Atomistic Modeling of the Isotopic Enrichment via Ion Irradiation of Silicon-28 Layers for Quantum Architectures

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Introduction

High fluence ion implantation with silicon-28 into natural silicon substrates has been shown to result in the depletion of the nuclear spin 1/2 silicon-29 isotope to below 3 ppm resulting in a close to spin-free matrix for donor-based quantum computer architectures. Optimisation of this enrichment process requires a detailed understanding of the atomic dynamics during the deposition process. Given that previous binary collision Monte Carlo simulations, employed to model experimental settings, lack the mechanistic detail needed for process optimisation, a more exhaustive description of the ion implantation process remains to be addressed. In this context, we employ molecular dynamics (MD) simulations, to examine the enrichment process by performing overlapping depositions of silicon-28 ions across a wide range of energies followed by a post-irradiation annealing, resulting in the overall enrichment of the sample with silicon-28, and reduced silicon-29 and silicon-30 isotopes. By comparing with experimental outcomes, we aim to validate and enhance the understanding of the silicon-28 enrichment process for future quantum computing architectures.

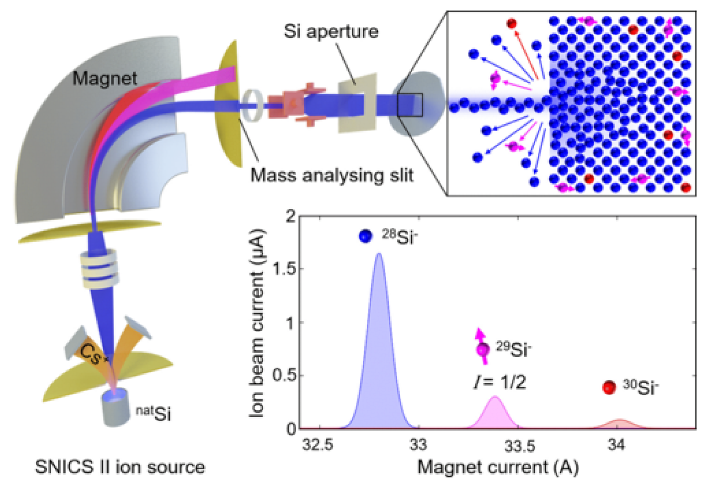

Figure 1: Ion beam used to istopically enrich a substrate[1].

Simulation details

In this study, we employed MD simulations to examine the isotopic enrichment of natural Si layers by performing overlapping depositions of silicon-28 projectiles. All of our MD simulations were performed using the LAMMPS code[2].

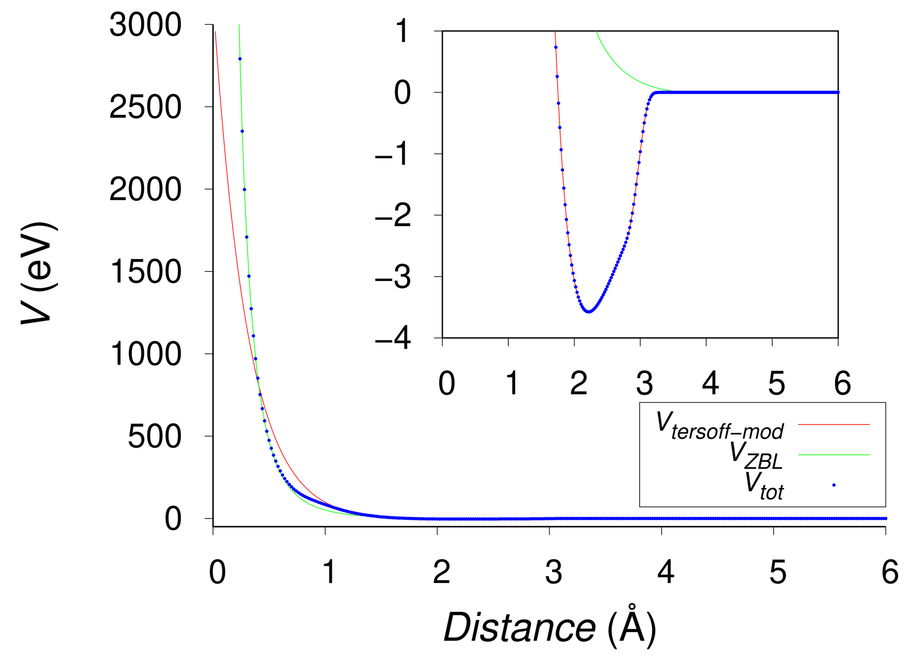

Figure 2: Si-Si pair potential (V) as a function of distance.

Details

- Atoms: 11'000'000
- Diamond rep: 50 × 50 × 550
- Variable timestep
- Incidence: 7°
- Charged-neutral projectiles
- Sufficiently large substrates
- Deposition: 2-10 ps
- Thermalisation: 50 ps
- Kumagai[3] joined to ZBL[4]

MD model

We employed ion implantation energies of 20, 30, and 45 keV. To emulate the ion implantation process, (charged-neutral) silicon-28 projectiles were launched into the material one by one. To reproduce a highly-irradiated material, i.e. high-fluence; we subjected the substrate to an amorphization process

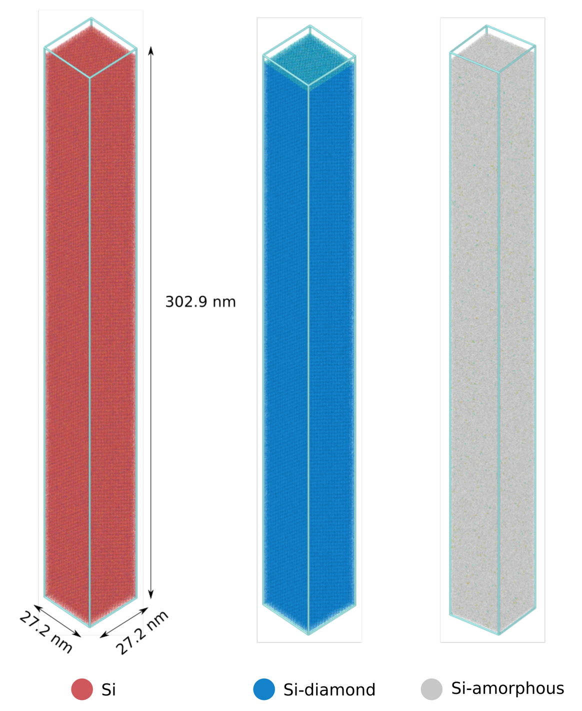

Figure 3: Substrates employed in this study.

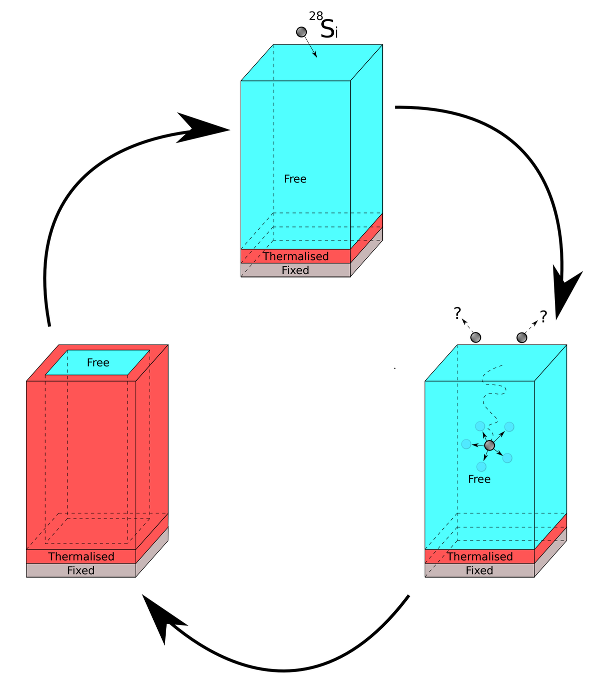

Figure 4: Schematic representation of the injection cycle.

Sputter yield and Implantation depths

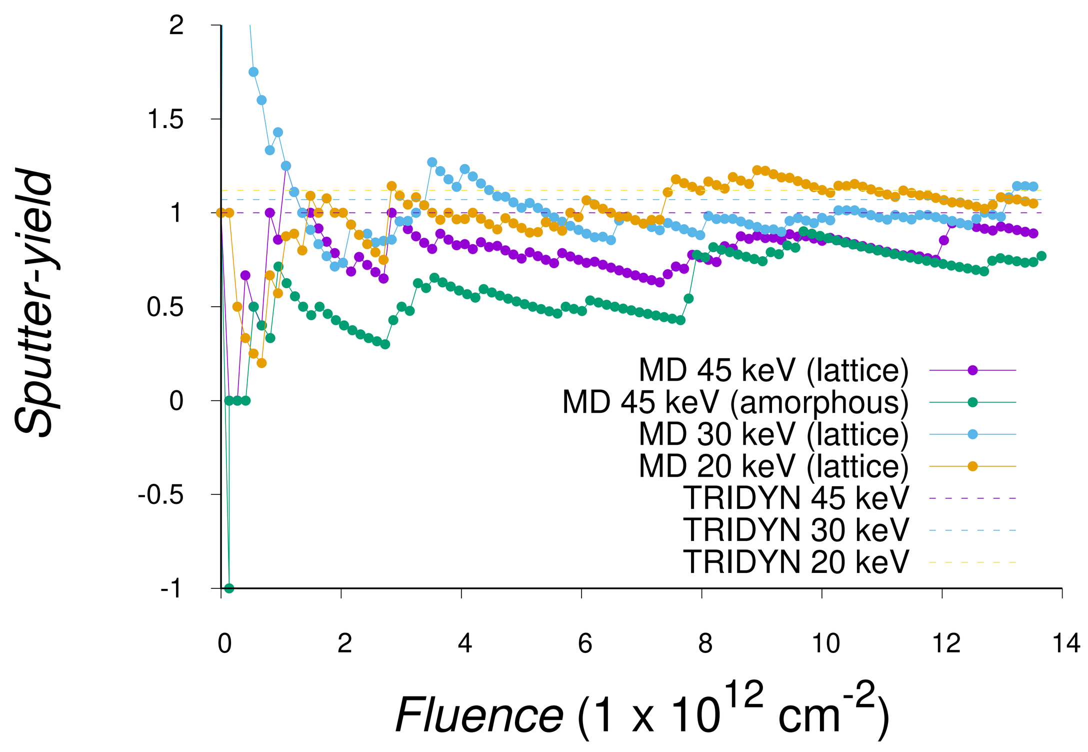

Figure 5: Sputter yield as a function of fluence, i.e. incident projectiles.

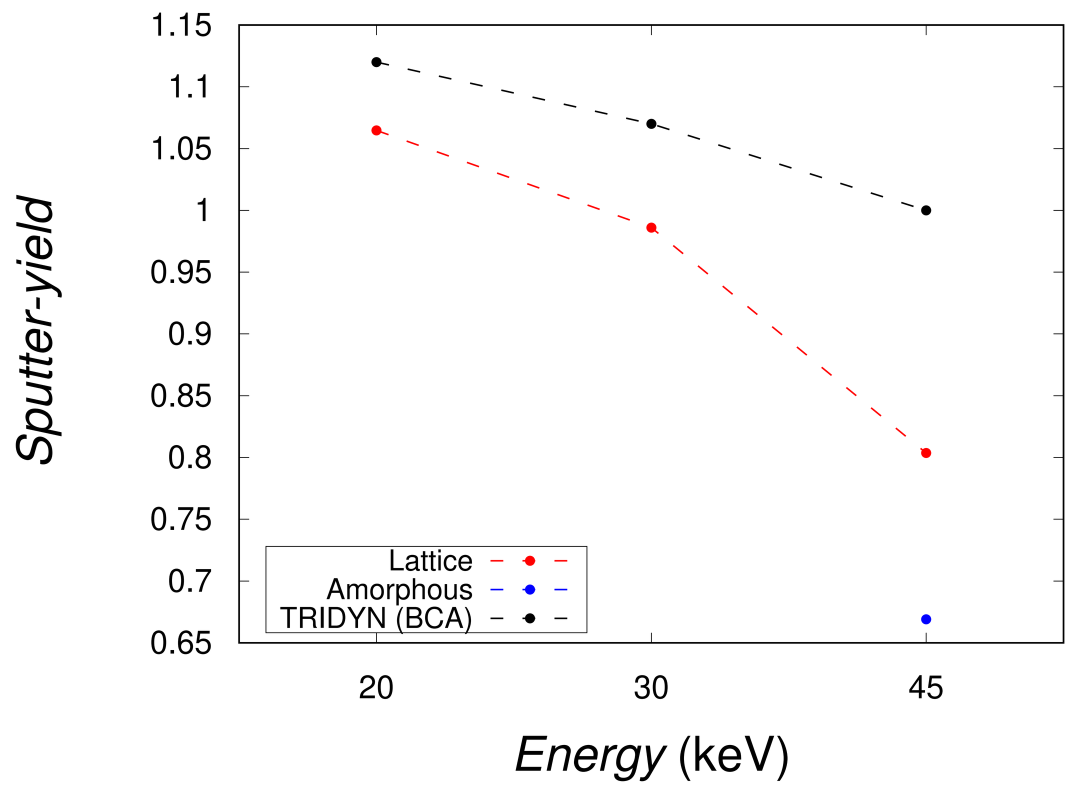

Figure 6: Sputter yield for different implantation energies, lattice structures, and simulation methodology.

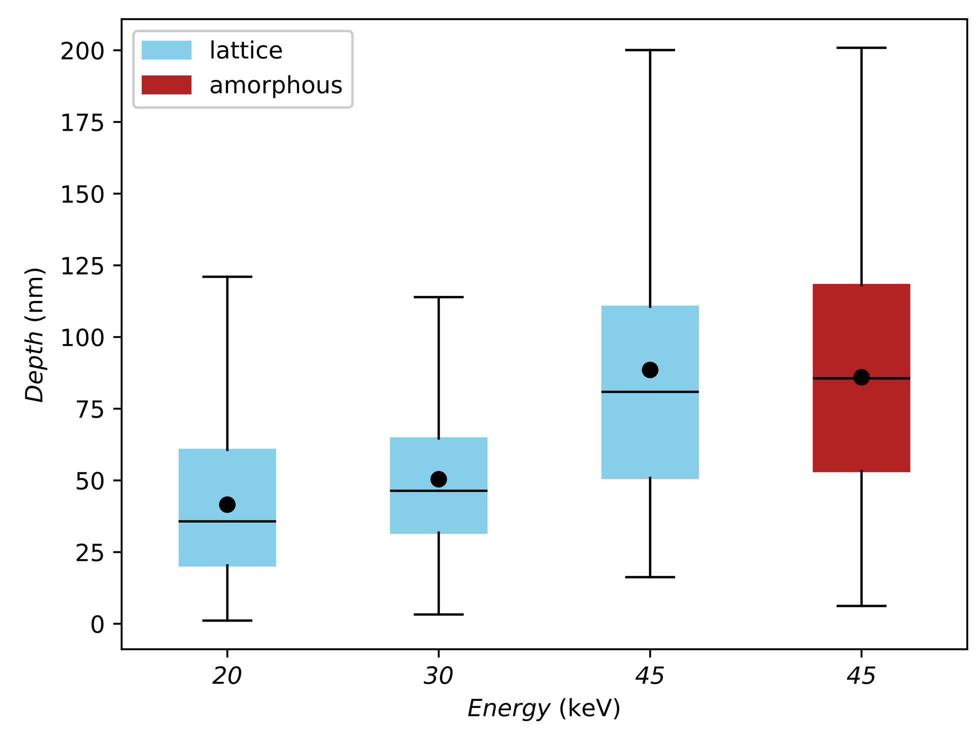

Figure 7: Distributions of the implanted silicon-28 for different implantation energies, and lattice structures.

High-fluence

To explore the enrichment of the silicon substrate at a high fluence, we model 9000 ion injection cycles corresponding to a fluence of ca. 3.052×10^{16} cm^{-2} with an ion implantation energy of 1 keV and normal angle of incidence.

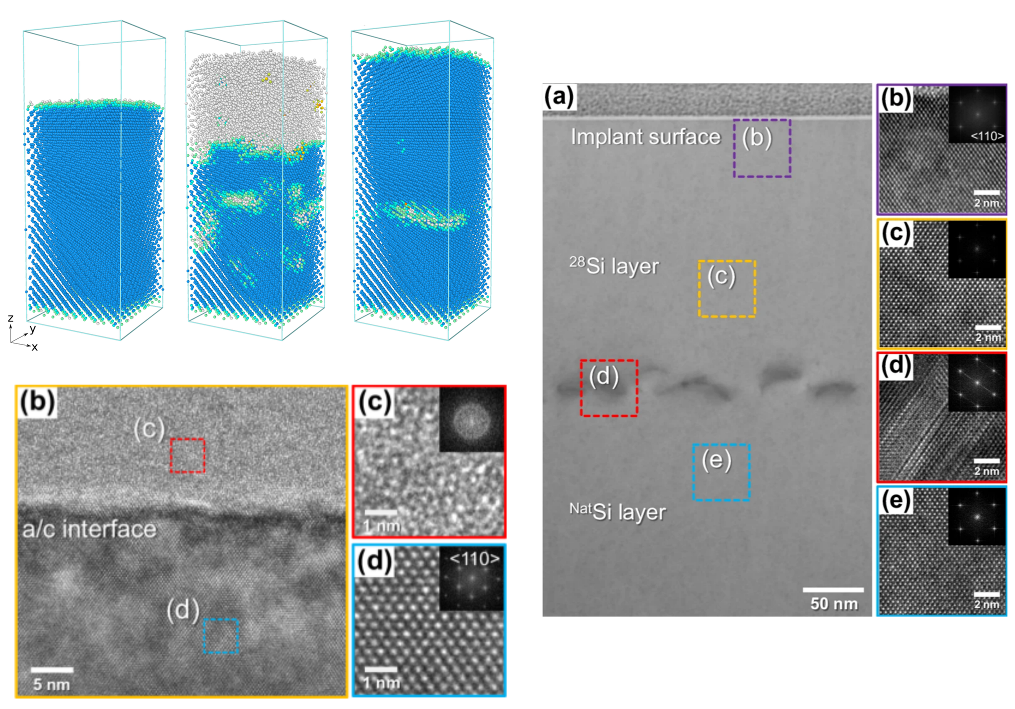

Figure 8: High-fluence irradiation compared to experiments. Experiments taken from [5]

Conclusions

- **MD is a valid methodology to study silicon enrichment via ion implantation.**
- **At high fluences, the amorphous material accumulates more projectiles, as indicated by a decreased sputter yield.**
- **The silicon substates transitions from recession to accumulation between 20 and 45 keV implantation energies.**
- **Remnant dislocation loops below the amorphous-crystalline interface result from unrecombined defects.**

References

1. D. Holmes et al. *Phys. Rev. Mater.* (2021).
2. AP. Thompson, *Comput. Phys. Commun.* (2022).
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4. JF. Ziegler, *The stopping and range of ions* (1985).
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