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Studying the parameters effect of the sputtering yield for polypropylene bombarding by ions of atmospheric background gases

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Abstract. Using the transport of ions in matter program which is the TRIM program that based on a Monte Carlo simulation method to calculate the sputtering yield for polypropylene, that was bombed with (N2, O2, and Ar) ions of gas in ions energy range (0.1-300) Kev and for different angles. It can be seen from the results of this study the sputtering yield depends on the incident angle, ions energy, and atomic number of incident ions, surface binding energy of the elements that make up the polypropylene (pp) and the atomic number of the elements that make up the polypropylene. It is noted that the sputtering yield increases with increasing Incident ions angle (ɵ), and this increase is slight when the angle of incident ions angle is less than 600, and the sputtering yield increases clearly and quickly when the incident ions angle is from 600 to 800 , and then decreases significantly when the angle is greater than 800 . In addition, the sputtering yield increases significantly with the increase in the detonation ion energy until it reaches the highest value and then decreases with increasing energy, due to the amount of energy transferred from the detonating ion to the polymer atoms. We note the sputtering yield increase with increasing atomic number of ions (N2, O2, and Ar) that bombardment the polypropylene.

Key words: Monte Carlo simulation (MCs), polypropylene, sputtering yield, atmospheric background gases, Ar ions, N_2 ions, O_2 ions.

1. Introduction

Sputtering is a process during which the atoms of the target materials are expelled when bombed with ions, surface erosion occurs when energy particles bombard the target surface [1-4]. The sputtering occurs because of the transfer of momentum from the bombing projectile to the target surface atom, which leads to a series of atomic collisions [5, 6]. The sputtering is considered to be an unwanted side effect as in wall of nuclear fusion reactor, since the bomber's ions create a collision of cascades in the target material. When the cascades reach the target surface, the atom will be released. This occurs when the bombarding ions have more energy than the surface binding energy of the target material atoms [7]. On the other hand, sputtering is widely used as drilling, surface cleaning, thin-film analysis and sedimentation [8, 9].

In this study, On the Monte Carlo simulation method, in particular the binary collision approximation, the calculations operations were performed using TRIM program. Its use of simulations because it is widely treated of theoretical calculations for the influence parameters of the incident ions and material of target.

The aim of this research is to study the parameters affecting of the sputtering yield, reduce the cost of the substitution by reducing the polymer corrosion and consequently capitalize from it for the longest potential interval because of its importance in using it in many implementations as Medical Applications, The Automotive Industry, Flexible and Rigid Packaging and Consumer Products. And thus work to reduce the wear of the polymer surface to reduce environmental pollution. In this study, using quasi-experimental equations, the fitting parameters of calculation for sputtering yield curves has been found.

2. Theory

Many programs develop a collision chain within the target bombarded by ions. TRIM is one of them, it simulates the process of sputter and calculates the sputtering yield and other parameters corresponding to it via a Monte Carlo collision code [10].

The following equation illustrates the most important parameter in the sputtering process, which is the deposited energy (E) and the ion incident angle (θ) on the surface [11, 12]:

$$Sp(E,\theta) = \lambda\beta N S nucl(E,\theta) \tag{1}$$

As that λ is factor associated with target material ,β is the correction factor , which is a function of the mass ratio between target mass to the mass of the particle projectile , N is atomic volume (atom/nm3), and $S_{nucl}(E, \theta)$is a nuclear stopping power, so it can be described sputtering yield [11,13].

$$Sp\ Y\ (E,\theta) = \frac{0.042\ \beta N S\ nucl\ (E,\theta)}{U} \tag{2}$$

U is the surface binding energy (eV/atom) and the nuclear stopping power can be represented by the following equation [14]:

$$S_{nucl}\ (E) = \frac{8.462 Z_1 Z_2}{\left(1 + M_2/M_1\right)\left(Z_1^{0.23} + Z_2^{0.23}\right)} S_N\ (\epsilon) \tag{3}$$

appear for Z_1, Z_2, atomic numbers and M_1, M_2 atomic mass of both the incident ion and the target, respectively, and $S_N(\epsilon)$ given by the equation [14, 15]:

$$S_N\ (\epsilon) = \frac{3.441 \sqrt[2]{\epsilon}\ \ln(\epsilon + 2.718)}{1 + 6.355\sqrt[2]{\epsilon} + \epsilon\left(6.88\sqrt[2]{\epsilon} - 1.708\right)} \tag{4}$$

ϵIs the reduced energy given by equation [11]:

$$\epsilon = \frac{(M_2\ E)/(M_1 + M_2)}{Z_1 Z_2\ e^2/4\pi\varepsilon_0\ C} \tag{5}$$

C is the parameter given by:

$$C = \sqrt[3]{\frac{9\pi^2}{128}} \frac{B}{\sqrt[2]{Z_1^{2/3} + Z_2^{2/3}}} \tag{6}$$

Where B is the Bohr radius [14, 15]. The total sputtering yields for multiple-component target defined with partial sputtering yields of ingredients $S_p Y$ as follows [16, 17]:

$$Sp\ Y = \sum_i Sp\ Y_i \tag{7}$$

3. Results and discussion

In this section, we show the results and calculations of the sputtering yield of polypropylene bombardment by (Ar, N2, O2) ions that obtained through the use of the TRIM 2013 program and discuss the factors affecting it. In addition, to show the behavior of the sputtering yield of the polypropylene used in this study, we used the Organ lab program and found the fitting parameter for the results obtained using different equations. The number of ions used for this study is (5000 ions) and the bombarded polypropylene width (1000 A0). This number of ions will collide with the target's atoms and the energy will transfer to atoms during successive collisions, and the atoms will be removed from the surface and the sputtering will occur. Energy is transferred from the incidence ions to the polypropylene atoms by elastic nuclear collisions (kinetic energy and momentum are conserved, atom-on atom "billiard" ball collisions), and inelastic electronic loses (electronic excitation, ionization, electron- electron collisions). Through this study, it was found that there are several factors that affect sputtering yield, including:

3.1. Impact of incident ion angle

The relationship between the sputtering yield for polypropylene (PP) and the angle of incident (θ^o_{inci}) of the bombard ions Argon, nitrogen and oxygen show it Figures (1-3).
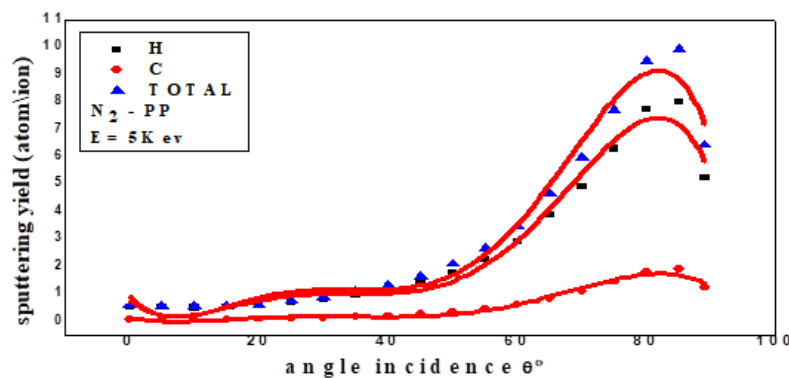

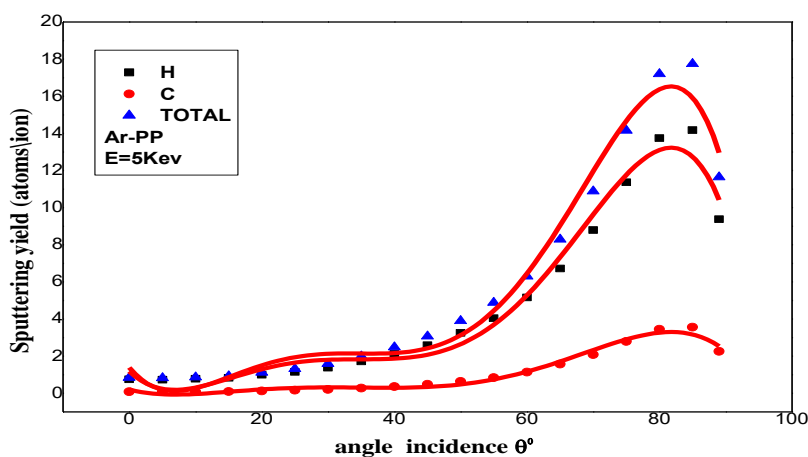**Figure 1.** S_pY dependence on θ^o_{inci} of (PP) bombard by Argon ion with (5kev).

Figure 2. S_pY dependence on θ^o_{inci} of (PP) bombard by Nitrogen ion with (5kev)
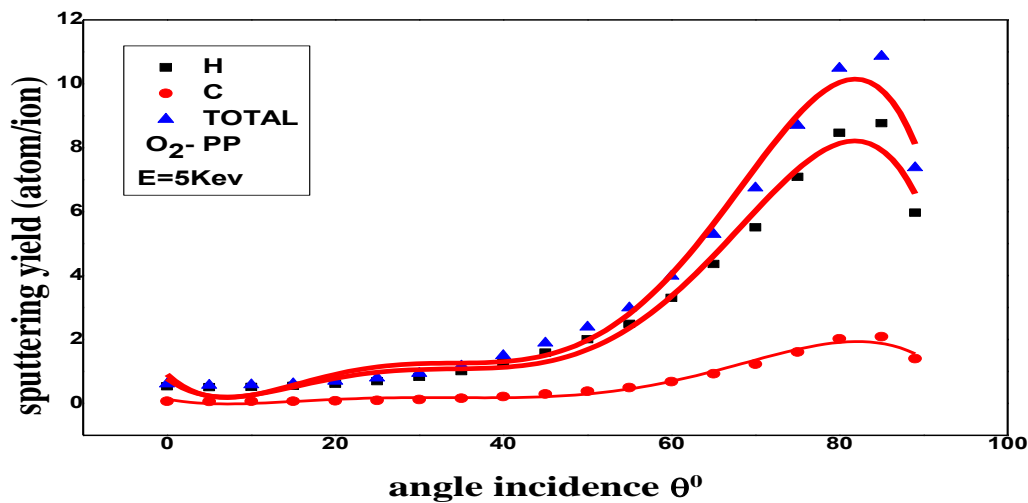
3

Figure 3. S_pY dependence on $\theta^o{}_{inci}$ of (PP) bombard by Oxygen ion with (5kev)

We notice from the above figures that the sputtering yield increases slightly with the angle of incident of the bombing ions increasing from (00) to (600) due to the amount of energy transmitted from the bombing ions to the target material atoms is small at these angles, The ejected atoms from the surface of the target material are few and consequently the increase is slight. As for the angles $85o\geq$ $\theta> 60o$, the sputtering yield increases in a clear and significant way, as the number of atoms removed from the polymer surface at these angles is large, due to the amount of energy transmitted from the bombing ions to surface atoms, and therefore we notice a clear increase in the sputtering yield. In general, it appears that the sputtering yield after the angle (850), which represents the angle corresponding to the greatest value of the sputtering yield begins to decrease rapidly due to the decrease in the amount of energy traveling from ions to the target surface atoms upon collision.

In figures (1, 2 and3) we have fitted the curves of the SPY dependence on θo inci by quasi- semi-empirical equation. The parameters values are given by:

$$SPY = \beta0 + \beta1\theta + \beta2\,\theta2 + \beta3\,\theta3 + \beta4\,\theta4 + \beta5\,\theta5 \tag{8}$$

Where (β_0, β_1, β_2, β_3, β_4 and β_5) are parameters depending for the incident ions angle.

3.2. Impact of ion energy

Figures (4-6) show the relationship between the sputtering yiled of (PP) and the energy of the incident ions.
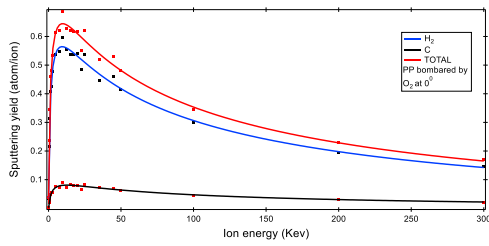
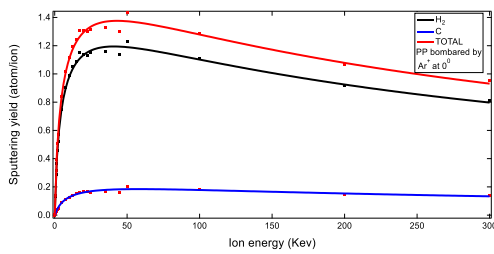**Figure 4.** Energy dependence of S_pY of incident Argon ions at (0^0) on PP

Figure 5. Energy dependence of S_pY of incident Nitrogen ions at (0^0) on   PP
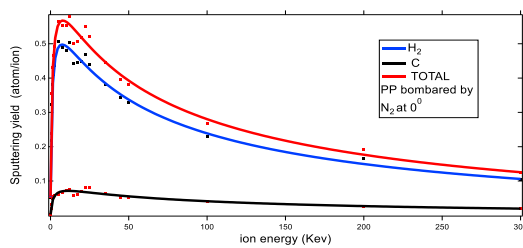

Figure 6. Energy dependence of S_pY of incident Oxygen ions at (0^0) on   PP

We notice in the above figures that the sputtering yield increasing by increasing the incident ions energy clearly and significantly increasing from (0.1-20) keV, This is due to the fact that the amount of energy traveling from the bombing ion to the target matter atoms is large, the sputtering yield increases rapidly .and then after that it is a very slight increase for it almost becomes a state of stability down to (50 kev), This is due to the fact that the energy of the bombing ion is very large, leading to the implantation of the bombing ions in the target material and thus the sputtering yield stabilizes almost then after that the sputtering yield begins to decrease rapidly that due to the fact that the ionic ion has a large energy that enables it to penetrate the target material, thus the sputtering yield decreases.. The parameters values for figures (4-6) We have fitted the curves of the S_pY dependence on E_{ions} by quasi-semi-empirical equation ,is given by:

$$S_p\ Y = \alpha + \gamma e^{-\left[\frac{\ln\frac{E}{\mu}}{\omega}\right]^2} \tag{9}$$

Where (α , γ, μ ° and w ω) are parameters depending on E_{ions}

3.3. Impact of atomic number of incident ions

The figure (7) shows the effect of the atomic number of bombing ions on the sputtering yield. The effect of the atomic number of the target material is shown when fixing the angle of fall and energy of the bombing ion.
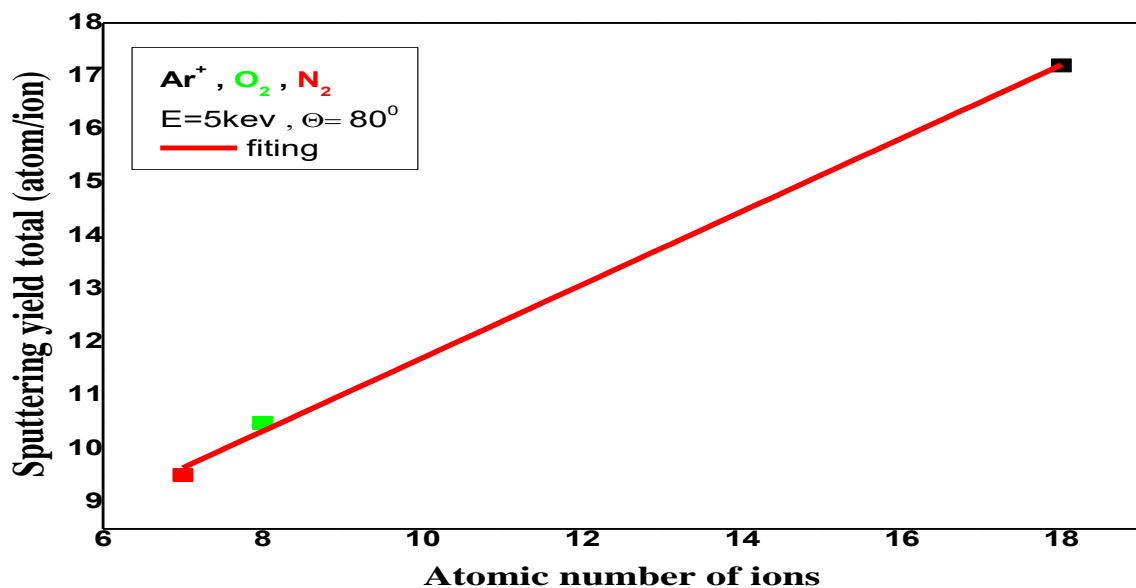

Figure 7. S.Y as a function atomic number of ions (Ar, N_2, O_2) that bombardment the Polypropylene PP with (5kev) at (80^0)

It appears that the sputtering yield of the polypropylene bombed with the (Ar) ion is greater than the sputtering of the same polymer when bombard by (O_2) ion and the last sputtering has a greater amount of sputtering when bombing with the ion (N_2). This is due to the atomic number (Z) of (ZAr> ZO2> ZN). Thus, we conclude that the sputtering yield increases with the increasing atomic number of the bombing ion. Because the energy traveling from the bombing ion to the target matter atoms increases, the more the atomic number of the bombing ion increases, Parameters fitting equation (10) is given by:

$$SpY \ = \ 4.83527 \ + \ 0.6877 \ Zion \tag{10}$$

Where (Z_{ion}) is the atomic number of ions.

3.4. The effect of the atomic number of components of polypropylene

The relationship between sputtering yield and the atomic number of the components of polypropylene is illustrated in Figs (8).
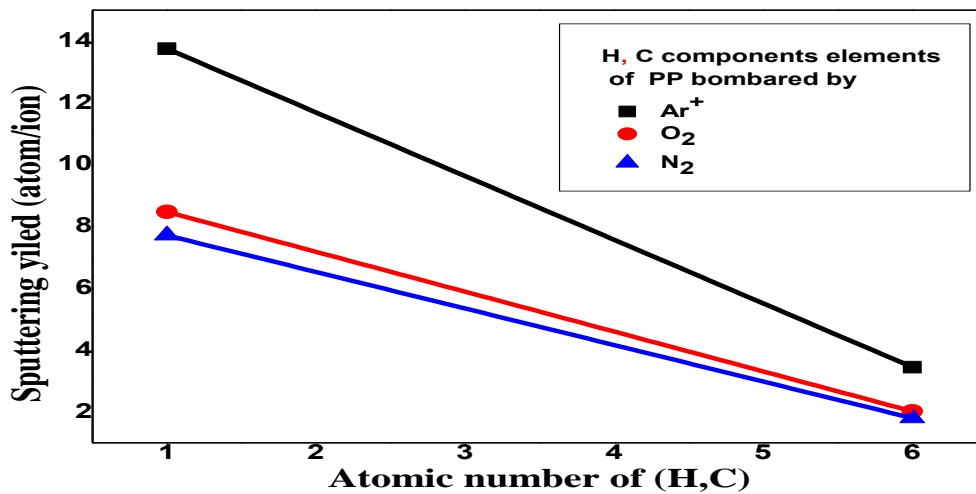

Figure 8. S_pY as a function atomic number of Polypropylene bombardment by (Ar, N_2 and O_2) ion with (5keV) at (80^0).

The figure (8) shows that the sputtering yield element of hydrogen is greater than the sputtering yield element of carbon, due to the atomic number(Z) of (ZH <ZC). From this we conclude that sputtering increases with the decrease in the atomic number of the constituent elements of polypropylene. The fitted data is given by:

$$SpY \ = \ \alpha0 \ + \ \alpha1 ZPP \tag{11}$$

Where α0 and α1 are constats fitting for the   eq 11 and depending on (Zpp) is the atomic number of the compenent elements (H, C) of PP, and Table 1 shows the values of these constants.

Table 1: parameters for equation (11) plotted in Figure (8) from (Ar, N_2, O_2) ions constants.

Ion	α_0	α_1
Ar	15.81	-2.06
O_2	9.76	-1.29
N_2	8.892	-1.182

3.5. The effect surface binding energy

Sputtering yield as a function of the surface binding energy of the polypropylene components when bombed with ions (Ar $^+$, N_2, O_2) with energy (5 kev) at 80^0 shown in Figur (9).
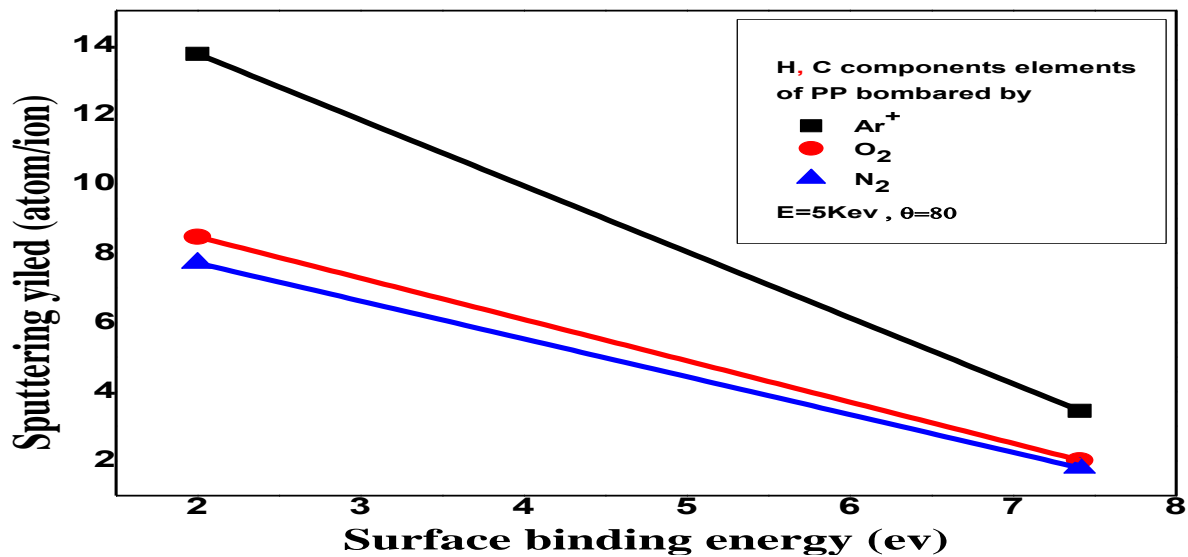
Figure 9. S.Y as a function surface binding energy of component for Polypropylene bombardment by (Ar, N_2 and O_2) ion with (5kev) at (80^0).

Polypropylene is made of hydrogen and carbon, and the surface binding energy both (2, 7.41) eV respectively. The noted from figures above that The sputtering yield of the hydrogen element to be larger than the sputtering yield of the carbon element, and this is because The surface binding of element (H) is greater than the surface binding energy of element (C), thus we conclude that sputtering increases with decrease of surface binding energy of the constituent elements of polypropylene and vice versa. .

Parameters fitting equation (12) is given by:

$$S.Y = K0 + K1Usb \tag{12}$$

Where K0 and K1are constants fitting for the eq 12 and depending on (Usb) is the surface binding energy of the component elements (H, C) of PP, and Table 2 shows the values of these constants

Table 2. parameters for equation (12) plotted in Figure (9) from (Ar, N_2, O_2) ion

Ions	K_0	K_1
Ar	17.55776	-1.90388
O_2	10.85447	-1.19224
N_2	9.89484	-1.09242

3.6. The normalized sputtering yield (NSY) vs. angle of incident ion

Figure (10) show how the reaction process between the incident ions and the constituent elements of polypropylene (PP) depends on the structure.
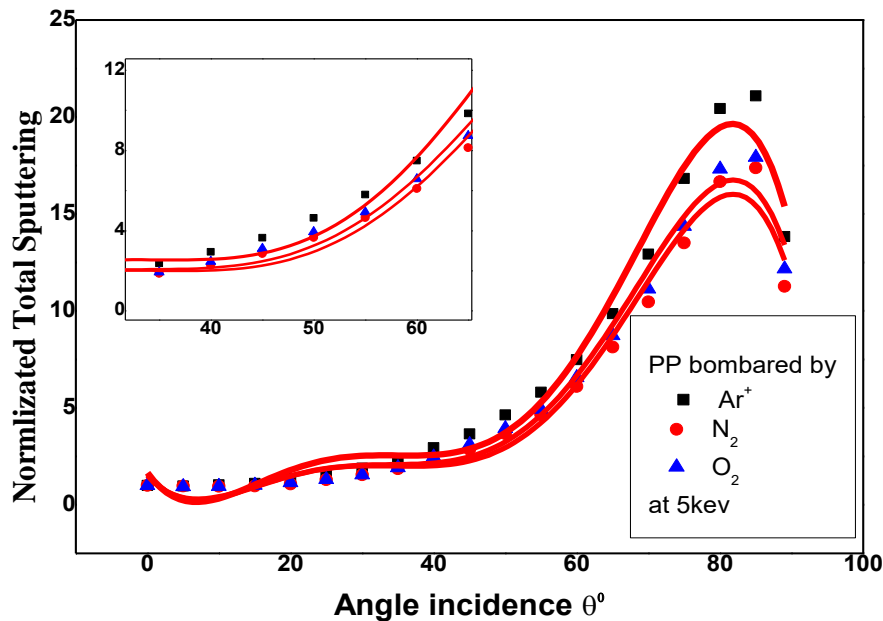
Figure 10. (NSY) vs. of the angle of ion incidence at Polypropylene bombardment by (Ar , N_2 and O_2) ion with (5kev).

Figure (10) represents the normlizated total sputtering yield, which is a total sputtering yield for angles (0^0-89^0) divided by a total sputtering yield of 0^0. It is often usually for the researchers in topic of sputtering to use normalized sputter yield rather than direct sputter yield as soon as they treat with ion angle of incidence dependence. The normalized sputter yield is the ratio of the value of sputter yield at certain angle with respect to that at normal incidence 0^0. If the general behavior is observed the total sputtering yield to depend on the incident angle of the ion.

4. Conclusions

In this research has been studying the parameters that affect the Sputtering yield and thus work to reduce the wear of the polymer surface to reduce environmental pollution and work to extend the life of the polymer and thus save time and effort to change the polymer used in many industrial and medical applications. In this study, the calculations of were fitting and found parameters of curves with quasi-experimental equations. The sputtering yield increases slightly with increasing angle from (0^0) to (60^0), then increases significantly and clearly from (60^0) to (85^0), and decreases rapidly at an angle greater than (85^0). Through the results, the effect of the bombing ion energy is clearly shown on the sputtering yield, as it increases with the energy of the bombing ions in energies less than 50 keV, after which the increase is very slight and almost stable, when the energy of the bombing ion reaches (50 keV). .The current study demonstrates the effect of the atomic number of accident ions on the sputtering yield, as it is directly proportional to it. While the sputtering yield is inversely proportional to atomic number of the constituent elements of polypropylene. The effect of surface binding energy on the sputtering yield can be observed, as it increases with decrease surface binding energy of the constituent elements of pp.

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