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Depth resolution studies in SiGe delta-doped multilayers using ultralow-energy Cs\(^+\) secondary ion mass spectrometry

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It is known that depth resolution can be improved by lowering the primary ion impact energy \(E_p\) and/or increasing the impact angle \(\theta\) up to a critical \(\theta\), beyond which surface roughening ensues. However, lower \(E_p\) is accompanied by lower secondary ion yield, and for ultralow-energy Cs\(^+\) primary beam, a poorly focused beam. In this study, the authors subject a Ge delta-doped Si sample to ultralow-energy (<1 keV) Cs\(^+\) bombardment over a wide range of impact angles (\(\theta\) \(\sim\) 0°–70°). The authors demonstrated high depth resolution with full width at half maximum (FWHM) of \(\sim\)1.9 and \(\sim\)2.5 nm with \(E_p\)\(\sim\)320 and \(\sim\)500 eV, respectively, at \(\theta\)\(\sim\)50° over a significant depth range (\(\sim\)120 nm). At a higher energy of \(E_p\)\(\sim\)1 keV, a FWHM of \(\sim\)2.5 nm is achieved at \(\theta\)\(\sim\)60°. The authors established that the relationship between improvements in depth resolution (FWHM) is linear and gradual with increasing \(\theta\). The decay lengths \(\lambda_d\) characterizing the trailing edge decreased with increasing \(\theta\) up to \(\theta\)\(\sim\)50°–60° throughout the depth evaluated, but \(\lambda_d\) decreased beyond \(\theta\)\(\sim\)60° only near the surface (\(\sim\)12 nm). The authors noted that good depth resolution is achievable with the following \(\theta\) ranges; \(E_p\)\(\sim\)320–500 eV/\(\theta\)\(\sim\)30°–50° and \(E_p\)\(\sim\)1 keV/\(\theta\)\(\sim\)40°–60°. Using the mixing-roughness-information depth model, the authors were able to differentiate the effect of atomic mixing and surface roughness on depth resolution of \(\delta\) layers. The impact of atomic mixing, surface roughness, and instrumental conditions (poor focus) on depth resolution is also discussed. © 2007 American Vacuum Society. [DOI: 10.1116/1.2429671]

I. INTRODUCTION

Secondary ion mass spectrometry (SIMS) is a sputter depth profiling technique widely used in the semiconductor industry because of its ability to detect all elements, high sensitivity (up to parts per 10\(^9\) levels), large dynamic range (10\(^9\)–10\(^5\)), excellent depth resolution (<1 nm), and minimal sample preparation.\(^1,2\) However, the technique is not without any shortcomings. Samples are damaged upon analysis and the lateral resolution is poor when compared to Auger electron spectroscopy.

Despite the disadvantages, SIMS has been a reliable tool for dopant depth profiling as well as contamination monitoring.\(^3,4\) As the semiconductor device geometry shrinks into the 65 nm range, so does the junction depth\(^5\) (13–30 nm) and the gate dielectric (1–3 nm for SiO\(_2\)/SiON gate oxides).\(^6,7\) This trend in device miniaturization demands an analytical technique with minimum surface transient and excellent depth resolution. High electron mobility transistors with multiple quantum wells require techniques with good depth resolution to be able to resolve adjacent quantum wells. High depth resolution is also essential for characterizing interfaces at nanoscale resolution.

Ultralow-energy SIMS has been developed to meet such analytical demands.\(^8\) We have previously reported approaches to minimize surface transient with ultralow-energy O\(_2\)\(^+\) and Cs\(^+\) SIMS (Refs. 9 and 10) and depth resolution on Si using O\(_2\) ultralow-energy SIMS.\(^11\) This work on depth resolution using Cs\(^+\) ultralow-energy SIMS completes this extended study. The concept of depth resolution, as defined by the ASTM E-42 committee, is the distance over which a 16%–84% (or 84%–16%) change in signal over an ideally sharp interface is measured (\(\Delta z\)).\(^12\) More recently, depth resolution is also taken to be a measure of the ability to discriminate between features in adjacent thin layers.\(^13\) Very often it is annotated by the full width at half maximum (FWHM) of signals from atomic layer delta-doped samples as well as decay length (\(\lambda_d\)), which is the distance over which the intensity drops by a factor of \(e\).

The attainable depth resolution is affected mainly by three factors: instrument related factors, sample characteristics, and ion-solid interactions.\(^1,14\) Non-uniform irradiation from a poorly focused beam and poor rastering quality cause erosion inhomogeneity (crater edge effects),\(^15\) resulting in a degradation of depth resolution with depth. Redeposition from crater walls (crater sidewall effects\(^2\)) has been known to affect the quality of the depth profiles. Intrinsic surface roughness on the sample will affect topography development as depth profiling progresses. Instrumental factors can be minimized with good ion source design and electronic or optical gating. Nearly atomically flat surfaces are now possible to achieve, thus minimizing sample roughness.

Among the three factors, ion-solid interactions cannot be completely eliminated as it is part of the sputtering process. Upon surface bombardment, ion-solid interactions cause atomic mixing, recoil implantation, radiation-enhanced diffusion, and chemically driven segregation.\(^15\) Atomic mixing or bombardment induced atom relocation is a dominant factor affecting depth resolution; ion bombardment induced roughness and segregation are other ion-solid interactions that af-
fect depth resolution. It has been suggested that to minimize the atomic mixing length, primary ion energy \( E_p \) < 500 eV and/or high incidence angle \( \theta \), typically \( \theta > 70^\circ \), should be used.\(^{16}\) To reduce bombardment induced surface roughness, sample rotation or oxygen flooding\(^{17}\) during sputtering and/or glancing ion incidence \( \theta > 80^\circ \) have been proposed.\(^{16}\) A list of basic profiling conditions to ensure minimum degradation of depth resolution has been suggested by Hofmann.\(^{16}\)

There are few reported studies on the influence of \( \text{Cs}^+ \) primary ion energy and impact angle on depth resolution. Most studies have been done using \( \text{O}_2^+ \) primary ions. Generally, beam induced broadening effects have been observed to decrease with the use of heavy primary ions,\(^{15}\) lower\(^{18,19}\) \( E_p \) and increasing\(^{20}\) \( \theta \) from 0° to 60° as it minimizes the width of the atomic mixing zone in the sample. However, these observations were made at higher beam energies of >1 keV. At ultralow-energy \( E_p < 1 \text{ keV} \), depth resolution improves by increasing \( \theta \) only to a certain critical\(^{21,22}\) \( \theta \) before the onset of surface roughening. Another consideration is that by lowering \( E_p \), the beam current density is lower and so is the sputtering yield. The consequence is a trade-off between depth resolution and detection limits.\(^{20}\)

At ultralow \( \text{Cs}^+ \) primary energy \( (\theta \sim 0^\circ – 75^\circ) \), Kataoka et al.\(^{22}\) observed an improvement in depth resolution [defined as resolution contrast \( R_z = (I_{\text{max}} - I_{\text{min}})/(I_{\text{max}} + I_{\text{min}}) \)] of Sb-\( \delta \) layers up to a critical angle of \( \theta \sim 50^\circ \) with \( E_p = 250 \text{ eV} \), \( \theta \sim 55^\circ \) with \( E_p \sim 500 \text{ eV} \), and \( \theta \sim 60^\circ \) with \( E_p \sim 1 \text{ keV} \). van der Heide et al.\(^{21}\) made similar conclusions based on observations of surface roughness while working on \( \text{B}-\delta \) layers. The deterioration in depth resolution is attributed to rapid ripple formation at oblique incidence.\(^{21,22}\) Kelly et al.\(^{23}\) observed best depth resolution on \( \text{B}-\delta \) layers at \( \theta \sim 50^\circ \) \( (E_p \sim 1 \text{ keV}) \). Similar resolution can only be achieved at \( \theta \sim 60^\circ \) when trapezoidal scan correction is used. This technique corrects for the sloping crater bottom caused by the projection of the beam raster and spot shape onto the sample at glancing angle, creating a rectangular projection on the sample.

Li et al.\(^{24}\) used ultralow-energy \( \text{Cs}^+ \) on \( \text{B}-\delta \) layers in Si at \( \theta \sim 45^\circ – 80^\circ \) and observed that the depth resolution (estimated from \( I_{\text{max}}/I_{\text{min}} \)) degrades as \( \theta \) is increased up to \( \theta \sim 70^\circ \). This observation, however, contradicts those made by Kataoka et al.\(^{22}\) and van der Heide et al.\(^{21}\) cited earlier, where depth resolution improves up to only \( \theta \sim 50^\circ – 60^\circ \). A similar conclusion could have been reached if profiles were done at \( \theta \sim 50^\circ \). Li et al. observed the worst resolutions at \( 70^\circ \) \( (E_p = 250 – 500 \text{ eV}) \) and \( \theta \sim 75^\circ \) \( (E_p \sim 1 \text{ keV}) \) before the "best" depth resolution was attained at \( \theta \sim 80^\circ \). Others have also observed good depth resolution at glancing angle \( \theta \sim 85^\circ \) using \( E_p < 1 \text{ keV} \).\(^{25}\) To obtain the best depth resolution while avoiding surface roughening, Kataoka et al.\(^{26}\) recommended the use of \( \theta \sim 45^\circ – 50^\circ \) \( (E_p \sim 250 \text{ eV}) \), \( \theta \sim 50^\circ – 55^\circ \) \( (E_p \sim 500 \text{ eV}) \), and \( \theta \sim 55^\circ – 60^\circ \) \( (E_p \sim 1 \text{ keV}) \).

In this work, we study the effect of ultralow-energy \( \text{Cs}^+ \) primary ion beam on depth resolution and dynamic range by varying the impact energy and impact angle. The depth resolution is systematically evaluated with established methods of FWHM and \( \lambda_d \) of delta layers to a depth of 120 nm. This work also examines the factors affecting depth resolution with the use of the mixing-roughness-information depth (MRI) model. From these observations, a relationship between improvements in depth resolution and impact angle is made and the optimum conditions for high depth resolution with good dynamic range is recommended.

II. EXPERIMENT

An Atomika 4500 SIMS depth profiler equipped with an ultralow-energy quadrupole SIMS with “floating” low-energy ion gun (FLIG™),\(^8\) capable of delivering stable ion beams down to 100 eV, was used for all depth profiles. The \( \text{Cs}^+ \) primary ion energies used were 1 keV, 500 eV, and 320 eV at incidence angles from 0° (normal incidence) to 70° at 10° intervals. The beam was rastered over an area of \( 300 \times 300 \mu \text{m}^2 \) for 1 keV and \( 400 \times 400 \mu \text{m}^2 \) for 500 and 320 eV, and the corresponding beam currents were 77, 40, and 40 nA, respectively. Crater edge effects were minimized by using a 6% area electronic gating. The secondary ions monitored were \( ^{30}\text{Si}^+ \), \( ^{59}\text{Si}^2+ \), and \( ^{98}\text{SiGe}^+ \).

The sample used was a Ge delta-doped \((\text{Ge}-\delta)\) Si sample comprising ten \( \text{Si}_{0.7}\text{Ge}_{0.3} \) delta layers of 0.4 nm thickness (nominally), grown by atmospheric pressure chemical vapor deposition at 700 °C. The first layer is at 12 nm and subsequent depths of the deltas are at multiples of 11 nm.\(^{27}\) The \( \text{Ge}-\delta \) layers serve as depth markers. The peak shape of \( ^{98}\text{SiGe}^+ \) profiles were evaluated for FWHM, \( \lambda_d \), and dynamic range. \( \lambda_d \) was calculated based on the following equation:

\[
I_z = I_1 e^{-((z - z_1)/\lambda_d)^2},
\]

where \( I \) is the secondary ion intensity, and \( z_2 \) and \( z_1 \) are the depth between which the decay length is determined. The dynamic range was calculated based on the ratio of peak intensity to the background intensity.

III. RESULTS

Figure 1(a) shows typical depth profiles of \( ^{30}\text{Si}^- \), \( ^{59}\text{Si}^2^- \), and \( ^{98}\text{SiGe}^- \) using \( E_p = 320 \text{ eV} \) and \( \theta \sim 50^\circ \). The dips in the depth profiles of \( ^{30}\text{Si}^- \) and \( ^{59}\text{Si}^2^- \) coincide with the peaks of \( ^{98}\text{SiGe}^- \) profile, which are the positions of the delta layers. The positions of the dips and peaks are used as depth markers for depth scale calibration. The \( ^{98}\text{SiGe}^- \) profile shows ten well-resolved \( \delta \) layers. However, before the trailing edge of the first peak reaches the background intensity level, the leading edge of the next peak begins. This is a result of the atomic mixing depth being comparable to the inter-\( \delta \) layer spacing. We also noted tailing at the base of the trailing edge, and the baseline appears to drift linearly upward with depth.

Similar profiles were done using different \( E_p \) and \( \theta \), but are not shown here.

Figure 1(b) shows an example of \( ^{98}\text{SiGe}^- \) profiles when \( E_p \) is varied, using \( E_p = 320 \text{ eV}, 500 \text{ eV}, \) and \( 1 \text{ keV} \) at \( \theta \sim 60^\circ \), normalized to the first peak of \( E_p \sim 500 \text{ eV} \) profile. The depth resolution is observed to be slightly better with
lower \( E_p \) at shallower depths (<23 nm), but the resolution deteriorates more quickly with depth as compared to the profile at \( E_p \sim 1 \) keV. This can be seen from the rapidly decreasing peak-to-valley ratio (PVR). The PVR is comparable at all \( E_p \) at the first delta but becomes smaller with depth, the deterioration being more severe at lower \( E_p \).

Figure 1(c) shows typical \(^{98}\text{SiGe}^-\) profiles when \( \theta \) is varied, using \( E_p \sim 320 \) eV with \( \theta \sim 40°-70° \), and normalized to the first peak at \( \theta \sim 40° \). We observe that the \( \theta \sim 50° \) profile has the narrowest peak, indicating the best depth resolution. The \( \theta \sim 40° \) profile has a gentler trailing edge, whereas the \( \theta \sim 60° \) profile has a gentler leading edge. Both \( \theta \sim 60° \) and \( \theta \sim 70° \) profiles show greater deterioration in depth resolution with depth compared to \( \theta \sim 40° \) and \( \theta \sim 50° \) profiles.

Figures 2(a)–2(c) show the depth resolution measured in terms of FWHM of the \(^{98}\text{SiGe}^-\) peaks obtained at \( E_p \sim 320 \) eV, 500 eV, and 1 keV and \( \theta \sim 0°-70° \) against depth. At \( E_p \sim 320 \) eV, good depth resolution is obtained at \( \theta \sim 30°-50° \) with FWHM of less than 2.4 nm throughout the analysis depth of 120 nm. The best depth resolution is observed at \( \theta \sim 50° \) with a mean FWHM of 1.9 nm. The difference in depth resolution from the first delta to the last delta is about 18%. At \( \theta \sim 60° \), the depth resolution is stable at FWHM of 2.6 nm up to a depth of 23 nm (second delta) before deteriorating linearly to 5.7 nm at the last delta. The worst depth resolution is at \( \theta \sim 70° \), beginning with a FWHM of 3.4 nm that degrades with depth.

The trends in depth resolution are similar at \( E_p \sim 500 \) eV with good depth resolution of less than 2.5 nm FWHM observed at \( \theta \sim 30°-50° \). The best depth resolution is at \( \theta \sim 50° \) with a mean FWHM of 2.2 nm throughout the analysis depth. The difference in depth resolution from the first delta to the last delta is about 17%. At \( \theta \sim 60° \), the FWHM at the first delta (depth of 12 nm) is 2.3 nm, but it deteriorates with depth to 2.5 times the initial FWHM at the last delta. The depth resolution is worst at \( \theta \sim 70° \), with a FWHM of 3.3 nm at the first delta and degrading thereafter.

Using \( E_p \sim 1 \) keV, we observe a different trend compared to that at lower \( \text{Cs}^+ \) primary ion energy. The depth resolution deteriorates with depth when profiled at \( \theta \sim 70° \) but not at \( \theta \sim 60° \). The best depth resolution is observed when profiled at \( \theta \sim 60° \), with a mean FWHM of 2.5 nm up to a depth of

![Fig. 1. Typical depth profiles: (a) \(^{98}\text{SiGe}^-\) profiles with \(^{30}\text{Si}^-\) and \(^{58}\text{Si}^2^-\), (b) \(^{98}\text{SiGe}^-\) profiles with various \( E_p \) at \( \theta \sim 60° \), and (c) \(^{98}\text{SiGe}^-\) profiles with \( E_p \sim 320 \) eV at various \( \theta \).

![Fig. 2. Depth resolution of Ge-\( \delta \) as a function of profile depth, measured by FWHM for (a) \( E_p \sim 320 \) eV, (b) \( E_p \sim 500 \) eV, and (c) \( E_p \sim 1 \) keV at various incidence angles.]
about 80 nm (seventh delta) before it deteriorates gradually by 34% at the last delta. At $\theta \sim 50^\circ$, the mean FWHM is 2.6 nm up to a depth of 103 nm (ninth delta), which is slightly worse than at $\theta \sim 60^\circ$ but constant to a greater depth.

Given the above observations, a good depth resolution of about FWHM 2 nm can be obtained at an ultralow-energy of 320–500 eV with $\theta=50^\circ$ throughout the depth analyzed. At a higher primary ion energy of 1 keV, the best depth resolution is achievable at a higher impact angle of $\theta=60^\circ$.

These observations with Ge- are similar to those made with Sb- and B-21,22. Beyond these impact angles, the depth resolution deteriorates severely, consistent with the data reported by Li et al.24. Generally, good depth resolution is achievable across a $20^\circ$ range of $\theta$, namely, at $\theta \sim 30^\circ$–$50^\circ$ for $E_p \sim 320$ or 500 eV and $\theta \sim 40^\circ$–$60^\circ$ for $E_p \sim 1$ keV.

Figures 3(a)–3(c) show the depth resolution (in terms of FWHM) of three representative Ge- at the near surface d1 (12.2 nm), intermediate depth d5 (57.8 nm), and deepest depth at d10 (114.8 nm) for all three energies investigated at $\theta \sim 0^\circ$–$70^\circ$. Generally, the depth resolution improves gradually as $\theta$ increases up to a critical angle before worsening considerably. The critical angle is $\theta \sim 50^\circ$ at $E_p \sim 320$ eV and $E_p \sim 500$ eV, and at $\theta \sim 60^\circ$ at $E_p \sim 1$ keV. Beyond the critical angles, the depth resolution degradation is more severe with depth as can be seen from the increasing slopes of d1, d5, and d10.

Figure 4(a) shows depth resolution in terms of FWHM of the first Ge- peak for all three Ep at $\theta=0^\circ$–$70^\circ$. It confirms that depth resolution improves with decreasing $E_p$ provided that there is no surface roughening. However, the improvement in depth resolution is marginal, about 1.3 times from 1 keV to 320 eV. This improvement is not as significant as that observed when using O$_2^+$, where the improvement in depth resolution was more than 2.5 times. 11

Figure 4(b) shows the plot of depth resolution in terms of FWHM denoted as $dz$ of the Ge- peak for d1, d5, and d10 against $\theta$ up to the critical angle for all three impact energies. At each impact energy, a linear relationship is observed as follows:

for $E_p \sim 320$ eV,  
\[ dz = -0.019\theta + 3.0; \]  
for $E_p \sim 500$ eV,  
\[ dz = -0.019\theta + 3.2; \]  
for $E_p \sim 1$ keV,  
\[ dz = -0.019\theta + 3.8. \]  

The incremental improvement in depth resolution (decreasing FWHM) with increasing $\theta$ is linear, gradual, and noticeably similar across all $E_p$.

Figures 5(a)–5(c) show the decay length for selected deltas using $E_p \sim 320$ eV, 500 eV, and 1 keV against $\theta$.
Generally, for the first delta, the $\lambda_d$ decreases as $\theta$ increases, similar to that observed at higher energy ($E_p \approx 8$ keV). For $E_p \approx 320$ eV, we observe $\lambda_d$ for the first delta decreasing with increasing $\theta$ ($\theta > 10^\circ$) from 2.7 nm/e to a minimum at a $\theta$ $\approx 60^\circ$–$70^\circ$. $\lambda_d$ values at the fifth and tenth deltas are correspondingly higher, also decreasing as $\theta$ increases, reaching a minimum at $\theta \approx 50^\circ$. At $E_p \approx 500$ eV, $\lambda_d$ at the first delta decreases with increasing $\theta$ from 2.5 to 1.1 nm/e at $\theta \approx 50^\circ$–$70^\circ$; at 1 keV, $\lambda_d$ decreases with increasing $\theta$ from 3.8 to 1.5 nm/e at $\theta \approx 70^\circ$.

Figure 5(d) compares the exponential decay of the first delta against depth for various $E_p$. At $E_p \approx 320$ eV, increasing $\theta$ beyond $50^\circ$ does not improve $\lambda_d$ significantly. Similarly for $E_p \approx 500$ eV, increasing $\theta$ beyond $60^\circ$ does not improve $\lambda_d$. However, an improvement is observed with $E_p \approx 1$ keV when $\theta$ is increased beyond $\theta \approx 60^\circ$ but limited to the near surface regions ($\approx 12$ nm) only, similar to that estimated by Wittmaack20 at $E_p \approx 8$ keV. This has been observed in the case of depth profiling of $^{75}$As implants,28 where using $E_p \approx 1$ keV/ $\theta \approx 75^\circ$ gives better depth resolution than at $\theta \approx 60^\circ$, when only the trailing edge is evaluated. It is clear that $\lambda_d$ decreases with $E_p$, but at ultralow energies ($E_p < 1$ keV) improvements in $\lambda_d$ beyond $ \theta \approx 50^\circ$–$60^\circ$ is negligible.

Figures 6(a)–6(c) show the overlay of profiles of the first Ge-$\delta$ obtained at various $\theta$ and $E_p$ normalized to the peak obtained at $\theta \approx 30^\circ$. The trailing edges at all three values of $E_p$ are always gentler than the leading edges due to knock-on and ion beam mixing effects. It can be clearly seen that at $E_p \approx 320$ eV, the depth resolution is best at $\theta \approx 50^\circ$ [Fig. 6(a)]. At $E_p \approx 500$ eV, the depth resolution is marginally better at $\theta \approx 50^\circ$ compared to $\theta \approx 60^\circ$ [Fig. 6(b)]. Even though $\lambda_d$ obtained when using $E_p \approx 500$ eV/ $\theta \approx 60^\circ$ is smaller than that at $\theta \approx 50^\circ$, the depth resolution at $\theta \approx 50^\circ$ is better as the FWHM is smaller, i.e., there is less ion bombardment induced peak broadening. At $E_p \approx 1$ keV, it is best at $\theta \approx 60^\circ$.

![Figure 5](image1.png)

![Figure 6](image2.png)
[Fig. 6(c)]. Therefore, based on FWHM and \( \lambda_d \) data, we conclude that the best depth resolution is achievable using \( E_p \sim 320 \text{ eV/}\theta \sim 50^\circ \), \( E_p \sim 500 \text{ eV/}\theta \sim 50^\circ \), and \( E_p \sim 1 \text{ keV/}\theta \sim 60^\circ \).

Figure 7 shows the dynamic range averaged over the first nine peaks. The dynamic range gives an indication of the range of concentrations that can be detected by SIMS. For all three primary ion energies studied, the dynamic range increases as \( \theta \) moves away from normal. A good dynamic range of more than three decades is obtained at \( \theta \sim 40^\circ –70^\circ \) with all impact energies studied. The results are summarized in Table I.

### IV. DISCUSSION

Lau et al.\(^{29}\) have successfully demonstrated with a similar SiGe \( \delta \)-doped sample that the surface roughening behavior during ion sputtering can be accounted for by the MRI model proposed by Hoffman.\(^{30}\) The model considers the contributions of three fundamental parameters, namely, atomic mixing, roughness, and information depth toward depth resolution. Atomic mixing is described by an exponential function, with a characteristic, mixing length \( \lambda \), as shown in Eq. (5).

Roughness is represented by a Gaussian term with standard deviation \( \sigma \), which corresponds to the root mean square surface roughness, as in Eq. (6); and information depth is represented by an exponential term with characteristic information depth \( \lambda \), as in Eq. (7). \( z \) is the sputtered depth and \( z_0 \) is the running depth parameter for which the composition is defined. For example, each monoatomic layer at a location \( z_0 \) gives a normalized contribution at a sputtered depth \( z \) that is described by\(^{31}\)

\[
g_{\sigma} = \frac{1}{\lambda} \exp \left( -\frac{(z - z_0)}{\lambda} \right) \tag{6}
\]

\[
g_{\lambda} = \frac{1}{\lambda} \exp \left( -\frac{(z - z_0)}{\lambda} \right) \tag{7}
\]

In the atomic mixing parameter, mixing is assumed to be instantaneous,\(^{32}\) complete, and extends to a depth \( w \). Therefore, roughness and atomic mixing are assumed to be independent of each other. The information depth parameter can be neglected as it is about 1–2 ML based on the secondary ion escape depth in low-energy SIMS.\(^{30}\) The roughness parameter consists of three components: the original interface roughness \( \sigma_i \), sputtering induced surface roughness \( \sigma_s \), and straggling of the mixing length \( \sigma_w \).\(^{30}\) The total \( \sigma \) parameter in the model is

\[
\sigma = (\sigma_i^2 + \sigma_s^2 + \sigma_w^2)^{1/2} \tag{8}
\]

Interface roughness can be neglected as the sample is assumed to have high quality interfaces. Contribution from mixing length straggling\(^{33}\) can be significant compared to the contribution of the original interface roughness and sputtering induced surface roughness but is difficult to determine. The rms value of \( \sigma_i \) can be obtained from atomic force microscopy (AFM) measurements.

Figure 8 shows the penetration depth of Cs\(^+\) primary ions at ultralow energies with \( \theta \sim 0^\circ –70^\circ \) using TRIM calculations.\(^{34}\) In Fig. 1(b), when \( E_p \) is increased at a con-
In Figs. 2 and 3, the increase in FWHM observed is a result of the onset of roughening occurring at θ = 60° for $E_p$ ~ 320 eV and ~500 eV, and at θ = 70° for $E_p$ ~ 1 keV. In Fig. 4(a), under conditions where surface roughening does not occur, peak broadening is expected since the penetration depth increases with $E_p$, causing a wider w and $\lambda_d$. This conclusion is also confirmed by analyzing Fig. 6.

In Fig. 5(d), the decrease in $\lambda_d$ near the surface (~12 nm) levels off when θ increases at θ = 50° with $E_p$ ~ 320 eV and θ = 60° with $E_p$ ~ 500 eV and $E_p$ ~ 1 keV. We propose two possibilities for this occurrence. As θ increases, the primary ion penetration depth becomes shallower, thus reducing atomic mixing and $\lambda_d$, but as surface roughening sets in, the decrease in $\lambda_d$ is offset by the broadening brought about by ripple formation. Alternatively, the decrease in penetration depth at oblique angles is not significant enough to cause a variation in $\lambda_d$. Another observation is that with $E_p$ ~ 320 eV [Fig. 5(a)] and 500 eV [Fig. 5(b)], $\lambda_d$ deteriorates (increases) with depth only at θ ~ 60°–70° onward, even though $\lambda_d$ is decreasing with increasing θ at the surface. We infer that the deterioration in $\lambda_d$ with depth is mainly attributed to the onset of roughening which begins at a depth of 12–23 nm. Similarly, at $E_p$ ~ 1 keV [Fig. 5(c)], the onset of roughening is experienced at θ ~ 70°. Figure 5(a) shows that only at $E_p$ ~ 320 eV, we observe a significant difference in $\lambda_d$ with depth represented by d1, d5, and d10. At θ ~ 50°–50° where no surface roughening is present, the wider $\lambda_d$ can be attributed to poor beam focus, which is commonly experienced using ultralow-energy Cs+ beams. Poor beam focus causes erosion inhomogeneity. We studied the profiles obtained at impact angles where surface roughening does not occur and conclude that the effect of poor beam focus is characterized by a linear increase in baseline with depth but with no change in the peak intensity [cf. Fig. 1(a)]. We noted, however, that an increase in baseline also occurs when there is surface roughening, but it is always accompanied by peak broadening and a decrease in peak intensity. In both situations, the PVR will decrease, but only in the case of surface roughening where a deterioration in depth resolution is obvious. Hence, PVR is not a conclusive measure of depth resolution. The deterioration in depth resolution caused by poor beam focus with depth is better understood with the following relationship:

$$dz = M + Uz,$$

(9)

where the $U$ term reflects instrumental problems (poor focus in this case) and the $M$ term represents the peak shape due to ion beam broadening, which like atomic mixing is independent of depth. While the drop in PVR with depth is obvious, the increase in $\lambda_d$ with depth does not affect the FWHM significantly (cf. Fig. 2).

Table II shows the best depth resolution obtained with Cs+ SIMS compared to that from a similar work done with O$_2^+$ primary ion SIMS. The penetration depth based on TRIM calculations for the θ with the best depth resolution is also included in the table. We find that with $E_p$ ~ 1 keV, Cs+ SIMS gives better depth resolution than O$_2^+$ SIMS. This is

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**Fig. 8.** Penetration depth of Cs+ primary ions at various incident angles calculated from TRIM.
expected as a higher mass primary ion will give a shallower penetration depth and hence narrower atomic mixing width. Penetration depth is determined by the rate of energy loss along the path of the ion. At constant energy, the bombarding ion with a higher mass (larger atomic number) will have a higher nuclear energy-loss rate in an elastic binary collision due to its higher nuclear cross section when penetrating the target. However, at lower $E_p$, the best depth resolutions are similar. This unexpected behavior can be explained by the contribution to depth resolution from a poorly focused Cs$^+$ beam. The Cs$^+$ beam with a diameter larger than the O$_2^+$ beam is more difficult to focus as it fills up the aperture as it enters the focusing lens in the ion gun column. Moreover, at ultralow energy, the beam is retarded as it enters the lens, which spontaneously expands the beam.

V. CONCLUSION

High depth resolution can be achieved with ultralow-energy Cs$^+$ SIMS. The trends in depth resolution are quite similar when using $E_p \sim 320$ eV and $E_p \sim 500$ eV, with high depth resolution of less than 2.5 nm FWHM observed at $\theta \sim 30^\circ$–$50^\circ$ throughout the depth range studied. The best depth resolution of FWHM of 1.9 nm is observed at $\theta \sim 50^\circ$ with $E_p \sim 320$ eV, and 2.2 nm with $E_p \sim 500$ eV. With $E_p \sim 1$ keV, depth resolution of less than 3 nm FWHM is observed at $\theta \sim 40^\circ$–$60^\circ$. The best is observed at $\theta \sim 60^\circ$ with a mean FWHM of 2.6 nm.

By considering the MRI model, we confirm that depth resolution can be improved by reducing atomic mixing and/or eliminating surface roughness. Atomic mixing is reduced by lowering $E_p$ and/or by increasing $\theta$ up to a critical impact angle of $\theta \sim 50^\circ$ at $E_p \sim 320$ and $\sim 500$ eV, and at $\theta \sim 60^\circ$ for $E_p \sim 1$ keV. Beyond the critical angle, the depth resolution deteriorates severely with depth due to the onset of surface roughening. However, a close examination reveals that the onset of surface roughening is present with $E_p \sim 320$ eV/$\theta \sim 60^\circ$ only after 23 nm and with $E_p \sim 500$ eV/$\theta \sim 60^\circ$ after 12 nm. The relationship between depth resolution (decreasing FWHM) and $\theta$ is ascertained to be linear and gradual with all $E_p$ evaluated.

The decay length decreases as $\theta$ is increased, with the narrowest $\lambda_d \sim 1.1–1.5$ nm/e obtained at oblique angles. We can extrapolate that narrower $\lambda_d$ can be achieved beyond $\theta \sim 70^\circ$, but only near the surface. However, at this $\theta$, the FWHM is broader. Hence smaller decay length do not necessarily indicate a better resolution. Under the conditions when $\lambda_d$ is narrow, it is useful for distinguishing interfaces. $\lambda_d$ also decreases with impact energy, but does not decrease significantly at ultralow energy ($E_p \sim 1$ keV). A small change in the penetration depth does not affect the atomic mixing length and therefore has little or insignificant impact on $\lambda_d$.

Using the MRI model, we can establish whether the broadening is dominated by surface roughening or atomic mixing. Surface roughening corresponds to a decrease in peak intensity and peak broadening, while atomic mixing corresponds to an increase in the exponential decay of the trailing edge but not a reduction in peak intensity. Another phenomenon that is observed in Cs$^+$ SIMS is poor beam focus. This is seen as a linear increase in profile baseline but without any change in peak intensity, provided there is no surface roughening.

Cs$^+$ SIMS gives better depth resolution than O$_2^+$ SIMS at higher impact energy, but not at lower energies below $E_p \sim 500$ eV due to the poor beam focus that causes uneven erosion. We suspect that poor beam focus limits the improvement in depth resolution at ultralow energy.

We recommend the use of $\theta \sim 40^\circ$–$50^\circ$ for $E_p \sim 500$ eV and $\theta \sim 40^\circ$–$60^\circ$ for $E_p \sim 1$ keV for high depth resolution without compromising dynamic range.

7S. Nakai et al., Tech. Dig. – Int. Electron Devices Meet. 2003, 11.3.1.

Table II. Primary ion penetration depth and FWHM at $\theta$ with best depth resolution.

<table>
<thead>
<tr>
<th>$E_p$ (eV)</th>
<th>O$_2^+$ (nm)</th>
<th>Cs$^+$ (nm)</th>
<th>O$_2^+$ (nm)</th>
<th>Cs$^+$ (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>250 eV</td>
<td>1.7 ($\theta$–$40^\circ$)</td>
<td>...</td>
<td>1.5</td>
<td>...</td>
</tr>
<tr>
<td>320 eV</td>
<td>...</td>
<td>1.7 ($\theta$–$50^\circ$)</td>
<td>...</td>
<td>1.9</td>
</tr>
<tr>
<td>500 eV</td>
<td>2.8 ($\theta$–$30^\circ$)</td>
<td>1.9 ($\theta$–$50^\circ$)</td>
<td>2.2</td>
<td>2.2</td>
</tr>
<tr>
<td>1 keV</td>
<td>4.6 ($\theta$–$20^\circ$)</td>
<td>2.0 ($\theta$–$60^\circ$)</td>
<td>3.5</td>
<td>2.5</td>
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</table>