Response function during oxygen sputter profiling and its application to deconvolution of ultrashallow B depth profiles in Si

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The secondary ion mass spectrometry (SIMS) response function to a B "δ surface layer" has been investigated. Using electron-gun evaporation combined with liquid nitrogen cooling of target, we are able to deposit an ultrathin B layer without detectable island formation. The B spatial distribution obtained from SIMS is exponentially decaying with a decay length approximately a linear function of the incident energy of the oxygen during the SIMS analysis. Deconvolution with the response function has been applied to reconstruct the spatial distribution of ultra-low-energy B implants. A correction to depth and yield scales due to transient sputtering near the Si surface region was also applied. Transient erosion shifts the profile shallower, but beam mixing shifts it deeper. These mutually compensating effects make the adjusted distribution almost the same as original data. The one significant difference is a buried B peak observed near the surface region. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1636269]

Shrinking dimensions of microelectronic devices require improved analytical techniques for B profiling in Si on the atomic scale.[1] However, the resolution of secondary ion mass spectrometry (SIMS) has approached its limit, with surface transient erosion and ion mixing being the most serious obstacles encountered.[2–4] These intrinsic features of SIMS cannot be eliminated, even if ultra-low-energy primary beams or clusters beams are used.[5] The atomic mixing during ion bombardment induces B-profile broadening and shifts from the true positions. Therefore, collected SIMS counts are not determined solely by the instantaneous B concentration. Instead, the SIMS signal $Y(z)$ at a depth z is given as a convolution of the true B-concentration distribution $C(z)$, with the SIMS response function $R(z)$:

$$Y(z)=\int_0^z C(z')R(z-z')dz'. \quad (1)$$

Since the SIMS response function is B-concentration independent, it is possible to recover the true B profile by deconvolution. Using the so-called "maximum entropy method,"[6] Chu and Dowsett have found a sample-independent response function[7] which, for a perfect δ layer, can be simplified to be

$$R(z)\approx\frac{1}{2\lambda_d}\{[1+\mathrm{erf}(\xi_d)]\exp[-z/\lambda_d+(\sigma/\lambda_d)^2/2]\}, \quad (2)$$

where σ is the primitive standard deviation, λ_d the decay length, and $\xi_d=(z/\sigma-\sigma/\lambda_d)^{1/2}$. However, the determination of the response function $R(z)$ has been a controversial subject for a decade. The issue is how perfect a δ layer can be obtained. Low-energy B implants, even in a preamorphized Si substrate, have a well-known Gaussian-like profile, and are unsuitable for the study. Recently, δ-doped B spikes formed by molecular-beam epitaxy (MBE) have been used to extract $R(z)$. However, the true B profile deviates from a perfect δ layer due to segregation and diffusion during MBE growth. B has a longer migration distance at lower temperatures and forms an exponential tail.[8] Any deconvolution based on a response function extracted from an imperfect δ layer will produce distorted information.

We have developed a technique to deposit a smooth B layer on a Si surface. Since the energy of B atoms in the vapor phase has a typical energy of ~1 eV, B penetration into Si is prohibited. We believe that the ultrathin B film formed by this procedure is the most δ-like distribution, compared with those used in previous studies. Furthermore, the smooth surface minimizes the signal deviation, which, resulting from sputtering-induced surface roughening, usually yields significant profile broadening beyond a depth of above 0.5 μm.[9] In this work, a boron layer (0.4 nm) was first deposited by e-beam evaporation onto an n-type (100) Czochralski-grown Si wafer. The deposition process was immediately preceded by a gaseous HF etch to remove the native oxide. Deposition was performed at a rate of 0.1 nm/s under a base pressure of 3×10^{-6} Torr. A liquid-nitrogen-cooled substrate holder was used to decrease the mobility of the deposited boron atoms and to avoid boron island forma-

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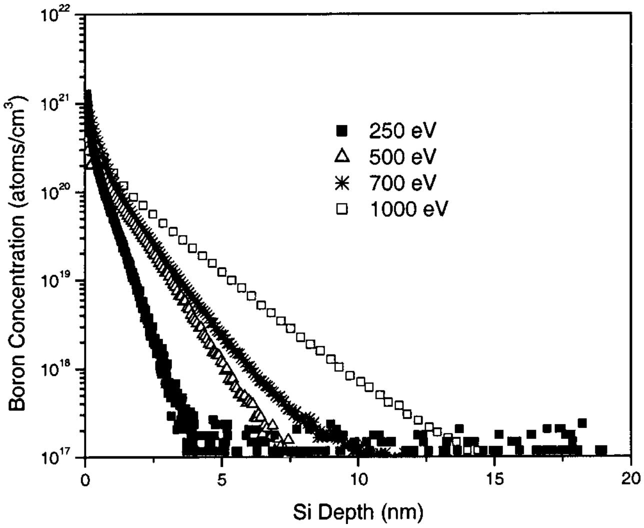

FIG. 1. SIMS profiles of boron measured at normal direction with oxygen flooding and incident oxygen beam at 250, 500, 700, and 1000 eV.

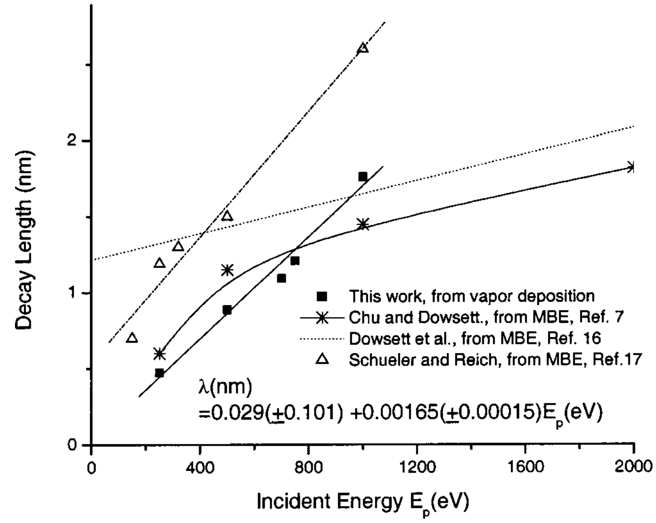

FIG. 2. Decay lengths obtained from this work and other groups.

tion. After deposition, nuclear reaction analysis was performed to confirm the amount of boron deposited. Atomic force microscopy (AFM) was used to examine the film uniformity. The surface roughness for a bare Si sample was 0.3 nm based on the AFM measurements. For the 0.4 nm boron layers, the roughness was still 0.3 nm if liquid-nitrogen-cooled substrates were used. This is to be compared with a 2.0 nm surface roughness when the B is deposited on substrates at room temperature. There was no boron island structure observed under AFM for cold deposition.

Figure 1 shows the B profile measured using an oxygen beam at normal incidence with oxygen flooding. The incident energies of oxygen were 250, 500, 700, and 1000 eV. All profiles can be well represented by exponential functions, characterized by a decay length λ. Long-range recoils created by primary ions and short-range secondary recoils produced by cascades can result in an exponential-like distribution. This has been discussed in our previous studies[10] based on the Lindhard–Scharff–Schiott approximation.[11,12] In addition to cascade mixing,[13] bombardment-induced dopant migration[14] can also result in considerable dopant relocation. We have no intention of giving a theoretical modeling here due to complexity of the phenomena, but would like to point out that these mechanisms may have been oversimplified in early theoretical treatment by assuming a fixed mean recoil distance.[15]

Figure 2 shows the comparison of decay length obtained from this work and other groups.[7,16,17] As suspected, previous studies somewhat overestimated the decay lengths for sub-keV SIMS due to the *intrinsic* non-δ characteristics of the calibration samples. Another important feature is that the trend from this work exhibits a monotonic decrease fitted by $\lambda\ (\mathrm{nm}) = 0.029(\pm 0.101) + 0.00165(\pm 0.00015) \times E_P\ (\mathrm{eV})$, instead of a power dependence of λ on the primary oxygen ion energy E_P proposed earlier.[7] To further determine the standard deviation σ, we have used buried δ layers with capped Si. We obtained that σ=0.3 nm for 500 eV SIMS at normal direction. However, by changing σ to a value approaching zero, there is no detectable difference for deconvoluted profile. Therefore, the most important and sensitive parameter is λ, and Eq. (2) can be further simplified to an exponential function without adjustment from σ.

We have applied the response function to reconstruct the spatial distribution of 0.5 keV B implants. Aside from the accurate determination of the response function, another issue is the transient sputtering of SIMS for the first few nanometers. This phenomenon has been investigated by various groups.[18–22] It results in a systematic shift in the deeper region of the profiles, and must be corrected. The sputtering rate of amorphous Si has been recently investigated via medium-energy ion scattering.[23,24] It shows that[24]

$$Z(z) = z + a[1 - \exp(-bz)], \quad (3)$$

where z is the eroded Si thickness obtained from constant profilometer measurements, and Z is the true value. Values of a=1.216 nm and b=8.56 (nm^{-1}) were extracted from Ref. 24.[25] With the understanding that the transient erosion rate may be different for different substrate conditions, we have performed the same preamorphization and the same SIMS conditions as described in Ref. 24. A (001) Si wafer was preamorphized by 5 keV Ge bombardment (dose of 1×10^{15} cm^{-2}), followed by a 0.5 keV B implantation.[26] SIMS was performed using a 500 eV O_2^+ primary beam at normal incidence with oxygen flooding.

A previous study has shown that the ionization probability of B remains almost constant near the surface region.[24] Thus, the deviation of B yield from the true value is caused predominantly by the sputtering ratio change. In order to give a same overall B yield integrated over depth, a change in depth scale requires a change in the scale of B yield.[24] We therefore made a yield correction by

$$Y[Z(z)] = Y(z)/[1 + ab \exp(-bz)]. \quad (4)$$

Fourier transformation was then applied to the deconvolution of Eq. (1). Figure 3(a) shows the original SIMS and the deconvoluted profile without correction for transient sputtering (CTS). The reconstructed profile is shallower, with a B peak present at the surface. Figure 3(b) shows the difference when CTS is included. With CTS only, the profile has shifted deeper by around 1.2 nm. With deconvolution, the profile shifts in the reverse direction. The net result is a

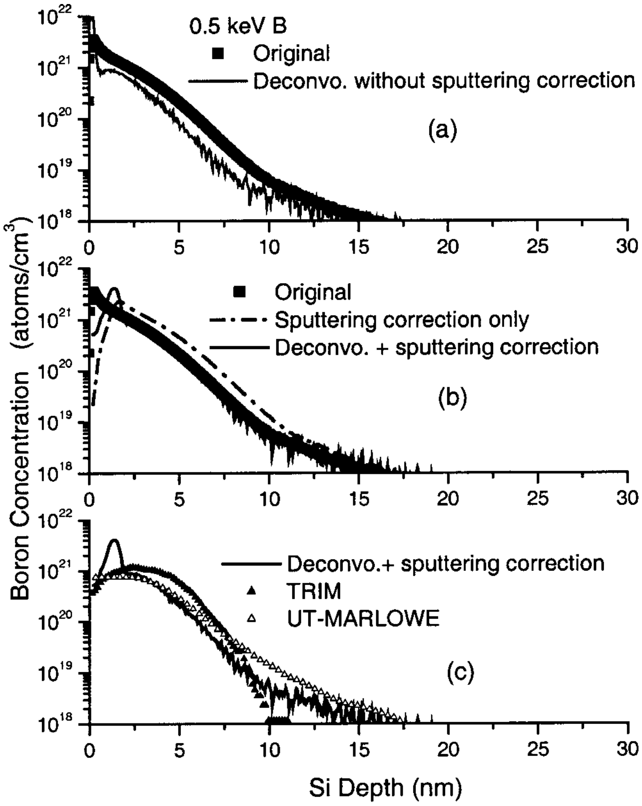

FIG. 3. Original SIMS boron profile, deconvoluted profiles, and simulated profiles. (a) Original SIMS profile and deconvoluted boron profile without sputtering correction, (b) original SIMS profile, deconvoluted profile with sputtering correction only, and profile with sputtering correction and deconvolution together, and (c) deconvoluted profile and simulated profiles from TRIM and UT-MARLOWE.

final profile close to the raw data. The only significant difference is the B distribution near the surface region: A shallow buried B peak is observed at a depth of $\sim$1.3 nm. This may be due to B migration and trapping at the native oxide layer. Experimental studies on this trapping feature are ongoing. Contrary to the raw data, the B concentration is low at the surface. It is also noteworthy that the deconvoluted profile is slightly steeper than original raw profile. In Fig. 3(c), a comparison is made between the deconvoluted curve (with erosion correction), and curve simulated from TRIM,[27] and UT-MARLOWE.[28] TRIM calculation was based on assumption of an amorphous substrate, and the result deviates from the deconvoluted profile both on peak and tail part. The UT-MARLOWE can predict the tail part reasonably, and is in good agreement at the peak region except for the trapped B peak. Obviously, the deconvolution can provide an important comparison/guidance for further improvement on modeling of sub-keV B implants.

In summary, we have studied the decay length of B yields by SIMS with a B δ layer deposited on the Si surface. The B spatial distribution shows an exponential-like profile, with the decay length as a linear function of the incident oxygen energy. When the effect of transient sputtering is considered, the profile shifts deeper, but it becomes shallower with beam mixing. These opposing effects make the corrected distribution close to the raw data itself in the deeper region. A sharp, buried B peak is observed at the surface.

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