Effects of Argon Ion Bombardment on Amorphous Silicon and Copper Indium Gallium Di-Selenide Solar Cells

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STEM High School for Boys – 6th of October,

October Gardens, Giza, Egypt

Abstract

Amorphous Silicon (a-Si) and Copper Indium Gallium Di-Selenide (CIGS) are two widely employed materials in thin-film solar cell technology due to their favorable photovoltaic and optoelectronic properties. This study aims to compare their sputtering yield, lateral ion range, and longitudinal ion range after the bombardment of argon ions to evaluate their stability and performance under different conditions. Simulations were conducted using TRIM technology at ion energies of 1 keV and 5 keV, with incidence angles ranging from 0° to 89°. The results indicate that CIGS has a higher sputtering yield, with its peak observed at an incidence angle of approximately 75°, while a-Si demonstrates superior lateral ion ranges. These findings suggest that a-Si offers better structural damage resilience, which is advantageous for long-term material stability, whereas CIGS is more suitable for applications where minimizing substrate damage is critical. The comparison of sputtering behavior and ion interactions in these materials provides valuable insights for optimizing ion-beam processing techniques in solar cell manufacturing. Such optimization is crucial for enhancing material selection, improving durability, and achieving better performance in thin-film solar cells. This study helps guide decisions in material choice and processing conditions, ensuring efficient, stable, and reliable solar cell technologies adjusted for specific manufacturing

requirements and environmental resilience.

Keywords: Amorphous Silicon (a-Si), Copper Indium Gallium Di-Selenide (CIGS), Collision Cascades, Thin-Film Solar Cells, Material Stability, Ion-Solid Interactions, Substrate Damage, Sputtering Yield, Ion Range

1 Introduction

The problem of climate change has many obvious harmful effects. The main reason that causes this problem is burning fossil fuels for energy production which results in the release of greenhouse gases which cause climate change. To create a greener environment and decrease the effect of this harmful phenomenon, cleaner sources of energy production should be considered. Solar energy is the most important one as it is nearly available everywhere. Thin-film solar cells are the most used source due to their cost-efficiency, lightweight design, and compatibility with flexible substrates. Amorphous silicon (a-Si) and copper indium gallium di-selenide (CIGS) stand out for their unique optoelectronic properties among the various materials used in this technology, in addition to their high performance in photovoltaic applications.

During the process of thin-film solar cells, ion-beam sputtering is involved. It is a process in which high-energy ions are being bombarded on the target materials, resulting in atoms' ejection which, consequently, forms a thin film. Sputtering has critical implications for the deposition and etching processes used in solar cell manufacturing. Factors like sputtering yield, which is the number of ejected atoms per ion bombarded, lateral ion range, the horizontal distance cut by the ion, and the longitudinal range, the penetration depth of the ion, are essential to understanding how materials behave under ion bombardment. These factors affect the structural stability of the materials, in addition to their performance and durability in photovoltaic devices.

While individual studies have investigated the ion-beam processing characteristics of a-Si and CIGS, a direct comparison of their sputtering behaviors under identical conditions remains limited. This comparison is essential to enhance material selection for specific fabrication techniques, such as precise etching, thin-film deposition, and energy-efficient solar cell manufacturing. Through this paper, this gap is aimed to be filled by evaluating and comparing the sputtering yield, lateral ion range, and longitudinal ion range of a-Si and CIGS when bombarded with argon ions. This evaluation is done through the simulation where SRIM/TRIM software is used to run this simulation. The simulation was conducted through 1 keV and 5 keV ion energies while varying the angle of incidence to consider various environmental conditions.

Previous research on ion-beam sputtering has established fundamental principles of ion-material interactions. Heavier atomic compositions, such as those found in CIGS, exhibit higher sputtering yields due to enhanced collision cascades. The influence of energy and angle on sputtering yields was further explored, showing that oblique angles often maximize material removal. Additionally, the importance of lateral and longitudinal ranges in determining material stability and damage profiles has been highlighted. According to these findings, this study hypothesizes that CIGS should have a higher sputtering yield since it has a higher density. Also, a-Silicon should have longer lateral ion ranges and greater resistance to ion bombardment-induced damage since it demonstrates superior structural stability.

Studying the effects of argon ion bombardment on a-Silicon and CIGS is crucial for advancing solar cell technology by understanding their sputtering characteristics. Using ion-beam processing techniques, the durability and efficiency of solar cells can be precisely controlled, which will result in reducing costs and environmental impact. This research not only provides practical guidelines for material selection in solar cell manufacture but also contributes to the general field of ion-beam material science, which will result in more innovations in renewable energy technologies.

2 Methods

Simulations were performed using the TRIM (Transport of Ions in Matter) software. This software is a molecular dynamic tool that simulates the interaction between ions and different materials. This includes collision cascades and energy deposition. TRIM gives precise results on sputtering yield and ion range, which makes it suitable to be used for this research.

The bombarded ions were chosen to be Argon ions (Ar^+) for their inertness and alignment with ion-beam techniques. The CIGS was implied by adding the elements: Copper, Indium, Gallium, and Selenium with a ratio of 1:0.5:0.5:2 respectively. The target thickness was set at 500 Å (50 nm) to ensure accurate simulation of surface interactions without significant substrate interference. The type of calculation was set to be Detailed Calculation with full Damage Cascades so that all collisional damage to the target is analyzed. The density of a-silicon was used as 2.28 g/cm^3, and that of CIGS as 5.75 g/cm^3.

The simulation was done twice for each material, one with 1 keV energy and the other with 5 keV. The sputtering yield, lateral range, and longitudinal range were measured by setting up each angle once, from 0° to 89°. Each simulation involved 1000 ions to achieve statistical significance. The outputs were visualized in graphs, comparing trends in sputtering yield and ion ranges for the two materials.

3 Results

The sputtering yield of a-Silicon and CIGS was collected for different energies and different incidence angles with the error bars. Generally, CIGS has higher values. When bombarded with ions of 1 keV, CIGS had a peak at 65° with a value of 5.191 atoms/ion. On the other hand, a-Si exhibited a peak at 75° with a value of 4.13 atoms/ion (Figure 1). When bombarded with 5 keV ions, CIGS had a peak at 72° with a value of 12.832 atoms/ion. While a-Si had a peak at 80° with a value of 10.21 atoms/ion (Figure 2).

The lateral range of bombarded ions was collected for both a-Si and CIGS for different energies and different incidence angles with the error bars. Generally, the lateral range was consistently increasing with a-Si having a higher lateral range. When bombarded with 1 keV, a-Si had a maximum value of 37 Ang while CIGS had a maximum of 26 Ang (Figure 3). When bombarded with 5 keV, on the other hand, a-Si had a maximum of 100 Ang, while CIGS had a maximum value of 68 Ang (Figure 4).

The longitudinal range of bombarded ions was collected for both a-Si and CIGS for different energies and different incidence angles with the error bars. Generally, the lateral range was consistently decreasing. When bombarded with 1 keV ions, a-Si decreases from 36 Ang. at 0° to 14 Ang. At 89°, while CIGS decreased from 25 Ang. at 0° to 15 Ang. at 89°

(Figure 5). On bombarding with 5 keV ions, the longitudinal range of a-Si decreased from 98 Ang. at 0° to 34 at 89°. While that of CIGS decreases from 98 Ang. at 0° to 34 Ang. at 88° (Figure 6).

Sputtering Yield

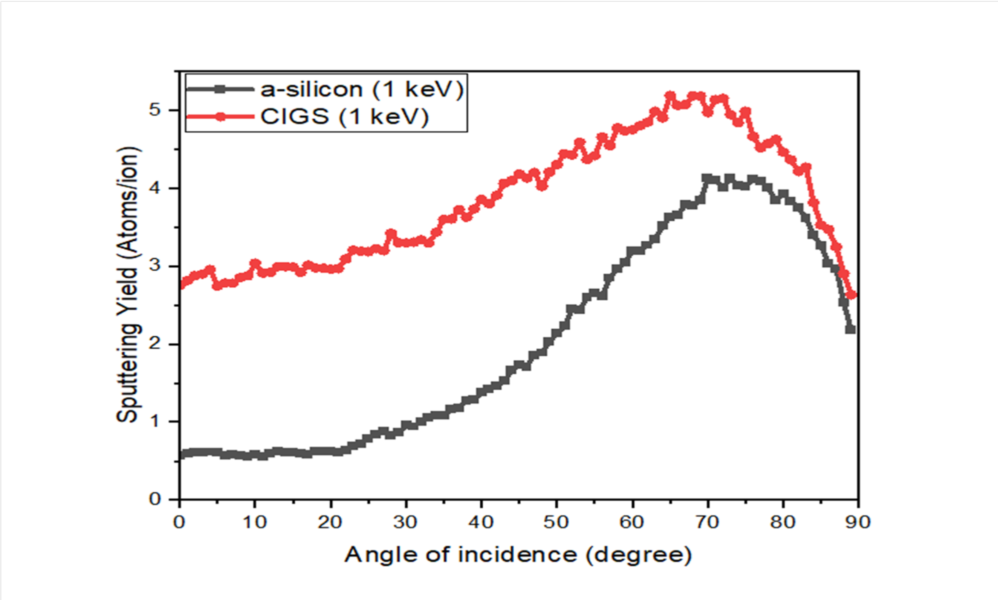

Figure 1: The sputtering yield of both a-Silicon and CIGS when bombarded with 1 keV ions.

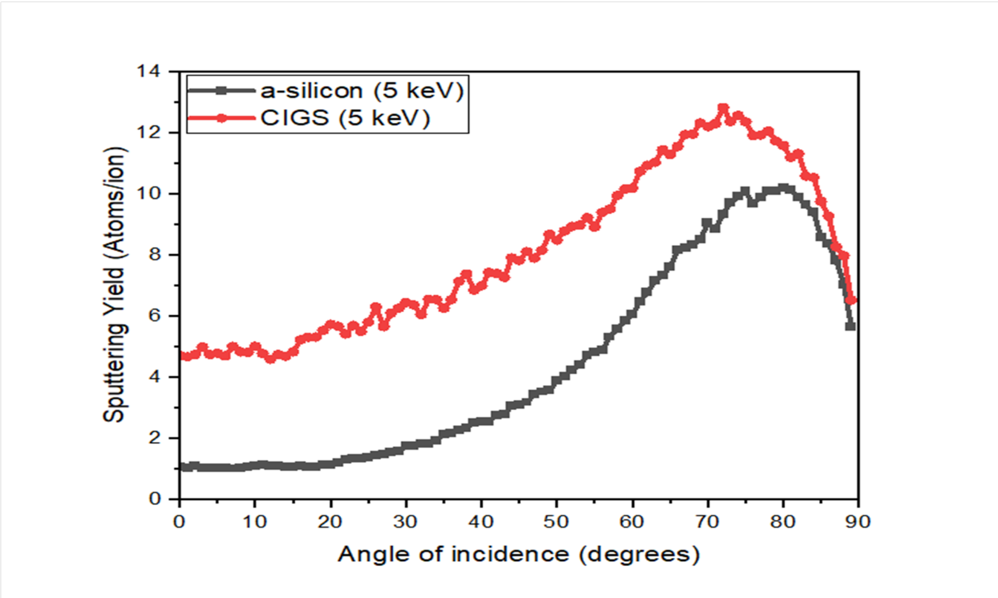

Figure 2: The sputtering yield of both a-Silicon and CIGS when bombarded with 5 keV ions.

Lateral Ion Range

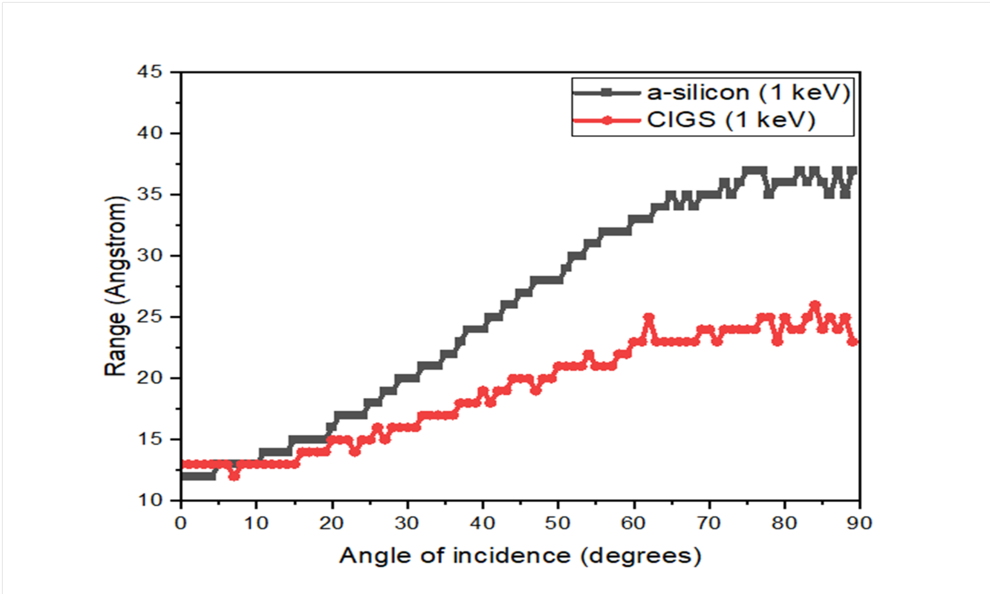

Figure 3: The lateral range of both a-Silicon and CIGS when bombarded with 1 keV ions.

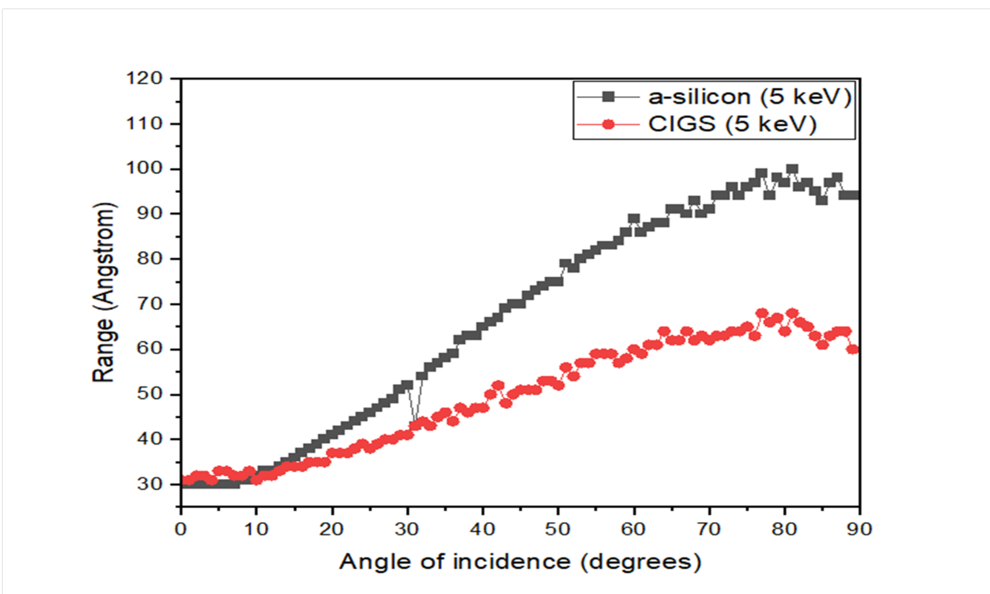

Figure 4: The lateral range of both a-Silicon and CIGS when bombarded with 5 keV ions.

Longitudinal Ion Range

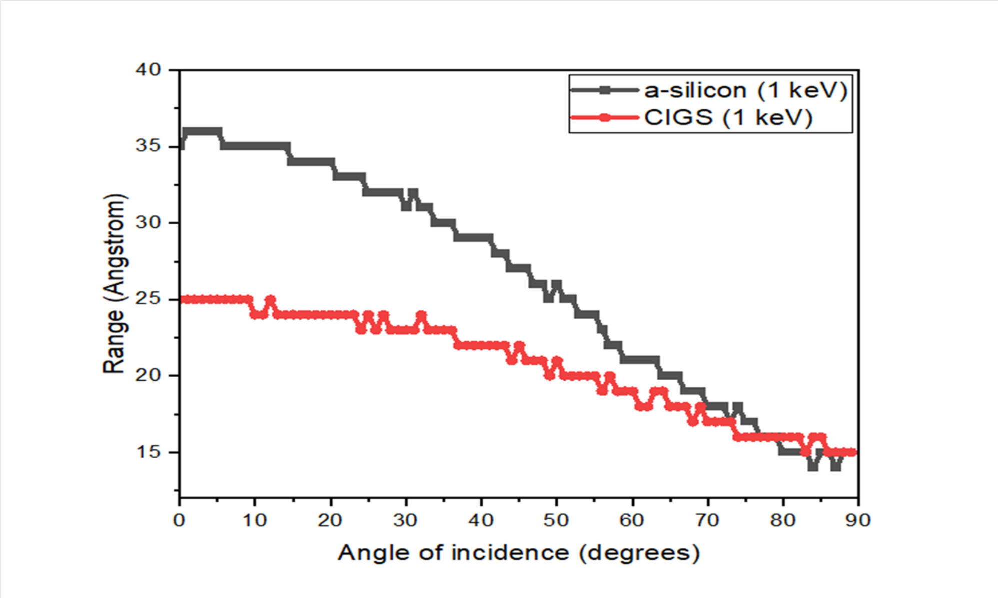

Figure 5: The longitudinal range of both a-Silicon and CIGS when bombarded with 1 keV ions.

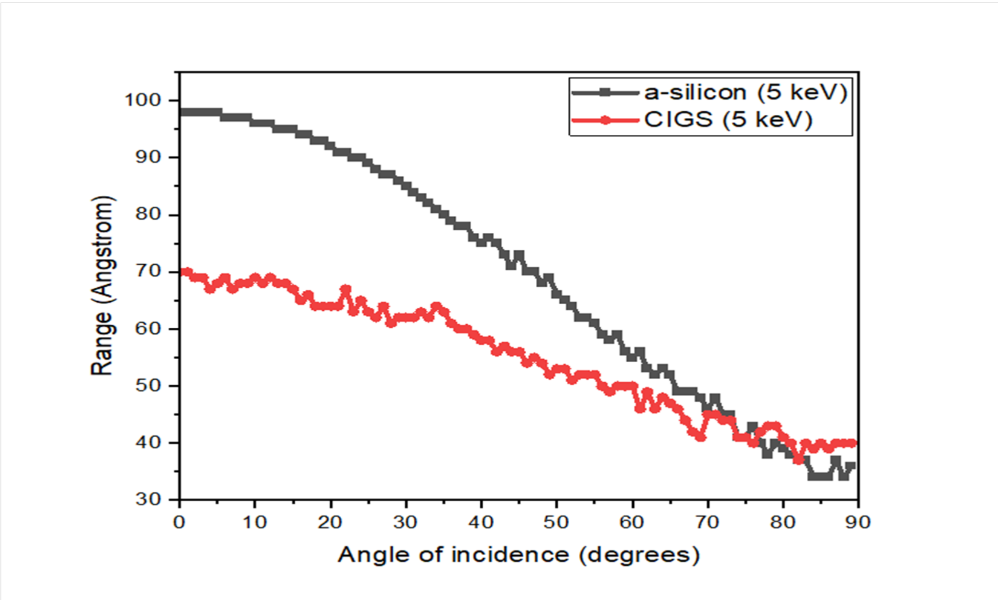

Figure 6: The longitudinal range of both a-Silicon and CIGS when bombarded with 5 keV ions.

4 Discussion

Sputtering yield measures the number of atoms ejected per ion bombarded on the material. It depends on the material's atomic structure, ion energy, and incidence angle. Higher sputtering yields indicate efficient material removal, which is advantageous for deposition or etching processes. CIGS exhibited a higher sputtering yield than a-Si. This behavior stems from its relatively heavier atomic composition (copper, indium, and selenium), which enhances the probability of collision cascades. Since a-Si has a lower sputtering yield, it has lower degradation, which improves long-term stability. Thus, CIGS is ideal for applications requiring high deposition rates, such as thin-film coatings, while a-Si is more suitable for precision etching or surface treatments in solar cells.

The lateral range is the horizontal distance cut by the ions within the material. It measures how the ions spread out laterally inside that material. This affects the material uniformity after bombardment. a-Si had higher lateral ranges than CIGS. This indicates better stability against structural damage caused by ion bombardment. Since CIGS has a lower one, this minimizes the associated damage to surrounding regions during sputtering. This confirms that CIGS is more suitable for precise, localized etching or deposition.

Longitudinal ion range measures the depth of ion penetration into the material. This impacts the substrate damage and energy transfer. The greater depth suggests a higher energy absorption capacity. This can be beneficial in processes like drug use or implantation where deeper ion penetration is necessary. Generally, a-Si had more longitudinal range than CIGS, especially at smaller angles where ions bombardment approaches to be perpendicular on the surface. This suggests that CIGS is more efficient in processes that require small subsurface manipulation.

To sum up, the higher sputtering yield of CIGS and its shorter ion ranges make it ideal for high-efficiency deposition or precise etching. On the other hand, a-Si is suitable for uniform surface treatments and processes requiring deeper ion implantation. These findings align with previous studies and emphasize the need for tailored ion-beam processing strategies based on specific application requirements.

5 Conclusion

This study simulated the collision of argon ions with thin-film solar cells of a-Si and CIGS with varying energies and incidence angles using SRIM/TRIM software. It focused on comparing the sputtering yield, lateral ion range, and longitudinal ion range. The results exhibited that CIGS has a higher sputtering yield specifically at an angle of 65° when bombarded with 1 keV ions and 72° for 5 keV bombarded ions. This makes it ideal for high-efficiency material removal in deposition and etching processes. On the other hand, a-Si exhibited higher lateral ranges and high stability against damage. This makes it suitable for precise surface treatments. Its deeper penetration indicates that it is more suitable for suitability for subsurface applications like ion implantation. The findings highlight the necessity of selecting materials based on specific processing requirements: CIGS for efficient and localized material removal, and a-Si for uniform surface treatments and more extensive energy transfer. This work is aimed at improving the understanding of ion-beam processing for thin-film solar cells and is intended to help optimize fabrication techniques that improve performance, durability, and efficiency.

References

1. Green, M. A., et al. (2019). Solar cell efficiency tables (version 54). *Progress in Photovoltaics: Research and Applications*, **27**(7), 565–575.

2. Solar Energy Technologies Office. `https://www.energy.gov/eere/solar/solar-energy-technolo`

3. Dharmadasa, I. M. (2020). Advanced Thin film materials for photovoltaic applications. *Coatings*, **10**(6), 562.

4. Behrisch, R., & Eckstein, W. (2007). *Sputtering by particle bombardment.*

5. Zhao, W., et al. (2023). Applied Surface Science, **622**, 156876.

6. James Ziegler - SRIM & TRIM. `http://www.srim.org/`

7. Oeba, D. A., & Mosiori, C. O. (2024). *European Journal of Applied Physics*, **6**(6), 1–13.

8. Barberet, P., et al. (2011). *Nuclear Instruments and Methods in Physics Research B*, **269**(20), 2163–2167.

9. Oyewande, O. E., & Akinpelu, A. (2018). *IOP Conference Series: Earth and Environmental Science*, **173**, 012045.

10. Ruzic, D. N. (1990). *The physics and technology of ion beams*. Wiley.