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Modelling of the similar depth profiles of two different kinds of ions, implanted to WC-Co tools, used in wood-based material machining

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Abstract: *Modelling of the similar depth profiles of two different kinds of ions, implanted to WC-Co tools, used in wood-based material machining*. An attempt was made to model the similar depth profiles of ions of two commonly used gases, i.e., nitrogen and argon, for the parameter values possible to obtain using classical implanters. Modelling was executed in two stages. Similar profiles were obtained for the acceleration voltage value of 35 kV in the case of nitrogen and the sum of the acceleration voltages of 65+32.5 kV in the case of argon. The difference in the obtained profile parameter values, such as: the peak volume dopant concentration of the implanted element, the projected range and the range straggling, was less than 1%.

Keywords: ion implantation, depth profiles, modelling, WC-Co tools, wood machining

INTRODUCTION

Ion implantation is a relatively simple and cheap method of the modification of near-surface regions of different materials, the machine elements or tools, including the tools used for wood-based material machining.

This low temperature method is used in material engineering processes to modify/change the physical and/or chemical properties of the near-surface regions of solid materials (targets) through the introduction of foreign element(s) ions. The introduced ions are accelerated in the electric field to an energy from several dozen to several hundred kiloelectronvolts, which corresponds to their velocity from hundreds to thousands of kilometres per second. The ion beam interacts with the modified material, introduces new atoms, damages its crystal lattice, creates vacancies and other defects up to total amorphisation. The modified region is not an additional layer, hence no adhesion problem occurs (no delamination), and the change of dimensions and of the surface finish of the implanted material is negligible.

This low temperature method can give spectacular results for tools used for a “mild wear” processing of soft materials, such as paper, rubber, and meat, despite the fact that only material surface is treated. Usually, the beam diameter exceeds 5 cm, thus enabling the treatment of relatively large surfaces.

There is little information regarding the application of classical ion implantation for the modification of tools for wood machining. This method is only briefly mentioned in some references (Raebel et al 1990; Ko 1998; Dearnaley and Arps 2006). More information about this can be found in our previous publications (Barlak et al. 2016, Barlak et al. 2017 Wilkowski et al. 2019).

The typical value of the range of the implanted ions usually spans from tens to hundreds of nanometers, but it is sufficient to increase the tool durability by a factor of 2-3 (Wilkowski et al. 2021).

The possible reason for the extended tool-life is the layer of amorphous carbon, which forms and self-regenerates on the implanted tool surface during the wood-based material machining (Wilkowski and Barlak 2022). The creation of this layer is not observed in non-modified tools (Wilkowski et al. 2022).

The implanted ions have different physical-chemical properties. In the simplest case, these can be inert and chemically active gas ions. The ions may have different kinetic energy, depending on their electric charge's product and the acceleration voltage's value. This problem complicates for the most ions implanted without mass separation, when the ion beam contains different fractions of the ions with different charges. In this case the depth profiles of the implanted ions is a sum of a few profiles, obtained for different ions.

The depth profile shape, the peak volume dopant concentration, the projected range and the range straggling are main parameters, that may affect the wettability. The profile shape and position influence on WC-Co tool life was presented in Ref. (Wilkowski et al. 2021). For example, the modelled nitrogen depth profiles obtained for the ion energies of 5, 50 and 500 keV and the implanted fluence of 5e17 cm^{-2}, gave the relative tool life on the level of: 1.03, 2.03 and 1.54, respectively. Therefore, it was decided to check the possibility of generating similar or identical depth profiles for two popular gases, used in laboratories and industry, i.e. chemically active nitrogen and inert argon. The atomic mass of these elements is: 14.0067 u for nitrogen, and 39.948 u for argon, so the difference is nearly 3-fold, which is evidently reflected in the positions of the depth profiles and their half-width.

The commonly available and freeware modelling programs were used throughout these works.

MATERIALS AND METHODS

Substrate materials used for the modelling

W-C-Co material including (at.%): 47.4% W, 47.4% C and 5.2% Co, i.e. in wt.%: 90.86% W, 5.94% C and 3.2% Co, with the density of 15.2 g/cm^3 was adopted as the substrate material to the modelling. The value of density was declared by the supplier of the e.g. KCR08 type knives (Ceratizit, Austria).

Ions used for the modelling of the implantation

Nitrogen and argon were used as implanted elements. In the case of direct implantation, i.e. without mass separation, nitrogen is delivered as two kinds of ions, i.e. N_2^++N^+, in ~1:1 ratio, so there are two elementary charges per three atoms. In the case of the N_2^+ molecule implanted e.g. with the acceleration voltage of 25 kV, each atom carries the energy of 12.5 keV, according to the energy conservation law. The fluence of the lower energy ions (12.5 keV) is 2-fold higher than the fluence of the ions with an energy of 25 keV (Barlak et al. 2019a). For simplicity, it is assumed that the argon beam contains only one type of ion, i.e. Ar^+. The depth profile for nitrogen will be obviously the sum of two profiles for both types of nitrogen implanted ions. Thus, for the same situation assumed for argon, it is necessary to apply the sum of the two profiles, obtained for two different values of the acceleration voltage, i.e. for some value of the acceleration voltage and a half of this value.

Modelling of the depth profiles and main peak parameters

The Stopping and Range of Ions in Matter (SRIM-2013.00), freeware type code, which is a collection of software packages which calculate many features of the transport of ions in matter, using the Monte Carlo method, was used for modelling (SRIM, Barlak et al. 2019b, Barlak et al. 2019c, Barlak et al. 2019d). This code is the most comprehensive program included. TRIM will accept complex targets made of compound materials with up to eight layers, each of different materials. It will calculate both the final 3D distribution of the ions and also all kinetic phenomena associated with the ion's energy loss: target damage, sputtering, ionization, and phonon production stromectol. All target atom cascades in the target are followed in detail. The programs are made so they can be interrupted at any time, and then resumed later. Plots of the calculation may be saved, and displayed when needed (SRIM).

The depth profile shape of nitrogen and argon ions implanted to W-C-Co material, projected range R_p, range straggling ΔR_p and peak volume dopant concentrations N_{max} were modelled using this code. The detailed explanation of the specific parameters was presented in Figure 1. The presented "SRIM units" in (atoms/cm^3)/(atoms/cm^2) are a special units of plot ordinate used in SRIM code results. With these units, by multiplying by the ion fluence (in atoms/cm^2), the ordinate values convert directly into a density distribution with the unit of atoms/cm^3. The maximum of SRIM units ($SRIM_{max}$) is a kind of equivalent of the peak volume dopant concentration (N_{max}), used for the profiles multiplied by the fluence of the implanted ions.

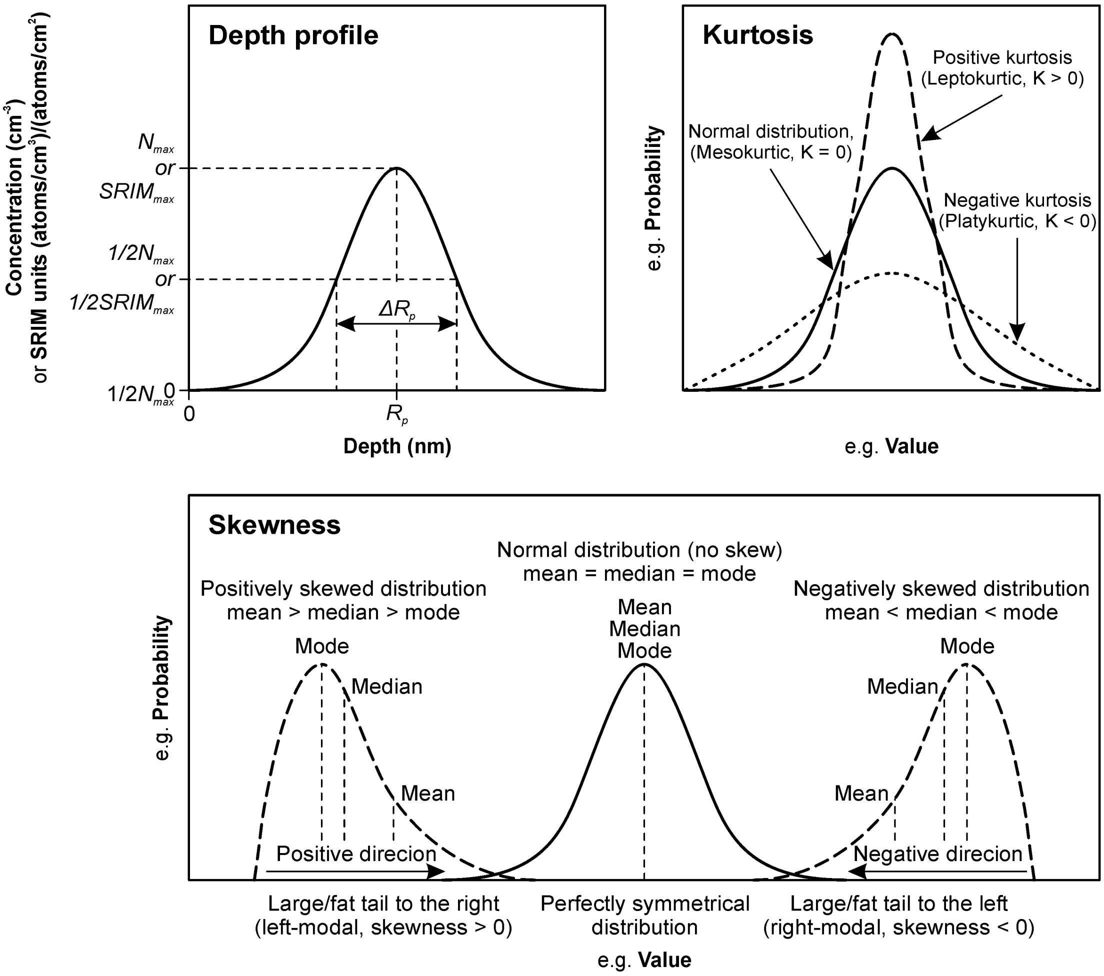

Figure 1. The graphical definitions of the main peak parameters, the kurtosis and the skewness

The modelling was performed for 100 000 implanted ions in each case. The ion incidence angle was defined as 0° (perpendicular to the implanted surface). The simulations were performed for room-temperature implantation. The modelling did not account for the phenomenon of substrate sputtering by the implanted ions, substrate damages and the chemical reactions between the implanted ions and the substrate components.

The theoretical values of the sputtering yield Y, defined as the average number of atoms sputtered (ejected) from the implanted substrate per incident ion, were calculated with the use of the quick ion implantation calculator SUSPRE, from the energy deposited in the surface region of the material using the Sigmund formula (SUSPRE).

The following energy of implanted ions was adopted for both cases in the first stage: 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65 and 70 keV. These values are classical for the typically used implanters. The similar shape and position profiles of nitrogen and argon were studied in the second stage, mainly by comparing the projected range and the range straggling values. Additionally, N^+ profile for 12.5 keV and Ar^+ profile for 32.5 keV were modelled. The total depth profiles were created in the second stage of the modelling, as a result of adding up the selected profiles and determining the amount of implanted argon ions. The assumed value of the fluence of nitrogen-implanted ions was 5e17 cm^{-2}. The sputtering values were omitted for simplicity, at this modelling stage.

RESULTS AND DISCUSSION

Depth profiles of the implanted ions

Figure 2 shows the modelled profiles of the implantation of singly ionized ions of nitrogen and argon to W-C-Co material, for an acceleration voltage of 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65 and 70 kV. Additionally, N^+ profile for 12.5 kV and Ar^+ profile for 32.5 kV, marked with dashed lines, were added. Due to the ions' single ionization, the ion kinetic energy values are numerically identical to the values of the accelerating voltage, i.e. 10 kV and 10 keV. Only a few selected profiles have been labelled, for better clarity in the figures.

It should be noted, that the adopted scale on the abscissa axis is the same for both gases for easier comparison of the profile position and the scale on the ordinate axis is twice as large for argon.

It is seen, that the profiles become lower and wider with the ion energy increasing. Moreover, the profiles' height and width strongly depend on the implanted ions' mass.

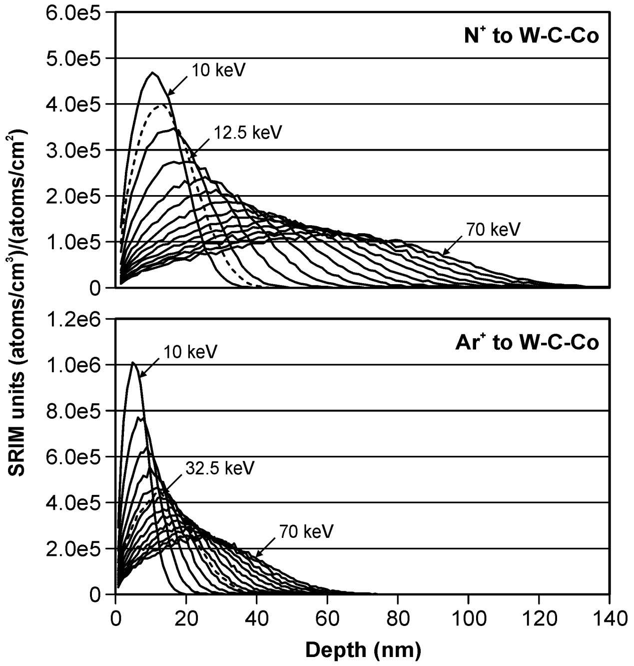

Figure 2. The modelled depth profiles of the implanted ions of nitrogen and argon

Main peak parameters

The modelling results of the acceleration voltage/ion energy-dependent change of the maximum of SRIM units, sputtering yield, projected range, range straggling, kurtosis and skewness are presented in Table 1, whereas their change is shown in Figures 3 and 4. Additionally, the trend lines, the equations and the values of the coefficient of determination R^2, determined using the Microsoft Excel 2010 spreadsheet, are presented in both figures. The determined equations can be potentially use to the values calculation of the peak parameters for the data not included in the modelling.

Table 1. The modelled values of the maximum of SRIM units, sputtering yield, projected range, range straggling, kurtosis and skewness

Acceleration voltage (kV) / Ion energy (keV)	Maximum of SRIM units, $SRIM_{max}$ (atoms/cm^3)/ (atoms/cm^2)	Projected range, R_p (nm)	Range straggling, ΔR_p (nm)	Kurtosis	Skewness	Sputtering Yield, Y (atoms/ion)
Nitrogen						
10	4.68e5	12	13	2.812	0.4792	0.52
12.5	3.99e5	**14.3**	**15,4**	2.7406	0.4546	0.52
15	3.46e5	16.5	17.6	2.7158	0.4225	0.52
20	2.74e5	20.7	21.8	2.6544	0.3845	0.52
25	2.42e5	**25**	**25.8**	2.5881	0.3259	0.52
30	2.13e5	29	29.8	2.5821	0.3151	0.5
35	1.88e5	33	33.4	2.5213	0.2759	0.49
40	1.7e5	36.9	37	2.4863	0.2405	0.47
45	1.56e5	40.6	40.2	2.4719	0.2153	0.46
50	1.49e5	44.4	43.8	2.4512	0.1969	0.45
55	1.4e5	48.3	46.6	2.436	0.1587	0.43
60	1.32e5	51.8	49.8	2.4132	0.1469	0.42
65	1.22e5	55.5	53	2.4082	0.1309	0.41
70	1.24e5	59	55.6	2.3992	0.1019	0.39
Argon						
10	1.01e6	5.9	6.6	3.0584	0.5764	1.69
15	7.71e5	7.9	8.8	2.9837	0.5467	1.84
20	6.41e5	9.8	10.8	2.9615	0.5332	1.92
25	5.55e5	11.6	12.6	2.9292	0.5165	1.97
30	4.65e5	13.3	14.4	2.8915	0.4956	2
32.5	4.47e5	**14.2**	**15.4**	2.8389	0.4708	2.01
35	4.47e5	15.1	16.2	2.8459	0.4716	2.01
40	4.22e5	16.8	18	2.8323	0.4559	2.02
45	3.79e5	18.3	19.6	2.8188	0.4479	2.02
50	3.45e5	20.1	21.4	2.7578	0.4205	2.03
55	3.21e5	21.7	23	2.753	0.4166	2.03
60	2.95e5	23.4	24.6	2.7487	0.4007	2.02
65	2.9e5	**25**	**26.2**	2.7084	0.382	2.01
70	2.58e5	26.6	27.6	2.7213	0.3805	2

It is seen, that the values of the maximum of SRIM units are more than 2-fold higher for argon implantation in comparison to the nitrogen one. It is different for the values of the projected range and the range straggling. In this case, the values of both parameters are about 2-fold higher for nitrogen. The kurtosis and skewness values are at a similar level for both elements. Unfortunately, the sputtering yield is about 3-5-fold higher for argon-implanted ions.

The acceleration voltage/ion energy-dependent curves for the maximum of SRIM units have an exponential character for both implanted ions. A 2nd-degree polynomial trend line can describe the curves for all other parameters. The coefficient of determination R^2 values are the highest for the proposed trend lines.

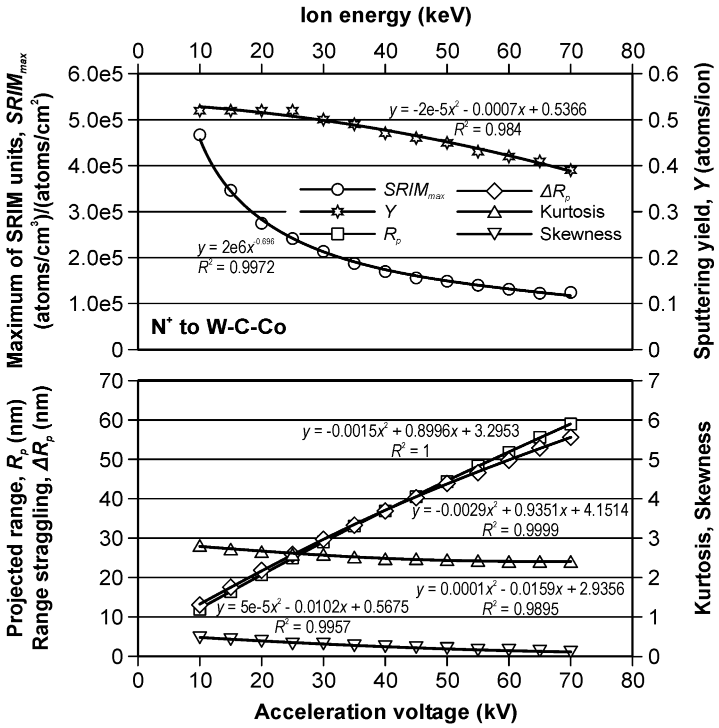

Figure 3. The modelled values of a maximum of SRIM units, sputtering yield, projected range, range straggling, kurtosis and skewness for the N^+ ions implantation to W-C-Co substrate

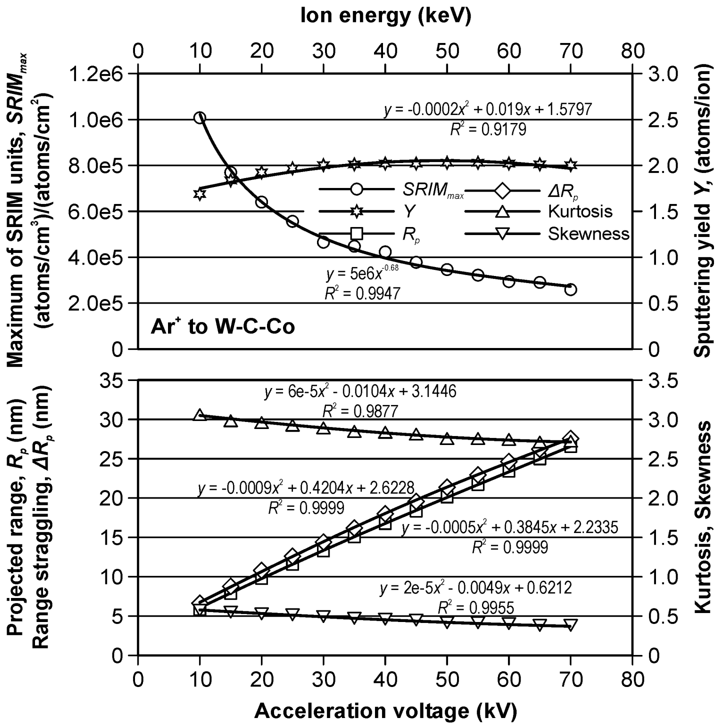

Figure 4. The modelled values of a maximum of SRIM units, sputtering yield, projected range, range straggling, kurtosis and skewness for the Ar^+ ions implantation to W-C-Co substrate

The selected values of the projected range and the range straggling, presented in Table 1 have been bolded. These values are similar for both implanted elements. The values obtained for 25 keV and 12.5 keV correspond to N^+ and N_2^+ ions in a nitrogen inhomogeneous beam, i.e. without mass separation, respectively. The values obtained for 65 keV correspond to Ar^+ ions in an argon homogeneous beam. As for nitrogen, the introduction of the additional ions with the energy of 32.5 keV was necessary to simulate the inhomogeneity of argon ion beam.

Similar depth profiles

Figure 5 presents the results of the second stage of modelling the similar depth profiles of nitrogen and argon implanted to W-C-Co material. The upper and middle parts of figure show the component (thin lines) and total (thick lines) profiles, with the applied parameters of the modelling. Additionally, the profile lines for argon are dashed for greater clarity, especially in the lower part. It is seen, that the total profiles for both implanted elements are very similar. Their parameter values and the percent difference in their values are presented in Table 2. This difference is less than 1% for the significant parameters, like the peak volume dopant concentration, the projected range and the range straggling.

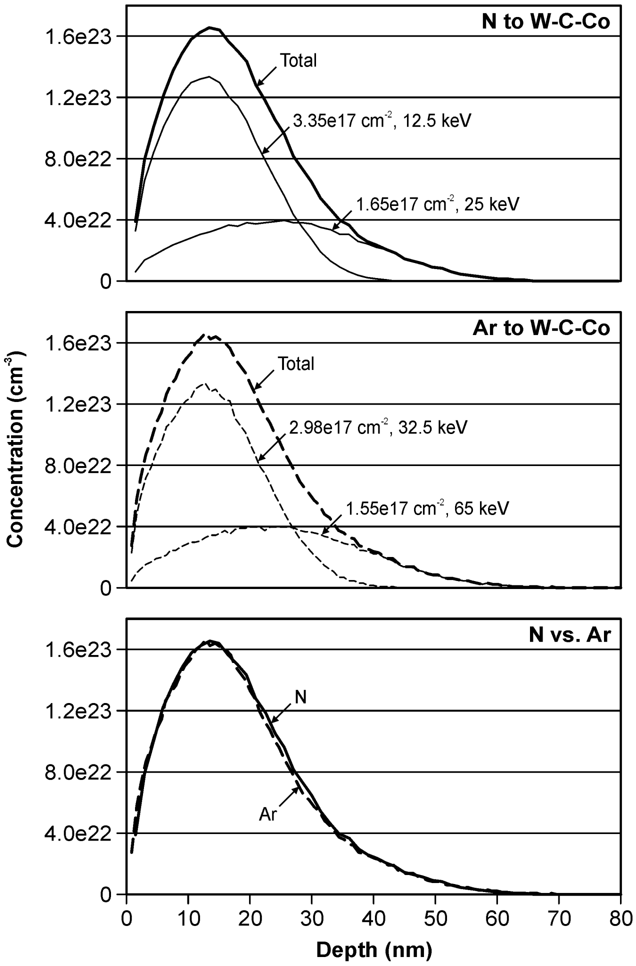

Figure 5. The modelling results of the similar/identical depth profiles of nitrogen and argon implanted in W-C-Co material

Table 2. The modelled values of the peak volume dopant concentration, sputtering yield, projected range, range straggling, kurtosis and skewness and the values of the percent difference in their values for both implanted elements

Parameter	Nitrogen (25 kV)	Argon (65+32.5 kV)	Difference N/Ar (%)	Difference Ar/N (%)
Peak volume dopant concentration, N_{max} (cm^{-3})	1.65e23	1.66e23	-0.57	0.57
Projected range, R_p (nm)	17.8	17.9	-0.56	0.56
Range straggling, ΔR_p (nm)	22	22.2	-0.91	0.90
Kurtosis	3.8995	4.0518	-3.91	3.76
Skewness	0.9376	0.9778	-4.29	4.11
Sputtering yield, Y (atoms/ion)	0.47	1.83	-289.36	74.32

CONCLUSIONS

Based on the results of the research, the following conclusions can be drawn:

- modelling of the similar depth profiles for the implanted ions of two popular gases, used in laboratories and in industry, i.e. nitrogen and argon, was successful,
- the differences for the obtained significant parameters, like the peak volume dopant concentration, the projected range and the range straggling, are less than 1%,
- it seems that such a solution may be problematic or impossible to achieve in the case of the ions with a greater difference in the atomic mass, especially for the parameters of typical implanters,
- the sputtering yield values should be considered in the next step for a better projection of the real processes.

The next stage of the investigation will be a practical verification of the influence of similar nitrogen and argon depth profiles in the WC-Co substrate for its wettability. We plan to carry out ion implantation processes, according to the modeling results, and determine the water contact angles of the modified substrates.

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Streszczenie: *Modelowanie podobnych głębokościowych profili dwóch różnych rodzajów jonów, implantowanych do narzędzi WC-Co, wykorzystywanych w obróbce materiałów* drewnopochodnych. Podjęto próbę modelowania tożsamych głębokościowych profili implantowanych jonów dwóch powszechnie stosowanych gazów, tj. azotu i argonu, dla wartości parametrów możliwych do uzyskania w przypadku klasycznych implantatorów. Modelowanie było prowadzone dwuetapowo. Tożsame profile zostały uzyskane dla wartości napięcia przyspieszającego na poziomie 35 kV w przypadku azotu i sumy napięć 65+32,5 kV w przypadku argonu. Różnica w wartości znaczących parametrów uzyskanych profili, takich jak: maksymalna koncentracja objętościowa implantowanego pierwiastka, zasięg rzutowany oraz rozrzut zasięgu, była mniejsza niż 1%.

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