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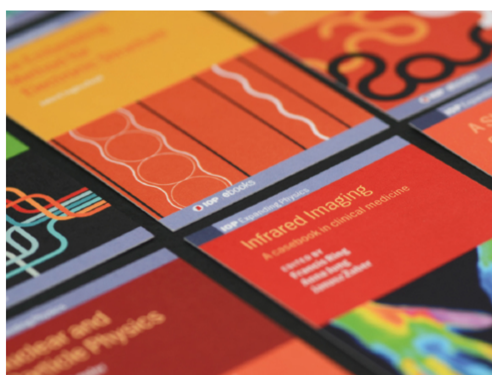

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Trends of Sputtering Parameters in Monte Carlo Simulations of Rare Gas Impingement of GaSb, AlSb and InSb

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Abstract. Binary alloys of Group III-V metals and metalloids, such as GaSb, InSb and AlSb, were recently found to be very promising spintronic materials. For such potentially innovative materials, the quantum spin properties of constituent electrons can be exploited, for better enhanced high-tech applications, than the particulate dynamics of the electrons as in current electronic device applications. Ion beam surface sputtering is a versatile tool for crystal and thin film growth in materials science and characterisation. Consequently, trends of some sputtering parameters were investigated through Monte Carlo simulations of the bombardment of the binary compounds GaSb, InSb and AlSb using Argon, Helium and Krypton ions. The sputtering parameters for the binary compounds were found to be inconsistent as the angle of incidence increased, which occurred for different ion and energy combinations. Also, the maximum sputtering yield did not occur at a particular angle but within a range of values, 65° - 85° and 75°- 85° for ion energies 1keV and 10keV respectively. The sputtering yield was also found to increase with an increase in the ion energy.

1. Introduction

Sputtering is the ejection of particles (atoms or molecules) from a solid material surface through the influence of highly energetic incident ions. The technique is an economic way of generating ordered nano-patterns on a material surface. It is useful in thin-film deposition and semi-conductor manufacturing [1, 2].

A number of theoretical approaches have been developed over the years to study the nano-structuring of material surfaces by ion beam sputtering. These approaches include the continuum models [3-19], Monte Carlo simulations [20-25] and molecular dynamics simulations [26, 27]. Group III-V compounds are useful in optoelectronic development [28]. For example, the group III-V compound, GaSb is highly useful in optoelectronic development, although, it was reported to swell when bombarded with either high energy ions or low energy caesium ions at 14.5 keV [29].

In molecular dynamics and Monte Carlo simulations of [26], He^+, Ne^+, Ar^+, Xe^+, Kr^+ and Rn^+ were used in the study of the group IV elemental materials, C, Si, Ge, Sn, Pb and the binary compounds InP and GaAs. Ion energies of 1 keV and 10 keV and incident angles 0°, 20°, 30°, 40°, 60° and 89.9° were employed. It was stated that the projected range and the longitudinal straggle decreased with increasing angle of incidence whereas the lateral straggle was found to rise with increasing angle of incidence. It was further stated that the sputtering yield was not consistent with an increase in the angle of incidence.

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However, generally for all target materials employed, the highest sputtering yield occurred at an incident angle of 60°.

The knowledge of the trend of different sputtering parameters of materials is highly relevant in thin film deposition which has applications in the manufacturing of semiconductor devices. In this paper, Monte Carlo simulations of the sputtering of binary compounds AlSb, GaSb and InSb have been performed to investigate the variation of various sputtering parameters when these materials are impinged with energetic noble gas ions.

2. Theoretical Background

In ion beam sputtering, the ions bombard the target and penetrate the surface of the substrate transferring part of their energy to the surrounding atoms. This triggers a collision cascade with secondary atoms [30]. This in turn leads to the ejection of a small percentage of atoms. The rate of removal of atoms from a point O is proportional to the power dissipated at that same point by the random distribution of the incident ions and the average energy released at O as a result of the incident ion is given in [30] as

$$Q(r) = \frac{\xi}{(2\pi)^{3/2} ab^2} \exp[-(r')^2/2a^2 - (p'^2 + q'^2)/2b^2] \tag{1}$$

where ξ is the total energy transferred by the incident ion, r' is the parallel axis while p' and q' are the perpendicular axes to the ion beam direction while a and b represent the longitudinal and lateral straggling respectively. The sputtering yield is given as

$$Y(\theta) = \frac{n\mu(\theta, R_y)}{F\cos\theta} \tag{2}$$

where n is the number of atoms per unit volume in the amorphous solid and F is the flux of the incoming ions. It was further stated that in [31], in the limit, $k/R_y \ll 1$, the erosion velocity is given as

$$\mu(\theta, R_y) = \frac{F}{n} Y_0[\cos(\theta) - \Lambda_y(\theta)k/R_y] \tag{3}$$

where Y_0 is the yield for a flat surface, *k* is the average range of ion penetration and $\Lambda_x = \sin^2(\theta)\sin^2(\theta/2) - \cos^2(\theta/2)$ (4)

Y₀ dependence on θ restricts the Bradley Harper theory to angles not close to grazing incidence angle.

3. Angular Dependence on Yield

Wei *et al.* (2008) [32] derived an expression for the angular dependence of sputtering yield, using Sigmund's theory. It was further stated that the peak of the sputtering yield is as a result of the interplay between the increased energy deposited on the surface via the incident ion and decreased depth traversed by the recoil atom which promoted and reduced the sputtering yield respectively. The equation for the normalized sputtering yield under symmetry was then given as

$$Y(E,\varphi) = Y(E,0)\cos\varphi \exp\left[\frac{b^2 \sin^2\varphi}{2\beta}\right] \tag{5}$$

where *φ* is the angle of incidence, b is the projected range, E is the ion energy and β is the energy range straggling along the longitudinal directions.

The yield would have a maximum value for an angle of incidence

$$\varphi_{\max} = \cos^{-1}\left(\frac{\beta}{b}\right) \tag{6}$$

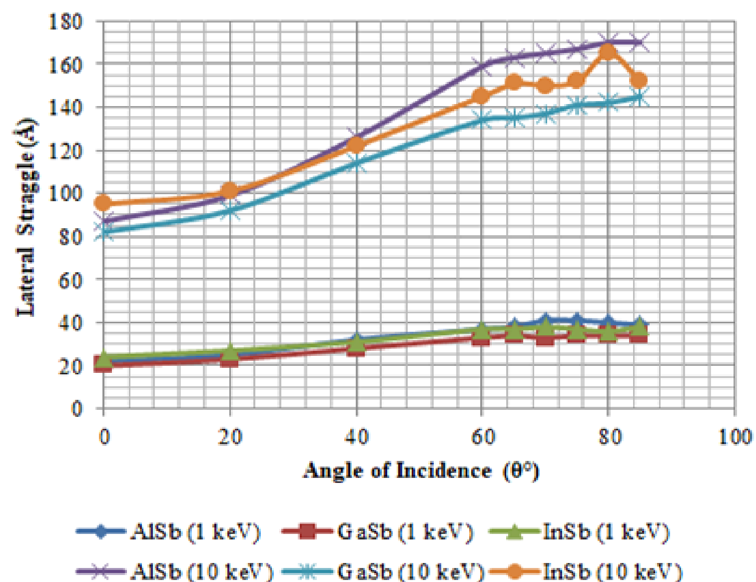
4. Method

Monte Carlo simulations of the sputtering process were done using SRIM and TRIM codes [33, 34]. The simulation was carried out on the binary compounds GaSb, AlSb and InSb which were bombarded with noble gas ions (Ar^+, He^+ and Kr^+) with energies of 1 keV and 10 keV at incident angles, 0°, 20°. 30°, 40°, 60°, 65°, 70°, 75°, 80° and 89.9°. The densities used for AlSb, InSb and GaSb were 4.2600 g/cm^3, 5.7747 g/cm^3 and 5.6140 g/cm^3 respectively which were obtained from a table of inorganic compounds [35]. The target width and the total number of ions were set to 10000Å and 1000 respectively. The target layer for the compounds was single layered. The damage type, detailed calculation with full damage cascades, was employed in the simulation. This monitors the energy of the recoil ions until they are incapable of causing sputtering [34]. The incident ions and recoils are monitored during the simulation in which their energy decreases until it is very low to cause sputtering or they are too far from the surface [26].

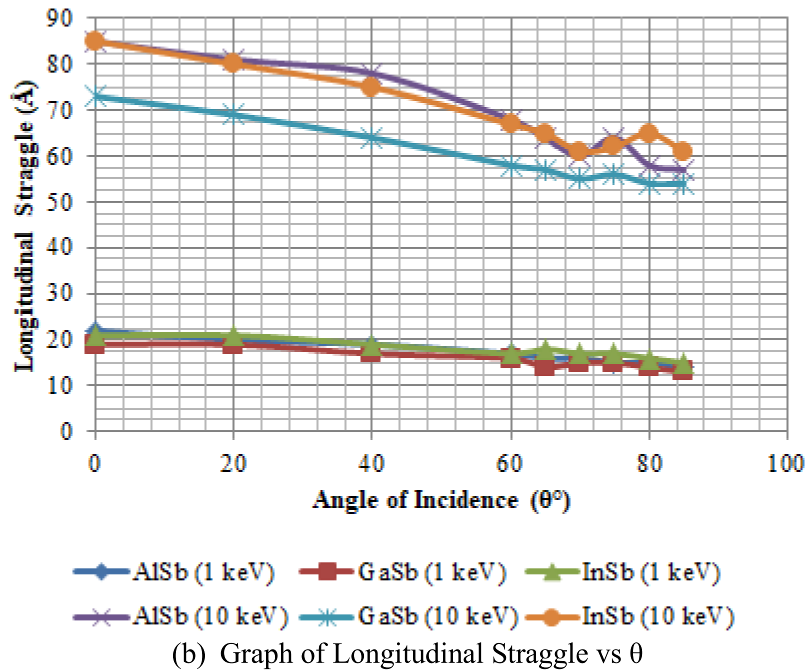
The sputtering parameters studied are projected the projected range, longitudinal straggle, lateral range, and lateral straggle. The projected range is the projection is the projection of the range in the direction of the incoming energetic ions. The probabilistic nature of the ions' collisions, having different stopping potentials and deflected at different angles leads to spreads in the projected range known as the longitudinal straggle and also a lateral straggle of the projected range [36].

5. Results and Discussion

From the results, it was found that at ion energies of 1 keV and 10 keV, the longitudinal straggle and projection range were not consistent but decreased in general with an increase in the angle of incidence whereas the lateral range and straggle increased in general with the angle of incidence for all incident ions. The highest projected range was recorded for He^+ at 10 keV. Generally, the values of the various sputtering parameters were the highest for He^+ compared to other ions except for the sputtering yield where it was the lowest. The increase in the sputtering yields was not also consistent as the angle of incidence increased. However, from 0° to 60°, the decrease and increase in the sputtering parameters were consistent which is similar to the result of [26] though the material-ion combinations used there differ from the ones employed in this paper. The maximum sputtering yield did not occur at a particular angle for all incident ion and compound combinations. Instead, in general, they were observed to occur within a range. At 1 keV, for all incident ions, the variation was between 65° and 85° while at 10 keV, they were observed between 75° and 85°. For all simulations, the maximum sputtering yield was found to be 19.720 atoms/ion and these occurred at an incident angle of 70° for Kr^+ at 10 keV on AlSb. Some of the plots obtained are shown in figures 1, 2 and 3 below.

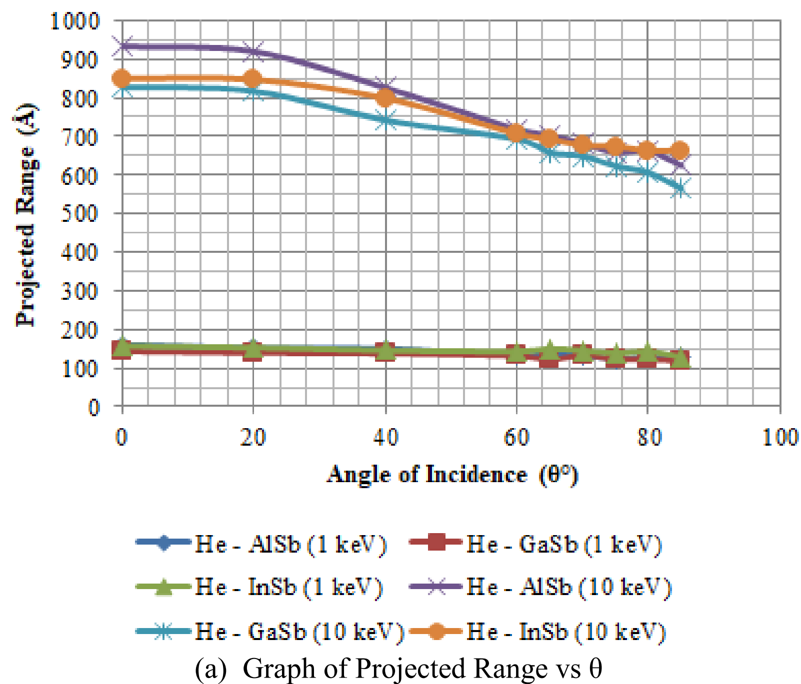


(a) Graph of Lateral Straggle vs θ

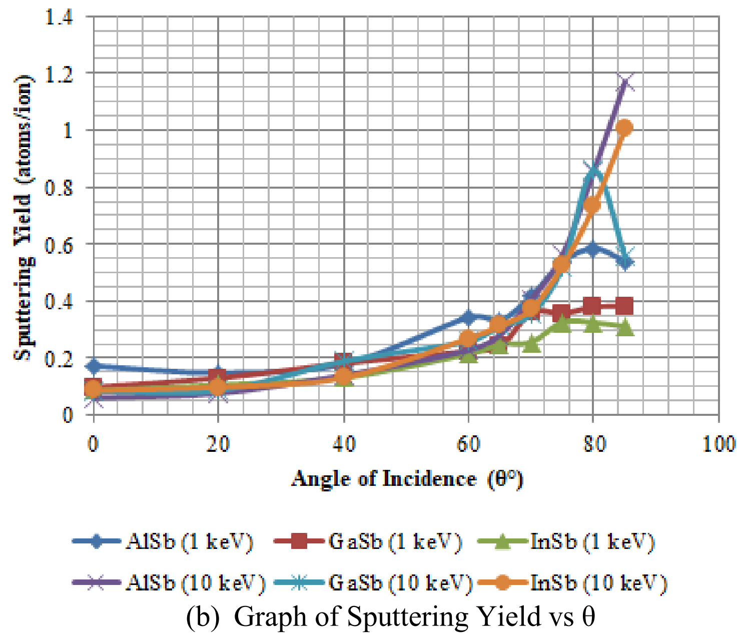


(b) Graph of Longitudinal Straggle vs θ

Figure 1. 1 keV and 10 keV He^{+} impingement of AlSb, GaSb and InSb

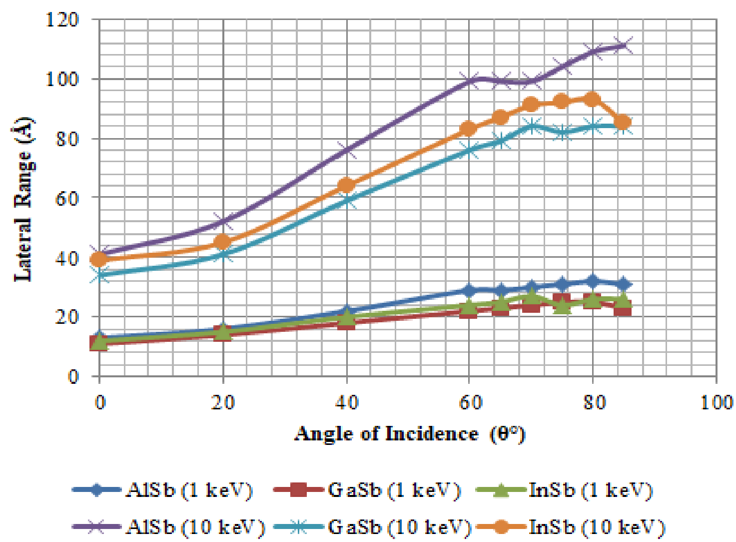


(a) Graph of Projected Range vs θ

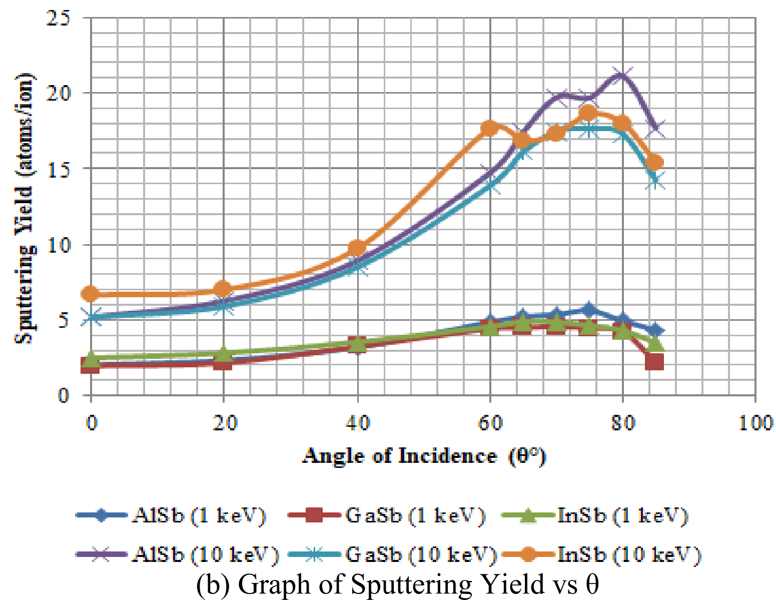


(b) Graph of Sputtering Yield vs θ

Figure 2. 1 keV and 10 keV Ar^+ impingement of AlSb, GaSb and InSb



(a) Graph of Lateral Range vs θ



(b) Graph of Sputtering Yield vs θ

Figure 3. 1 keV and 10 keV Kr^+ impingement of AlSb, GaSb and InSb

6. Conclusion

From the Monte Carlo simulation performed, it was found that for the various binary compounds, the maximum sputtering yield did not occur at a particular angle but within a range of 65° and 85° for ion energy of 1keV and between 75° and 85° for ion energy of 10keV. Also, as the energy was increased, the sputtering yield also increased which shows a direct dependence of the ion energy on the sputtering yield.

Furthermore, for ion energy of 10 keV, the changes in the sputtering parameters were rapid as opposed to when the ion energy was set to 1 keV where the changes were slight. Also, Kr^+ resulted in highest sputtering yield at 10 keV.

Thus, where the interest is in high sputtering parameters for the binary compounds AlSb, GaSb and InSb, a high energy heavy noble gas ion should be utilized.

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