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Optimization of the Cathodic Sputtering Process for Fabricating Thin Film Materials used in Modern Photovoltaic Applications

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Abstract: This study aims to optimize cathodic sputtering techniques to produce high-quality thin films for modern photovoltaic (PV) applications. Sputtering is a widely utilized deposition method known for its ability to generate superior thin films, thus potentially improving the performance of PV devices. This research focuses on investigating materials such as cadmium sulfide (CdS), copper-indium-gallium-selenium (CIGS), and perovskites (CH3NH3PbI3), which possess optical, electrical, and structural properties suitable for PV applications. The primary aim of this study is to enhance our understanding of cathodic sputtering by examining key parameters that influence thin film deposition. Various factors, including vacuum chamber energy, incidence angles, and gas composition, were analyzed to determine their effects. Our findings demonstrate that the sputtering yield is superior when employing Argon gas compared to Nitrogen and Xenon. Additionally, increasing the incidence angle and bombardment energy produces a proportional boost in the sputtering yield until an optimum value is reached. These parameters significantly contribute to the quality of the obtained thin films. Furthermore, our results are consistent with previous research, thus providing validation for our calculations.

Keywords: Thin films deposition; sputtering process, Photovoltaic materials; CdS, CIGS, perovskites.

1 Introduction

Thin film deposition is a sophisticated and precise technique employed in various industrial applications to deposit ultrathin layers of material onto substrates or previously deposited layers. These layers, typically on the nanoscale, are crucial in producing compounds that cannot be easily manufactured through traditional chemical mass production methods. Industries such as optics, electronics, packaging, and even contemporary art benefit from the capabilities of thin film deposition technology [1-3].

One significant area where thin film deposition plays a critical role is in modern photovoltaic cell technology. Photovoltaic cells, which convert sunlight into electricity, have gained prominence as a clean and sustainable energy solution. Thin film deposition techniques have enabled the fabrication of thin films tailored explicitly for photovoltaic applications, offering distinct advantages over traditional bulk silicon-based solar cells [4-5].

The deposition process involves carefully depositing a thin material layer onto a substrate or previously deposited

layers, achieving precise layer thicknesses in the nanometer range. Various deposition techniques and parameters are optimized to ensure uniformity and compositional accuracy, producing thin films with desired properties [6-7].

In the context of photovoltaic cells, thin films offer significant benefits. They exhibit exceptional light absorption characteristics and can be engineered to convert sunlight into electricity efficiently. Commonly used semiconducting materials in thin film photovoltaic cells include amorphous silicon (a-Si), cadmium telluride (CdTe), copper indium gallium selenide (CIGS), and organic compounds. These materials provide flexibility and lightweight design options, broadening the possibilities for integrating photovoltaic cells into various applications. The use of thin films in photovoltaic cell fabrication brings several advantages.

Firstly, it enables cost-effective production processes by minimizing material usage compared to traditional siliconbased solar cells. This reduction in material requirements



translates to lower manufacturing costs and enhanced scalability of photovoltaic technologies [8-10].

Furthermore, the versatility of thin film deposition techniques allows for the deposition of films on diverse substrates, including flexible materials. This versatility opens new avenues for integrating solar cells into buildingintegrated photovoltaics, portable devices, and wearable electronics. In addition, thin film photovoltaic cells exhibit superior performance in low-light conditions, making them suitable for areas with suboptimal sunlight exposure. Their lightweight nature facilitates easier installation and integration into various surfaces, expanding their practical applications [11].

Ongoing research and development efforts in thin film deposition techniques aim to continuously improve the efficiency and durability of thin film photovoltaic cells. Emphasis is placed on enhancing stability and longevity, ensuring these cells' long-term viability and sustainability. Overall, using thin films in modern photovoltaic cell technology represents a significant milestone in the renewable energy sector. These advanced cells offer higher efficiency, cost-effectiveness, and innovative design possibilities. The widespread adoption of thin film photovoltaic cells drives the transition to solar energy as a clean and viable power source for a sustainable future

2 Cathodic sputtering process

Understanding the process of surface sputtering is crucial to the operation of fusion energy devices. Cathodic sputtering involves expulsing high-atomic-number materials from surfaces into the plasma, leading to contamination, increased plasma charge, and inefficient fuel heating.

From a plasma-wall interaction standpoint, cathodic sputtering is undesirable as it contaminates the plasma and erodes the surrounding walls. However, sputtering is also widely utilized in various applications.

Controlled removal of surface layers at an atomic scale and submicron spatial resolution can be achieved through sputtering, particularly when employing a wall-focused ion beam.

Thin film deposition on diverse substrates stands out as one of the primary applications of sputtering. Thus, it is crucial to present an empirical and analytical formula that can quickly determine the sputtering yield for any ion-target combination [12].

3 Findings and Discussion

3.1. Sputtering yield of ions according to the energy of the atom

In the figures below, we present the results of the sputtering yield obtained using SRIM software based on the Monte Carlo method. The sputtering yield of CIGS ions is higher than that of CdS and the perovskite.

The presence of these metallic vapors in the discharge will enhance the sputtering in the cathode. In Figures 1(a, b, c and d), we distinguish five areas representing the variations of sputtering yield Y(E) as an energy function. In the first area, energy is too low in order that sputtering takes place.

There are no sputtering levels. The energy limits that do not match a "cut-off value" are introduced to simplify calculations or at a maximum below which the measuring devices cannot detect sputtering particles. In the second area, sputtering becomes possible.

The incident particles have enough energy in order that atoms can break the links binding the surface. The coefficient increases rapidly for a slight variation in energy. In the third area, the coefficient increases linearly with the energy of incident particles.

These coefficient values are sufficiently high to be able to produce deposits. In the fourth area, the incident particles penetrate more deeply into the target when its energy increases and the recoil atoms are created in more significant quantities.

The sputtering yield is greater than 1. So, there are more particles ejected than incident particles. The sputtering yield reaches a maximum in the fifth area. The penetration depth of the incident particles is sufficiently large to cause the reduction of this coefficient. The incident particles penetrate so deeply into the target that the recoil atoms cannot escape.





Figure 1: Sputtering yield as a function of energy for photovoltaic cells of Cds, CIGS, and Perovskite materials bombarded by (a) Argon, (b) helium, (c) Neon, (d) Xenon gases

3.2. Influence of the incidence angles

Each collision cascade highlights the interactions of the incident particles with the target surface, showing the trajectories and subsequent collisions.

These collision cascades are essential for understanding the processes of atom ejection during sputtering. They make it possible to visualize how the energetic particles interact with the target, leading to the ejection of the atoms of the surface. By using these collision cascades based on specific angles of incidence, it is possible to understand better the mechanisms involved in the ejection of atoms during the cathodic sputtering, thus contributing to the optimization of the process and improving the performance of the thin films obtained.







Figure 2: Sputtering yield as a function of angle of incidence for photovoltaic cells of Cds, CIGS, and Perovskite materials bombarded by (a) Argon, (b) helium, (c) Neon, (d) Xenon gases

The variation in angles also plays a role in determining the quality of the Thin-film obtained.

According to the results in Figure 2 from the SRIM simulation, the optimal angle to obtain the best sputtering yield is 75 degrees (argon, helium, neon) and 85 degrees (Xenon).

Indeed, energy and angle are the two key factors influencing the production of optimum spray performance according to SRIM results. The table below shows the values for energy and angle of incidence necessary to obtain the maximum ejection of atoms from the target.

 Table 1: Energies, incidence angles and maximum sputtering yields obtained by SRIM

		Cds	CIGS	Perovskite
Argon (Ar)	Energy (Kev)	10	10	10
	Angle (Degree)	75	75	75
Helium (He)	Energy (Kev)	10	10	10
	Angle (Degree)	75	75	75
Neon (Ne)	Energy (Kev)	10	10	10
	Angle (Degree)	75	75	75
Xenon (Xe)	Energy (Kev)	1000	1000	1000
	Angle (Degree)	85	85	85

4 Conclusion and Recommendations

This study highlighted using SRIM software to analyze ion interactions, atom ejection and implantation during the cathodic sputtering process of modern materials such as CdS, CIGS and perovskites.

This simulation tool has played an essential role in understanding the mechanisms underlying thin film formation and its qualities.

The results obtained have made it possible to deepen our knowledge of the processes of atom ejection and their deposition, as well as their impact on the quality of the thin films deposited.

We could identify optimal deposition conditions to obtain high-quality thin films through these obtained results.

This approach provided additional information to guide our future research in sputtering and its applications, the development of thin-film solar cells and other emerging technologies.

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