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Materials Innovations for Next-Generation Photovoltaic Manufacturing

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Abstract **–** The next generation of photovoltaic cells holds great promise to revolutionize the solar energy landscape. Advanced materials have shown exceptional efficiency and potential for scalability. By incorporating these next-gen photovoltaic cells, we can further enhance the efficiency and performance of solar energy conversion. Therefore, research endeavors exploring the synthesis and deposition of these cutting-edge photovoltaic materials through processes like DC sputtering are of utmost importance for the future of sustainable energy. Our study proposes an advanced simulation to investigate the thin film formation of Cu2ZnSnS4, Si, and CuInxGa(1−x)Se2 semiconductor materials used in today's PV cells based on the Monte-Carlo method, where Argon is utilized as the bombardment gas in the vacuum chamber during this simulation. We aim to identify the most efficient sputtering yield by systematically varying the bombardment energies and incidence angles. Our findings reveal that an incident angle of 85° gives the optimal sputtering yield, with CZTS exhibiting superior performance compared to Si. Building upon these results, we proceed to apply this specific angle (85°) during the sputtering process for Cu2ZnSnS4 and CuInxGa(1−x)Se2. By meticulously varying the bombardment energy, we examine the total ejected atoms from the constituent elements of these materials. As a result, we deduce that the sulfide (S4) and selenide (Se2) elements significantly contribute to the overall sputtering yield obtained from these materials. The insights gained from this research can potentially pave the way for optimizing the deposition of nextgeneration photovoltaic materials, thereby propelling the solar energy industry towards unprecedented levels of efficiency and sustainability.

Keywords – Next-Gen PV, Sputtering Process, Thin Films, CIGS, CZTS

I. INTRODUCTION

Photovoltaic (PV) technology has emerged as a transformative solution to meet the world's escalating energy demands in the quest for sustainable and renewable energy sources. As the world transitions towards a greener future, advancing solar energy conversion efficiency and the scalability of PV manufacturing processes have become pivotal goals. The key to achieving these goals lies in the realm of materials innovations [1–4].

Materials Innovations for Next-Generation Photovoltaic Manufacturing represents a groundbreaking exploration into materials science's cutting-edge advancements and transformative potential in solar energy generation. This field of research seeks to revolutionize the entire PV landscape by harnessing the power of novel materials, engineering techniques, and manufacturing processes, With the rising focus on sustainability and a pressing need to curb greenhouse gas emissions, the demand for cost-effective, efficient, and eco-friendly solar cells has never been greater. Pursuing materials innovations has become imperative for the PV industry to realize its full potential and establish itself as a major player in the global energy landscape [5-7].

This paper delves into the most promising materials innovations key to the next generation of photovoltaic manufacturing. From developing high-efficiency photovoltaic materials such as

Cu_2ZnSnS_4, Si, and $CuIn_xGa_{(1-x)}Se_2$ to exploring novel manufacturing techniques that optimize resource utilization and reduce waste, this research aims to present a comprehensive overview of the advancements reshaping the solar energy paradigm.

Solar cells utilizing semiconductor materials have demonstrated commendable and intriguing efficiency levels, reaching approximately 23.35%, as recently reported in [8-10]. However, a significant concern arises due to the relative rarity and high cost of this material's elements Ga (gallium) and In (indium). Consequently, the feasibility of photovoltaic cell applications relying on next-generation materials may need to improve profitability in the future.

On the other hand, those next-gen materials are emerging as a promising alternative for thin film-based solar cells. It boasts advantageous optoelectronic characteristics as a direct band-gap semiconductor with an efficient absorption coefficient. CZTS stands out as an abundant, cost-effective, and environmentally friendly material. Despite this, the highest conversion efficiencies achieved by CZTS thin film solar cells currently hover around 9.2%. Nonetheless, its unique properties position CZTS as a rising star for large-scale applications, including solar cells. Certain material properties tend to enhance with larger grain sizes, presenting opportunities for further optimization and efficiency improvements in CZTS-based solar cells.

II. PHYSICAL VAPOR DEPOSITION (PVD) THEORY

PVD is an alternative term used to describe the process of sputtering. Physical Vapor Deposition encompasses various techniques, including sputtering, that involve the deposition of thin films onto surfaces through the physical vaporization of materials. Sputtering is a key method within the broader realm of PVD, and it involves bombarding a target material with energetic ions to release atoms or molecules from its surface. These ejected particles then condense on a substrate to form a thin film. The PVD theory comprehensively explains the principles and mechanisms governing the sputtering process. It is a fundamental aspect of thin-film deposition and various technological applications such as semiconductor manufacturing, optical coatings, and thin-film solar cells. [11-16].

A. *Sputtering yield*

Sputtering yield, often denoted by the Y, is a fundamental parameter in the sputtering process. It refers to the number of atoms or molecules ejected from the target material's surface per incident ion or particle. The sputtering yield is a crucial factor determining material removal efficiency during the sputtering process [17,18].

The sputtering yield depends on various factors, including the energy and mass of the incident ions, the properties of the target material (such as its composition, crystal structure, and binding energies), and the angle of incidence of the ions. Higher incident ion energies and masses generally lead to higher sputtering yields. The sputtering yield can also vary for different target materials and ion species. For example, heavier ions tend to have higher sputtering yields than lighter ones. The angle of incidence can also affect the sputtering yield, with higher yields often observed at glancing angles.

Understanding the sputtering yield is essential for optimizing the sputtering process in various applications, including thin film deposition, surface modification, and microfabrication. By controlling the sputtering conditions and target material properties, researchers and engineers can tailor the yield to achieve desired thin film thicknesses, deposition rates, and material characteristics [19-21].

B. *The Evolution of Sigmund's Hypothesis in Linear Collision Cascade Theory*

Developing the Sigmund hypothesis in the linear collision cascade theory was pivotal, enhancing our understanding of the interactions between energetic ions and amorphous targets. This theory extended the linear collision cascade model to describe ion behavior in amorphous materials. By employing Boltzmann's transport equations, it analyzed ions undergoing multiple collisions with atoms in amorphous targets during the early stages of collision processes. Sigmund's work shed light on energy deposition, ion range, and damage formation in amorphous targets, crucial for practical applications like ion implantation and radiation damage studies in semiconductors. This development provided a comprehensive framework for studying ion-solid interactions in amorphous materials, significantly impacting ion beam physics and materials science [22].

III. SRIM SIMULATION BASED ON MONTE-CARLO METHOD

The Monte Carlo simulation program SRIM (Stopping and Range of Ions in Matter) is a powerful and widely used computational tool in ion-solid interactions and materials science. Developed by James F. Ziegler and his colleagues, SRIM is designed to predict the behavior of energetic ions as they traverse through matter and interact with atoms in a target material [4-6].

SRIM simulates individual ion interactions using the Monte Carlo method, a probabilistic numerical technique. It considers various physical processes such as nuclear and electronic stopping, scattering, energy loss, and ion range calculations. These simulations provide valuable insights into ion penetration depth, energy deposition, and the creation of collision cascades in materials [23].

Researchers and engineers across diverse disciplines, including semiconductor technology, radiation damage studies, nuclear physics, and materials characterization, heavily rely on SRIM to predict the effects of ion bombardment and develop an understanding of the underlying physical mechanisms.

With its user-friendly interface and extensive database of material properties, SRIM allows users to input ion parameters (e.g., ion species, energy, angle of incidence) and material properties (e.g., density, composition) to generate comprehensive ion trajectories and energy loss profiles. This information is crucial for designing experiments, interpreting results, and optimizing ion implantation processes in various applications.

IV. FINDINGS AND DISCUSSION

A. *Dependence of sputtering yield on bombardment energies at fixed angles of incidence*

The figure 1 showcase the results of three-dimensional curve analyses derived from Monte-Carlo simulations, explicitly focusing on sputtering yield calculations. These simulations were conducted at three distinct angles of incidence (θ = 40°, 60°, and 85°), where the sputtering yield was evaluated across a range of energies. The target materials subjected to bombardment were Cu2ZnSnS4 and Si, while the incident ions employed were Argon ions.

The results depicted in Figure 1 reveal that, for each semiconductor, an angle of 85° yields the highest sputtering efficiency. Moreover, an interesting observation arises when increasing the bombardment energy, as a distinct peak, denoted as Emax, is observed. Beyond this peak value, the sputtering yield decreases. Thus, achieving optimal outcomes requires careful consideration of both the incidence angle and bombardment energy.

The presented curves can be categorized into three distinct zones:

- Zone 1: At low bombardment energies, the sputtering process remains inactive, as the argon gas ions lack sufficient energy to reach the target.
- Zone 2: Upon reaching a certain threshold energy level, the sputtering process initiates, with argon ions bombarding the target and causing the ejection of target atoms. During this phase, the bombardment energy can be increased up to the limit of Emax.
- Zone 3: The sputtering process reaches its maximum efficiency, and any additional energy leads to a decline in the yield. In this case, the ions possess extremely high energy, causing them to penetrate deeply into the target, preventing recoil atoms from escaping.

By considering these zones, researchers can optimize the incidence angle and bombardment energy to achieve the most favorable sputtering results in ion-solid interactions, which are vital for numerous applications in materials science and semiconductor technology.

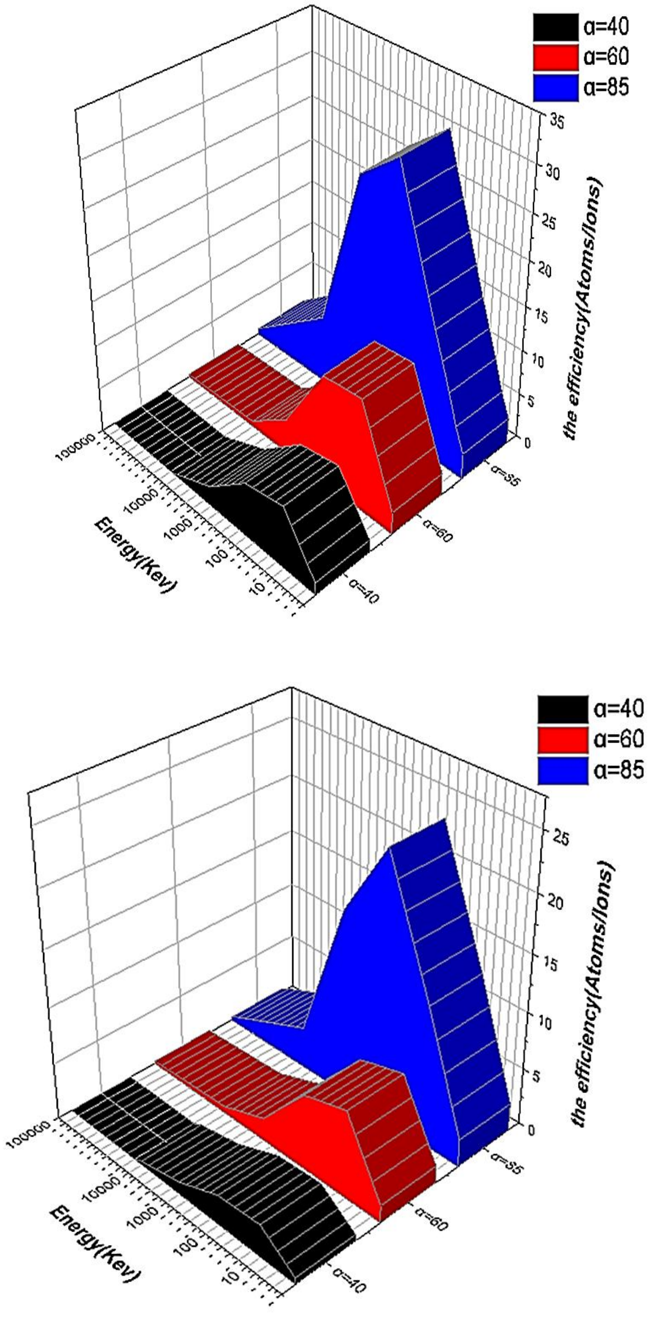

Figure 1: Sputtering yield as a function of the energy of the bombardment ions (Ar) on three incidence angles θ = [40°, 60°, 85°] calculated by the MC method for a: Cu2ZnSnS4 and b: Si.

B. *Dependence of sputtering yield on angles of incidence at fixed bombardment energies*

In this section, we examine the impact of varying energies (E) on the sputtering yield while considering the incidence angle. Energies of 10 keV, 100 keV, and 1000 keV are utilized, and the sputtering yield is assessed for each energy level. The same gas and target materials are consistently used throughout the bombardment experiments. The outcomes are graphically represented in Figure 2. Notably, employing a bombardment energy of 100 keV yields the most favorable performance. As the incidence angle increases, the sputtering yield also experiences growth, reaching a peak value labelled αmax. However, exceeding this threshold results in a decline in the sputtering yield. Conversely, opting for low bombardment energy leads to fewer atoms being ejected from the target, resulting in an inferior sputtering yield.

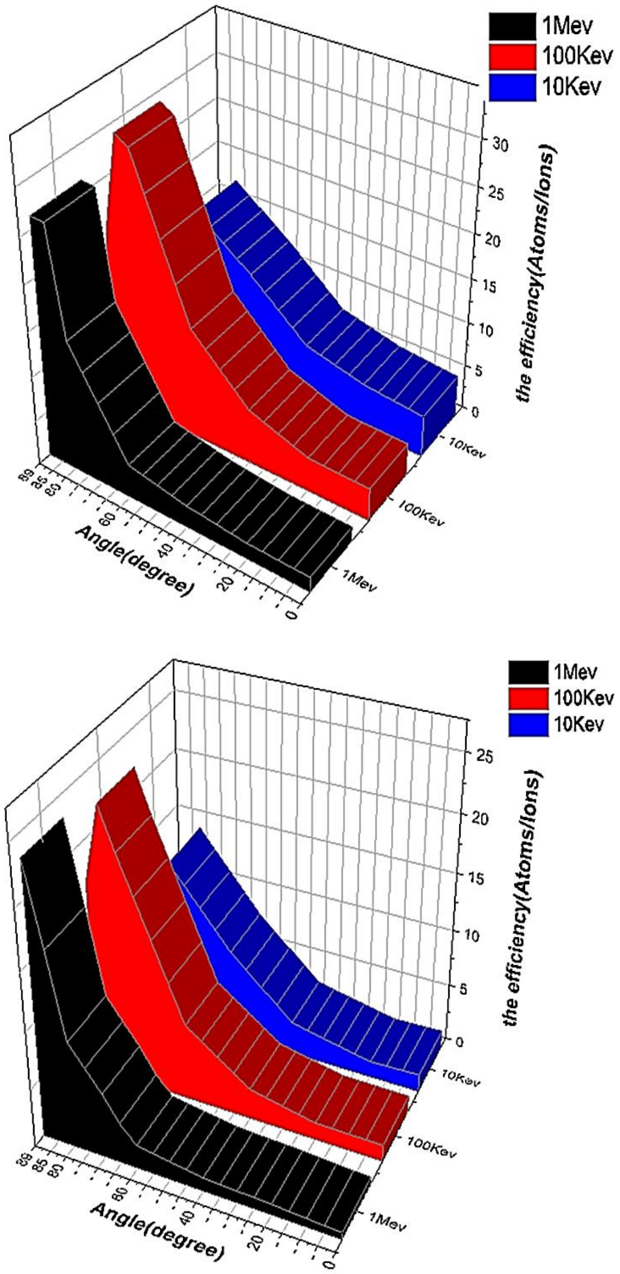

Figure 2: Sputtering yield as a function of incidence angles on three energies E = [10 keV, 100 keV, 1 MeV] calculated by the MC method for a: Cu2ZnSnS4 and b: Si.

C. *Comparison between Cu2ZnSnS4 and Si semiconductors*

Figures 3 and 4 present a comparative analysis between the two semiconductors, Cu2ZnSnS4 and Si, to determine their relative performance. We draw insightful conclusions by visualizing the previously obtained results as three-dimensional curves.

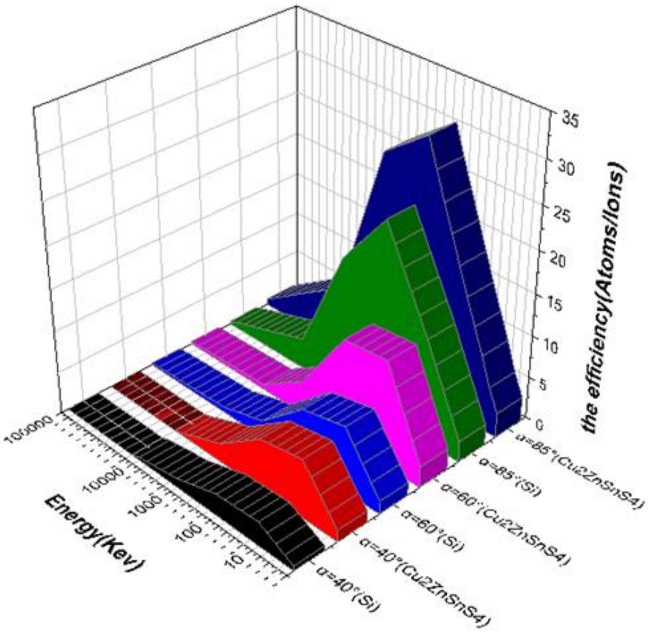

Figure 3: Comparison of sputtering yield as a function of the energy of the bombardment ions on three incidence angles θ = [40°, 60°, 85°] calculated by the MC method between Cu2ZnSnS4 and Si

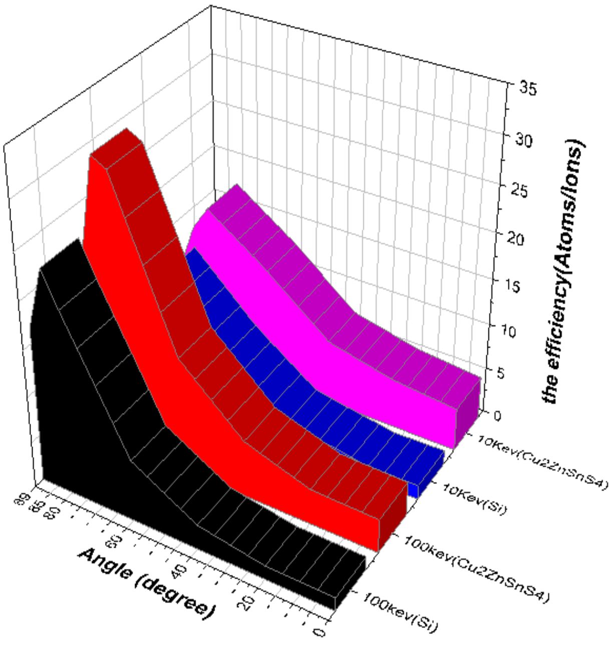

Figure 4: Comparison of sputtering yield calculated by the MC method between Cu2ZnSnS4 and Si as a function of incidence angles on three energies E = [10 keV, 100 keV, 1 MeV]

V. CONCLUSION

The next-generation photovoltaic cells based on CZTS and CIGS materials are experimental but hold immense promise in energy production. In this research, we have investigated the development of semiconductor cells using thin films of Si, Cu2ZnSnS4, and CuInxGa(1−x)Se2 through the sputtering method.

Through rigorous analysis and simulations, we have discovered that the optimal conditions for achieving the highest sputtering yield involve an incidence angle of 85° and bombardment energy of 100 keV. These parameters result in the most efficient ejection of atoms for both Cu2ZnSnS4 and Si semiconductors. Notably, surpassing these specific values of energy or angle leads to decreased sputtering efficiency.

Our findings have revealed that Cu2ZnSnS4 outperforms silicon in terms of sputtering yield, making it a more promising material for photovoltaic cell applications. These insights contribute to developing advanced semiconductor devices and pave the way for potential breakthroughs in renewable energy technology.

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