ATOMISTIC SIMULATIONS OF ION IMPLANTATION: THE SPUTTERING EFFECT ON DEPTH DISTRIBUTIONS

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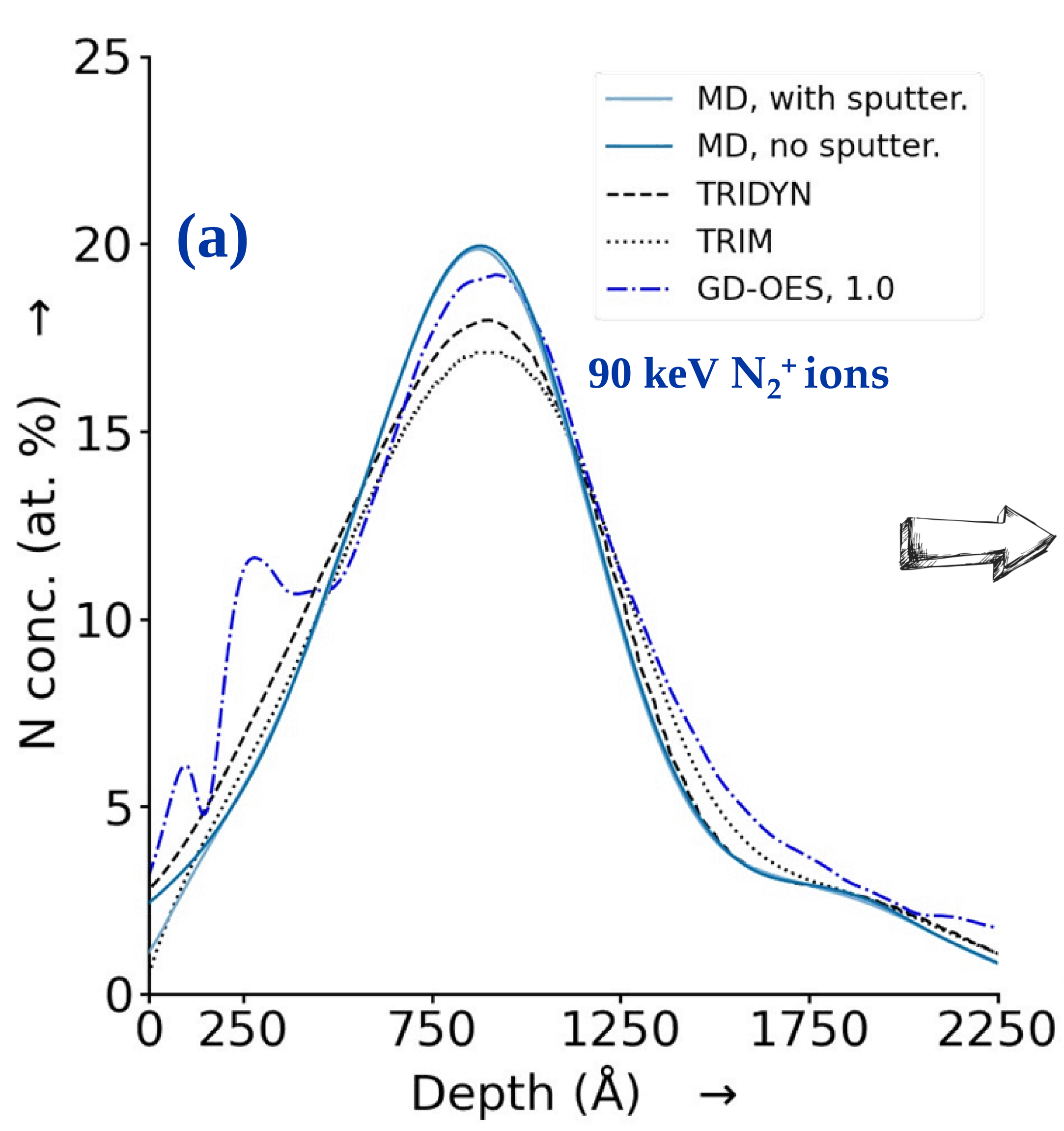
INTRODUCTION

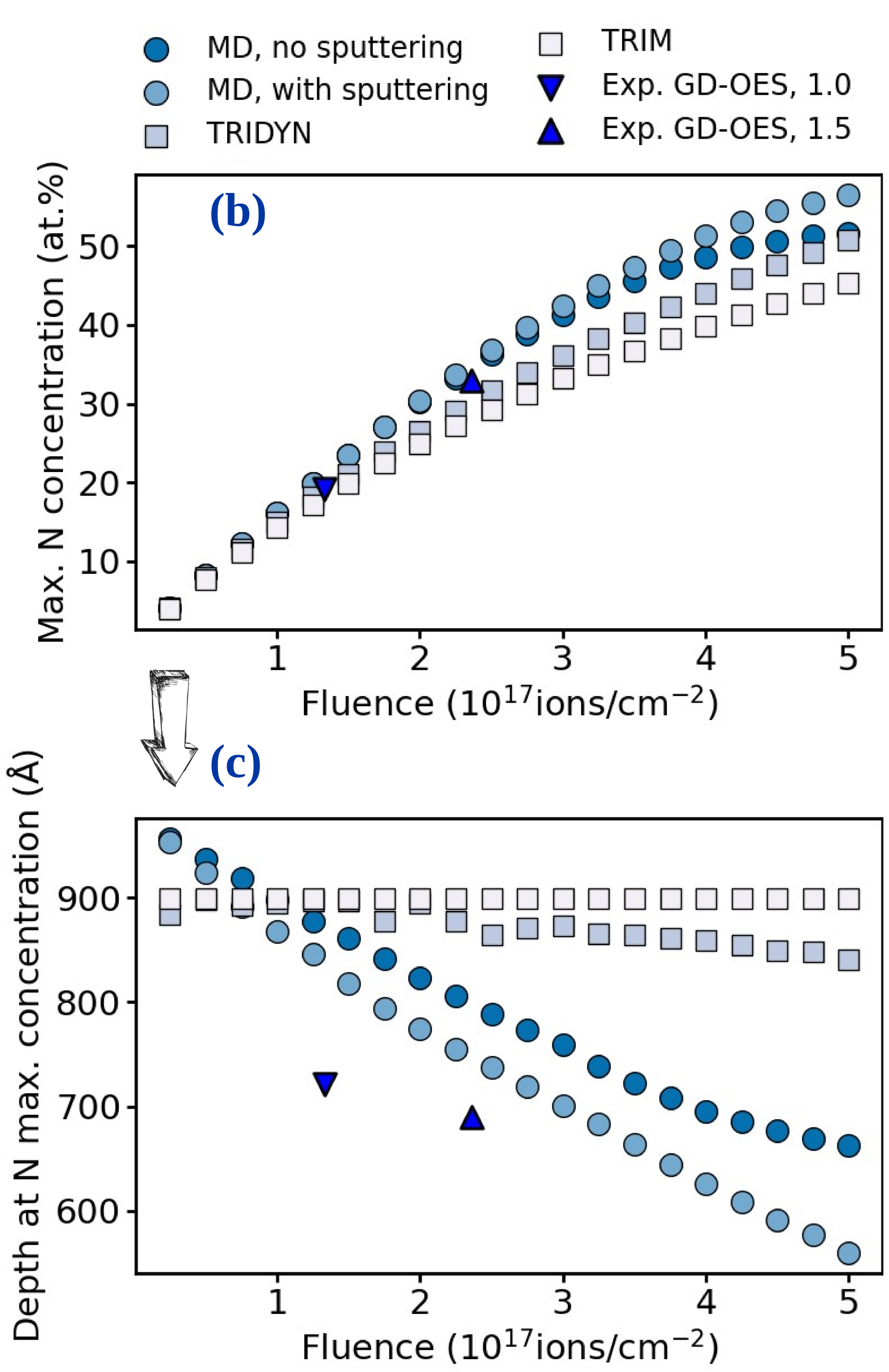
- Molecular dynamics (MD) suitable for studying ion implantation.
- Sputtering effect incorporation important for surface properties.
- **Problem:** High computational demands due to many atoms.
- **Solution:** Innovative integration of sputtering from TRIDYN into LAMMPS.
- This integration reduces computational time for MD simulations.
- Algorithm tested on N particle depth distributions in α-Ti target.
- Compared with/without sputtering and TRIM, TRIDYN, GD-OES data.
- Demonstrated efficient approach for predicting high-dose ion implantation.

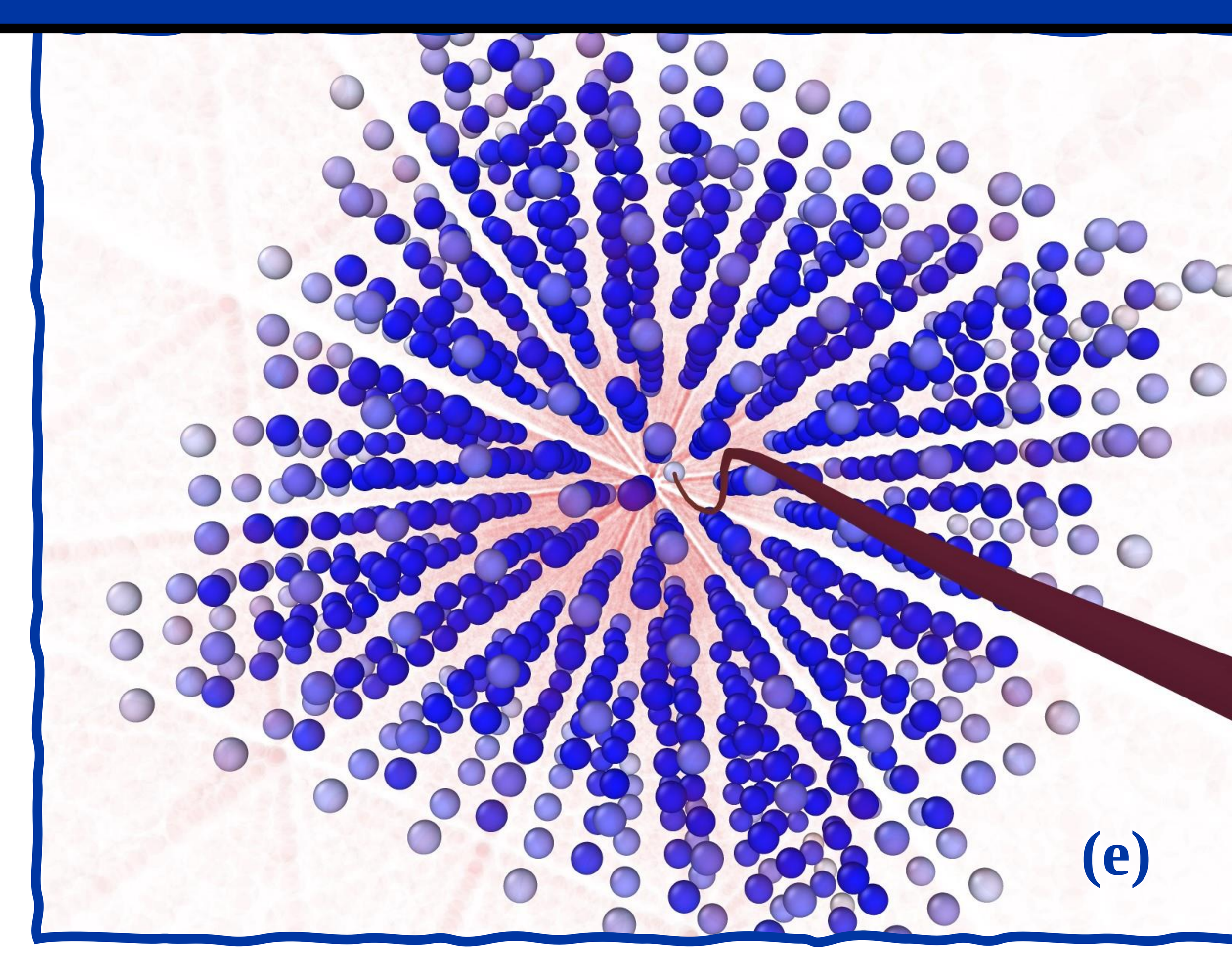
KEYWORDS

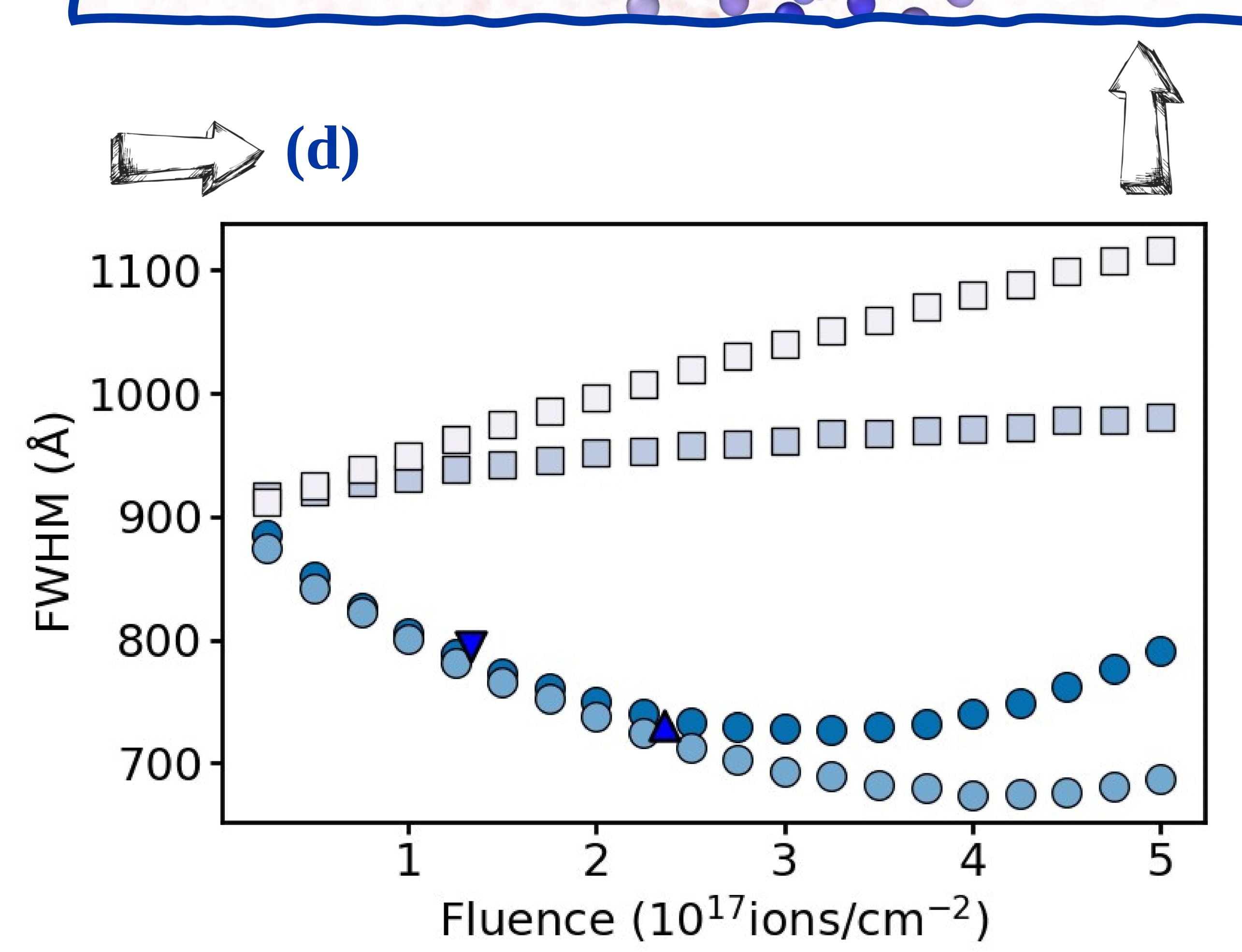
- Ion implantation
- Nitrogen in α-titanium
- Depth distributions
- Sputtering effect
- Molecular dynamics
- MC TRIM and TRIDYN

RESULTS









Figures:
(a) Implanted N distributions in α-Ti.
(b) N concentration maxima.
(c) Depth positions of N maxima.
(d) FWHM.
(e) Efficient MD simulation algorithm.

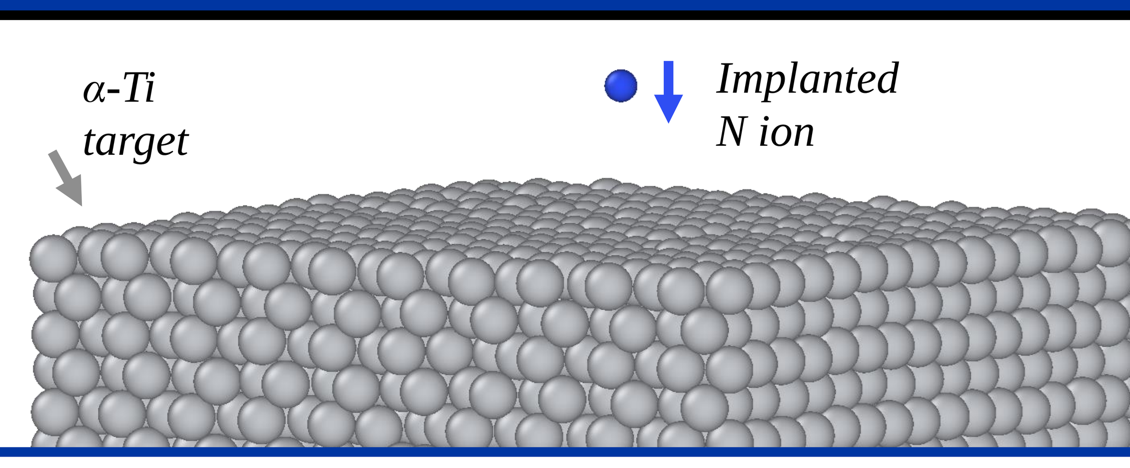
CONCLUSIONS

- Using MD simulations with and without sputtering, MC TRIM and TRIDYN, N depth distributions in α-Ti target were predicted as a function of implanted N fluence.
- The sputtering is shown to have an important effect for higher fluences and was succesfully implemented for middle-to-high fluences into MD LAMMPS using an in-house algorithm.
- Algorithm's practicality demonstrated for N depth distributions in Ti. The MD incorporating sputtering align better with experiments, providing more reliable predictions.

METHODS

Molecular dynamics simulations

#LAMMPS
#efficient algorithm for ion implantation [1]
#2NN-MEAM + ZBL [2] potentials
#SRIM electronic stopping power
#adaptive timestep
#velocity Verlet algorithm
#periodic boundaries (x, y), fixed boundary (z)
#α-Ti models from Atomsk



References:
[1] Lebeda, M et al., MD simulation of nitrogen ion into α-titanium target. In preparation.
[2] Kim, Y. M. and Lee, B. J. (2008), Acta Materialia, 56(14), pp. 3481–3489.

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