Atomistic simulation of nitrogen ion implantation into α-titanium target

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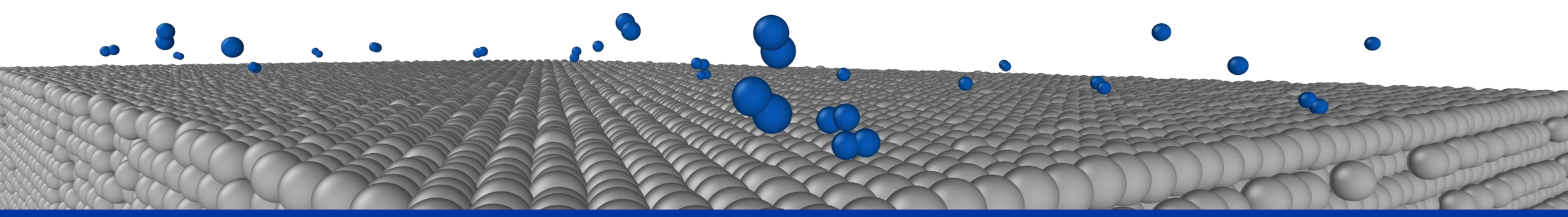
INTRODUCTION

We present a molecular dynamics simulation of N ion implantation with 90 keV impact energy into α-Ti target as a function of N fluence using our in-house time-saving algorithm, and compare the simulation with corresponding experiments.

- Implantation of N ions into Ti-based materials changes (improves) their properties such as hardness, corrosion resistance, and elastic moduli.
- Changes are connected to the number of introduced point defects and potentially formed new phases, which can be expected from N depth distributions.
- Depth distributions are experimentally studied by, e.g., Glow Discharge-Optical Emission Spectrometry (GDOES) or Secondary Ion Mass Spectrometry (SIMS), however, each of them is subjected to different analytical limits.
- To provide valuable comparison to the experiments, computer simulations are being advantageously used.
- We used molecular dynamics (MD) method to simulate N ion implantation into α-Ti target for a wide range of N fluences and we compared the results with our experimental results evaluated by GDOES and SIMS experiments.



RESULTS

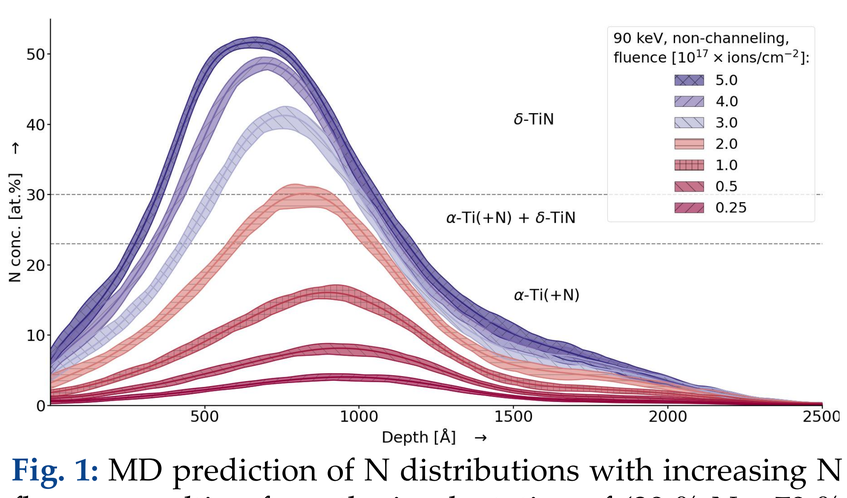


Fig. 1: MD prediction of N distributions with increasing N fluence resulting from the implantation of (30 % N + 70 % N_2) particles into a non-channeling surface of α-Ti matrix. The expected phases for given N concentration are illustrated.

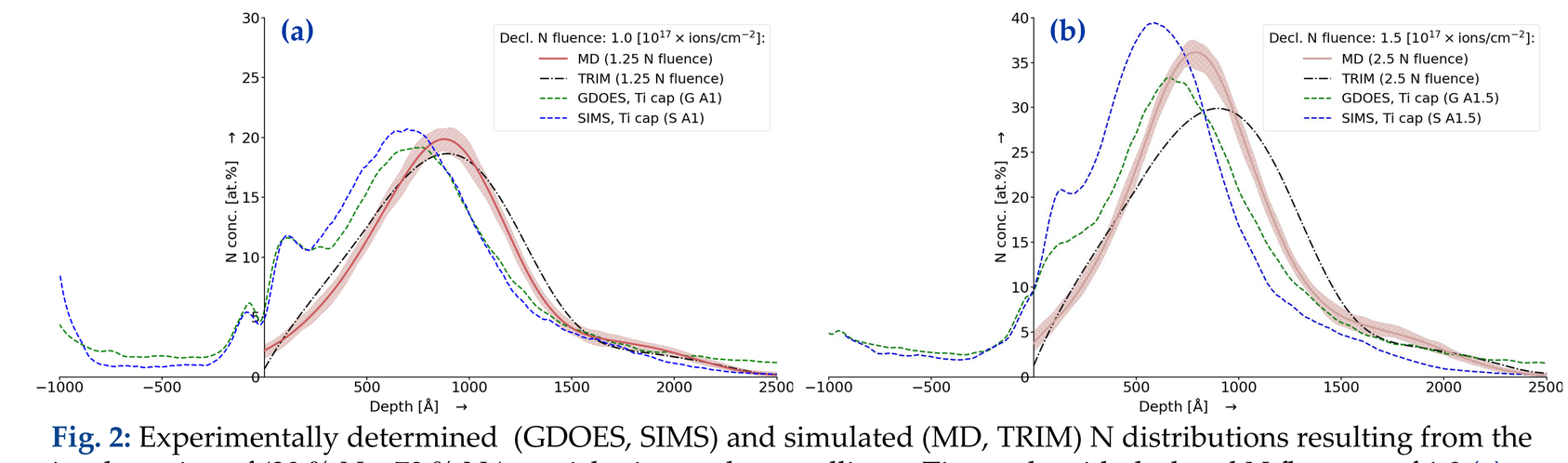


Fig. 2: Experimentally determined (GDOES, SIMS) and simulated (MD, TRIM) N distributions resulting from the implantation of (30 % N + 70 % N_2) particles into polycrystalline α-Ti sample with declared N fluences of 1.0 **(a)** and 1.5 **(b)** × 10^{17} ions/cm^2.

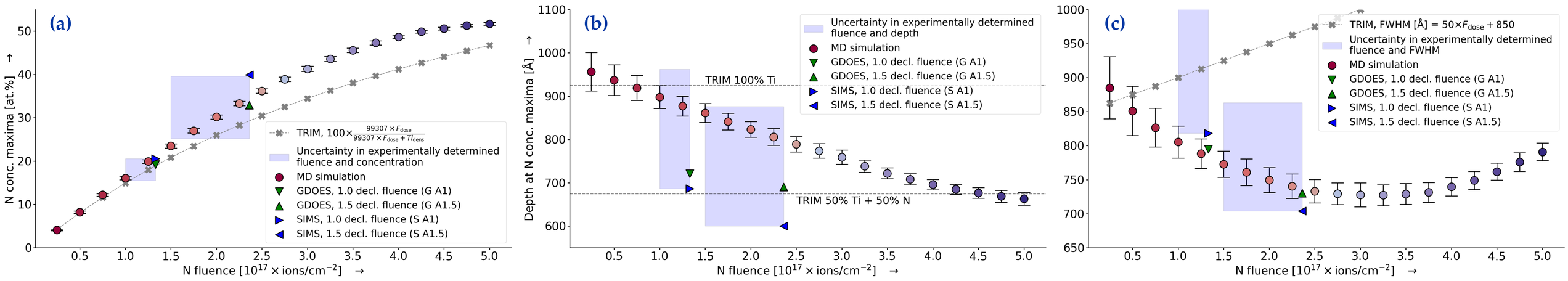


Fig. 3: MD, TRIM and experimental (SIMS, GDOES) N concentration maxima **(a)**, corresponding depths **(b),** and full width at half maxima **(c)** determined from N distributions (**Fig. 1** and **Fig. 2**.).

CONCLUSIONS

- We predicted N depth distributions in α-Ti target resulting from N ion implantation using molecular dynamics for a wide range of N fluences and with the accelerating voltage of 90 kV (**Fig. 1**).
- We determined characteristics of obtained N distributions: N concentration maxima increase non-linearly as a function of N fluence **(Fig. 3, a)**, the corresponding depths exhibit linear decrease (up to 4.50 × 10^{17} ions/cm^2) (**Fig. 3, b**), and full width at half maxima (FWHM) decrease up to 2.75 × 10^{17} ions/cm^2, have a plateau up to 3.50 × 10^{17} ions/cm^2 and then start to increase, meaning that more N ions are being captured closer to the surface around the concentration maxima rather than deeper (**Fig. 3, c**).
- We achieved good agreement between MD N distributions and experimentally determined distributions by SIMS and GDOES **(Fig. 2** and **Fig. 3**).

METHODS

- **Computer simulation methods:**
  - Molecular dynamics (in LAMMPS with our time-saving script for ion implantation technique (**Fig. 4**), using 2NN-MEAM + ZBL [1] interatomic potentials and electronic stopping power [2])
  - Monte Carlo (in TRIM)
- **Samples and experimental methods:**
  - Samples prepared from commercially pure Ti grade II
  - Tecvac implanter using 90 keV N particles with 1.0 and 1.5 × 10^{17} fluences
  - Glow Discharge-Optical Emission Spectrometry (GDOES)
  - Secondary Ion Mass Spectrometry (SIMS)

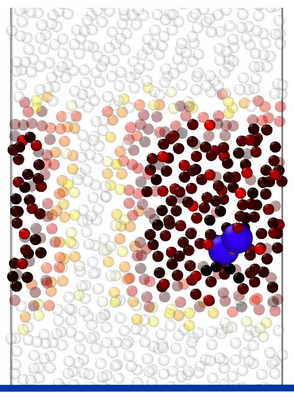


Fig. 4: Demonstration of our ion implantation simulation technique. For illustrative purposes, the implanted N ions are enlarged (blue color) compared to the titanium atoms (the rest). At one timestep, MD computations were performed only on the colored particles inside the box of arbitrarily chosen dimensions. The colored but transparent particles were fixed (forces acting on them were set as zeroes), but their pairwise interactions were taken into account. The remaining particles (non-colored and transparent) were kept frozen and were not considered during the calculation step.

References:

[1] Kim, Y. M. and Lee, B. J. (2008), Acta Materialia, 56(14), pp. 3481–3489.

[2] Nordlund, K. (1995), Computational materials science, 3(4), pp. 448–456.

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