The influence of target film material and coating on neutron yield and sputtering yield

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Abstract

The long-life, high yield deuterium-deuterium (D-D) neutron tube has become one of the research hotspots. Here, deuterated polyethylene target, heavy water target and titanium target were investigated by Stopping and Range of Ions in Matter (SRIM). The calculation showed that the deuterated polyethylene target, which was a potential target material, had the highest yield at an incident energy of 120 keV. Further, considering the unfavorable factors such as impurity ions and high temperature, the coating was used to protect the target material. Diamond, boron carbide, boron nitride, silicon carbide, and aluminum carbide were selected. The simulation results showed that the diamond composite deuterated polyethylene film had the best sputtering resistance, and the aluminum nitride composite heavy water target film had the lowest sputtering yield. The two coating materials shield the target, reduced the energy loss of incident ions, and provided a new method for the research of high yield and long life neutron tube.

1. Introduction

Neutron tube has been widely used in nuclear physics, reactor physics, radiochemistry and medicine, cancer treatment, neutron radiography, on-line neutron activation analysis, and nuclear data measurement [1–5]. Neutron tube is a kind of small accelerator neutron source, which seals ion source, acceleration system, target and pressure regulating system in a ceramic tube, forming a compact electric vacuum device. There are two kinds of neutron tubes. One is D-D neutron tube, which mainly reacts: \( \text{D} + \text{D} \rightarrow \text{n} + ^3\text{He} \); The other is D-T neutron tube, which mainly reacts: \( \text{D} + \text{T} \rightarrow \text{n} + ^3\text{He} \). Compared with D-T neutron tube, D-D neutron tube has no pollution to the environment because it does not use radioactive tritium, which is more in line with the concept of green and sustainable development and more conducive to the promotion of use. The principle of neutron tube is simple, but the manufacturing process is complex. The yield, lifetime, and stability of D-D neutron tubes are affected by the performance of various components in the neutron tube. The neutron tube target is an important part of the neutron tube, and also greatly affects the maximum neutron yield. As we all know, the target is composed of a target film and a target substrate. The target film, which is the reaction interface between deuterium and deuterium, is used to store deuterium or tritium gas. Obviously, the target film plays an important role in the yield and life of the neutron tube. Traditional target film materials (titanium, lanthanum, yttrium, zirconium, scandium, and erbium) have made important contributions to increasing neutron yield [6–9]. However, pure titanium has defects as a neutron tube target material. The plasticity, flexibility, and tensile strength of titanium are greatly reduced after hydrogen absorption. The hydrogen embrittlement or many cracks can be generated, pure titanium target becomes less flexible and is subject to more cracking and failures, which affects the lifetime and output of D-D neutron tubes.

Many encouraging advances have been made to solve the above problems [10–15]. For example, Shi et al [16] studied the molybdenum–titanium alloy film, which could reduce carbon pollution. In addition, the material improved resistance to embrittlement caused by hydrogen (created in fusion reaction). Huang et al [17] prepared D-D neutron tube target with molybdenum, which had good mechanical strength and better
conductivity. The D-D neutron yield reached $1 \times 10^8$ n s$^{-1}$. Scandium titanium alloy is also a potential alloy target, which has high neutron yield and strong sputtering resistance ability. Guo et al [15] studied scandium titanium alloy target, and the neutron yield (D-D neutron tube) could reach $6.73 \times 10^7$ n s$^{-1}$. Falabella et al [18] developed a metal palladium coating, that was used to prevent the titanium target film from being oxidized.

Although many promising advances have been made, some problems remain. For example, Tritium contamination of D-T targets causes environmental pollution. Alloying targets (due to high atomic number) have a high energy loss, which leads to a decrease in the neutron yield. D-T target is used to store tritium gas inside neutron tube and is also the interface of deuterium-tritium nuclear reaction. The high atomic number of metal coatings increases the energy loss of incident ions and reduces the neutron yield. Therefore, high-yield, long-life, and environmentally friendly target films are urgently needed.

Herein, based on the idea of maximizing neutron yield, deuterated polyethylene target and heavy water target were studied by SRIM 2013. The experimental results showed that the neutron yield of deuterated polyethylene target had been significantly improved (compared with the current best scandium titanium alloy material). When the incident particle energy was 120 keV, the simulated neutron yield was $9.6 \times 10^8$ n s$^{-1}$. In order to improve the high temperature resistance of deuterated polyethylene target, boron nitride, boron carbide, diamond and silicon carbide were used as protective layers. Compared with the previous coating materials [19, 20], the above materials have lower energy loss. The above research is helpful to promote the research and development of high-yield neutron tube, and provides important reference for the research of target materials and protective layer materials.

2. Neutron yield calculation

In the calculations which follow, the equation (1) was used to calculate the D-D neutron tube yield [20].

$$Y(E) = \frac{AR \cdot I_0 \cdot N_T}{e} \sum_{k=1}^{3} k \cdot f_k \int_{E/k}^{E_{max}/k} \sigma(E) \left(\frac{-dE}{dx}\right) dE$$

Where $Y(E)$ is the integrated neutron yield, $AR$ is the atomic ratio of the deuterium in the target, $I$ is the incident D beam intensity, $N_T$ is the density of deuterium atoms in the target. The integrals represent the contributions of each ion species. $k = 1, 2$ and 3 correspond to monatomic ion, diatomic ion, and triatomic ion, and $f_k$ is the proportion of certain ion. $\sigma(E)$ is the neutron production cross section of the reaction D-D (figure 1). The $-dE/dx$ is the energy loss of the deuterium ion in the target and is also described the molecular stopping power of the target material loaded with deuterium. Material energy loss was calculated by the Stopping and Range of Ions in Matter (SRIM 2013, figure 2). $E$ is the initial accelerating ion energy. In addition, single-energy ion beams with different energy values of 40 keV, 50 keV, 60 keV, 70, 80 keV, 90 keV, 100 keV, 110 keV, 120 keV, 130 keV, 140 keV, 150 keV, 160 keV, 170 keV, 180 keV are selected as the initial accelerated ion energy.
3. The neutron yield with different materials target

The neutron yield calculations for deuterated polyethylene target were based on equation 1, and stopping power calculated by SRIM. The deuterium beam current was 200 $\mu$A. There are two reasons. First, the neutron tube we designed is a small portable neutron tube, so the current must be small enough. Secondly, with the current technical level of our laboratory, the beam current of 200 $\mu$A can make the neutron tube work stably. And the incident deuterium ion beam energy was in the range of 40–180 keV. Similar calculations were completed for heavy water target and the pure titanium target by the above formula. Pure titanium target film is prone to be oxidized to form oxide layer during transportation and storage. TiO, Ti$_2$O$_3$, TiO$_2$ are composed oxide layer mainly. However, due to different oxidation conditions, it is difficult to determine the composition ratio of oxide layer. In this paper, assuming the oxide layer was TiO$_2$, and the thickness was 200 nm. The neutron yield of titanium target with oxide layer was calculated by SRIM.

When the intensity of the incident beam current was constant (in a certain range of deuterium ion energy), the neutron yield increased exponentially with the increase of incident energy. When the incident energy was the same, the oxide layer of the target had an important influence on the neutron yield. It could be seen that the

![Figure 2](image1.png) **Figure 2.** Relationship between deuteron Energy and $D^+$ ionization stopping power in three targets. At the same energy, the energy loss of pure titanium target is the highest compared with deuterated polyethylene and heavy water target, which will reduce the neutron yield.

![Figure 3](image2.png) **Figure 3.** Neutron yields in different target films. At the same incident energy, the neutron yield of deuterated polyethylene target is higher than that of high water target and pure titanium target.
growth trend of the neutron yield of deuterated polyethylene target was rapid. The neutron yields of heavy water targets, pure titanium targets and titanium targets with oxide layers gradually decrease (in a certain range of deuterium ion energy). When the incident deuterium ion energy was 120 keV, the neutron yields of deuterated polyethylene target, heavy water target, pure titanium target and titanium oxide target were $9.6 \times 10^8 \text{ ns}^{-1}$, $8.8 \times 10^7 \text{ ns}^{-1}$, $6.34 \times 10^7 \text{ ns}^{-1}$ and $4.03 \times 10^7 \text{ ns}^{-1}$, respectively (figure 3).

The target material has an important influence on the neutron yield of neutron tube. The neutron production efficiency of target film material largely depends on its ability to retain and inhibit deuterium. The increased deuterium retained will increase the fusion reaction between the ions and the deuterium. The lower stopping power of materials, the less energy that ions will lose (when interacting with materials). The absorption rate of deuterium in the target material and the energy loss of the incident ion are also important. Materials with good thermal stability and mechanical strength are optimal. For two reasons, the neutron yield of pure titanium target is lower than that of titanium target with oxide layer. First, the oxide layer affects the transmittance of deuteron. The transmittance of deuteron decreases as the oxide thickness increases.
deuteron decreases as the oxide thickness increases. Secondly, due to the high hydrogen absorption density of titanium, hydrogen embrittlement is easy to occur. So, titanium as a target material has many defects. Fortunately, due to the small atomic number of deuterated polyethylene, its energy loss is low, leading to an increase in neutron yield. The theoretical analysis is consistent with the simulation results.

4. The sputtering yield of targets with different coatings

The target life of neutron tube is one of the important factors to determine the quality of neutron tube. The life of the neutron tube target is affected by many factors, such as the thickness of the target film, the high target temperature is caused by the bombardment of the deuterium ion beam; the sputtering and contamination of the target film by impurity ions (C, N, O, etc.). Coating on the surface of the target film to shield the target from the impurity ions in the beam. Diamond, boron carbide, boron nitride, silicon carbide and aluminum nitride were selected as coating materials. In order to study the influence of the coating on the sputtering resistance of the

![Figure 6](image1.png)

**Figure 6.** The relationship between sputtering yield of deuterium atom and different coatings: (a) AlN coating, (b) BN coating, (c) B₄C coating (d) diamond coating (e) SiC coating. The target material is deuterium polyethylene.

![Figure 7](image2.png)

**Figure 7.** The relationship between sputtering yield of deuterium atom and different coatings: (a) AlN coating, (b) BN coating, (c) B₄C coating, (d) diamond coating (e) SiC coating. The target material is heavy water.
target material, the sputtering yields of five coating materials were simulated by SRIM. The incident ions were C⁺, N⁺, and O⁺ (the energy was 40 keV–120 keV).

As shown in figure 4, diamond, boron carbide, boron nitride, silicon carbide and aluminum nitride were coated. The sputtering yield of carbon atoms (in deuterated polyethylene target) was not linear with the energy of incident ions. As shown in figure 5, when the above five materials were coated, there was no linear relationship between the energy of incident ions and the oxygen atoms in the heavy water target. When the five materials were used as coating, the deuterium atoms (in the deuterated polyethylene target and the heavy water target) had a linear relationship with the energy of the incident ions (figures 6 and 7). The sputtering yield of deuterium atom decreased with the increase of incident ion energy.

The sputtering yields of deuterated polyethylene target and heavy water target were linear with the energy of the incident ions (figures 8 and 9). In addition, the sputtering yield decreased with the increase of the incident ion energy. When the incident energy was the same, the incident ions are C⁺, N⁺, O⁺, the sputtering rate of diamond coated deuterated polyethylene target was the lowest (figure 8). Under the same conditions, the sputtering rate of heavy water target was the lowest when aluminum nitride was used as coating (figure 9).

Figure 8. The relationship between sputtering yield of deuterium polyethylene target and coating at different energies. This showed that under the same incident energy, Diamond composite deuterated polyethylene film had the best sputtering resistance.

Figure 9. The relationship between sputtering yield of heavy water target and coating at different energies. This showed that under the same incident energy, Aluminum nitride composite heavy water film had the best sputtering resistance.
5. Conclusion

In this paper, the effect of different target materials on the neutron yield of D-D neutron tube was studied, and the sputtering resistance of the target with coating on the target surface was studied. The neutron yields of the three target materials were calculated by equation (1). The neutron yield of the deuterated polyethylene target was as high as $9.6 \times 10^6$ n s$^{-1}$, the neutron yield of the heavy water target was $8.8 \times 10^7$ n s$^{-1}$, and the neutron yield of the pure titanium target was $6.3 \times 10^7$ n s$^{-1}$ (when the incident ion energy was 120 keV). Therefore, the deuterated polyethylene target is a potential neutron tube target membrane material. Further, the influence of different coatings (diamond, boron carbide, boron nitride, silicon carbide, aluminum carbide) on the sputtering resistance of target materials (deuterated polyethylene, heavy water, metallic titanium) was simulated by SRIM. The results showed that Diamond composite deuterated polyethylene film had the best sputtering resistance and Aluminum nitride composite heavy water target film had the lowest sputtering yield (within a certain energy range of the incident ion). The above research provides the possibility for the development of high yield and long life neutron tube, and makes exploratory research for the wide application of neutron tube. Although this research has made some progress, there are still some problems to be solved in material manufacturing. We have reason to believe that with the progress of manufacturing technology, deuterated polyethylene is expected to be used as a target material and play an active role in explosive detection, nuclear medicine, and other fields.

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Data availability statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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