The Sputtering Problem

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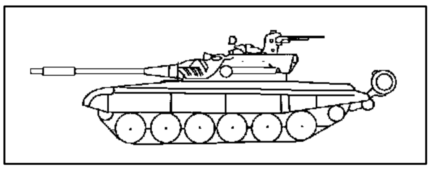
I propose to consider first the various elements of the subject, next its various parts or sections, and finally the whole in its internal structure. In other words, I shall proceed from the simple to the complex.

Carl Von Clausewitz

Introduction



Gun tubes produced for Army weapons systems, such as tanks and artillery pieces, are designed to fire a specific number of rounds before they are considered unsafe and must be replaced. The exact round count for a gun tube is so critical that detailed records are kept for each tube in every Armor and Artillery unit in the Army. Frequent replacement of gun tubes is undesirable not only for obvious fiscal reasons, but also due to the manpower and firepower drain it places on a unit in combat. One method of increasing the number of rounds a gun tube can safely fire is to place a metal lining inside the tube. One of the techniques for placing a lining inside a gun tube is called sputtering.

Sputtering is a process where a cylindrical metal bar is inserted inside a gun tube, centered, anchored in place, and connected to a power source. The tube and rod are placed inside a chamber where all air is evacuated and replaced with a noble gas. When electricity is run through the source rod, a magnetic field develops and atoms from the metal source rod are broken away and literally fly across the gap from the source rod to the inside of the gun tube. During flight, the metal atoms collide with atoms of the noble gas that separate the source rod from the inside wall of the gun tube. Each collision with a noble gas atom causes the metal atom to change the direction of its flight and lose energy. In developing the sputtering process, the Army used three mathematical models to create computer simulations of the sputtering process.

The computer simulations were used to quickly and inexpensively predict the effects of different materials and experimental conditions on the sputtering results. One model was used to simulate initial direction and energy of a sputtered atom. A second model was used to analyze the effects of an atom colliding with the inside of the gun tube wall. This chapter deals with the third mathematical model, which was developed to analyze the flight of a metal atom from the source rod to the inside of the gun tube.

In order to model this portion of the problem, it is necessary to analyze the flight of an atom from the source rod (cathode) to the inside of the gun tube (anode) in small steps. Each step represents an important event in the flight. The first event is when the atom breaks away from the cathode. The initial velocity vector of the atom as a result of this event is given as an initial condition. The second event is determining the location of the sputtered atom's collision with a neutral gas atom. Locating a collision site involves determining a free path length for the atom and applying the free path length along the direction of the initial velocity vector. The third step is examining the effects of the collision on the energy and flight path of the sputtered atom. To simplify this step, the collision is examined in a center of mass frame of reference. The fourth and final step in the process involves determining the location and energy of the metal atom when it impacts with the inside wall of the gun tube (anode). Because a sputtered atom might collide with multiple neutral gas atoms during its flight from the source rod to the wall of the gun tube, steps two and three may be repeated several times for each atom before calculating the terminal effects in step four.

Geometry

We begin with an explanation of the geometry of our model. The gun tube will be treated as a hollow right circular cylinder with a radius equal to **R**. The source rod is also a right circular cylinder with a radius equal to **r**. Both cylinders are centered on the z axis so that the straight line distance from the source rod to the inside of the gun tube is equal to **R-r**. (See Figure 1)

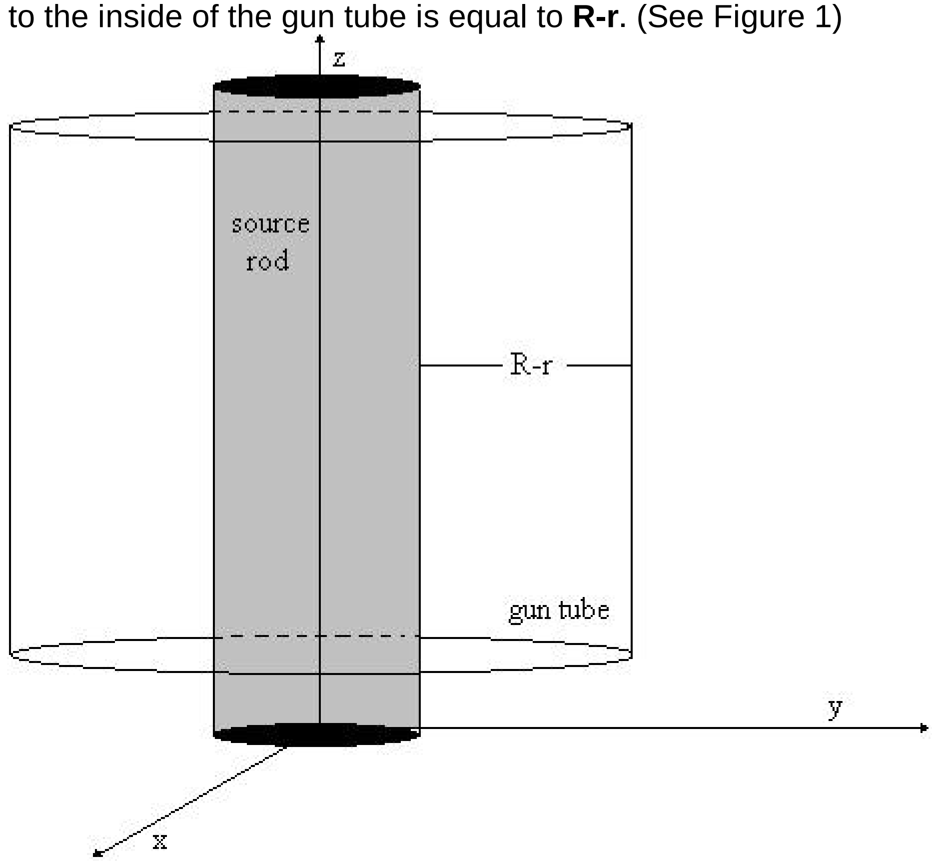


Figure 1

Step 1 - Initial Velocity Vector

We will use vectors in spherical coordinates to describe the flight of the sputtered metal atom. We use the angle q to describe the rotational angle in the x,y plane and the angle f to describe the elevation of the atom above the x,y plane. Thus a unit direction vector for the sputtered atom will be of the form:

$$Direction = \left\langle \cos(q)\cdot\sin(f), \quad \sin(q)\cdot\sin(f), \quad \cos(f) \right\rangle$$

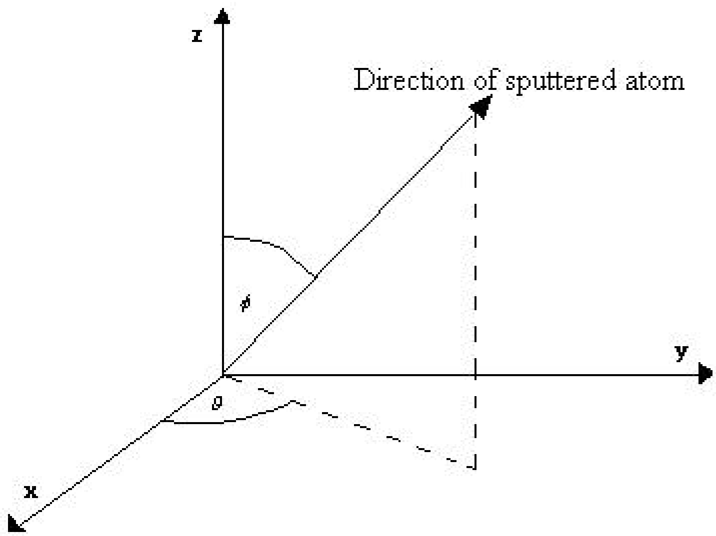


Figure 2

The unit direction vector is then multiplied by the initial speed to generate an initial velocity vector for the atom.

Step 2 - Locating Collision Sites

The location of an atom's collision is determined by moving a specific distance along the direction of its velocity vector. The distance moved is called the free path length. The free path length changes for each atom after each collision. The free path length is based on a distribution about an atom's mean free path length. The mean free path length for an atom is the average distance that the atom will travel before it has a collision with a neutral gas atom. The mean free path length for all sputtered atoms of the same element remains constant as long as the density of the neutral gas remains unchanged.

The mean free path length is calculated by examining the relation between the density of the neutral gas and the distance a sputtered atom would travel in a unit of time if it were allowed to travel unimpeded. The radius of the sputtered atom and the distance it travels in a unit of time are used to create a cylinder through which an atom travels during the unit of time. The volume of the cylinder is calculated and multiplied by the density of the neutral gas to determine the average number of atoms that occupy a cylinder of that size. The length of the cylinder is then divided by the number of atoms that occupy the cylinder and the result is a reasonable approximation for the length of the mean free path (See Figure 3).[1]

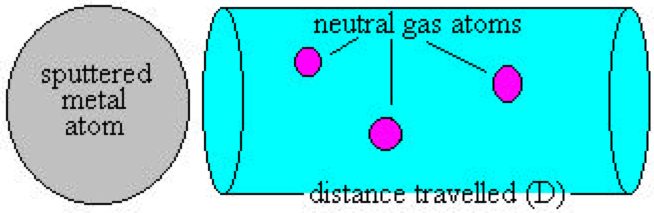


Figure 3

This method yields the following equation: $L = \frac{D}{p\ r\ r^2}$. Where L is the mean free path length, D is the distance traveled, r is the density of the neutral gas, and r is the radius of the sputtered metal atom.

Once the mean free path is determined, the graph in figure 4 is created using the equation $\frac{n}{N} = e^{\frac{-x}{L}}$ to define the curve.[2] The ratio $\frac{n}{N}$ represents the percentage of free path lengths that are at least as long as the corresponding number of mean free path lengths from the graph. In the graph, free path length is measured in terms of the number of mean free path lengths a sputtered atom will travel prior to a collision (DIST/L).

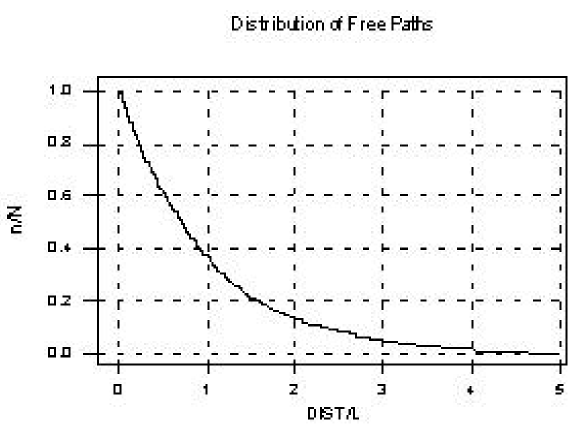


Figure 4

The free path length for a specific atom at a specific moment in time is then created by applying a uniform distribution to the n/N axis (randomly choosing a number between 0 and 1) and then finding the corresponding DIST/L coordinate on the graph in figure 4. The DIST/L term is multiplied by the atom's mean free path length to yield the distance to the atom's next collision.

Now that the distance to the collision has been determined, the actual location of the collision is found by multiplying distance to collision by a unit vector in the direction of the sputtered atom's velocity vector and adding the resulting vector to the sputtered atom's old position vector.

Step 3 - Effects of a collision

Moving to a Center of Mass Frame of Reference

When a sputtered atom collides with a neutral gas atom, the sputtered atom will change direction and speed. The analysis of a collision is best made in a center of mass frame of reference. A center of mass frame of reference means that the origin of the coordinate system used in making calculations is fixed on the center of mass of the two atoms involved in the collision. Thus the center of mass does not move (as it would in the laboratory frame of reference). Using the center of mass frame of reference makes the calculation of the changes in direction and speed of the sputtered atom less complicated because the changes are measured against a "stationary" point.

Change in direction

Since we are working in spherical coordinates, the direction change forced upon a sputtered atom as the result of a collision with a neutral gas atom is best examined in terms of an angle of rotation and an angle of deflection. The angle of rotation is determined by examining the collision from directly behind the sputtered atom. The key to the collision effects is the relative positions of the centers of mass of the sputtered atom and the neutral gas atom at the moment of impact. In figure 5, we see that a circle of radius equal to the sum of the radii of the neutral gas atom and the sputtered metal atom (b_{max}) can be drawn centered on the neutral gas atom. In order for a collision to occur, the center of mass of the sputtered metal atom must be located within the circle of radius b_{max}.

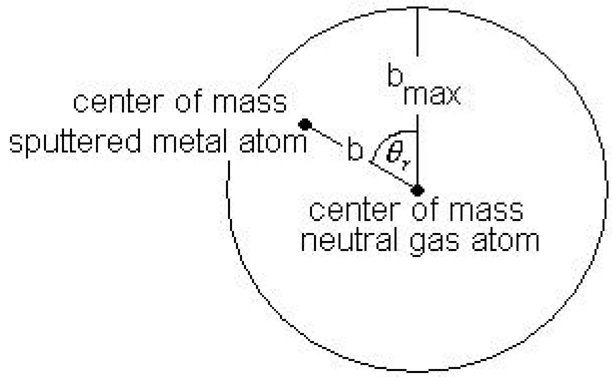


Figure 5

We will assume that the relative positions of the centers of mass at the moment of collision are completely random. Therefore, we need only apply a uniform distribution over the circle of radius b_{max} to randomly determine the locations of the centers of mass of the two atoms. Measuring the angle of rotation, q_r , then becomes a simple trigonometry problem.

Calculation of the angle of deflection, c , is made by examining the collision in two dimensions as viewed from a position orthogonal to both the pre collision and post collision velocity vectors of the sputtered atom (figure 6).

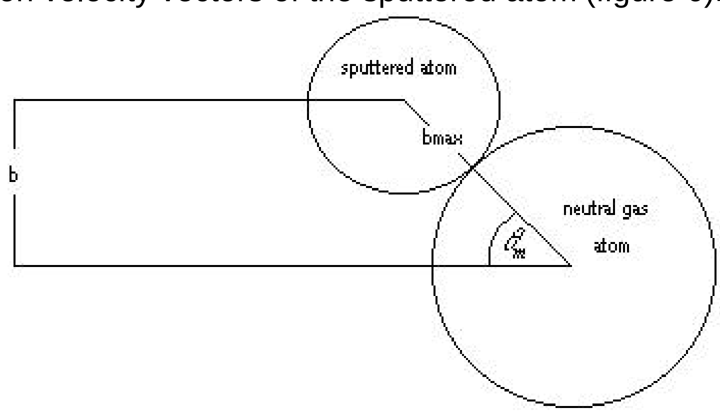


Figure 6 (pre collision)

The distance, b (measured in the previous step) is the controlling parameter in the determination of c . Using trigonometry, the incoming angle for the collision, q_m , is defined by the equation $q_m = \sin^{-1}\left(\frac{b}{b_{\max}}\right)$.

The angle of interest, c , is equal to p minus two times q_m in the center of mass frame of reference.[3]

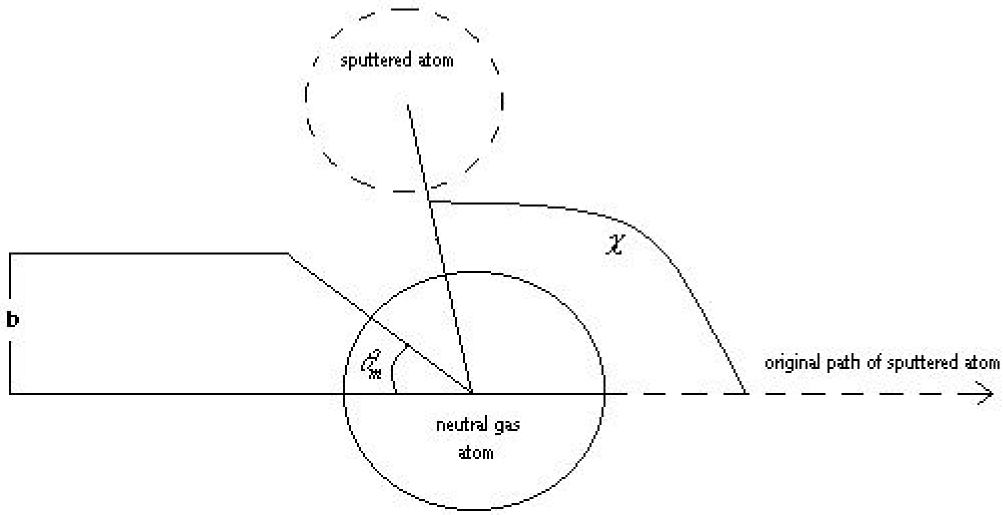


Figure 7 (post collision)

Once the angles q_r and c are determined, spherical coordinates are used to create a unit vector for the direction of the sputtered atom in the revised new system. The unit direction vector is: $\langle \sin(c)\cos(q_r), \sin(c)\sin(q_r), \cos(q_r)\rangle$.
The unit direction vector must then undergo a linear transformation (rotation about origin) so that it can be used in the standard coordinate system in the center of mass frame of reference. The revised coordinate system is aligned so that its z axis is on the pre-collision path. As a result, the parameters for the transformation, a and b, come from measuring the angles of the pre-collision direction of the sputtered atom in the standard system of coordinates (Figure 8).

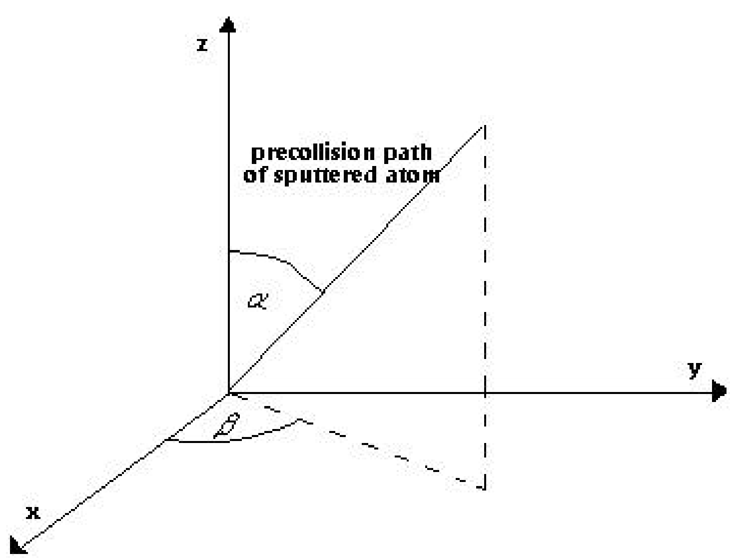


Figure 8

The linear transformation aligns the pre collision path of the sputtered atom with the standard z axis and thus brings the post collision direction vector into the standard system of coordinates. The matrix for this transformation is:

$$C = \begin{bmatrix} \cos(a)\cos(b) & \cos(a)\sin(b) & -\sin(a) \\ -\sin(b) & \cos(b) & 0 \\ \sin(a)\cos(b) & \sin(a)\sin(b) & \cos(a) \end{bmatrix}$$

The post collision direction vector in the revised system of coordinates is multiplied by C to yield the post collision direction vector in the standard coordinate system.[4,5]

$$\left\langle x_{revised}\ , y_{revised}\ , z_{revised} \right\rangle \cdot C = \left\langle x, y, z \right\rangle$$

Change in Speed

The outgoing speed of a sputtered atom equals the incoming speed of the sputtered atom in the center of mass frame of reference. The laws of conservation of momentum and conservation of energy can used to demonstrate why this is true. The proof of this concept is left as an exercise for the reader. See exercise 2.

Returning to a Normal Frame of Reference

Now that the speed and direction for the post collision sputtered atom have been determined, the post collision unit direction vector for the sputtered atom is multiplied by the post collision speed of the sputtered atom to find a new velocity vector in the standard coordinate system in the center of mass frame of reference. To find the post collision velocity vector in the laboratory frame of reference, the vector v_{cm} is added to the post collision velocity vector in the center of mass frame of reference.

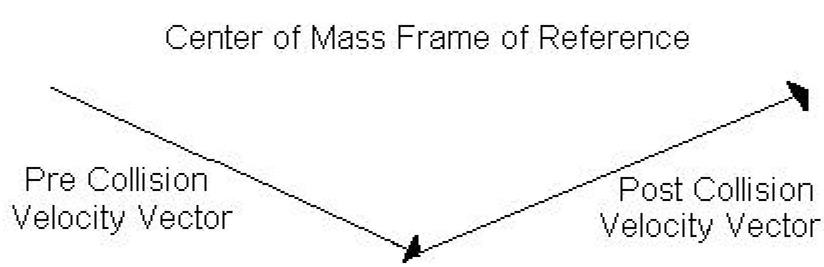


Figure 9

Figure 9 represents the view of the collision in the center of mass frame of reference. The speed of the sputtered metal atom remains unchanged and therefore, the velocity vectors before and after collision are of the same magnitude. Thus the collision in the center of mass frame of reference effects only the direction of the sputtered metal atom. The loss of velocity is accounted for when the system is moved back to the laboratory frame of reference. Movement from the center of mass frame of reference to the laboratory frame of reference is accomplished by adding the velocity vector for the center of mass (VCM) to the post collision velocity vector as depicted in Figure 10.

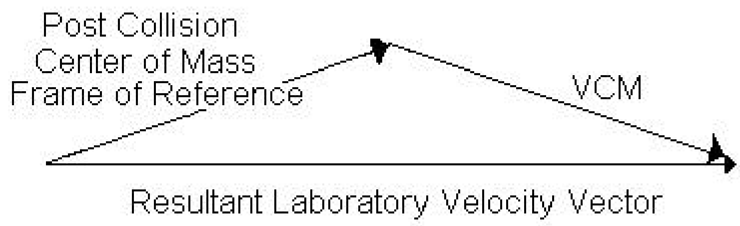


Figure 10

Step 4 - Determining the Impact Location and Energy of a Sputtered Atom

Determining the location where an atom impacts the inside wall of the gun tube is done by keeping track of its position vector throughout its multiple movements and collisions. When the radial movement of the atom equals the inside radius of the gun tube, its position vector coordinates are used to plot its location on the gun tube wall. The height of the atom as it strikes the gun tube is equal to its z coordinate at the time of impact. The radial location is calculated using the equation:

$$Radial\ location = \cos^{-1}\left(\frac{x\ coordinate}{gun\ tube\ radius}\right)$$

The kinetic energy of the atom at the moment of impact with the gun tube is calculated using $\frac{1}{2} mass \cdot (speed)^2$ where the speed is equal to the magnitude of the velocity vector at the moment of impact.

Example: The flight of one atom

In this example we will follow the flight of one atom from the source rod (r = 10 mm) to the inside of the gun tube wall (R = 50 mm) and compute the terminal effects of the atom at the gun tube wall. We will assume several conditions that would actually be computed using random numbers and probabilistic models.

Step one is to find an initial velocity vector. The initial speed is estimated based on the energy and mass of the metal atom. Let's start with an initial speed of 20,000,000 mm/sec. Assume initial launch angles of $q = 25^\circ, \quad f = 80^\circ$. This yields an initial velocity vector of

$$20000000 \left\langle \cos(25^\circ)\sin(80^\circ), \quad \sin(25^\circ)\sin(80^\circ), \quad \cos(80^\circ) \right\rangle$$

or

$$V = \left\langle 1.785\times10^{7}, \quad 8.324\times10^{6}, \quad 3.473\times10^{6} \right\rangle \text{mm/sec}$$

Step two is to find the location of a collision. The collision location is based on an initial location of $\langle 10, \; 0, \; 2000 \rangle$mm (this location will place the atom on the outside wall of the source rod). We randomly generate a free path length based on the exponential distribution of free path lengths, figure 4. Assuming a free path length of 30 mm we can compute the time it takes until a collision.

$$time = \frac{dist}{speed} = \frac{30}{20000000} = 1.5\times10^{-6} \text{ sec}$$

Now we can easily determine the location of the collision using vectors.

Collision location = **initial location** + **velocity**(time)

Collision location = $\langle 36.78, \; 12.49, \; 2005 \rangle$

Looking at the x and y components of the collision location vector, we can determine if our collision would be outside the gun tube wall

$$radius = \sqrt{36.78^2 + 12.49^2} = 38.84 \; mm$$

Our inside gun tube radius was 50 mm, thus this collision is before we reach the gun tube wall.

Step three is to determine the velocity of the center of mass and the effects of the collision in the center of mass frame of reference. When determining the velocity of the center of mass, our model only considers the sputtered atom to be moving. Therefore, the velocity of the center of mass is in the same direction as the velocity vector, but has a different speed. If the neutral gas atom has a mass of 50 Atomic Mass Units (AMU) and the sputtered atom has a mass of 200 AMU

$$\vec{V}_{cm} = \vec{V} \cdot \frac{mass(sputtered)}{mass(sputtered) + mass(neutral\ \ gas)}$$

For our example we have

$$\vec{V}_{cm} = \vec{V} \cdot \frac{200}{50+200} = \left\langle 1.428\times 10^{7},\ 6.659\times 10^{6},\ 2.778\times 10^{6} \right\rangle$$

We now determine the effects of the collision. Assume collision parameters of $q_r = 10^\circ$ *and* $c = 15^\circ$. The pre collision velocity vector of the sputtered atom, as seen in the center of mass frame of reference, is $\vec{V} - \vec{V}_{cm}$. The post collision velocity vector has the same magnitude(*speed*), but it's direction is determined using spherical coordinates and a coordinate system oriented with the z axis pointing parallel to our velocity vector.

$$V'_x = speed\ \sin(c)\cos(q_r) = 4\times 10^{6}\ \sin(15^\circ)\cos(10^\circ) = 1.020\times 10^{6}$$
$$V'_y = speed\ \sin(c)\sin(q_r) = 4\times 10^{6}\ \sin(15^\circ)\sin(10^\circ) = 1.798\times 10^{5}$$
$$V'_z = speed\ \cos(c) = 4\times 10^{6}\ \sin(15^\circ) = 3.864\times 10^{6}$$

We must now perform a rotation about the origin to move us to the standard x-y-z axis. The angles we rotate are determined from our velocity vector,

$$a = \arccos\left(\frac{z\ component\ of\ \vec{V}_{cm}}{magnitude\ of\ \vec{V}_{cm}}\right) \qquad b = \arctan\left(\frac{y\ component\ of\ \vec{V}_{cm}}{x\ component\ of\ \vec{V}_{cm}}\right)$$

For our example we have:

$$a = \arccos\left(\frac{6.946\times 10^{5}}{4\times 10^{6}}\right) = 1.396\ radians \qquad b = \arctan\left(\frac{1.665\times 10^{6}}{3.570\times 10^{6}}\right) = 0.4363\ radians$$

Now to complete the rotation we multiply the vector $\vec{V}'$ by the direction cosine matrix. The direction cosine matrix, C, is determined by taking the cosine of the angle between the standard x-y-z axis and the new axis (z-axis pointing in the direction of $\vec{V}$).

$$C = \begin{bmatrix} \cos(a)\cos(b) & \cos(a)\sin(b) & -\sin(a) \\ -\sin(b) & \cos(b) & 0 \\ \sin(a)\cos(b) & \sin(a)\sin(b) & \cos(a) \end{bmatrix}$$

Thus we have

$$\langle 1.020\times10^6, 1.798\times10^5, 3.864\times10^6\rangle \begin{bmatrix} \cos 1.396 \cos 0.4363 & \cos 1.396 \sin 0.4363 & -\sin 1.396 \\ -\sin 0.4363 & \cos 0.4363 & 0 \\ \sin 1.396 \cos 0.4363 & \sin 1.396 \sin 0.4363 & \cos 1.396 \end{bmatrix}$$

$$= \langle 3.533\times10^6, 1.846\times10^6, -3.331\times10^5\rangle$$

This is our post collision velocity vector in the center of mass frame of reference in the standard x-y-z coordinate system. Now to return to the laboratory frame of reference we simply add $\vec{V}_{cm}$.

$$\langle 3.533\times10^6, 1.846\times10^6, -3.331\times10^5\rangle + \langle 1.428\times10^7,\ 6.659\times10^6,\ 2.778\times10^6\rangle$$
$$= \langle 1.781\times10^7,\ 8.505\times10^6,\ 2.445\times10^6\rangle$$

Repeat step two. We must now find the time until our next collision. We again randomly generate a free path length, say 43 mm for this iteration. We find the time until our next collision. Our post collision speed is 1.986×10^7 mm/sec.

$$time = \frac{dist}{speed} = \frac{43}{1.986\times10^7} = 2.162\times10^{-6}\ \text{sec}$$

We now determine the location of the 2nd collision using vectors.

2nd Collision location = **1st Collision location** + **velocity**(time)

Collision location = $\langle 75.28,\ 30.87,\ 2010\rangle$

Looking at the x and y components of this we can determine if our collision would be outside the gun tube wall

$$radius = \sqrt{75.28^2 + 30.87^2} = 81.37\ mm$$

Since our inside gun tube radius was 50 mm, this collision cannot occur because the atom will impact the inside of the gun tube wall prior to reaching the collision location.

Step four is to calculate the terminal effects. We have already determined the arrival velocity $\langle 1.781\times10^7,\ 8.505\times10^6,\ 2.445\times10^6\rangle$ and speed 1.986×10^7 mm/sec. Now we must determine the arrival energy.

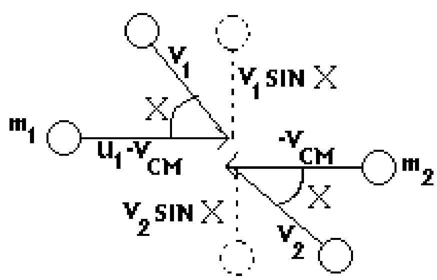
$$\text{Energy} = \frac{1}{2}mv^2 = 410.1\ \text{EV}$$

Exercises

1. Using dimensional analysis, find the conversion factor used to convert the terminal energy of the sputtered atom from $AMU\left(\frac{mm}{\sec}\right)^2$ to electron volts.

2. We have stated that in the center of mass frame of reference the pre-collision speed and the post collision speed are equal. Prove this statement using conservation of energy and conservation of momentum.

Hint: Momentum is conserved as a vector quantity. Note: the momentum in the y component was zero prior to the collision and therefore must be zero after the collision. In this sketch $\mathbf{u_1}$ is the pre collision speed of the metal atom in the laboratory frame of reference. $\mathbf{v_1}$ and $\mathbf{v_2}$ are the post collision speeds of mass 1 and 2 respectively.



3. Verify the transformation matrix $C = \begin{bmatrix} \cos(a)\cos(b) & \cos(a)\sin(b) & -\sin(a) \\ -\sin(b) & \cos(b) & 0 \\ \sin(a)\cos(b) & \sin(a)\sin(b) & \cos(a) \end{bmatrix}$ by breaking the transformation into two steps. A rotation of angle a and a rotation of angle b. These two transformation matrices A and B are then multiplied to yield C. Discuss the difference if any caused by the order of performing the rotations (What is the relationship between AB and BA).

4. Write an algorithm to find the impact location of the metal atom against the gun tube wall.

5. Construct the flight of an atom from launch to wall impact. Use the following parameters.

$$r = 10\ mm$$
$$R = 100\ mm$$
$$initial\ speed = 20{,}000{,}000\ mm/\sec$$
$$launch\ angles \quad q = 20^\circ \quad f = 75^\circ$$
$$free\ path\ length = 25, 54, and\ 32$$
$$Neutral\ gas = 50\ AMU$$
$$Metal\ gas = 100\ AMU$$
$$Collision\ parameters \quad q = 30^\circ \quad c = 20^\circ$$
$$q = 215^\circ \quad c = 75^\circ$$

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