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Comparative study of the sputtering yield and photovoltaic efficiency in photovoltaic materials

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Abstract

The comparison of the results obtained from argon ions and those obtained from neon ions in various photovoltaic materials in this work led to the identification of factors influencing the ionic sputtering deposition method as well as the effect of the used ion beam type. The SRIM simulation software was used in the study. According to the results, the sputtering yield increases proportionally with the angle and energy of incidence up to a certain point, then decreases. Furthermore, the value disparity confirmed the close relationship between the spraying process and the material structure. The same findings were made when the electronic and nuclear stopping powers were calculated. Solar cells were then simulated using the materials under consideration.

Keywords: SRIM software, Sputtering process, Solar cell, Modelling and Simulation.

1. Introduction

At the nanoscale, the manipulation of matter is the subject of an increasing number of research projects thanks to technological advances concerning the development and characterization of nano-materials [1]. The considerable development of nanotechnology allows the production of very small objects, which have different properties from their massive counterparts [1]. Various deposition techniques have been used for the thin layer formation, among which are chemical vapor deposition (CVD), low pressure chemical vapor deposition (LPCVD), plasma enhanced chemical vapor deposition (PECVD), catalytic chemical vapor deposition (Cat-CVD), and ion sputtering [2-5]; The deposition parameters strongly control the physical properties of the obtained layers. Therefore, the simulation of the deposition step is necessary to define the material with the appropriate properties.

Methods for simulating thin film deposits at the atomic scale complement traditional theoretical and experimental approaches. Indeed, these methods make their best contribution in cases where the discrepancy between the experimental measurements and the theoretical explanation is considerable. In particular, the Monte Carlo method allows the exploration of the evolution and properties of a wide range of problems and systems at the nano- and micro-scale [6-7]. It is a powerful tool for modeling the deposition process, which involves the growth of a film on the substrate surface.

Thus, the present work fits as part of the thin layer formation study conducted by the TRIM simulation software in SRIM [8-9], based on the Monte Carlo method notions [6-7]; The aim is to characterize the parameters influencing the ion spray deposition process in photovoltaic materials. Then, the simulation of the operation of a solar cell based on these same materials and of the same size was carried out.

2. Methodology

In this work, the SRIM software is used to simulate ion-matter interactions. Various phenomena, such as ion energy loss, electronic shutdown power, nuclear shutdown power, and sputtering yield estimation, will be treated. Their variation curves as a function of the angle and energy of ion incidence on the surface of different semiconductor materials will be investigated. The following materials with a thickness of 180 nm were selected, and their characteristics are represented in Table 1. The incident ion beam gas is argon, which is commonly used in sputtering experiments because of its inert nature and low reactivity with the sputtered target. During the simulation, 1000 incident ion particles were used.

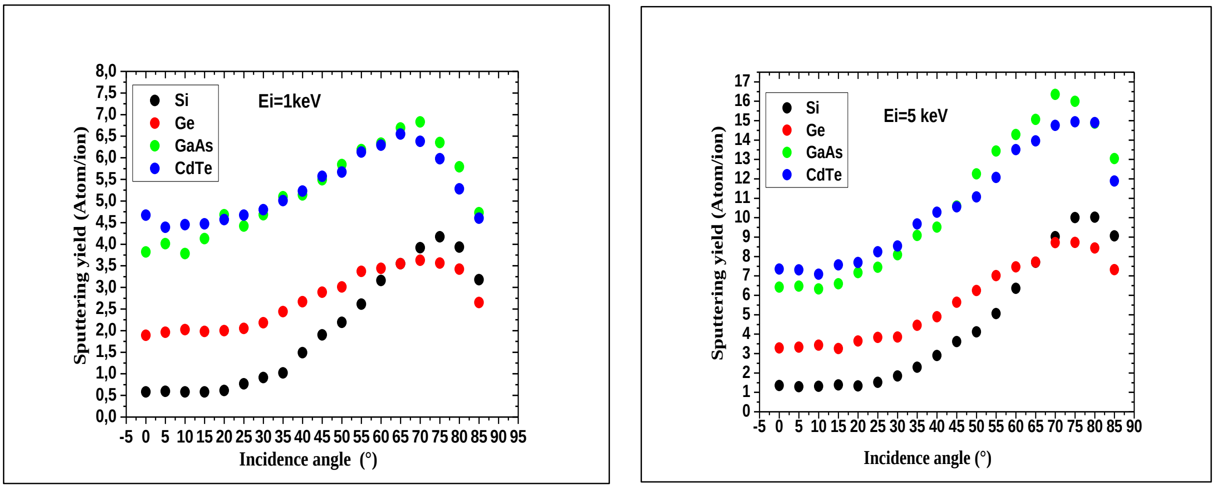
Table 1. Materials characteristics

Material	Structure	Gap (eV)	Volume Density (g/cm^3)	Mesh Parameter (Å)
Si	Cubic crystalline	1.12	2.33	5.43
Ge	//	0 .61	5.323	5.66
GaAs	//	1.43	5.32	5.6533
CdTe	//	1.5	5.85	6.4805

3. Results and discussion

3.1 Sputtering yield

In our work, the two used values for incident energy are 1 keV and 5 keV. For the incidence angle, a sweep from 0° to 85° was performed with a 5° pitch; the obtained results are shown in the following figures.



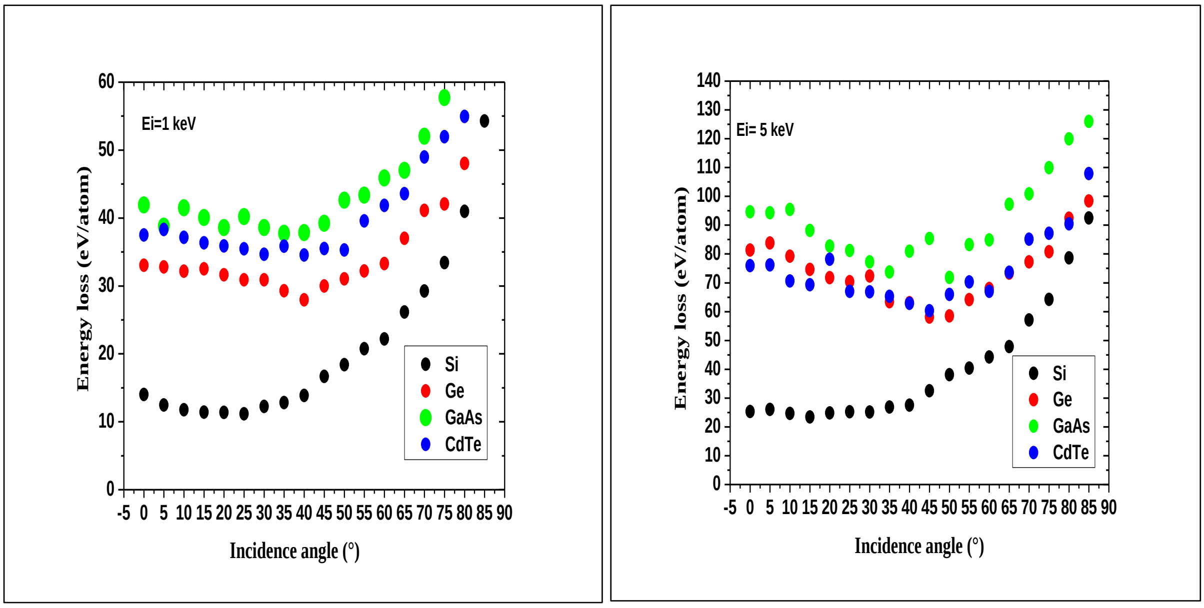
(a) (b)

Fig 1. Sputtering yield, (a): 1 keV and (b): 5 keV.

Target argon ionic bombardment causes ionic removal at the surface. The phenomenon depends on several parameters, namely: the energy and angle of ion beam incidence; the nature and mass of the ions; the mass of the material constituting the target; and the structure and chemical composition of the material. Thus, according to the results shown in Fig 1. (a) and (b), the obtained yield values depend closely on the nature of the material to be sprayed. It should be noted that the curves of compound materials are very close and evolve in the same way; similarly, the Ge. In silicon, the values are lowest compared to those obtained in other materials at low incident angle values and become higher compared to those obtained in germanium at high incidence angle values. This can only be explained by the chemical and structural composition of the sputtered materials since they have been subjected to the same sputtering conditions [10].

3.2 Energy loss

In the two cases of 1 keV or 5 keV incidence energies represented in Fig 2., the superposition of the obtained curves shows that the important values of the energy loss are observed in the composite materials and the low values are seen in silicon. In the other materials, practically the same energy loss per atom is obtained.



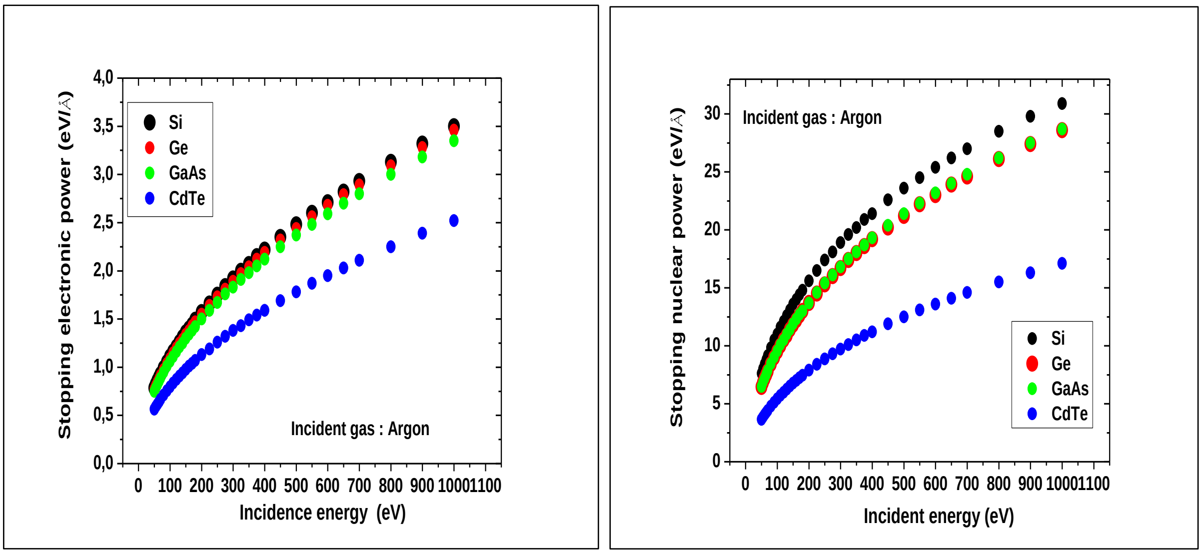
(a) (b)

Fig 2. Energy loss, (a): 1 keV and (b): 5 keV.

3.3 Electronic and nuclear stopping power

The energy loss can be divided into two parts: the energy transferred by the ions to the electrons of the target (called electronic stopping power or inelastic energy loss) and the energy transferred by the ions to the nuclei of the target (called nuclear shutdown power or elastic energy loss). The stopping powers of evolution in the materials under consideration are shown in Fig 3.

The results show that the nuclear stopping power is always higher than the electronic stopping power for the various materials considered. This can be explained by the fact that in a certain range of energy, from a hundred eV to a few keV, the ions' path in the matter is weak, and it is the first atomic layers that participate in the sputtering. The impact of the ions mainly causes the emission of neutral atoms (ionic sputtering), and the ejection requires a sequence of collisions to change the amount of incidental motion, directed towards the inside of the material, towards the surface. However, this does not prevent the ejection of ions (secondary ion emission), photons (luminescence), and secondary electrons. For higher energies (from a few keV to a few MeV), the incident ion penetrates much deeper into the solid (a few tenths of microns at 100 keV); this is the ion implantation phenomenon that is used to implant dopants in a material [1].



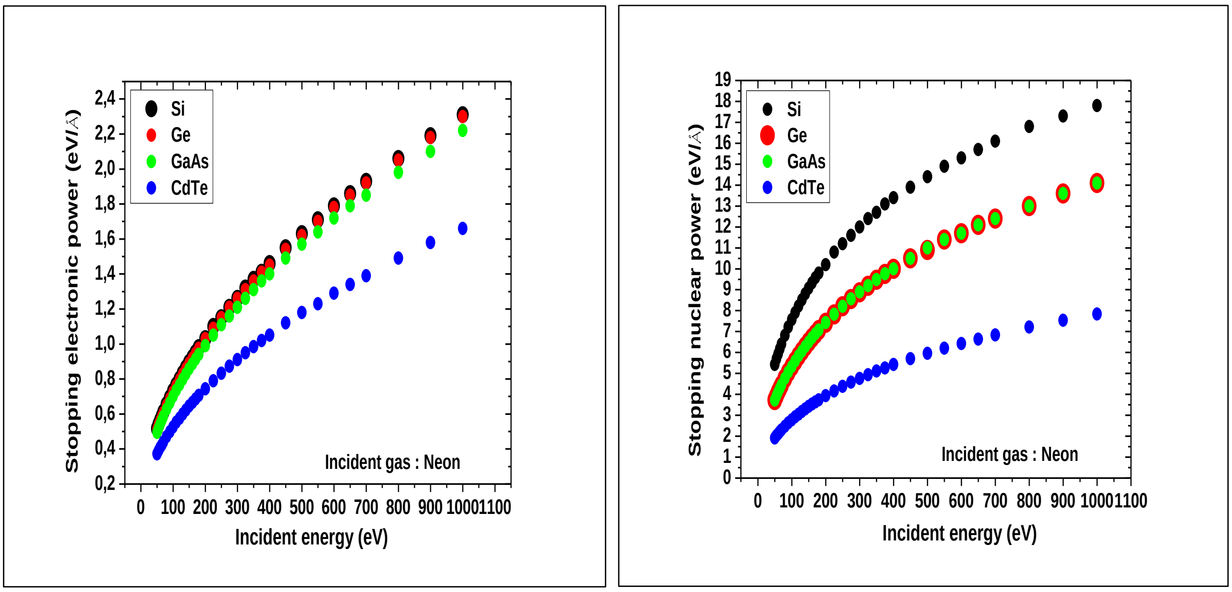
(a) (b)

Fig 3. Stopping power (argon incident gas), (a): electronic and (b): nuclear.

It can also be seen that the obtained values of the powers depend closely on the structural morphology of the material to be sprayed. A visible discrepancy is observed in the curves of the four materials as a function of the incidence energy evolution. It can be noticed that, compared to CdTe (cadmium telluride), in the case of electronic stopping power, the curves are almost identical for materials such as Si (silicon), GaAs (gallium arsenide), and Ge (germanium). A slight shift of the silicon curve and a significant shift of the CdTe (cadmium telluride) curve are observed in the case of nuclear stopping power.

To confirm the obtained results, the gas constituting the bombardment ions was substituted by neon; in Fig 4., the evolution of the stopping powers as a function of the incidence energy in the previous materials is represented, where the same observations are made, and this can only be explained by the material characteristics represented in Table 1.

Although the physical process of sputtering is the same for all materials, the regular arrangement of atoms in a crystalline structure produces effects that are not seen in disordered structures. For crystals, the sputtering efficiency also depends on the crystal plane that is subjected to ion bombardment. When the bombardment is carried out according to certain privileged crystallographic directions, the penetration depth in the crystal is much more important than, for example, in the amorphous case; the atoms' alignment in the crystals provides real "ways" for the incident ions with the same direction. As it encounters few obstacles, the ion energy loss is much lower (the silicon case; see Fig. 2). This results in a lower sputtering efficiency because the collisions occur at a deeper level and the atoms have a lower probability of being ejected. This phenomenon is known as the "channeling effect."



(a) (b)

Fig 4. Stopping power (neon incident gas), (a): electronic and (b): nuclear.

On the other hand, when the bombardment is carried out perpendicular to the planes of high atomic densities, the sputtering yield is higher. For diatomic materials (such as GaAs and CdTe), which meet more impediments, the ion energy loss is much higher (see Fig 2.). The variation in sputtering yield of the different components of the material will lead to the formation of a surface layer called an "altered layer," typically a few nm thick, enriched with the component with the lowest sputtering yield (differential sputtering) [11]. As the sputtering continues, the surface concentration of the component with the highest yield will decrease [12].

4. Modelling and Simulation

In this part of our study, the simulation of the performance of four solar cells designed from previous materials is presented. To simulate the solar cell, the Silvaco TCAD simulator was used. It is made up of two main parts: Athena, which is used to design the solar cell structure, and Atlas, which is used to simulate the operation of any semiconductor device in order to extract the electrical characteristics [13].

The doping concentration of the p-type silicon region layer is about 1×10^{16} (cm^{-3}), with a thickness of about 2.82 (μm), and 180 (nm) for the n-type region, which is doped with 5×10^{18} (cm^{-3}). Thus, a one-dimensional simulation program of solar cells is performed based on the planar electrodes, ITO/Germanium, silicon, CdTe, or GaAs structures shown in Fig 5. The AM 1.5 standard sunlight spectrum with a power of 1.32 mw/cm^2 is used for illumination.

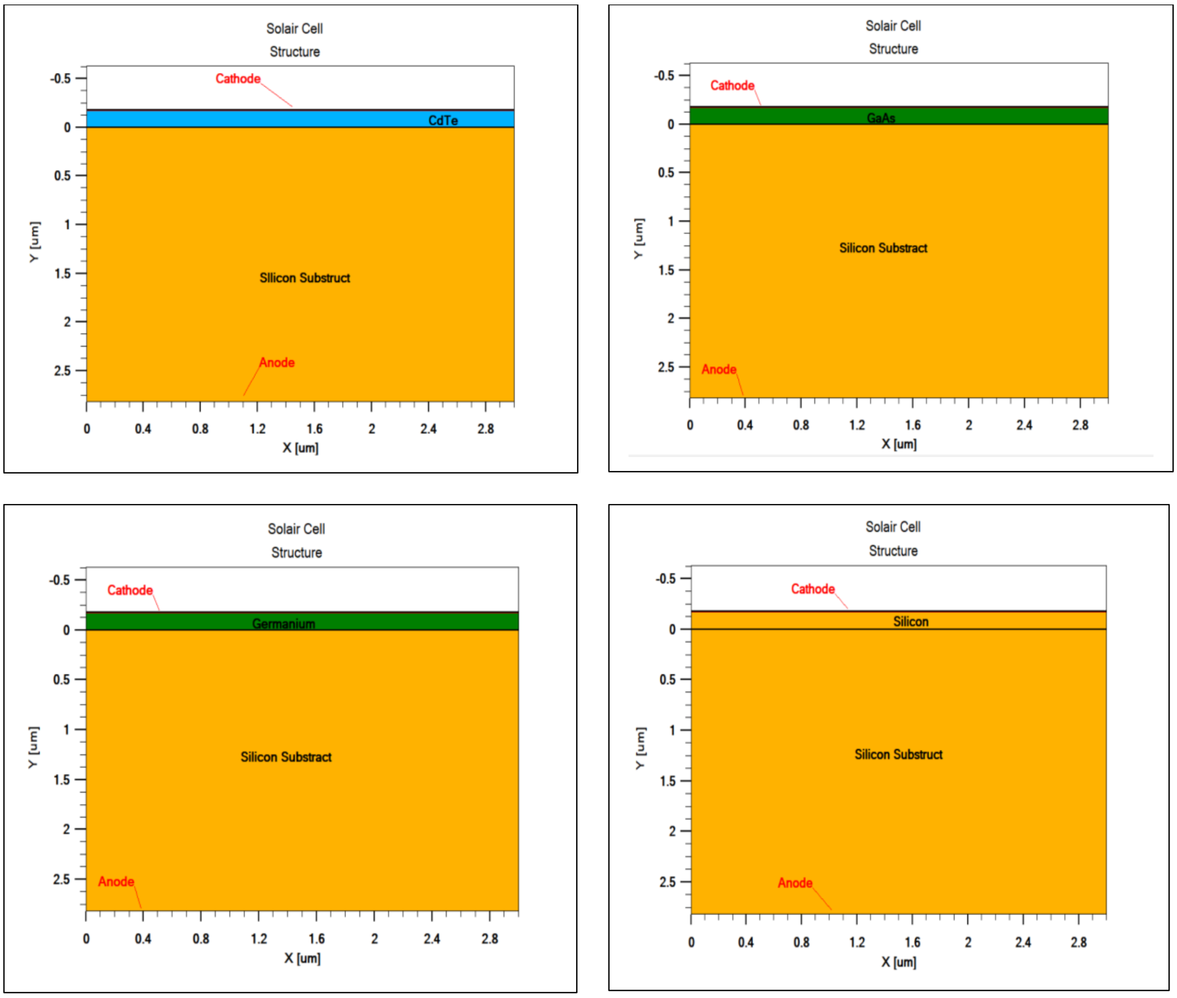
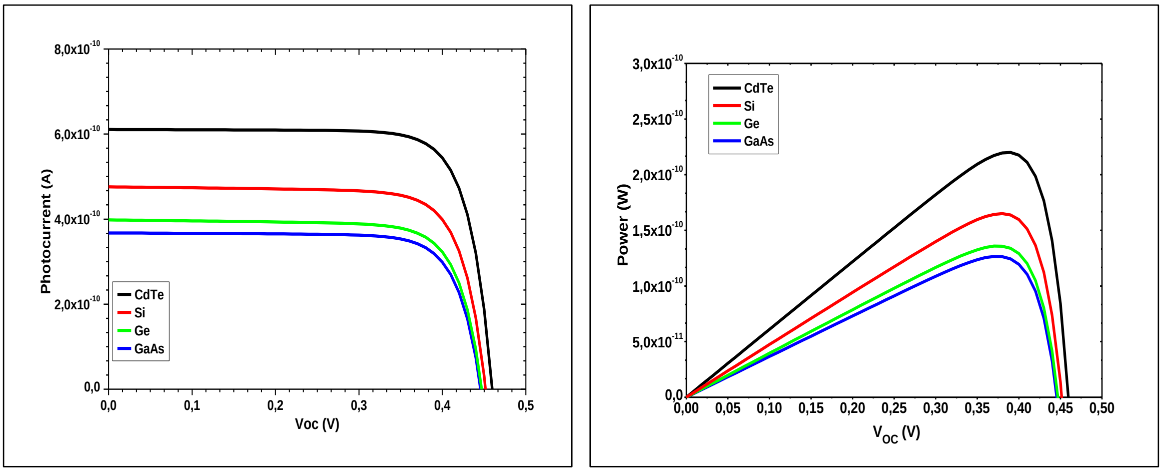


Fig 5. Simulation of the structures of solar cells with: (a) CdTe, (b) AsGe, (c) Ge, (d) Si.

According to the results shown in Fig 6., the photocurrent and photovoltaic power of CdTe are greater than those of other materials, which can be explained by its high absorption coefficient compared to others, which makes it effective at absorbing more photon energy [14].



(a) (b)

Fig 6. Photocurrent (a), and photovoltaic power (b) versus the open circuit voltage.

5. Conclusion

In this work, the evolution of many parameters has been studied as a function of the variation of incidence angle and energy in many photovoltaic materials during the sputtering deposition process carried out by simulation, such as sputtering efficiency, energy loss, and electronic and nuclear stopping powers.

With respect to the obtained results, the spraying efficiency evolves proportionally with the incidence angle up to a certain value, then it decreases for the different materials considered. The difference in the obtained values in these materials confirmed that this process is strongly dependent on the material structure to be sprayed, which was verified when we proceeded with the same energy and angle of incidence. The same observations were made when the electronic and nuclear stopping powers were calculated. In addition to the above, the comparison of the obtained results from argon ions and those obtained from neon ions shows that the ion beam nature is a crucial parameter. As the sputter yield obtained from argon is higher than that obtained from neon, this justifies the usual and preferential use of argon in sputtering. The simulation of the solar cell operation based on the considered materials showed that the photovoltaic efficiency of cells simulated from CdTe and silicon is the highest compared to that obtained in AsGa and germanium cells.

6. Acknowledgements

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7. References

[1] Tzitzios V, Synthesis, Development and Characterization of Magnetic Nanomaterials. *Nanomaterials*. 2022, 12(7):1036. doi.org/10.3390/nano12071036.

[2] Jilani A, Abdel-wahab M S, Hosny Hammad A, Advance Deposition Techniques for Thin Film and Coating, in Modern Technologies for Creating the Thin-film Systems and Coatings. London, United Kingdom: IntechOpen; 2017. doi: 10.5772/65702.

[3] Eriksson A, Zhu J, Ghafoor N, Johansson M, Sjölen J, Jensen J, Odén M, Hultman L and Rosén J, Layer Formation by Resputtering in Ti-Si-C Hard Coatings during Large Scale Cathodic Arc Deposition. Surface & Coatings Technology. 2011, 205(15), 3923-3930. doi.org/10.1016/j.surfcoat.2011.02.007.

[4] Madadi M, Heiska J, Multia J, Karppinen M, Atomic and Molecular Layer Deposition of Alkali Metal Based Thin Films. ACS Applied Materials & Interfaces. 2021, 13 (48), 56793-56811. doi: 10.1021/acsami.1c17519.

[5] Malik S, Tripathi CC, Thin Film Deposition by Langmuir Blodgett Technique for Gas Sensing Applications. Journal of Surface Engineered Materials and Advanced Technology. 2013, 3(3) Article ID:34491,7. doi:10.4236/jsemat.2013.33031.

[6] Frenkel D, Introduction to Monte Carlo Methods, Computational Soft Matter: From Synthetic Polymers to Proteins. Lecture Notes, John von Neumann Institute for Computing, Julich, NIC Series, 23, ISBN 3-00-012641-4, pp. 29-60, 2004.

[7] Martin-Bragado I, Borges R, Pablo-Balbuena J, Jaraiz M, Kinetic Monte Carlo simulation for semiconductor processing: a review. Progress in Materials Science, 2017. doi: 10.1016/j.pmatsci.2017.09.

[8] Zeigler F, Beirsack JP, Littman U, 1985, The Stopping and Range of Ions in Solids. Pergamon Press, New York; version 2013.

[9] Martinie S, Saad-Saoud T, Moindjie S, Munteanu D, Autran J, Behavioral modeling of SRIM tables for numerical simulation. Nucl. Instrum. Meth. Phys. Res. B; 2014, 322, 2–6. doi:10.1016/j.nimb.2013.12.023

[10] Attaf A, Benkhedir ML, Aida MS, Influence of substrate bombardment on sputtered a-Si:N thin film properties. Physica B: Condensed Matter, 2005, 355 (1–4), pp. 270-279. doi:10.1016/j.physb. 2004.11.004

[11] Alfonso JE, Olaya J, Cubillo G, Thin film growth through sputtering technique and its applications. In: Rubens M, Andreeta B, editors. Crystallization. Rijeka, Croatia: Intech Open; 2012. pp. 397-432. doi: 10.5772/35844.

[12] Javier MO-G, Luis VZ, Mario C, Raú LG, Andre S.R.-C, Ana M.-B, Rodolfo C, Self-organized nanopatterning of silicon surfaces by ion beam sputtering. Materials Science and Engineering R, Nucl. Inst. Meth. Phys. Res. B, 2014, 86, 1–44. doi :10.1016/j.mser.2014.09.001

[13] Muzaffar Imam M, Askari SSA, Das M K, Effect of grain boundary orientation on the recombination in polycrystalline materials: a theoretical and simulation study. Applied Physics A, 2022, 128.10 : 891. Doi : 10.1007/s00339-022-06027-5

[14] Thivakarasarma T, Lakmal AAI, Dassanayake BS , Velauthapillai D, Ravirajan P, Thermally Evaporated Copper Iodide Hole-Transporter for Stable CdS/CdTe Thin-Film Solar Cells. Nanomaterials 2022, 12, 2507. Doi :10.3390/nano12142507