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Comparison of experimental and theoretical results of nitrogen implantation in AISI 304 stainless steel

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Abstract

Depth and distribution of implanted ions play an important role in electrical and mechanical properties of implanted surfaces. In this study nitrogen implantation at 30 keV with different doses in the range of 1×10^{17}–1×10^{18} ions/cm^2 on AISI 304 stainless steel samples has been performed. The experimental and theoretical depth profiles of nitrogen-implanted samples are investigated. Experimental depth profile using secondary ion mass spectrometry (SIMS) is compared with theoretical analysis (TRIM simulation). By considering the presence of N_2^+ in the implanting ion beam and sputtering effects, the TRIM and SIMS results were modified to good agreement. The proper ratio of N_2^+/N^+ is evaluated by a curve fitting procedure.

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Keywords: Nitrogen implantation; SIMS; Simulation; Stainless steel; Depth profile

1. Introduction

Ion implantation is one of the well known techniques for modification of physical and chemical properties of material surfaces. In this process, ions with different energies and doses are accelerated towards the sample surface. The implanted surface properties are a function of energy, dose and type of ions and also surface composition of the sample. [1].

Because of unique properties of stainless steel, it has many practical applications. Nitrogen ion implantation improves surface properties of stainless steel such as corrosion resistance, hardness and wear [2,3].

In this research AISI 304 stainless steel samples were implanted by nitrogen ions at different doses. The experimental nitrogen depth profile using Secondary ion mass spectrometry (SIMS) analysis has nearly Gaussian distribution shape, which can be compared with theoretical TRIM simulation [4].

SIMS technique is a powerful tool for characterization of chemical structure and surface components

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of materials because of its good combination of high detection and high sensitivity. Depth profiling is one of the important applications of SIMS, which provides composition properties with a high depth resolution.

2. Experimental details

The AISI 304 stainless samples (area = 6 × 18 mm^2, thickness = 1 mm) were mechanically polished and ultrasonically cleaned. The nitrogen implantation was performed at 30 keV with a ion current density of 50 μA/cm^2 and doses of 8 × 10^{17} to 1 × 10^{18} ions/cm^2. SIMS depth profile analysis of nitrogen has been carried out by CAMECA IMS 6F instrument. In this analysis Cs^+ was used as the primary ion beam and negative secondary N^- ions were detected. Impact energy of primary ions and primary ion current were 15 keV and 2 nA, respectively. The scanned area was 200 × 200 μm^2 and the analyzed area was 60 μm^2.

3. Results and discussion

This investigation was carried out on implanted samples with 8 × 10^{17} and 1 × 10^{18} ions/cm^2 doses. Nitrogen distribution at low dose implantation in absence of special orientation is Gaussian form but at high doses (>10^{17} atoms/cm^2) due to sputtering effect will be semi-Gaussian [5].

Beside the sputtering effects at high doses, the other factor that affects on shape of depth profile to deviate from Gaussian is existence of N_2^+ ions in ion beam. Under ideal conditions N_2^+ ions split into two N^+ ions with half of the original energy (E/2) and result in less penetration into the sample surface. To be realistic in depth profile analysis one must take into account the existence of N_2^+ ions in TRIM simulations.

The slight deviation of SIMS results from Gaussian shape is shown in Fig. 1. The results of TRIM simulation for 15 and 30 keV energies are Gaussian shape as shown in Figs. 2 and 3 respectively. As Shown in Figs. 1–3 the *x*-axis scale of TRIM and SIMS profiles are different.

The difference between TRIM results and SIMS depth profile is due to sputtering effects and also the existence of N_2^+ ions in implanted ions. In order to fit the TRIM results on SIMS depth profile, we have to consider both 15 and 30 keV TRIM simulations. A linear combination of TRIM data at 15 and 30 keV has been used for take into account the existence of N_2^+ ions to get a good curve fitting of TRIM simulation and SIMS data. The incident nitrogen flux is composed of both N_2^+ and N^+ ions. We define the fraction

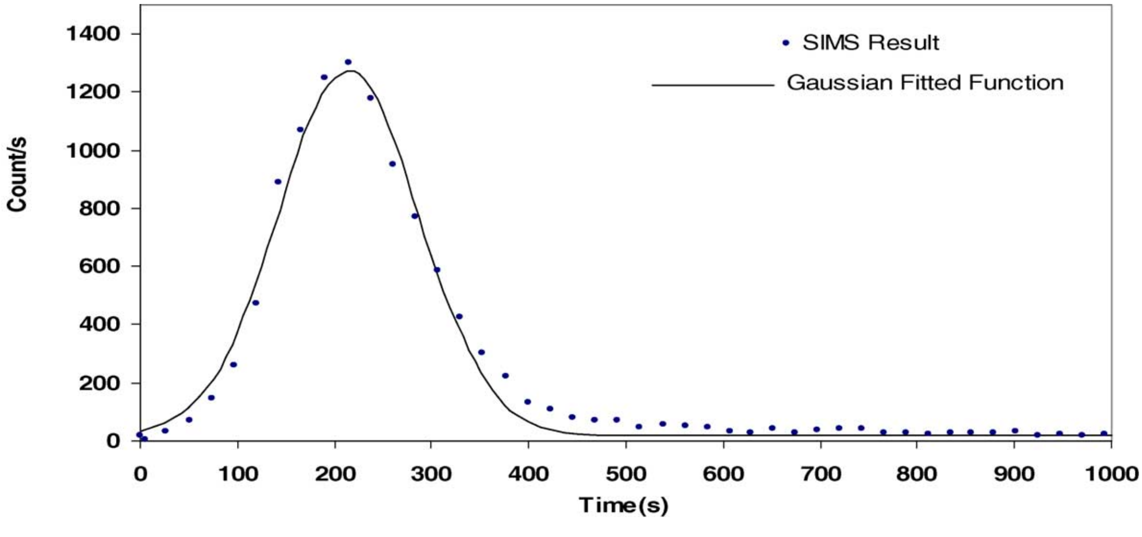

Fig. 1. SIMS depth profile of nitrogen implanted into stainless steel with a Gaussian fit.

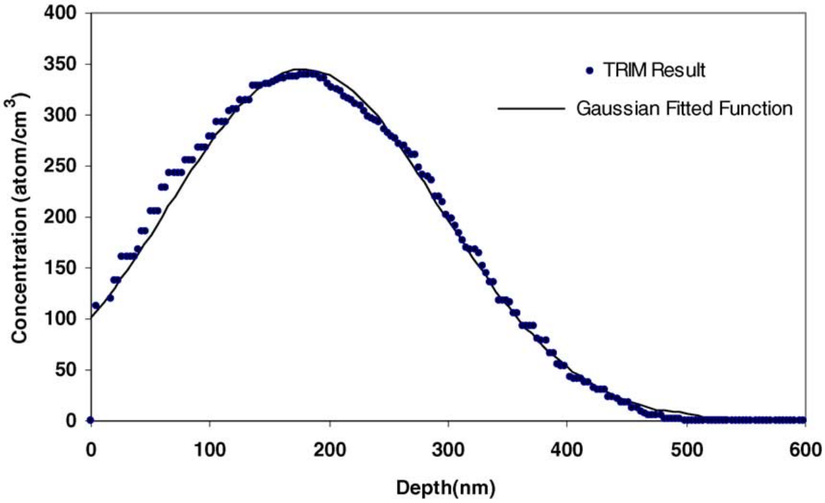

Fig. 2. TRIM simulation of nitrogen implanted into stainless steel at 15 keV energy with a Gaussian fit.

of N^+ ions in implanting ion beam as f, then its depth profile will be [6]:

$$N(E,x) = \frac{2(1-f)N(E/2,x) + fN(E,x)}{2-f} \quad (1)$$

where $N(E, x)$ is the normalized depth profile, E is ion energy and x is depth.

Another problem in this curve fitting is to take into account the effect of ion implantation and SIMS sputtering effect. This problem was resolved by shifting the depth profile. In the other word by considering various combinations of TRIM results at 15 and 30 keV with respect to Eq. (1) and also by changing the origin and scale on SIMS profile we can obtain a good agreement between experimental SIMS results and theoretical TRIM simulation.

We denote SIMS and TRIM results by N_{SIMS} and N_{TRIM}. In SIMS profile, $N_{\mathrm{SIMS},}$ is modified by change

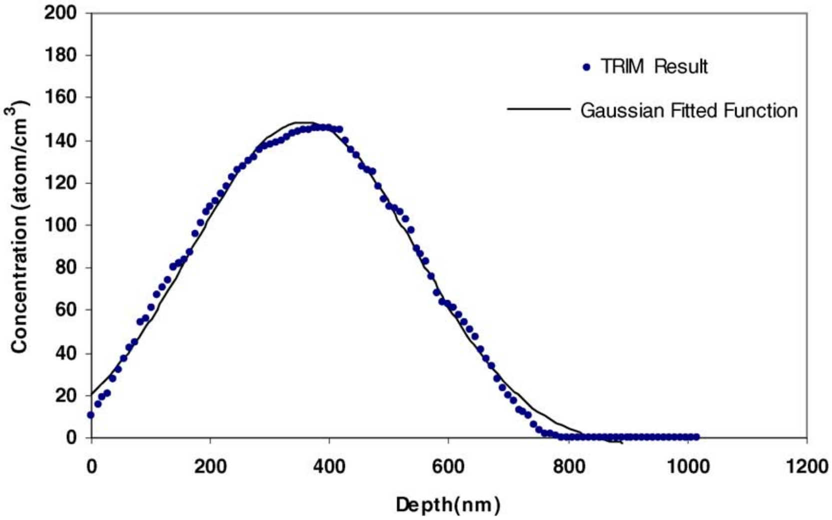

Fig. 3. TRIM depth profile of nitrogen implanted into stainless steel at 30 keV energy with a Gaussian curve fit.

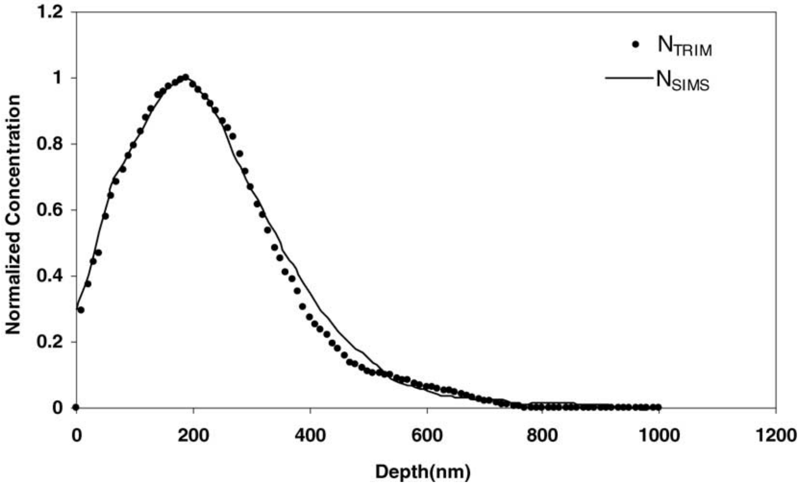

Fig. 4. Modified TRIM simulation and SIMS results depth profiles.

of origin and scale as:

$$N_{\mathrm{SIMS}}(x) \longrightarrow \text{Scale and origin transformation} \quad N_{\mathrm{SIMS}}(ax+b)$$

and N_{TRIM} as:

$$N_{\mathrm{TRIM}}(E,x) = \frac{2(1-f)N(E/2,x) + fN(E,x)}{2-f}$$

where $E = 30$ keV

Least square method is applied in curve fitting to obtain suitable values for *a* and *b*. Where *b* is related to change in origin due to sputtering effects and *a* is related to scale transformation from time into depth scale in SIMS data. It should be considered that all profiles were normalized to one before applying the above curve fitting.

Fig. 4 shows a good agreement between TRIM and SIMS data by using above procedure. The result of curve fitting gives the values of $a = 1.9$, $b = 301$ and $f = 0.24$. The projected range of ions from modified TRIM is evaluated to be about 190 nm (Fig. 4). It is considerable that *f*-value has good agreement with other reports [7].

4. Conclusion

In this work a good agreement between TRIM simulation results and experimental SIMS data has been obtained by scale transformation in SIMS depth profile and a suitable combination of TRIM result for 15 and 30 keV energies. It has been concluded that the existence of N_2^+ with N^+ ions simultaneously in implantation ion beam and the effect of surface sputtering deviate the nitrogen profile from Gaussian. By choosing of the proper ratio of N_2^+/N^+ it has been shown that a good fit to SIMS depth profile using TRIM simulation can be obtained. It should be noted that *f*-value obtained from curve fitting is in good agreement with previous reports. One of the applications of this research is depth calibration of SIMS raw data without a direct measurement. This work also suggests, future development and application of TRIM simulator.

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