

Angle-Dependent Implantation and Damage Characteristics of 60 keV Nitrogen Ions in Zirconium: A SRIM/TRIM Simulation Study

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Abstract

The implantation geometry of energetic ions controls their penetration, reflection and collision-cascade morphology. Here, the influence of incidence angle on 60 keV nitrogen-ion implantation into zirconium was evaluated with the Monte Carlo Binary Collision Approximation implemented in SRIM/TRIM. For each angle (0° , 6° , 12° , 18° and 24° , measured from the surface normal), 100,000 incident ions were simulated using a zirconium displacement energy of 25 eV, lattice binding energy of 3 eV and surface binding energy of 6.33 eV. Increasing the angle from 0° to 24° reduced the longitudinal projected range from 102.9 to 96.8 nm (5.93%) and increased the number of backscattered ions from 7,966 to 10,223 (28.33%), corresponding to backscattering fractions of 7.97% and 10.22%. In contrast, the lateral projected range increased from 48.4 to 57.5 nm (18.80%), the radial range from 76.0 to 83.3 nm (9.61%), the lateral straggle from 59.8 to 70.4 nm (17.73%), and the radial straggle from 37.0 to 39.9 nm (7.84%). Vacancy production remained 314.7 vacancies per ion through 18° and decreased slightly to 311.4 vacancies per ion at 24° . These results show that modestly oblique incidence redistributes the collision cascade toward a shallower, laterally broader near-surface volume while increasing ion reflection, without substantially changing the gross displacement yield. The findings provide a quantitative basis for selecting implantation geometry in zirconium surface modification; however, experimental validation and crystal-aware simulations are required before inferring retained nitrogen concentration, phase formation or property enhancement.

Keywords: SRIM/TRIM; nitrogen ion implantation; zirconium; incidence angle; projected range; straggling; backscattering; vacancy generation; Binary Collision Approximation.

1. Introduction

Ion implantation modifies the near-surface composition and defect structure of solids without requiring a deposited coating. The implanted depth, retained-ion distribution and radiation-damage field depend on ion mass, energy, target composition, displacement thresholds and beam geometry. In a collision-cascade description, energetic nitrogen ions lose energy through

interactions with target electrons and through elastic collisions with zirconium nuclei; the latter generate recoils and lattice displacements when the transferred energy exceeds the adopted displacement threshold [1–5].

Zirconium and its alloys are important in nuclear, chemical and biomedical technologies because of their corrosion behaviour, low neutron-capture cross-section and biocompatibility. Nitrogen implantation has been investigated as a route to produce nitrogen-enriched or nitride-containing surface layers and thereby alter hardness, wear and corrosion response. Experimental studies on Zircaloy-4 and Zr-containing alloys have reported phase formation and changes in tribological or corrosion performance after nitrogen implantation [6–9]. Those outcomes are dose-, temperature- and microstructure-dependent and cannot be predicted from ion-range data alone.

Incidence angle is a particularly useful processing variable because it can change the component of ion motion normal to the surface and the probability of near-surface reflection. The present study therefore quantifies the angle dependence of backscattering, vacancies, ranges and straggling for 60 keV N ions incident on Zr at 0–24°. The objectives are to (i) compare depth and transverse cascade descriptors, (ii) quantify relative changes with angle, (iii) visualize the reported first-moment and spread parameters in two and three dimensions, and (iv) identify conclusions that are supported—and limitations that remain—within a static SRIM calculation.

2. Methodology: SRIM/TRIM simulation

2.1 Simulation design

The calculations used the Transport of Ions in Matter module of SRIM, a Monte Carlo code based on sequential binary collisions and semi-empirical stopping relations [5,10]. A monoenergetic 60 keV N beam was directed onto elemental Zr at 0°, 6°, 12°, 18° and 24°. Throughout this paper, angle is defined relative to the surface normal. A total of 100,000 incident ions was used at every angle. The target parameters supplied for all runs were: displacement energy, 25 eV; lattice binding energy, 3 eV; and surface binding energy, 6.33 eV. All other settings should be reported exactly as selected in the original SRIM input file when the manuscript is submitted, including target density, layer thickness, calculation mode and SRIM version/build.

2.2 Extracted quantities and analysis

The reported outputs were the number of backscattered ions, vacancies per incident ion, longitudinal projected range, longitudinal straggle, lateral projected range and straggle, and radial range and straggle. Lengths were converted from ångström to nanometre using $1 \text{ Å} = 0.1 \text{ nm}$. The

backscattering fraction was calculated as $N_{bs}/100,000$. Relative change was calculated as $100[X(24^\circ) - X(0^\circ)]/X(0^\circ)$. No inferential uncertainty was supplied by the exported dataset; accordingly, the discussion treats the values as simulation estimates rather than experimentally measured quantities.

3. Theoretical background

3.1 Nuclear and electronic energy loss

The stopping power may be written as $-dE/dx = S_n(E) + S_e(E)$, where S_n is nuclear stopping and S_e is electronic stopping. Elastic nuclear encounters transfer kinetic energy to Zr atoms and can initiate recoil cascades. Electronic stopping represents inelastic energy transfer to the target electron system. At each binary encounter, scattering is evaluated using a screened interatomic potential; repeated stochastic events generate a distribution of terminal positions rather than a single range [1,4,5].

3.2 Range, straggling and angular geometry

The longitudinal projected range R_p is the mean penetration component along the chosen depth direction, while longitudinal straggle ΔR_p characterizes its statistical spread. Lateral and radial measures describe transverse dispersion. With increasing tilt from the surface normal, the normal component of a nominal straight trajectory scales approximately with $\cos \theta$; real trajectories additionally undergo multiple scattering. Therefore, a reduction in normal projected range can coexist with increased transverse spread and backscattering. The approximation is qualitative because collision trajectories are neither straight nor identical.

3.3 Vacancy estimate

A vacancy is counted when the recoil-transfer sequence satisfies the displacement criterion used by the code. The resulting vacancies-per-ion value is a prompt displacement estimate. It is not the surviving defect concentration after recombination, thermal diffusion, dynamic annealing, cascade overlap or dose accumulation. The classical NRT framework and later assessments emphasize that displacement counts are model quantities whose relationship to stable defects depends on material and irradiation conditions [3,4,11].

3.4 Basis of the 2D and 3D imaging

Because raw ion-coordinate and recoil-coordinate files were not provided, an authentic SRIM trajectory image or three-dimensional collision-cascade cloud cannot be reconstructed. For visualization only, the depth distribution at each angle was represented by a normalized Gaussian

$p(z, \theta) = \exp\{-[z - R_p(\theta)]^2 / [2\Delta R_p(\theta)^2]\}$, using linear interpolation between the reported R_p and ΔR_p values. The resulting 2D contour and 3D surface preserve the supplied mean depth and longitudinal spread, but they do not constitute additional SRIM output, a concentration profile, or a prediction of retained dose.

4. Results and discussion

Table 1: Numerical results: Angle-dependent SRIM outputs for 60 keV N ions in Zr. Lengths were converted from Å to nm; backscatter percentages assume 100,000 incident ions per run.

Angle (°)	Backscattered ions	Backscatter (%)	Vacancies/ion	Long. range (nm)	Long. straggle (nm)	Lateral range (nm)	Lateral straggle (nm)	Radial range (nm)	Radial straggle (nm)
0	7966	7.966	314.7	102.9	48.3	48.4	59.8	76.0	37.0
6	8231	8.231	314.7	102.6	48.0	48.9	60.5	76.3	37.2
12	8477	8.477	314.7	101.3	48.1	50.8	62.7	77.9	38.0
18	9315	9.315	314.7	99.6	47.6	53.8	66.1	80.1	38.9
24	10223	10.223	311.4	96.8	47.2	57.5	70.4	83.3	39.9

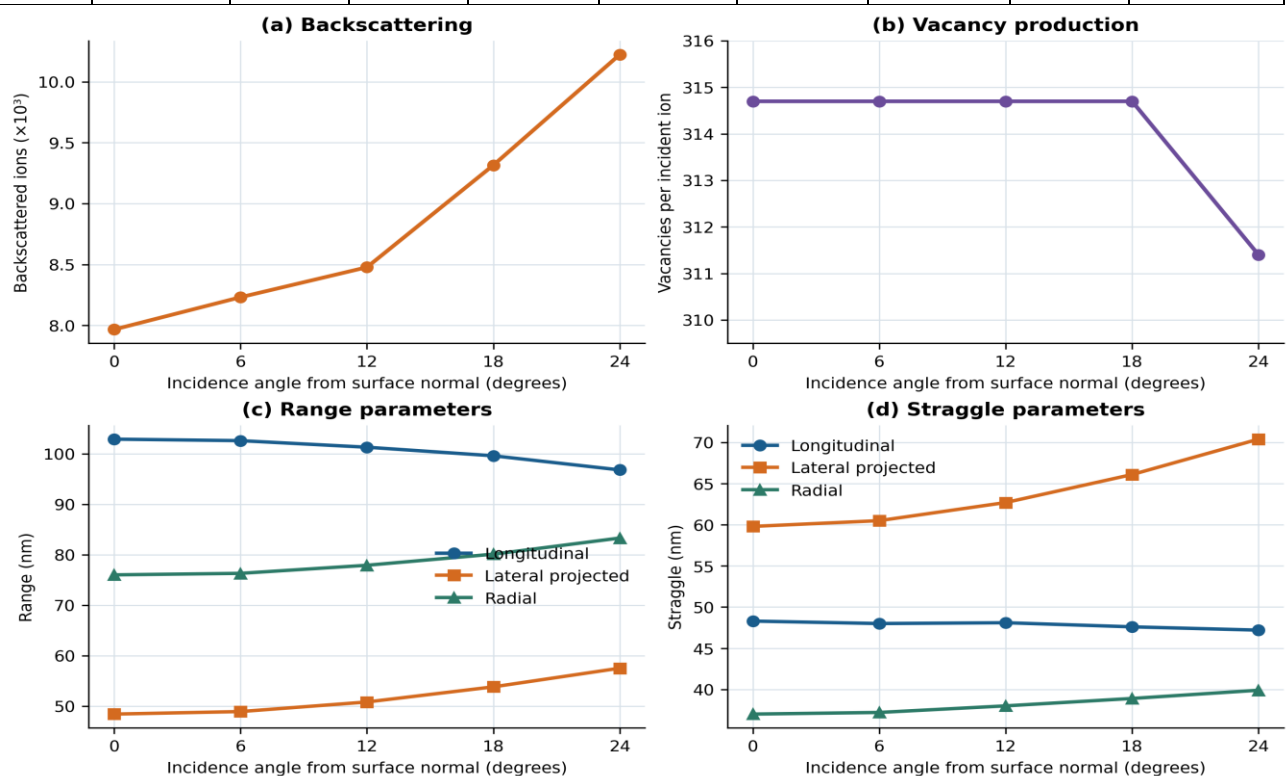


Figure 1. Dependence of (a) backscattering, (b) vacancy yield, (c) range and (d) straggle parameters on incidence angle. Points are the supplied SRIM values; connecting lines guide the eye.

4.1 Backscattering and depth contraction

The number of backscattered ions increased monotonically from 7,966 at normal incidence to 10,223 at 24°, raising the reflected fraction from 7.966% to 10.223%. This is an absolute increase of 2.257 percentage points and a relative increase of 28.33%. Simultaneously, R_p decreased from 102.9 to 96.8 nm, a reduction of 6.1 nm or 5.93%. A simple geometric projection $R_p(0)\cos 24^\circ$ gives 94.0 nm, close to but lower than the simulated 96.8 nm. The difference is physically reasonable because R_p is an ensemble moment shaped by scattering, energy loss and preferential loss of reflected trajectories, not merely a projected straight-line path.

4.2 Lateral and radial broadening

The depth contraction was accompanied by systematic transverse broadening. The lateral projected range increased by 18.80% (48.4 to 57.5 nm) and its straggle increased by 17.73% (59.8 to 70.4 nm). Radial range and radial straggle increased by 9.61% and 7.84%, respectively. Thus, oblique incidence redistributes the implanted population and collision cascade: it becomes shallower in the surface-normal direction but broader parallel to the surface. This is relevant when lateral uniformity or proximity of damage to a free surface is important.

4.3 Longitudinal straggle and vacancy production

Longitudinal straggle changed only modestly, from 48.3 nm at 0° to 47.2 nm at 24° (−2.28%), with small non-monotonic variation among intermediate angles. Vacancy production was exactly 314.7 vacancies per ion in the supplied outputs from 0° through 18°, then decreased to 311.4 at 24° (−1.05%). Consequently, within the resolution of these outputs, angle mainly changes where the damage is distributed and how many ions escape; it does not materially change the prompt gross displacement yield over 0–18°. The slight 24° reduction is consistent with increased reflection and reduced energy deposition in the target, although recoil and energy-partition files would be required to demonstrate that mechanism directly.

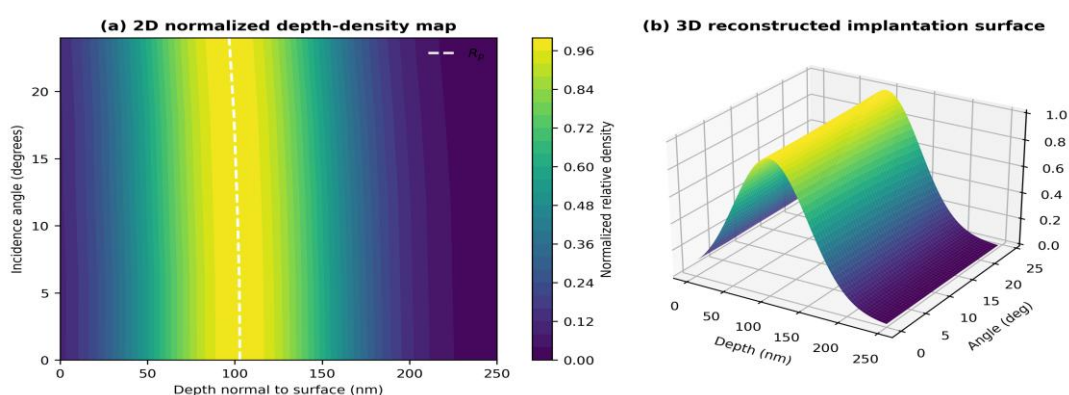


Figure 2. Data-derived imaging based on a normalised Gaussian reconstruction from the reported longitudinal range and straggle: (a) 2D depth–angle contour and (b) 3D surface. These are visualisations of first moments, not raw SRIM trajectories or absolute concentration maps.

4.4 Interpretation in relation to zirconium surface modification

The predicted depth scale (approximately 97–103 nm for the mean range) places the implanted population within a nanoscale surface layer. Prior experimental work has shown that nitrogen implantation can form ZrN/Zr–O–N-related phases and modify wear or corrosion response in zirconium alloys [6–9]. The present simulations complement those studies by isolating an angular transport effect at fixed energy. They do not establish phase formation: chemical state depends on fluence, temperature, oxygen activity, diffusion and post-implantation treatment. Nor do the data support the aluminium-based applications stated in the preliminary abstract; the simulated target is zirconium, so all material-specific claims have been corrected accordingly.

4.5 Model limitations and reproducibility

Several constraints delimit the conclusions. Standard SRIM treats the target through an amorphous/random-collision approximation and does not explicitly reproduce crystallographic channeling, evolving composition, dose-dependent sputter erosion, cascade overlap, defect recombination or long-time diffusion. Comparisons with experiment show that SRIM range estimates can exhibit material- and energy-dependent offsets [12]. Crystal-aware BCA or molecular-dynamics calculations are preferable when orientation and near-surface atomistic effects are central [13,14]. For reproducibility, a final submission should archive the SRIM version, input file, target density, layer thickness, detailed calculation mode, random seed policy and all output files. Independent repeated runs would also permit numerical confidence intervals.

5. Conclusions

A SRIM/TRIM study of 100,000 60 keV N ions incident on Zr at 0°, 6°, 12°, 18° and 24° predicts a clear angular redistribution of ion transport. Between 0° and 24°, the longitudinal projected range decreases from 102.9 to 96.8 nm, while backscattering increases from 7.97% to 10.22%.

The lateral projected range and lateral straggle rise by 18.80% and 17.73%, respectively; radial range and radial straggle also increase. Oblique incidence therefore produces a shallower but laterally broader affected region. Vacancy production remains 314.7 vacancies per ion up to 18° and falls only 1.05% at 24°. The angle dependence is therefore stronger for cascade geometry and reflection than for gross prompt displacement yield. The 2D and 3D reconstructions visualise the supplied range moments but must not be interpreted as raw trajectory images or absolute nitrogen concentration. Experimental depth profiling, phase

analysis and mechanical/corrosion tests are needed to validate the predicted trends and connect them to functional properties.

Data availability and declaration

The numerical dataset analysed in this study is reproduced in Table 1. No external funding or conflict of interest was declared. This manuscript reports a computational study; no human participants, animals or biological samples were involved.

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