, the distributions of the final positions of implanted ^{28}Si projectiles, i.e., their implantation depths

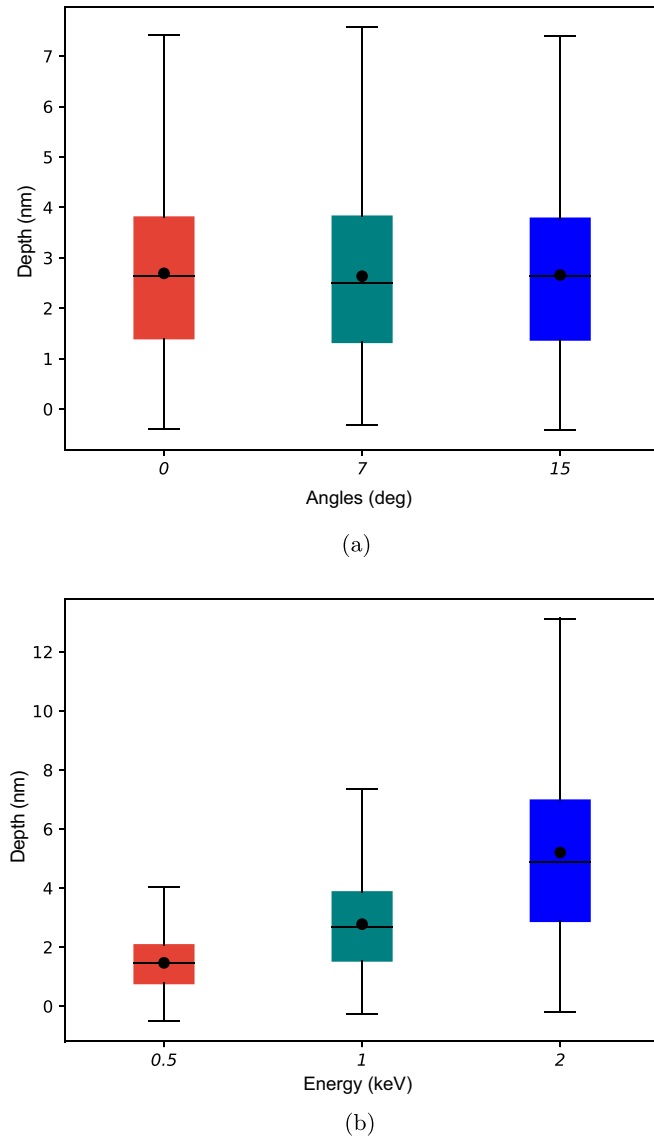


FIG. 6. Final positions of the implanted ^{28}Si ions after the irradiation process, for different (a) angles of incidence and (b) implantation energies, as described in Table II. The lower bounds of the boxes are the first quartile values, the horizontal black lines are the medians, and the upper bounds are the third quartile values. The black dots represent the means. The T-shaped whiskers indicate the last points, which are within 1.5 times of the interquartile range.

are examined. Figure 6 shows the implantation depths of the injected ions for different [Fig. 6(a)] angles of incidence and [Fig. 6(b)] implantation energies. First, Fig. 6(a) shows that the distributions of the implantation depths appear consistent across different angles of incidence. This is in agreement with the kinetic energy dissipation rates during the irradiation depicted in Fig. 5. Further, as expected, Fig. 6(b) indicates that ions penetrate and settle deeper into the material as the implantation energy increases. Consequently, our results suggest that the energy of the projectile has a greater impact on the implantation depth than the angle of incidence. This implies that while the angle of incidence could be adjusted

to achieve the desired sputter yield, the implantation depth should primarily be controlled by the energy of the projectile.

C. Enrichment

In this subsection, we present the results of enriching a Si sample through the cumulative deposition of ^{28}Si and the sputtering of ^{29}Si and ^{30}Si isotopes. We examine the extent and depth of enrichment in the substrate in its postirradiated and postannealed states. We model 9000 ion implantation events corresponding to a fluence of $3.052 \times 10^{16} \text{ cm}^{-2}$ with ion implantation energies of 1 keV and normal incidence. Note that as the system is in the accumulation regime ($Y < 1$), the substrate increases in its height during the ion irradiation. Figure 7 shows atoms classified by their diamond structure type, namely, cubic diamond and noncubic diamond (which include defects and amorphous material), at different configurations. From Fig. 7(b), we observe that there is a well-defined interface that separates the amorphous Si volume and the original crystalline Si below. This is in agreement with the transmission electron microscopy (TEM) images reported by Acharya *et al.* [19], where they observed an amorphous-crystalline interface on a sample that was irradiated with ^{28}Si projectiles with an ion incidence energy of 45 keV and a fluence of $1 \times 10^{19} \text{ cm}^{-2}$. To locate the amorphous-crystalline interface, the simulation box is divided into rectangular bins of height 0.2 nm, and for each bin we compute the fraction of atoms exhibiting cubic-diamond structure. Bins in which this fraction falls below 30% are classified as belonging to the amorphous volume of the substrate, as this threshold reliably distinguishes amorphous and crystalline regions. Thereafter, the position of the amorphous-crystalline interface is defined as the deepest bin, i.e., the bin with the lowest position along the z axis within the amorphous phase of the substrate. We find that this interface Fig. 7(b) is located at $8.7 (\pm 0.2) \text{ nm}$ along the positive z axis in the simulation box. Moreover, we employ the Wigner-Seitz defect analysis as integrated in Ovito [52] to characterize atomic disorder in the irradiated layer. Using the initial (preirradiation) configuration as the reference structure, we analyze the volume containing atoms located above 7.2 nm along the z axis to identify interstitials and vacancies. From these defect counts, we then determine the fraction of displaced atoms, computed as the ratio between the total defects and the total number of atoms in the volume, $([N_{\text{vac}} + N_{\text{int}}]/N_{\text{total}})$. We find that at a fluence of $3.866 \times 10^{14} \text{ cm}^{-2}$, the layer above 7.2 nm exhibits a vacancy concentration of approximately 20% and a fraction of displaced atoms of 0.39. These values identify the conditions under which the crystal phase transitions to an amorphous structure within this volume.

Following the irradiation process, an annealing procedure is used to recover the amorphous volume resulting from the ion implantation. Here, the system is annealed at 1273 K (1000°C) for 10 ns. We find that the number of atoms classified as cubic diamond types increased from 9618 (48.9%) to 17 895 (91.1%) after the annealing. This indicates the efficacy of the annealing procedure in facilitating the recovery of the diamond cubic structure in the substrate. Figure 7(c) shows the substrate in the postannealed state. From this figure, we observe remnant defects located below the

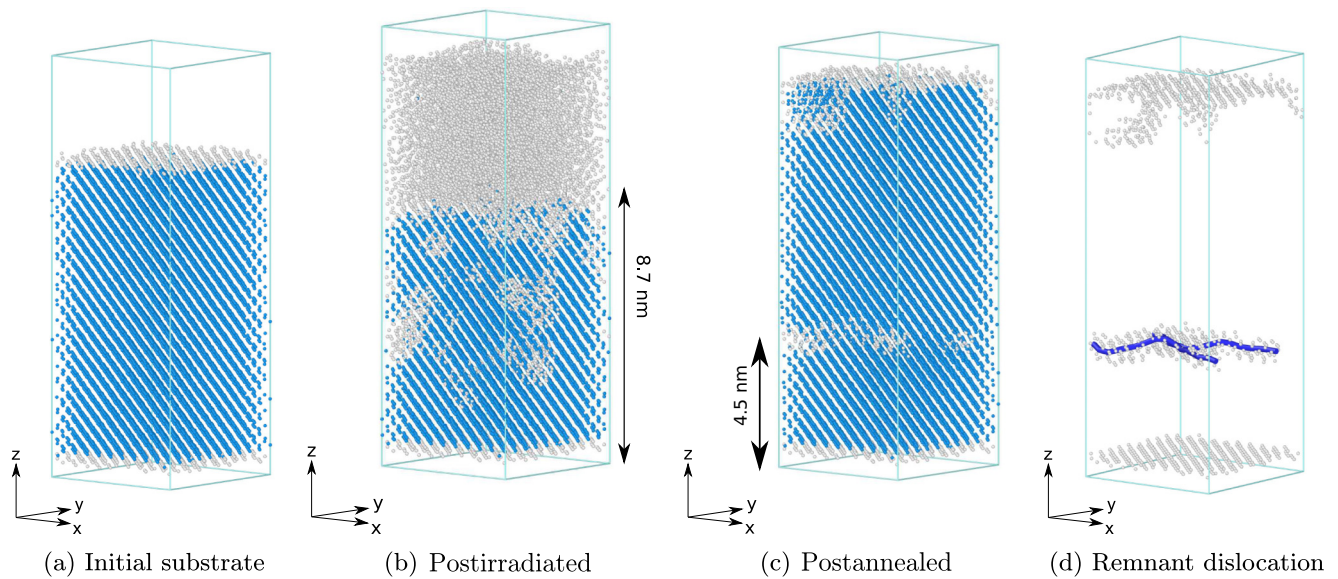


FIG. 7. Atom structure types in the MD model across different states. (a) The initial MD model before performing overlapping depositions of ^{28}Si ions. (b) The MD model after the implantation of 9000 ^{28}Si projectiles with an incident energy of 1 keV and normal angle of incidence. (c) The MD model after the implantation of 9000 ^{28}Si ions and subsequent annealing. (d) Remnant dislocation (blue) lines in the postannealed configuration. The blue spheres represent atoms identified as being of the cubic diamond structure type. The white spheres represent atoms with a noncubic diamond structure type, which includes defects and amorphous material.

amorphous-crystalline interface depicted in the postirradiated configuration Fig. 7(b). Our results reveal that these defects result from the partial recombination occurring below the amorphous-crystalline interface. Moreover, Fig. 7(d) shows that these defects consist of two periodic dislocation lines with burger vectors of $1/2\langle 110 \rangle$. These results agree with the most frequent dislocation found in Si [57,58] and with the extrinsic dislocation loop observed in the postannealed enriched sample by Acharya *et al.* [19].

To perform a more detailed analysis of the enrichment process, we probe the distributions of implanted ions and the location of the amorphous-crystalline interface in the postirradiated state at different fluences. Figure 8 depicts the mean (vermillion squares), median (teal triangles), the 3rd quartile (blue circles) of the final positions of the implanted ^{28}Si ions, as well as the location of the amorphous-crystalline interface (black asterisks) measured along the positive z axis in the simulation box. We observe a linear increase in both the positions of the implanted ^{28}Si ions and the location of the amorphous-crystalline interface, which results from the substrate's increase due to the accumulation of material. Moreover, beyond fluences of $2.03 \times 10^{16} \text{ cm}^{-2}$, the amorphous-crystalline interface is located above the 3rd quartile (blue circles), and at $3.05 \times 10^{16} \text{ cm}^{-2}$, it is positioned near the mean implantation depth during the start of the irradiation process. Thus, the ^{28}Si ions implanted at the start of the irradiation process remain below the amorphous-crystalline interface due to an increase in the thickness of the substrate, enabling isotopic enrichment in this region.

Figure 9 shows the depth profiles of the measured isotopic ratios for each of the three Si isotopes, normalized by dividing each by their total count, for the postannealed configuration of the substrate. Here, the isotopic ratios are calculated based on data collected from rectangular bins with a height of 0.5 nm

during the NVE ensemble, after the annealing has taken place. The vermillion, blue, and amber lines represent the isotopic ratios of ^{28}Si , ^{29}Si , and ^{30}Si , respectively. From this figure, we find that ^{28}Si displays its highest abundance at the surface layers, followed by a decline. Indeed, we observe that the abundances of the different isotopes above the amorphous-crystalline interface oscillate around the values of 97.42, 1.55, and 1.01 for ^{28}Si , ^{29}Si , and ^{30}Si , respectively. Moreover, at depths below 10 nm, the isotopic ratios oscillate around 92.23, 4.67, and 3.1, indicating that the Si isotopes return to their natural abundances. These results show a residual

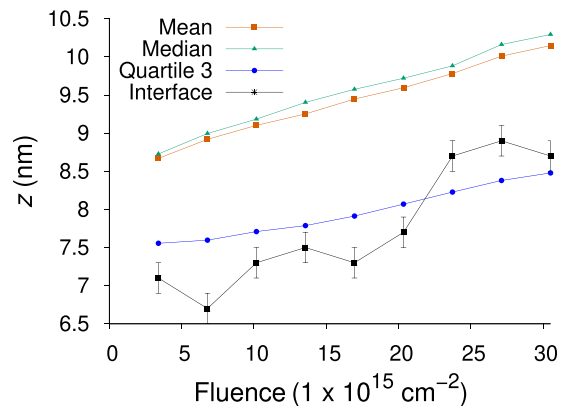


FIG. 8. Distributions of ion implantation locations and the amorphous-crystalline interface in the simulation box at various fluences. The vermillion squares, teal triangles, and blue circles represent the mean, median, and 3rd quartile positions of the implanted ions. The black asterisks represent where the amorphous-crystalline interface is located. Each point corresponds to positions evaluated after 1000 ^{28}Si implantations ($3.39 \times 10^{15} \text{ cm}^{-2}$).

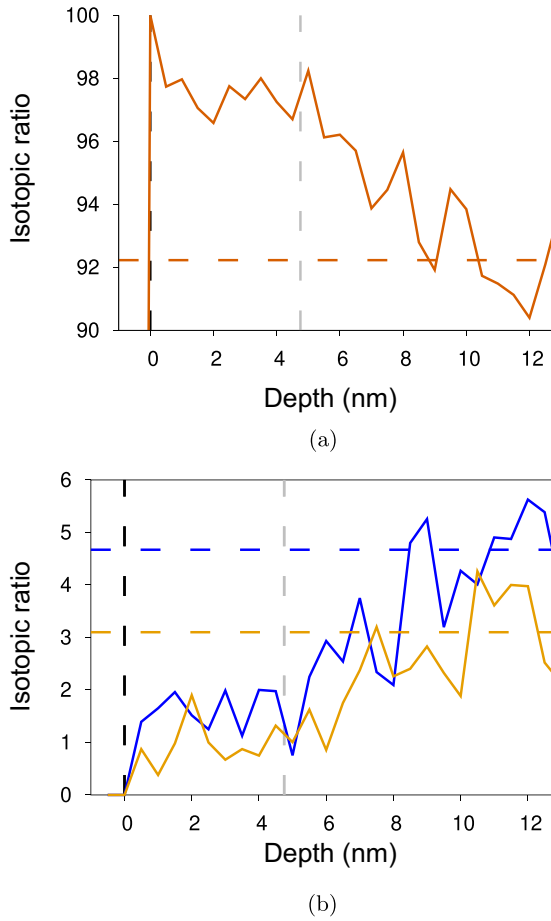


FIG. 9. The isotopic ratios of Si isotopes as a function of depth below the surface. The substrate is the postannealed configuration. The vermillion, blue, and amber lines represent the isotopic ratios of ^{28}Si , ^{29}Si , and ^{30}Si , respectively. The colored horizontal dashed lines represent the natural abundance of the three Si isotopes. The black and gray vertical dashed lines represent the substrate surface and the location of the amorphous-crystalline interface depicted in Fig. 7(b). (a) ^{28}Si profile, (b) ^{29}Si and ^{30}Si profile.

enrichment of ^{28}Si extending from below the amorphous-crystalline interface (indicated by the dashed gray lines) to a depth of 10 nm. From Figs. 8 and 9, we conclude that the isotopic enrichment observed at implantation depths below the amorphous-crystalline interface is primarily caused by implanted projectiles during the initial stages of the irradiation process, followed by the subsequent displacement of the interface as the deposition of ^{28}Si projectiles increases.

To examine the level and depth of the enrichment throughout the irradiation process, we evaluate the ratio for each of the three Si isotopes. Figure 10 shows the isotopic ratios for each of the three Si isotopes above the amorphous-crystalline interface, as a function of fluence. From this figure, we find that the isotopic ratio of ^{28}Si isotopes on the substrate displays a monotonic increment from 92.2 in the initial sample to 97.4 in the final state. Conversely, the abundances of ^{29}Si and ^{30}Si decrease to 1.55 and 1.01, respectively, demonstrating the efficiency of isotopic enrichment in accumulation regimes. Furthermore, if we approximate the enrichment trend with a logarithmic function ($y = 2.228 \times \log(x + 1) + 12.5080$),

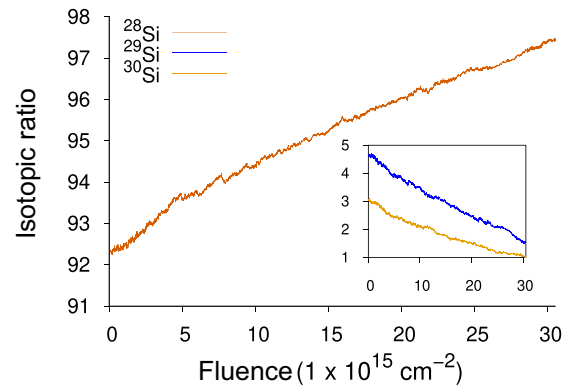


FIG. 10. Isotopic ratios for each of the three Si isotopes above the amorphous-crystalline interface, as a function of fluence. The main figure displays the enrichment of ^{28}Si . The inset displays the depletion of ^{29}Si and ^{30}Si .

this model predicts an enrichment ca. 99.999% above the amorphous-crystalline interface (i.e., within the enriched volume) would be achieved at fluences exceeding $1.133 \times 10^{17} \text{ cm}^{-2}$. However, it is important to note that as the fluence increases, the sputtering yield of ^{29}Si and ^{30}Si decreases. This reduction in yield leads to a diminished rate of enrichment, suggesting that even higher fluences may be required in practice to achieve such isotopic enrichment.

The enrichment depths observed in this work are not expected to vary strongly with the substrate temperature, although the enrichment levels may be influenced. Previous MD simulations of hydrogen ion implantation in Si [59] showed that the depth distribution of implanted projectiles is primarily governed by the implantation energy. In particular, the position of the maximum hydrogen concentration was found to be insensitive to implantation temperature. Nonetheless, higher implantation temperatures can lead to increased defect production due to enhanced atomic mobility during collision cascades [60]. Consequently, the level of enrichment may be influenced by variations in surface atom sputtering associated with defect formation. As the substrate surface becomes amorphous under continued ion impact, this influence should diminish as the fluence increases.

To gain further analysis of the postirradiated and postannealed configurations, we compute the in-plane stress, $\tau_{||} = \frac{\tau_{xx} + \tau_{yy}}{2}$. For this particular calculation, we compute the components of the stress tensor (τ_{xx} and τ_{yy}) implementing an atomistic approach based on data collected from rectangular bins with a height of 0.5 nm. The approach described by Thompson *et al.* [61] is used to calculate the virial contribution to the pressure, while the stress tensor is calculated as the sum of the kinetic and virial components. Figure 11 depicts the in-plane stress ($\tau_{||}$) as a function of depth for the (vermillion) postirradiated and (blue) postannealed configurations. From this figure, we observe a decay of surface $\tau_{||}$ and the relaxation of the underlying substrate layers as the system transitions from the postirradiated to the postannealed state. Moreover, we observe the effect of the dislocation loop in the cumulative stress at a depth of approximately 9 nm in the postannealed configuration.

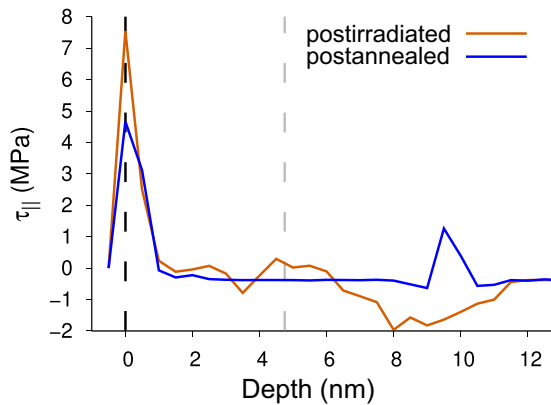


FIG. 11. The in-plane stress ($\tau_{||}$) as a function of depth for the (vermilion) postirradiated and (blue) postannealed configurations. The black and gray vertical dashed lines represent the substrate surface and the location of the amorphous-crystalline interface.

IV. CONCLUSIONS

MD simulations were conducted to carry out ^{28}Si ion implantations and produced the isotopic enrichment of Si layers. We discussed the role of implantation energy and angle of incidence on sputtering yield and implantation depths. At relatively low energies (≤ 3 keV), the substrate showed net deposition of material, and the sputtering yield increases with incident ion energy, in qualitative agreement with BCA models and experiments. However, BCA models reported larger sputtering yield values than those obtained from our all-atom MD calculations. This difference highlights the ability of MD simulations to capture the complex many-body collisions that occurred during the implantation and sputtering processes. Furthermore, the distributions of implanted ^{28}Si projectiles showed similar implantation depths for different angles of incidence, suggesting that the depth was predominantly determined by the projectile's kinetic energy. In the range of incident energies modeled in this work, the mean implantation depth of projectiles was shallower than the optimal donor (^{31}P) placement required for effective qubit operation. Nonetheless, due to the ongoing accumulation of material, the irradiation process at these energies can achieve the desired thickness for donor implantation for spin qubits at fluences greater than $1 \times 10^{17} \text{ cm}^{-2}$.

In agreement with cross-sectional TEM images of postirradiated and postannealed samples irradiation by 45 keV ^{28}Si ions, we observe the formation of an amorphous-crystalline interface and the presence of a dislocation array resulting from the partial recombination of defects beneath this interface. Moreover, we find that the location of this amorphous-crystalline interface changes with the increase in thickness of the substrate. This displacement explains the presence of isotopic enrichment beyond the interface at the end of the irradiation process. Overall, our results demonstrate the applicability of MD simulations for studying the enrichment process of Si layers via localized FIB implantation. Nonetheless, the time and space limitations of the MD approach make it difficult to achieve the required fluences and enrichment levels at higher implantation energies. Additionally, to explore results comparable to those obtained using higher-energy FIB hardware in other studies on localized ^{28}Si -enriched layers, the role of electrons, in particular electronic stopping, must be addressed, as it plays a key role in the energy exchange of fast-moving atoms, which becomes significant important at higher implantation energies.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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