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Spectroscopic Ellipsometry of Ion-Implantation-Induced Damage

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1. Introduction

In modern semiconductor manufacturing ion implantation requires precise control and such a control is impossible without adequate measurements of the implanted media. As the global trend of miniaturization dictates continuous decrease of the energy and dose of the implants, the measurement precision should match stricter requirements.

Well-established analysis techniques, including secondary ions mass-spectrometry (SIMS) (Benninghoven et al., 1987; Brundle et al., 1992; Alford et al., 2007), high-resolution transmission electron microscopy (HRTEM) (Hirsch et al., 1977; Horiuchi, 1994; Williams & Carter, 2009) allow direct observation of the effect of ion implantation, although they suffer from being destructive, time consuming and unusable for real-time in-line monitoring of ion implantation process or to measure uniformity. Some of the more common methods, like sheet resistance measurements (four-point probe, FPP) (Keenan et al., 1985; Johnson, 2001; Schroder, 2006) and thermal-wave technology (TW) (Smith et al., 1985; Guidotti & van Driel, 1985; Smith et al., 1986), are fast and relatively inexpensive, but require special efforts in order to get reliable information and exclude measurement errors. Ideally, the technique should be non-destructive to the sample, fast, accurate and precise to be used for routine process monitoring and control.

Among various characterization methods, ellipsometry is a fast, non-intrusive and informative technique that is sensitive to changes in optical properties and thicknesses of thin films. As ion implantation significantly changes optical properties of many materials (especially, crystalline), the ellipsometry is one of the most suitable technique for monitoring the results of ion implantation with no special sample preparation requirements. Ellipsometric analysis is able to detect and characterize the degree of crystallinity in buried layers as well as depth profiling in the sample. Besides the crystalline substrates, the ellipsometry is able to measure crust, formed on top of photoresist during masked ion implantation. The crust often poses a problem in post ion implantation photoresist strip and its characterization is important for optimization of strip processes.

Ellipsometry of implanted crystalline substrates is based on the fact that those substrates are amorphized and amorphous medium has very different optical properties from the crystalline one. In traditional models, ion-beam-induced amorphization occurs as a phase transition induced by adequate number of point defects created by individual ions (point-

defect concentration exceeds some critical value; homogeneous amorphization) or the formation of continuous amorphous layer is due to overlapping of isolated damaged regions (heterogeneous amorphization) (Pelaz et al., 2004). Despite numerous studies, the mechanisms of amorphization by ion implantation are still under intensive investigations. Currently, various numerical simulations for ion implantation processes, like Monte-Carlo (MC) and molecular dynamics (MD) techniques, have been widely used to reconstruct the amorphization profiles (Sigmund, 2004; Ziegler et al., 2010; Nordlund, 1995; Beardmore & Grønbech-Jensen, 1998).

The amorphization depends on the crystalline medium, implanted elements, energy and dose of the implantation. There are number of papers describing dependence of the optical properties and depth of the amorphized layer on the processing conditions. However, the recent results indicate that even for rather low-energy low dose implants (with energy of several keV, dose around 10^{15} ions/cm²), which do not cause amorphization, the changes of the optical properties of the implanted crystalline semiconductor are significant and can be detected by ellipsometry. The implantation depth measured by ellipsometry corresponds to direct observations of distorted crystalline lattice by TEM. These results allow extension of the ellipsometry capabilities toward the lower limits of energy and dose, where no amorphization occurs.

Ellipsometric measurements of the photoresist crust formation are based on the fact that energetic ions remove lighter photoresist fraction leaving behind graphite-like carbon-rich layer. Having optical properties different from those of the bulk photoresist, such a layer could be measured by ellipsometry. It should be noted, however, that with reduction of dose and energy of the ion implantation, the formation of this layer is less pronounced and it causes less issues in post ion implantation photoresist strip.

In the chapter, a short overview of ellipsometry principles is given in section 2. The application of ellipsometry to investigate ion implantation of crystalline and polycrystalline silicon is reviewed in section 3. The recent results obtained on very shallow low-dose implantation are also presented. Finally, summary and future perspectives are presented in section 4.

2. Fundamentals of ellipsometry

In this section, a very brief overview of the ellipsometry principles is presented. For much more extended and detailed up-to-date discussion on fundamental principles of ellipsometry, instrumentations, data analysis as well as multiple applications, see (Tompkins, 1993; Tompkins & McGahan, 1999; Tompkins & Irene (Eds.), 2005; Fujiwara, 2007; Losurdo et al., 2009; Azzam, 2010).

Ellipsometry (reflection polarimetry; single-wavelength as well as spectroscopic) is an optical measurement technique for evaluation geometrical and material properties of substrates, thin films and multilayer structures. Determination of fundamental optical properties (complex dielectric functions (ϵ) or complex refractive indexes (N)) gives an opportunity to characterize other important material properties such as composition, phase structure, doping, stress, uniformity, electrical properties, etc. The principles of this technique as well as first applications have been established in the late 19th century but it

became widely utilized only in 1960s and 1970s due to significant developments in the instrumentation, computers and data analysis algorithms (Azzam & Bashara, 1977; Rzhanov et al., 1979; Theeten & Aspnes, 1981; Riedling, 1988; Azzam (Ed.), 1991).

Ellipsometry measures the changes in the polarization state of light upon reflection from a sample surface at non-normal (oblique) incidence (although transmission ellipsometry at normal incidence can be used for optically anisotropic samples) and those changes typically expressed in terms of two values (ellipsometric angles) called Psi (Ψ) and Delta (Δ). These represent an amplitude ratio and relative phase shift between p- and s-components of the polarized light¹ which are induced by reflection from the sample (see Fig. 1).

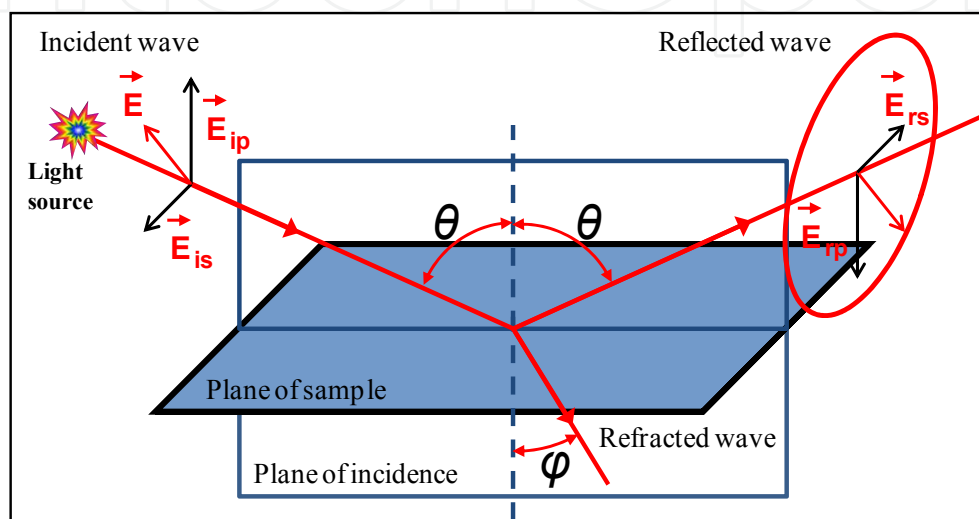


Fig. 1. Scheme showing the basic principle of ellipsometry: linearly polarized light with p- and s-components at oblique incidence is reflected and it becomes elliptically polarized. The parameters of the resulting ellipse depend on the initial direction of polarization, the angle of incidence and the optical properties of the surface. E_{ip} , E_{is} , E_{rp} , and E_{rs} represent the p- and s-components of the incident (i) and reflected (r) light waves.

The measured quantities Ψ and Δ are described by the fundamental equation of ellipsometry

$$\rho \equiv \tan(\Psi)e^{i\Delta} \equiv \frac{R_p}{R_s} \equiv \left(\frac{E_{rp}}{E_{ip}} \right) / \left(\frac{E_{rs}}{E_{is}} \right), \quad (1)$$

where R_p and R_s are the Fresnel reflection coefficients for the p- and s-polarized light, respectively. The reflection coefficients are directly related to the optical properties of the sample. In the simple case of single thin film on substrate (see Fig. 2), ρ can be described as a function

$$\rho \equiv \tan(\Psi)e^{i\Delta} = f(N_0, N_1, N_2, \theta_0, d), \quad (2)$$

¹ The term "p-polarization" was taken from the German word "parallel" since this component of the electric field \mathbf{E}_p is parallel to the plane of incidence. The component perpendicular to this plane, \mathbf{E}_s , was named "s-polarization" and derived from the German word "senkrecht" (perpendicular).

where $N = n - ik$ is the complex index of refraction.²

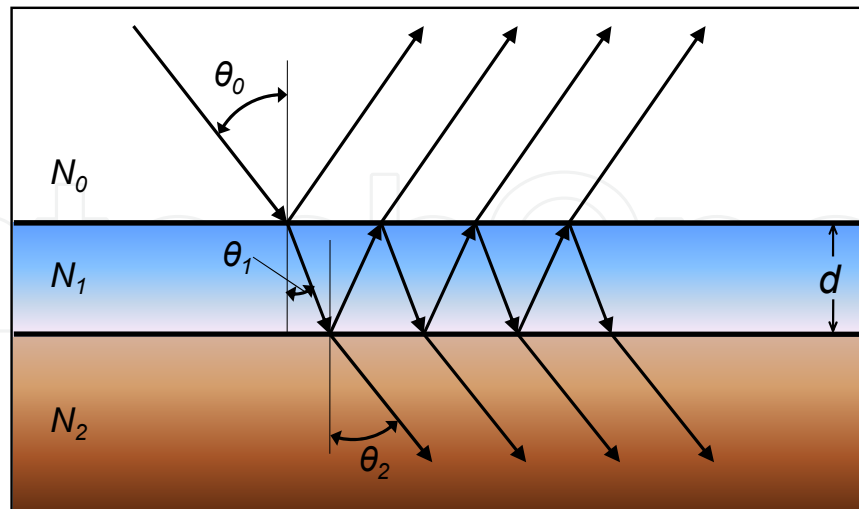


Fig. 2. Three-phase (ambient/film/substrate) optical model.

There are two major flavours of ellipsometric technique. Single-wavelength ellipsometry (SWE) uses a monochromatic light source (typically, high-intensity probe beam from HeNe laser with a wavelength of 632.8 nm) which results in only single set of ellipsometric parameters (Ψ, Δ). Multi-wavelength approach or spectroscopic ellipsometry (SE) involves measurements of Ψ and Δ as functions of wavelength (Tompkins & McGahan, 1999; Fujiwara, 2007). Therefore, the SE determines the complex index of refraction as a function of wavelength λ (material dispersion; $N = f(\lambda)$). This is definitely an advantage of the SE as compared with SWE since knowledge of the n and k spectra is very helpful in establishing the correlations to various physical and chemical properties of the materials (for instance, the ultraviolet (UV) range of the n and k spectra allows us to determine the degree of crystallinity in polycrystalline silicon or, together with visible range, to ascertain SiGe stoichiometry). In variable-angle spectroscopic ellipsometry (VASE), a variant of the SE, the ellipsometric angles Ψ and Δ are measured as functions of both wavelength and angle of incidence (AOI) which results in higher sensitivity and accuracy due to additional optical paths for various AOI's (Woollam, 1999 ; Woollam et al., 1999 ; Johs et al., 1999).

The real part of N , namely n , is the conventional refractive index. The imaginary part of N , namely k , is called the extinction coefficient and it is directly related to the absorption coefficient of the medium:

$$\alpha = \frac{4\pi k}{\lambda}$$

where λ is the free-space wavelength of light.

These two wavelength-dependent quantities are often called the “optical constants” of the material, although they are not constants in fact but depend, in addition to the λ (or light

² Here we follow the traditional ellipsometric convention which defines the imaginary part of N with a „minus“ sign („The Nebraska Convention“, 1968; see (Muller, 1969; Holm, 1991; Bennett, 2010)). In other areas of physics the complex index of refraction is defined with a „plus“ sign.

frequency), also on material's conditions. The "optical constants" can be considered as *intrinsic* properties of the material which completely characterize material's optical response.

There is an equivalent approach to describe the optical properties in terms of the complex dielectric function ε (sometimes also called "complex dielectric constant"):

$$\varepsilon = \varepsilon_1 - i\varepsilon_2.$$

The complex index of refraction N and complex dielectric function ε are related to each other through the following relation derived from Maxwell's equations:

$$\varepsilon = N^2.$$

Therefore,

$$\begin{aligned}\varepsilon_1 &= n^2 - k^2, \\ \varepsilon_2 &= 2nk\end{aligned}$$

and

$$\begin{aligned}n &= \frac{1}{\sqrt{2}} \left(\varepsilon_1 + \sqrt{\varepsilon_1^2 + \varepsilon_2^2} \right)^{1/2}, \\ k &= \frac{1}{\sqrt{2}} \left(-\varepsilon_1 + \sqrt{\varepsilon_1^2 + \varepsilon_2^2} \right)^{1/2}.\end{aligned}$$

The fact that ellipsometry measures the changes in polarization (rather than the absolute light intensity or absolute phase) makes it highly accurate, robust and very reproducible technique. Presence of "phase" information (Δ) also makes ellipsometric measurements extremely sensitive for the analysis of surfaces.

Experimentally, the ellipsometric parameters Ψ and Δ can be determined with very high precision. However, the next step, namely, extraction of required information (the optical constants n and k and film thickness(-es)) from those measured values, requires adequate optical model for calculations and it might be quite complicated to construct one in some cases. Thus, the ellipsometric technique is the *indirect* characterization method.³ Then using linear regression analysis technique the film stack parameters are determined by minimizing fitting errors to the measured spectroellipsometric data using various error functions (for more details on data analysis procedure see, for instance, (Jellison, 1993, 1998; Fujiwara, 2007)).

3. Spectroscopic ellipsometry measurements on implanted silicon wafers

In the past few decades the spectroscopic ellipsometry was extensively used to investigate ion implantation (Si^+ , Ge^+ , B^+ , P^+ , As^+ , Ar^+ , Xe^+ , and N_2^+) of crystalline and polycrystalline silicon (Ibrahim & Bashara, 1972; Adams & Bashara, 1975; Adams, 1976; Jellison et al., 1981; Ohira & Itakura, 1982; Lohner et al., 1983; Vasquez et al., 1985; Vedam et al., 1985; Nguyen &

³ Direct n and k extraction from the ellipsometric parameters Ψ and Δ is only possible in case of flat, isotropic and homogeneous substrates (medium of semi-infinite thickness).

Vedam, 1990; Miyazaki & Adachi, 1993; Fried et al., 1992, 2004; Müller-Jahreis et al., 1995; Shibata et al., 1999, 2010; Giri et al., 2001; Tsunoda et al., 2002; Petrik et al., 2003; Yoshida et al., 2005; Stevens et al., 2006; Lioudakis et al., 2006a, 2006b; Petrik, 2008; Matsuda et al., 2010; Mohacsi et al., 2011). One of the motivations of that was to get non-contact, non-destructive and rapid measurement technique with high accuracy and sensitivity for industrial applications (in particular, for integrated circuits (IC) manufacturing). For instance, Vanhellemont et al. ([Van91], as cited in Petrik, 1999) claim that spectroscopic ellipsometry “can be considered as a non-destructive, cheap poor man's optical Rutherford backscattering spectrometer and even as a one-dimensional optical high-resolution microscope”. With a proper optical model, calibrated to other analytical techniques, it is possible to non-destructively characterize damage depth profiles with various degrees of crystallinity as well as effects of subsequent annealing of ion-implanted Si layers.

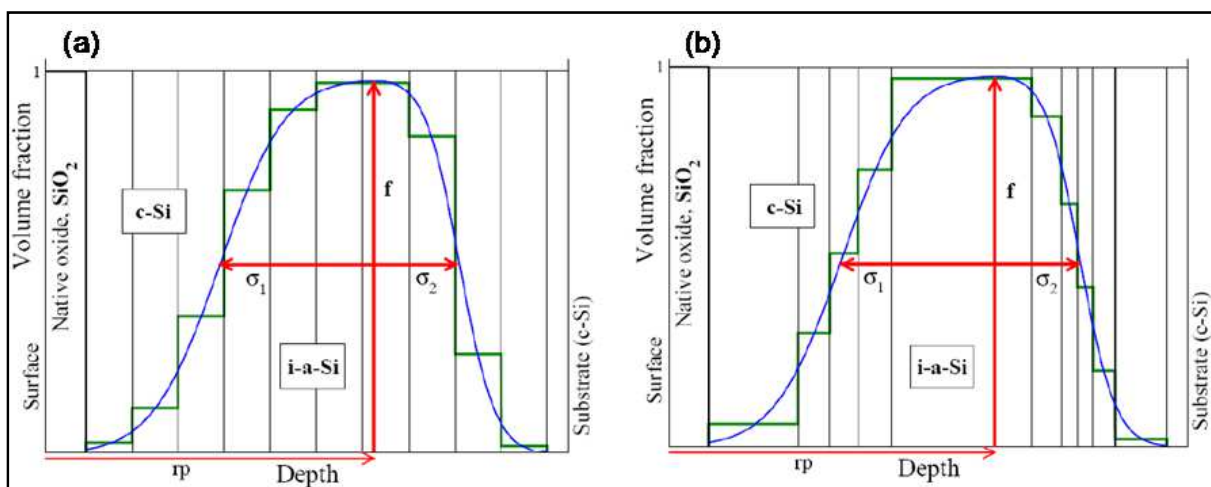


Fig. 3. Realistic damaged depth profile models where the damaged regions are divided into sublayers: (a) with fixed thicknesses (Fried et al., 1992); (b) with thicknesses inversely proportional to the slope of the profile (Petrik et al., 2003) (reprinted from (Petrik et al., 2008), with permission from Dr. P. Petrik).

The usual way of describing the ion-implanted media includes two constituents. At first, the parametrization of the amorphization profile needs to be established. For instance, typical layer structure for ion-damaged crystalline or polycrystalline Si consists of native oxide on the top, an extensively damaged region where amorphization exceeds critical amorphization density, and partially amorphous layer underneath. Those damaged regions can be divided in sublayers with various ratios for crystalline and amorphous components. Very sophisticated damaged depth profile models were introduced (Fig. 3) in which coupled half-Gaussian functions used to describe the damage levels in the sublayers with fixed thicknesses (Fried et al., 1992) or with thicknesses inversely proportional to the slope of the profile (Petrik et al., 2003). Secondly, it is necessary to describe the optical properties of the disordered layers or, in other words, parametrize the complex dielectric functions of such layers (sublayers). Typically, it can be modeled as a composition of crystalline (c-Si) and amorphous, ion-induced damaged (i-a-Si), phases using self-consistent Bruggeman effective medium approximation (B-EMA). Since dielectric functions of the amorphous silicon are not unique, various optical models can be selected to obtain its optical properties (for example, well-established Tauc-Lorentz (TL) optical model (Jellison & Modine, 1996a, 1996b) which

has been the most widely used parametrization of the optical functions for amorphous materials).⁴

However, even a simple model of the ion-damaged Si layer could be used for characterization of ion-implanted Si for semiconductor manufacturing, where the robustness and the speed of measurements are the key factors. The measurements are based on the fact that the top part of the crystalline Si is amorphized by high energy ions and since amorphous Si (a-Si), crystalline Si (c-Si) and SiO₂ (which inevitably exists on top of Si after exposure to air) have very distinctive optical properties, as shown in Fig. 4.

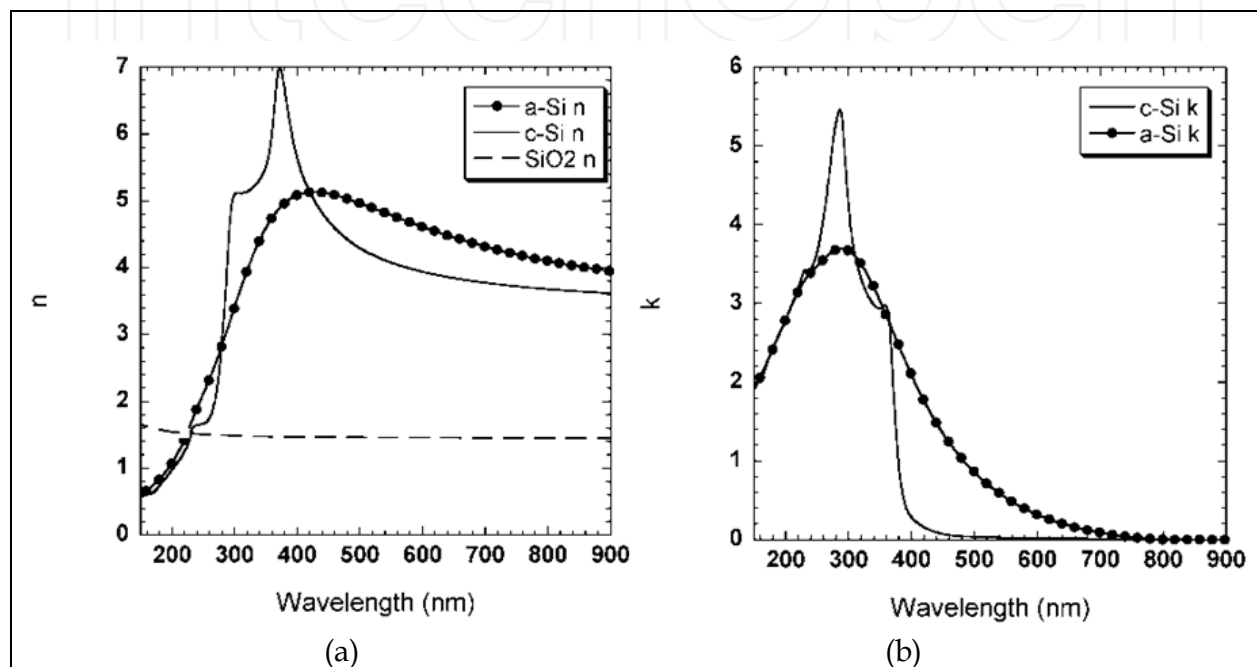


Fig. 4. Dispersions of the refractive index n (a) and the extinction coefficient k (b) of crystalline Si, amorphous Si and SiO₂. Extinction of SiO₂ is zero in the plotted range.

Significant difference in optical properties of those three layers allows thicknesses measurement of both the amorphized layer and SiO₂ on top of the crystalline Si substrate after ion implantation. It should be noted that the implantation energies in the aforementioned works are rather higher (10 keV or more) while modern ultra-shallow junctions require implantation energy close to 1 keV or even less. At such low energies Si might not be amorphized but only damaged. However, recently published papers (Shamiryan et al., 2010; Radisic et al., 2009, 2010) demonstrated that spectroscopic ellipsometry can be used for implanted Si measurements even in the case of low energy ion implantation, when no Si amorphization is observed.

Si implanted with B and As species at low energies (as specified in Table 1) was measured by spectroscopic ellipsometry with a spectral range of 150–895 nm. The optical model consisted of a Si substrate and two layers: SiO₂ on top and a damaged Si (d-Si) layer at the

⁴ Recently, Ferlauto et al. suggested the Cody-Lorentz dispersion model which has a few advantages over TL model and better describes the optical properties of some amorphous materials (see details in (Ferlauto et al., 2002)).

bottom. The SiO₂ model was taken from library since the optical properties of SiO₂ were considered not modified by ion implantation as it has been reported that the change of refractive index of silica upon ion implantation does not exceed 1-2% (Bayly & Townsend, 1973; Webb & Townsend, 1976). This could be easily explained by the fact that, unlike Si substrate, the SiO₂ layer is already amorphous prior to ion implantation and energetic ions do not significantly change its state. The model for the damaged (implanted) Si layer was based on the a-Si model represented by a set of harmonic oscillators. In order to fit the model to the measured spectra, the thickness of both SiO₂ and d-Si were varied as well as optical properties of the d-Si layer. After the implantation, besides ellipsometry, the samples were also inspected by transmission electron microscopy (TEM). This technique allows direct observation of the crystallinity of the layers and determination of their thicknesses using interatomic distance as a reference.

Element	Energy, keV	Dose, cm ⁻²	Tilt, degrees
B	0.5; 1; 3	1.5x10 ¹⁵	7
As	1; 1.5	1.5x10 ¹⁵	7

Table 1. Ion implantation conditions.

After fitting of the two layer model to the ellipsometric data obtained after ion implantation it was found that the top damaged layer is indeed similar in optical properties to amorphous Si. Fig. 5 shows the *n* and *k* dispersions for As- and B-doped Si along with the dispersions for a-Si taken from the library. One can see that the dispersions of both implanted layers are closer to the a-Si than to c-Si (cf. Fig. 4).

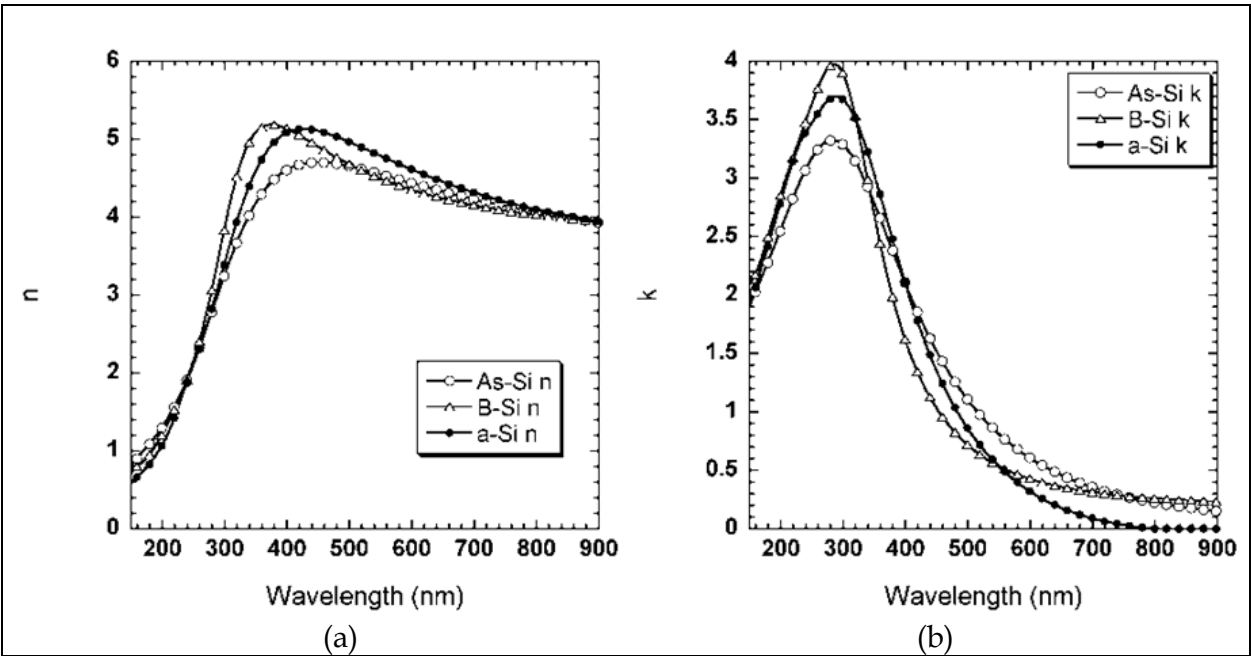


Fig. 5. Dispersions of *n* (a) and *k* (b) for a-Si (solid curve – taken from KLA-Tencor library) and for As (1 keV, 1.5x10¹⁵ cm⁻²)- and B (0.5 keV, 1.5x10¹⁵ cm⁻²) -doped Si (circles and triangles, respectively) as measured by SE.

TEM micrographs (Fig. 6) reveal that for implantation of B with energies of 0.5 keV and 1 keV the Si substrate is not amorphized. However, the top implanted layer is still visible on TEM images due to strain induced by ion implantation. The thickness of this strained layer is in a good agreement with SE measurements. As implantation energy of B increases to 3 keV, TEM images show two layers: a bottom strained layer and a top amorphous layer. The total thickness of these two layers is in agreement with SE measurements. Similar results were obtained for As, but the top layer was amorphized even for the lowest studied implantation energy of 1 keV. Summary of TEM measurements and SE measurements is shown in Table 2. One can see that both d-Si and SiO₂ measurements are in a good agreement with TEM data.

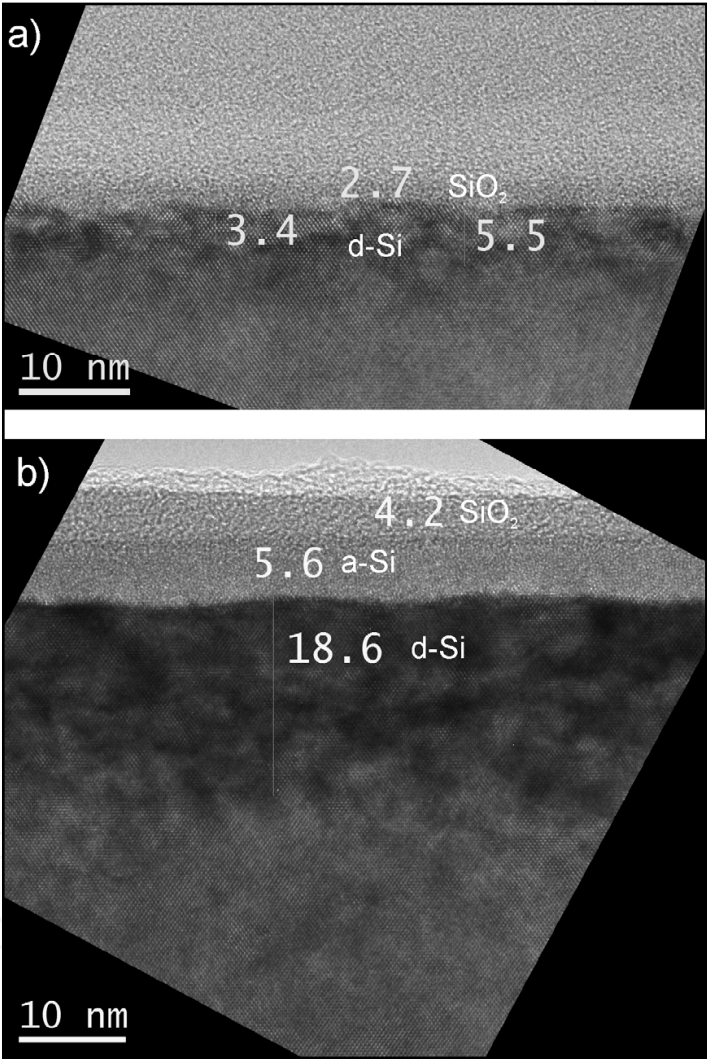


Fig. 6. TEM images of Si implanted with B at 0.5 keV (a) and 3 keV (b), the dose is 1.5×10^{15} in both cases. All measurements on the images are in nm.

From the comparison of the TEM and SE measurements we can make two important conclusions:

1. Even when the implanted Si is not amorphized, its optical properties change significantly, so it can be easily distinguished from c-Si.

2. Since the optical properties of the d-Si are close to those of a-Si (see Fig. 5) ellipsometry can hardly distinguish between those two layers when they both are present at higher implantation energies.

Therefore, it is possible to measure thickness of the implanted Si layer even though it might be impossible to tell whether the implanted layer is just strained or amorphized.

Technique	B implantation energy, keV			As implantation energy, keV
	0.5	1	3	1.5
SiO ₂ thickness (nm)				
TEM	2-2.7	2.4-2.6	2.1-2.9	2.3
SE	2.8±0.1	2.4±0.1	2.5±0.1	2.7
Damaged Si thickness (nm)				
TEM	3.5-5.5	7-10	20-24	7-10
SE	4.7±0.1	7.4±0.1	23.5±0.2	6.0

Table 2. Summary of TEM and SE measurements of thickness of the implanted Si substrates.

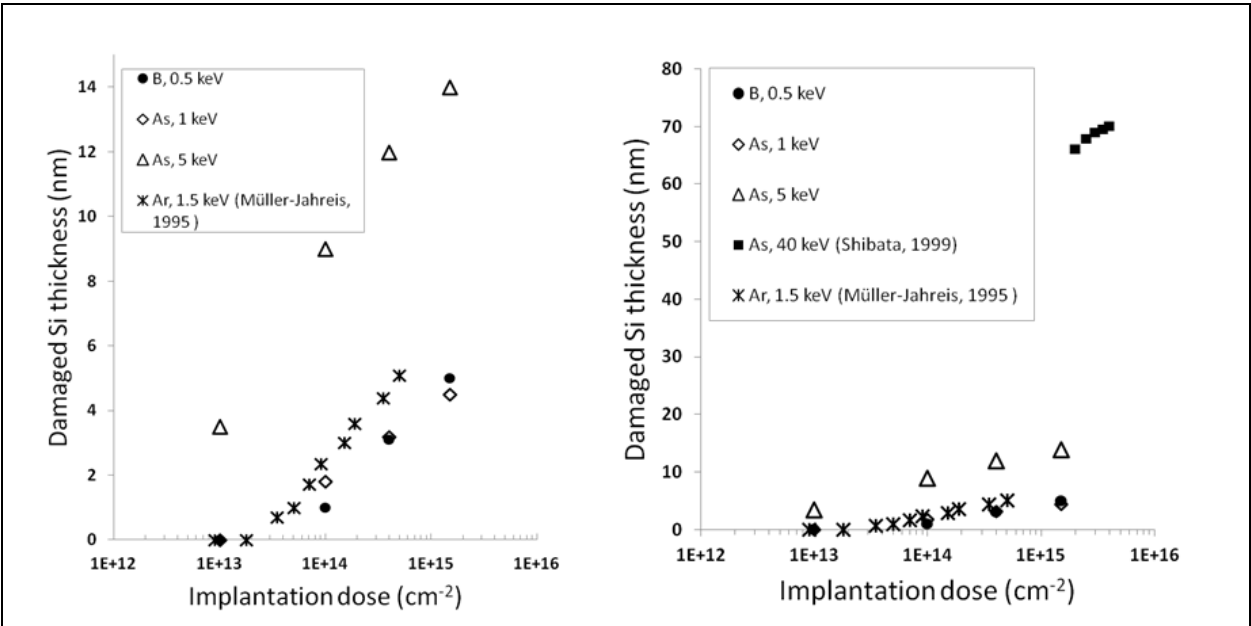


Fig. 7. Depth of the damaged Si as function of the implantation dose, as measured by ellipsometry. The left panel shows all data, the right one shows the data obtained for low energies (less than 10 keV).

The results of the ellipsometric measurements of ion-implanted monocrystalline Si are shown in Figures 7 and 8. One can see that there are detection limits above which the ellipsometry can detect damaged Si layer. The detection limits depend on the dose, energy and ion mass. The dependence of the damaged layer thickness on dose is logarithmic (the thickness is proportional to the logarithm of the dose; see Fig. 7), while the dependence of the damaged thickness d on the ion energy E exhibits power dependence in the form

$$d = A \cdot E^x,$$

where A is a constant related to the implanted element, and x is the power factor in the range of 0.7-0.8 (see Fig. 8).

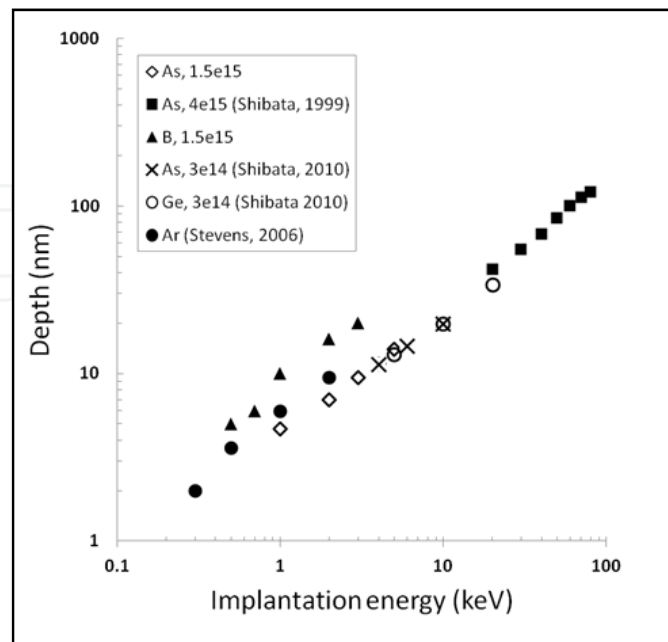


Fig. 8. Depth of the damaged Si as function of the ion implantation energy, as measured by ellipsometry.

4. Conclusion

In this chapter the basic principles of ellipsometry as well as application of spectroscopic ellipsometry to investigate ion implantation of crystalline and polycrystalline silicon have been reviewed. Spectroscopic ellipsometry can be used for characterization of ion-implanted crystalline substrates before anneal. Ion implantation creates a damaged Si layer, whether amorphized (for higher implantation energies) or just strained with a distorted lattice. SE can measure this damaged layer since its optical properties in both cases (amorphization or lattice distortion) are similar and significantly different from the crystalline Si. Due to similarity in optical properties, SE cannot distinguish between amorphized and distorted Si layer.

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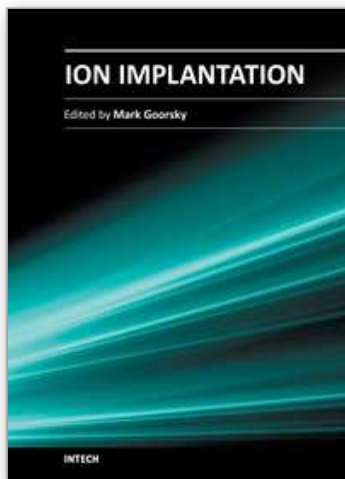
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