

Damage profiling of very shallow implanted silicon

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An attempt is made to bring together the measured damage depth profiles of very low energy Ge⁺ and B⁺ implants in crystalline silicon by spectroscopic ellipsometry and simulations using the ATHENA code, version 5.0. A global and original calibration methodology has been used to provide the physical set of parameters for simulations. The measured depth profiles (damage and concentration) of very low energy Ge implants in c-Si allow the identification of realistic values of some defect species in the implanted region, and depth profiles of the displaced atoms. It is shown that the complementary use of SE and suitable calibration algorithms could be an effective tool for a reliable conversion between damage and concentration depth profiles in very low energy Ge⁺ implants. The SE damage depth profile of 5keV Ge ions, $1 \times 10^{15} \text{cm}^{-2}$ in c-Si shows a different shape of the tail, below the amorphous/crystalline boundary, in comparison to other profiles of Ge⁺ with energies from 2keV to 20keV and doses of $1 \times 10^{15} \text{cm}^{-2}$, optimized for very low energy B⁺ implants and preamorphization (PAI) in deep submicron CMOS. Probably, the different shape of the damage profile of 5keV Ge, $1 \times 10^{15} \text{cm}^{-2}$, is one of the reasons for the least amount of transient enhanced diffusion for B⁺ implants in PAI silicon.

(Received November 1, 2006; accepted December 21, 2006)

Keywords: Ion implantation, Shallow, Ellipsometry, Simulations, Damage, Profile, Silicon

1. Introduction

The realization of ultrashallow silicon p⁺source/drain structures confined within a few tens of nanometers from the surface is the current challenge for ion implantation technology. As the ion energy required (for boron $\leq 1 \text{ keV}$) is reduced due to device shrinkage, the use of a high tilt angle (typically 7-10 deg) becomes ineffective in suppressing channeling. The formation of a thin amorphous layer in Si, close to the surface, prior to the B⁺ implantation, has shown to be very efficient in eliminating channeling. Such layers can be formed using a germanium implant, and the thickness of the amorphous layers can be varied with the Ge⁺ ions energy [1] and dose. However, Ge⁺ itself introduces point defects. During the annealing of implantation damage, ion-implanted boron exhibits transient enhanced diffusion (TED), which greatly exceeds the equilibrium diffusivity. It is found that the magnitude of the diffusion enhancement and the time duration of the enhancement are related to the type and depth profile of the damage produced.

Unfortunately, many of the details of the as-implanted defect structure are still unknown. Each generation requires a large effort in research and development, where technological computer aided design (TCAD) can play a key role [2]. In the state-of-the-art atomistic simulations of the implantation processes, phenomenological models for very shallow as-implanted damage have to be employed. At low energies, the accumulation effect of dopant ions and defects on its depth profiling must be taken into account. Although the complete models cover a wide range of physical interactions, they are straightforwardly usable thanks to a comprehensive set of parameters obtained using original, experimental calibration

algorithms and methodology for very shallow implants in Si.

Spectroscopic Ellipsometry (SE) [3] is a non-destructive and rapid optical technique for the characterization of thin films, multilayer structures and material surfaces with monolayer sensitivity. Defects created in crystalline Si(c-Si) by ion implantation alter its complex dielectric function. Therefore, SE has been used to extract physical information on the damage in the implanted region -the real and imaginary parts. The last relates to inelastic scattering processes in the materials.

Variable angle of incidence spectroscopic Ellipsometry (VASE) may determine both parts of the dielectric function independently.

The VASE measurements and the implanted damage depth profiles are not evaluated directly. The interpretation is based on a simulation and regression program that minimizes the difference between the measured and calculated data from models. Usually, the implanted region is modeled as a mixture of crystalline (c-Si) silicon and amorphous (a-Si) silicon, by the effective medium approximation (EMA). Mainly, two methods are used for parameterization of the damage profiles using EMA. One of them uses a number of layers with constant damage levels. The other uses a given function or functions for the damage depth, depending on a few unknown parameters.

Our group developed and published [4] new algorithms, based on some ideas of the inverse scattering theory for extracting the damage profile from ellipsometric experimental data. The Newton-Kantorovich method for solving of nonlinear operator equations was used to construct the numerical algorithm for depth profiling from SE and VASE data, under the general assumption that the unknown profile is a smooth function of depth. The

calculations run without any assumptions about the number of layers or the damage level depth functions. Our previous publications^[5,6] were devoted to the depth profile characterization of 10 keV B⁺ and 60 keV Ge⁺ at low dose rates and doses (below the threshold ones) by VASE measurements and Monte Carlo BCA simulations-ATHENA code, SILVACO TCAD.

In the present paper, the energies of the implanted ions were chosen to match the use of dopant in CMOS devices below 0.13 μm. We report on VASE and simulation study of damage profiles in Si after very low energy Ge⁺ ion-implantations. The doses of implanted Ge⁺ ions were well above the threshold one, in order to produce thin amorphous layers prior to the implantation of very low energy dopants such as boron.

2. Experimental

Czochralski-grown (001) n-type Si wafers were used in the study. Implantation was done at room temperature, with special care to avoid the heating, with a dose rate around $5 \times 10^{11} \text{ cm}^{-2} \text{ s}^{-1}$. Typically, the wafer orientation was 7 deg tilt, relative to the incident beam. In the experiments for comparison, the implantation conditions were kept constant for all samples investigated. The wafers were amorphized using either a deep or a shallow scheme. In the shallow amorphization scheme, Ge⁺ implantation was carried out at range 2 keV to 20 keV with doses of $1 \times 10^{15} \text{ cm}^{-2}$. Boron ions of 1 keV, $1 \times 10^{15} \text{ cm}^{-2}$ were implanted in c-Si or in PAI samples-preamorphized by implantation. For the deep damage depth profiling and amorphization by 40 keV Ge⁺, with doses above the threshold, RBS/channeling was used as an experimental method. The typical depth resolution in RBS is ~10 nm and this does not allow us to use this method in the case of very low energy ion implantations. RBS depth profiling was used in the present studies only as a checking procedure, as a starting step, for comparison between the measured and simulated profiles to a depth of 100 nm.

The damaged and atomic concentration depth profiles for very low energy ion implantation were studied by VASE measurements and by ATHENA, 5.0 simulations of TCAD-SILVACO.

The VASE measurements were performed using a J.Woollam Co Int. rotating analyzed-type ellipsometer from 1.5 eV to 3.2 eV at 11 equally spaced incidence angles, with wavelengths around the pseudo-Brewster angle. The random errors of the VASE data were < 0.002. The error bounds of 0.03 ÷ 0.005 in the retrieved damage profiles were obtained from the residuals with the real error estimations. A variation of 1 nm in the thickness leads to a difference in the profile within the estimated error bound. Since the penetration depth of the light from 1.6 eV to 3.4 eV is comparable to the penetration and disturbed depth of the very low energy Ge⁺ and B⁺ ions in Si, the VASE results are able to provide information about the implanted layers, in their overall depth. The implanted, damage layer was modeled as a structure of a thin top silicon oxide layer (a native, unknown oxide and

roughness of the surface) and an inhomogeneous substrate (damaged Si with a depth < 40 nm). The oxide (the thickness and dielectric functions) was a fitting parameter. We applied a Newton-Gauss [4] type algorithm developed for the VASE profiling of inhomogeneous layers, previously published and used in the case of higher energy Ge⁺ and B⁺.

In order to simulate the radiation induced damage by ATHENA, 5.0, the new models account for all collision events within the collision cascade. Up to 80% of the created interstitial-vacancy (I-V) pairs can annihilate, due to recombination, so the local arrangement of the displaced atoms and vacancies becomes important when spontaneous recombination has to be taken into consideration. It is not only the number of defects but their initial distribution which influences the residual damage after very shallow ion implantation. The value of the vacancy capture radius has to be carefully chosen so that the amount of residual damage in depth is comparable to the measured damage depth profile with techniques like VASE. The output of the new BCA with a comprehensive solution for simulating ultra shallow as-implanted and damaged regions was compared with two separate SIMS measurements (SILVACO framework).

3. Results

As a demonstration of the effectiveness and applicability of VASE measurements and our numerical algorithm for data interpretations, the as-implanted SE damage depth profiling of 40 keV Ge⁺ ions in c-Si is shown in Fig.1. The damage depth profile obtained by RBS/channeling is also shown in the figure, for a convenience.

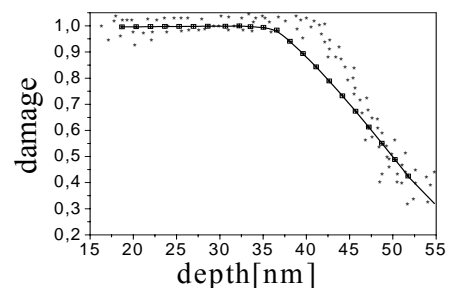


Fig.1 Damage profile of 40keV Ge⁺, $2.5 \times 10^{14} \text{ cm}^{-2}$ reconstructed from VASE data- the line. Profile of the RBS/channelling- symbols.

For lower energies of Ge⁺ implants (< 20 keV), with doses above the threshold ones, the reconstructed SE damage profiles from VASE data are compared with the simulated profiles.

SE profiles of 10 keV Ge⁺ doses: $2.5 \times 10^{14} \text{ cm}^{-2}$ and $1 \times 10^{15} \text{ cm}^{-2}$ are shown in Fig. 2 as curves 1 and 3. The SE damage = 1 is the damage of full, 100% amorphization of the crystal by ion intervention. For comparison, curve 2 shows the ATHENA, 5.0 simulated profile for $1 \times 10^{15} \text{ cm}^{-2}$.

SE damage <1 means a disturbed crystalline structure. An amorphous/crystalline (a/c) boundary depth is well recognized. The measured a/c depths are in a linear relation to the energies of the Ge⁺ ions [6,7].

The depth positions achieved from VASE profiles are shallower than the a/c depths from simulated profiles. This tendency is less pronounced in the case of very low energy Ge⁺.

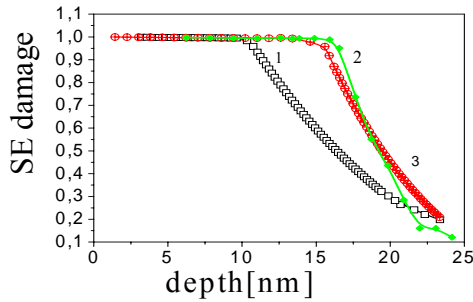


Fig. 2. SE damage profiles for Ge⁺10 keV: curve 1 - $2.5 \times 10^{14} \text{ cm}^{-2}$; curve 3 - $1 \times 10^{15} \text{ cm}^{-2}$ and curve 2- simulated profile for $1 \times 10^{15} \text{ cm}^{-2}$.

The SE damage depth profiles retrieved by our algorithm are reconstructed with higher accuracy around the extrema of the curves. The problem of the “end” of the Ge damage profile was solved in our previous paper[6] by implantation of B⁺ into the investigated damage region. The energy of the B⁺ was chosen so, that the B⁺ dopant profile was within the region disturbed by the Ge⁺. As was demonstrated, than the “end” damage depth was recognized pretty well.

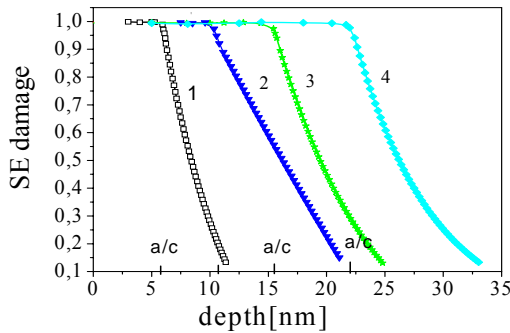


Fig. 3. The reconstructed SE damage profiles by Ge⁺: curve 1 - 2keV; curve 2 - 5keV, curve 3 - 10 keV, curve 4- 20keV; doses of $1 \times 10^{15} \text{ cm}^{-2}$, RT.

Fig. 3 shows the SE damage profiles of Ge⁺ with very low energies: 2 keV, 5 keV, 10 keV and 20 keV, as well as the exact positions of the a/c boundaries. Their depths are in agreement with the simulated positions of a/c. The measured damage depth profile for 5keV Ge⁺, $1 \times 10^{15} \text{ cm}^{-2}$, shows a different shape of the damage below the a/c, in comparison with the other profiles. This profile is smoother in a shape and has a longer tail. Special care was

devoted to give confidence in the measurements, but the difference in the tail shape was easily recognized in all our SE measurements. For reasons not understood, a 5 keV Ge⁺, $1 \times 10^{15} \text{ cm}^{-2}$ implant (as a PAI tool) appears to result in the least amount of boron TED [8]. As time progresses, the VASE results are continuing to be refined even further to take into account the reliable measurements by other methods for damage profiling- medium energy ion scattering.

For practice purposes, it will be very useful to know the damage depth profile by measuring the atomic concentration depth profile. A direct evaluation of the functional relationship- *damage/atomic concentration* is a most complex physical and mathematical task. In the present work an attempt to relate the above quantities was made by comparing the experimental results of SE.

Fig. 4 shows the simulated atomic concentration profile of Ge ions- 5keV, $1 \times 10^{15} \text{ cm}^{-2}$ implanted in Si<100>, tilt 7deg/30 rot. One may see the position in depth of the a/c boundary and of the “damage end”, measured by the VASE damage profile. It is not difficult to estimate the Ge atomic concentration limit for achieving full amorphization.

It is in a range- $(3.5 \div 2.5) \times 10^{20} \text{ cm}^{-3}$ implants into the Si target(7deg tilt/30deg rot). The lower Ge atomic concentrations belong to the tail region of the measured SE damage with the ”end” around $(7 \div 8) \times 10^{18} \text{ cm}^{-3}$.

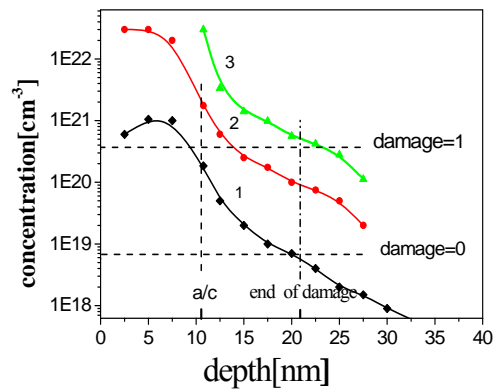


Fig. 4. Simulated depth profiles of the atomic Ge concentration- 5keV Ge⁺ in Si<100>, tilt 7deg/ rot 30deg; $1 \times 10^{15} \text{ cm}^{-2}$ - curve 1 and the simulated average number of different defect species: displacements - curve 2; disorders - curve 3.

The calculated displacements/cm³ values in the tail region are shown in the Fig. 4. The tail profile starts at $(2 \div 2.5) \times 10^{21} \text{ cm}^{-3}$ and ends $\sim 8 \times 10^{19} \text{ cm}^{-3}$, following curve 2 in the figure. Curve 3 presents the profile of the disorder.

The presented simulations demonstrate the usefulness of SE damage profiling. It provides the physical pickets for achieving realistic values of some defect species in the very shallow as-implanted region.

4. Conclusions

It is shown that VASE measurements with a suitable algorithm for data interpretation are a useful tool for quantitative damage profiling in very shallow implanted Si. The retrieved damage depth profiles for Ge implants with very low energies in c-Si provide exact information for the depth of the a/c boundaries, the “end” of the SE damage, and the shape of the tail regions in the profiles. A useful set of values for the relevant parameters of simulations by the Monte Carlo, new BC Algorithms, implemented within the SILVACO framework has been obtained from the measured SE damage profiles. An attempt was made to obtain for a reliable conversion between the damage and concentration depth profiles in very low energy Ge⁺ implants in c-Si.

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