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Amorphous silicon layer characteristics during 70–2000 eV Ar⁺-ion bombardment of Si(100)*

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Spectroscopic ellipsometry (SE) has been applied to characterize the damaged, amorphous silicon (*a*-Si) layer created by Ar⁺-ion bombardment in the ion energy range of 70–2000 eV impinging at 45° angle of incidence on Si(100). The dielectric functions of *a*-Si during ion bombardment have been determined using the Tauc-Lorentz model for the dielectric functions ϵ_1 and ϵ_2 . The dielectric functions resemble literature reports on *a*-Si-like dielectric functions. The *a*-Si layer thickness under ion bombardment conditions reaches values from ≈ 17 Å at 70 eV up to ≈ 95 Å at 2000 eV. These values compare reasonably well with SRIM and molecular dynamics simulations. The surface roughness, as determined with SE, is typically 5–15 Å during ion bombardment, with a minimum roughness at $E_{\text{ion}}=250$ eV. The creation of the amorphous silicon top layer upon 70 eV Ar⁺-ion bombardment with an ion flux of 0.07 ML s⁻¹ has been resolved using real-time spectroscopic ellipsometry. The creation of the amorphous layer shows a double exponential ion-dose dependence: a fast, initial period of *a*-Si creation, with $1/e$ constant $\Delta\tau_1=2$ ML, and a slower period, $\Delta\tau_2=9$ ML, until the matrix is fully amorphous after ~ 30 ML of Ar⁺ dosing. Relaxation of the *a*-Si top layer has been observed after the ions are switched off and has been analyzed with a stretched-exponential decay as a function of time, which is characteristic for a defect-controlled relaxation in the bulk *a*-Si layer. The corresponding time constant τ is found to be ~ 360 s, which is typically observed for self-annealing in amorphous silicon materials. © 2006 American Vacuum Society. [DOI: 10.1116/1.2244535]

I. INTRODUCTION

Ion bombardment plays a key role in fabrication processes of semiconductor and optical devices. Ion bombardment is, e.g., used to manufacture extremely low roughness x-ray mirrors^{1,2} and to implant dopants.^{3,4} In plasma etching ions are known to enhance etch rates⁵ and for their ability to etch highly anisotropic nanometer scale structures. The ion energy ranges of interest for these type of applications are $E_{\text{ion}}=10$ –500 eV for radio frequency or inductively coupled etch plasmas, 100–1000 eV for ion-polishing applications, and ~ 1000 –2500 eV for shallow implantation of dopants. Ions penetrate to a certain depth into a substrate depending on their energy, thereby creating a damaged amorphous layer. This ion damage layer will especially have an increasing influence on semiconductor device performance as device dimensions are steadily reducing. On the other hand the change from a crystalline to an amorphous surface layer is beneficial in plasma etching. The modified atomic bonding configuration allows chemically reactive species to adsorb more easily, and ion bombardment promotes the release of etch products.^{5–7} The amorphous ion damage layer has not had much attention in fundamental beam etching studies, although a few theoretical studies^{8,9} and a number of experimental studies report on the Ar⁺-ion damage aspects in the ion energy range <2500 eV on silicon, such as the damage

layer thickness^{10–12} or surface morphology.^{13,14} Characterization of the ion damage layer could aid in a better understanding of etch mechanisms.

A diagnostic tool that can be employed *in situ* to characterize optical properties and thicknesses of thin films is spectroscopic ellipsometry (SE). Here, we report on the use of SE to characterize amorphous silicon (*a*-Si) layers created by Ar⁺-ion bombardment of Si(100) in the 70–2000 eV ion energy range. SE has been used previously to study Ar⁺-ion bombarded silicon substrates with ion energies up to tens of keV.^{3,15} The experiments presented here have been performed in an Ar⁺/XeF₂ beam etching apparatus designed to study fundamental aspects of ion-assisted etch mechanisms.

Not only the saturated amorphous layer thickness under ion bombardment conditions but also the surface roughness and the dynamics of creation and relaxation of the damaged, amorphous layer as a function of ion energy have been investigated using SE. In addition, the ion energy range down to 70 eV will be explored, ultimately to close the existing experimental gap between beam etching and plasma etching studies.

After addressing the experimental details (Sec. II), the multilayer dielectric modeling and dielectric properties of the damaged, amorphous silicon will be described in Sec. III and will be compared to other *a*-Si-like dielectric functions reported in the literature. The *a*-Si layer thickness and surface roughness during ion bombardment are presented in Sec. IV. Also, a comparison is made between the measured *a*-Si layer thickness as a function of ion energy and SRIM and molecular

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FIG. 1. Experimental setup in horizontal cross-section. Samples can be exchanged between a rotatable sample holder and the sample storage in the load lock with a linear magnetic drive. The sample is mounted in a rotatable sample holder (1) that can be operated manually via an external drive. The XeF_2 source (2) and Ar^+ -ion source (3) are at 52° and 45° from surface normal, respectively. Etch products are detected in a separate detector chamber perpendicular to the sample surface. The spectroscopic ellipsometer is incident at 74.3° from the sample surface normal. The SE consists of a broadband light source, polarizer (P), rotating compensator (RC), analyzer (A), and a fiber-coupled charge-coupled device array detector (D).

dynamics simulations. In Sec. V, it will be shown that real-time SE can be used to monitor the creation and the relaxation of the *a*-Si top layer produced by ion bombardment.

II. EXPERIMENTAL DETAILS

A. Experimental setup

The experimental setup has been described extensively in previous publications.^{16–18} In Fig. 1 a top-view cross section of the setup is shown. The setup is equipped with a load-lock system for storage and easy sample exchange, a single-wavelength ellipsometer, and a mass spectrometer for etch product monitoring. The spectroscopic ellipsometer is a Woollam M2000U with an infrared extension covering the photon energy range of 0.7–5 eV (250–1700 nm). The angle of incidence of the light is typically 74.3° off the surface normal and the light is focused onto a 1 mm^2 area of the sample. Each measured spectrum is an average over typically 100 spectra recorded by the ellipsometer resulting in a time resolution of typically 5 s. The spectroscopic ellipsometry data are analyzed with EASE™ software version 1.98.

A low energy (10–2000 eV) ion beam source (Nonsequitur Technologies, customized version of Model LEIG-2) has been installed recently to access the lower ($<500 \text{ eV}$) energy range. The ion beam diameter is set to 3 mm full width at half maximum for all ion energies. The ions impinge onto the silicon surface at a 45° angle with respect to the surface normal. The ion flux is determined from the measured, total current on the sample. From calibration a sample current of $1 \mu\text{A}$ relates to an ion flux of 0.09 ML s^{-1} , which is equal to $0.6 \times 10^{14} \text{ cm}^{-2} \text{ s}^{-1}$ ($1 \text{ ML} = 6.86 \times 10^{14} \text{ cm}^{-2}$). The maximum fluxes that can be achieved with this source are typi-

FIG. 2. Pseudodielectric functions of the measured steady-state spectra during Ar^+ -ion bombardment with 70, 300, and 1000 eV ion energy and an ion flux of 0.07 ML s^{-1} . For reference, the dielectric functions of silicon are also shown (solid lines).

cally 0.1 ML s^{-1} for ion energies below 100 eV and 1 ML s^{-1} for ion energies above 1000 eV ion energy.

B. Si(100) samples

The silicon samples used in this study are *n*-type Si(100) with a resistivity of $10\text{--}30 \Omega \text{ cm}$. The $10 \times 10 \text{ mm}^2$ Si substrates are pretreated to remove the native oxide in a 2% hydrofluoric acid (HF) solution for 2 min after ultrasonic cleaning with ethanol at 40°C . This leads to a mono-, di-, and trihydride-terminated Si substrates with mostly dihydrides¹⁹ with an initial roughness of typically 0.6–1.0 nm measured with SE and $\sim 0.15 \text{ nm}$ root-mean-square roughness measured with atomic force microscopy (AFM) (NT-MDT Solver P47) in noncontact mode (scan size: $1.5 \times 1.5 \mu\text{m}^2$).

C. Measured pseudodielectric functions

On three Si(100) samples, SE spectra have been collected *in situ* and in real time for ion energies from 70 up to 2000 eV by increasing the ion energy stepwise and waiting until the measurement reached a steady state. The ion flux was 0.07 ML s^{-1} for each ion energy.

Figure 2 shows examples of steady-state pseudodielectric functions $\langle \epsilon_1 \rangle$ and $\langle \epsilon_2 \rangle$ measured with SE on substrates during 70, 300, and 1000 eV Ar^+ -ion bombardment. For reference the dielectric functions ϵ_1 and ϵ_2 for *c*-Si have been shown.²⁰ Pseudodielectric function spectra $\langle \epsilon_1 \rangle$ and $\langle \epsilon_2 \rangle$ are derived from the measured ellipsometric angles Ψ and Δ

FIG. 3. Multilayer dielectric model that has been used to analyze the measurements, consisting of an *a*-Si layer on a semi-infinite *c*-Si substrate and a top layer consisting of 50% void and 50% *a*-Si, which represents the surface roughness.

assuming a two-phase (ambient/substrate) layer model, where the ellipsometric angles Ψ and Δ are defined as $\tan \Psi \exp(i\Delta) = r_p/r_s$ with r_p and r_s the complex amplitude reflection coefficients of the electric field components parallel and perpendicular to the plane of incidence, respectively. The *c*-Si dielectric functions show the typical critical-point (CP) resonances related to E'_0/E_1 (3.36 eV) and E_2 (4.30 eV) electronic interband transitions.²¹ Ion bombardment results in the loss of crystallinity and, thus, the distortion or disappearance of the CP resonances of *c*-Si in a layer penetrated by the ions. Consequently, a shift to lower energies and a broadening of the pseudodielectric functions can be observed due to a top layer of amorphized silicon (*a*-Si) with a characteristic broad spectrum of Si–Si bond energies and disordered bond lengths and angles.¹⁵

To obtain information regarding dielectric properties or the thickness of the *a*-Si layer, a multilayer model is chosen. The unknown parameters within the multilayer model are the curve-fit variables to match the calculated pseudodielectric functions to the measured spectra in order to obtain either unknown dielectric properties or layer thickness defined in the layer model. With a linear regression analysis method the fit variable values are optimized by reducing the absolute value of χ^2 of the fit,

$$\chi^2 = \frac{1}{2N - P} \sum_{j=1}^N \left[\frac{(\langle \epsilon_1 \rangle_j^{\text{calc}} - \langle \epsilon_1 \rangle_j^{\text{expt}})^2}{\sigma_{\langle \epsilon_1 \rangle}^{\text{expt}}} + \frac{(\langle \epsilon_2 \rangle_j^{\text{calc}} - \langle \epsilon_2 \rangle_j^{\text{expt}})^2}{\sigma_{\langle \epsilon_2 \rangle}^{\text{expt}}} \right], \quad (1)$$

where N is the number of measurement points ($N=662$), P is the number of fit variables (typically $P \sim 2-6 \ll N$), and $\sigma_{\langle \epsilon_1 \rangle}^{\text{expt}}$ and $\sigma_{\langle \epsilon_2 \rangle}^{\text{expt}}$ are the experimental standard deviations for $\langle \epsilon_1 \rangle$ and $\langle \epsilon_2 \rangle$, respectively. The experimental standard deviation is typically $\sigma_{\langle \epsilon_1 \rangle}^{\text{expt}} = \sigma_{\langle \epsilon_2 \rangle}^{\text{expt}} = 0.1$. The next section discusses the multilayer model choice and dielectric functions ϵ_1 and ϵ_2 ($\tilde{\epsilon} = \epsilon_1 - i\epsilon_2$) of the layers.

III. MULTILAYER DIELECTRIC MODELING

To obtain the thickness and/or optical properties of one or more layers on a sample, a multilayer model is defined and for each separate layer either known dielectric functions or

FIG. 4. Dielectric function of *a*-Si obtained in this work and other amorphouslike silicon materials reported in literature: (a) 150 keV implanted *a*-Si (Ref. 15), (b) 50–250 keV implanted *a*-Si (Ref. 3), and (c) chemical vapor deposited *a*-Si (Ref. 23).

model dielectric functions are assigned. The multilayer model that will be used throughout this article consists of a semi-infinite *c*-Si substrate with an *a*-Si overlayer and a surface roughness layer, as shown in Fig. 3.

The dielectric functions for *c*-Si have been taken from literature.²⁰ The dielectric functions of the surface roughness layer are approximated using a Bruggemann effective medium approximation under the assumption that the effective dielectric function of the roughness layer can be described by a random mixture of 50% void and 50% *a*-Si. The dielectric functions of amorphous silicon are, however, not unique and are subject to specific processing/production methods, whether after ion bombardment (static equilibrium), during ion bombardment (dynamic equilibrium), or chemical-vapor deposition has been used.^{3,15,22} Since dielectric functions for *a*-Si during ion bombardment are not reported in literature, a full scale analysis of SE spectra measured in dynamic equilibrium has been undertaken to obtain dielectric functions of *a*-Si and to investigate a potential dependence on ion energy and ion flux, as described in the Appendix. To obtain dielectric functions of *a*-Si the Tauc-Lorentz (TL) model has been used (see Appendix), which has been proposed by Jellison, Jr. and Modine²³ and has been used successfully to model dielectric functions of amorphous materials.^{15,22–25}

The dielectric functions ϵ_1 and ϵ_2 of *a*-Si during ion bombardment are shown in Fig. 4. As can be seen the dielectric functions reveal a single broad spectral feature unlike the specific resonance features observed for crystalline silicon. This single, broad resonance spectrum is characteristic for a broad spectrum of Si–Si bond energies and disordered bond lengths. By comparing these dielectric functions with dielectric functions for different types of amorphous silicon reported in the literature, it can be concluded that the dielectric

FIG. 5. (a) Amorphous layer thickness d_{a-Si} and (b) roughness layer thickness d_r as a function of ion energy. The variance in layer thickness at a specific ion energy are caused by differences in ion flux and sample-to-sample fluctuations.

functions obtained in this study show good agreement with the literature dielectric functions for amorphous silicon. The observed differences can be ascribed to differences in the way the amorphous silicon has been generated.

The dielectric functions of *a*-Si, presented in Fig. 4, have been used to analyze all SE measurements presented in this article. A possible ion energy dependence of the TL parameters has been investigated with two multilayer models that include TL parameters as fit variables, in addition to (a) d_{a-Si} and (b) d_r and d_{a-Si} as described in the Appendix. A short summary of the Appendix is given here to give support to our choice of modeling of the ellipsometry measurements.

An ion energy dependence of TL parameters has been observed, but it cannot be excluded that correlations between TL-model parameters are responsible for the observed trends. The amorphous layer thicknesses resulting from the various multilayer models, with and without including TL-parameters in the curve fit, show identical trends as a function of ion energy. At ion energies $E_{ion} \geq 300$ eV no difference in absolute values of $d_{a-Si}(E_{ion})$ and $d_r(E_{ion})$ are observed for the various multilayer models. Below 300 eV the variations in $d_{a-Si}(E_{ion})$ are within a factor of 2, that is because the amorphous material in rough layer is not accounted for. This can be taken care of by introducing the effective amorphous layer thickness $d_{eff} = d_{a-Si} + 0.5 \cdot d_r$, which varies only by a factor of 1.3 between the various multilayer models at a specific ion energy. Sample-to-sample variations and variations in fit results for different ion fluxes at a fixed ion energy are found to be small ($<10\%$) and are therefore ignored. Furthermore, multilayer models including TL parameters as fit variables resulted in curve fits with $\chi^2 \approx 2.5$ whereas using the simplified multilayer model with

FIG. 6. Effective amorphous layer thickness ($=d_{a-Si} + 0.5 \cdot d_r$) as a function of ion energy. Molecular dynamics simulations (Ref. 8) (diamonds) and SRIM simulation (lines) are shown for comparison. The lines are labeled by numbers that correspond to the vacancy level for which the amorphous layer thickness is determined from the SRIM simulations in units of vacancies/Å.

only two fit variables, being the amorphous layer thickness d_{a-Si} and the roughness layer thickness d_r , resulted in values of $\chi^2 = 3-4$. This difference in χ^2 is negligibly small. For these reasons, the TL-model parameters are not included in the curve-fit analysis of the SE measurements presented in this article, which simplifies the curve-fit analysis to a multilayer model with only two fit variables.

IV. *a*-Si LAYER THICKNESS AND ROUGHNESS

The surface roughness d_r and *a*-Si layer thickness d_{a-Si} as a function of ion energy have been derived from SE measurements using the multilayer dielectric model described in Sec. III. The results are shown in Fig. 5.

The amorphous layer thickness increases with ion energy. Ions with a higher ion energy penetrate deeper into the sample and create, therefore, a thicker amorphous silicon layer. The surface roughness is found to be extremely small, typically between 5 and 15 Å, with a minimum roughness at approximately 250 eV. AFM measurements of 70, 200, 1000, and 2000 eV ion bombarded samples resulted in a root-mean-square roughness $\sigma = 0.9 \pm 0.2$ Å. The AFM roughness is lower than the SE roughness, because AFM measures the root-mean-square deviation σ of the height distribution on an area defined by the scan size, whereas SE measures the rough layer thickness which corresponds to a larger fraction of the height distribution, typically two to six times larger than σ .¹⁶ Furthermore, SE samples a larger (1 mm²) area than the AFM (1.5 × 1.5 μm²) and thus height fluctuations on length scales larger than 1.5 μm are measured by SE but not by AFM. The trend is difficult to corroborate with AFM measurements due to the extremely low roughness values. These absolute roughness values are typically observed on Si samples after ion bombardment.^{2,14,26}

Figure 6 shows the comparison between the effective *a*-Si layer thickness d_{eff} , defined as $d_{eff} = d_{a-Si} + 0.5 \cdot d_r$, and predictions from SRIM simulations²⁷ performed by the authors and molecular dynamics simulations performed by

FIG. 7. Time-resolved creation of *a*-Si, modeled as the change in amorphous fraction, as a function of time (bottom ordinate) and Ar^+ dose (top ordinate) for 70 eV Ar^+ -ion bombardment with an ion flux of 0.07 ML s^{-1} .

Humbird and Graves.⁸ The SRIM simulations were performed using Ar^+ ions impinging onto a Si substrate at a 45° angle from the surface normal. The creation of vacancies is chosen to be the measure for permanent damage of the *c*-Si. The thickness of the *a*-Si layer has been derived from the depth distribution of vacancies created by an ion impact. SRIM calculates the average number of vacancies generated at a certain depth by an ion given a specific ion energy. The number density of vacancies decreases with the depth in the target, since the probability of ions with sufficient energy left to cause the creation of a vacancy decreases with target depth. Now, by defining a minimum level of vacancies as being sufficient such that the material can no longer be considered crystalline, a corresponding depth can be derived being the *a*-Si layer thickness. Figure 6 shows the *a*-Si layer thickness (lines) as a function of ion energy for the vacancy levels 10^{-1} , 10^{-2} , 10^{-3} , and 10^{-4} vacancy/ $\text{\AA}$ averaged over 10^6 single ion impact calculations. As can be seen, the agreement between the measurements and the SRIM simulations is remarkably good. Almost all measured layer thicknesses fall within the SRIM simulations for 10^{-1} and 10^{-2} vacancy/ $\text{\AA}$. Below 100 eV ion energy the measurements coincide with SRIM simulation at lower vacancy levels.

The measured *a*-Si layer thickness also shows good qualitative agreement with molecular dynamics (MD) simulations for $E_{\text{ion}} < 200 \text{ eV}$ by Humbird and Graves. Although the absolute values differ at lower energies, the trend is similar and coincides nicely with the measured *a*-Si layer thicknesses at higher ion energies.

V. DYNAMICS OF Ar^+ BOMBARDMENT

A. Time-resolved amorphization

The creation of the amorphous layer is a fast process as has been observed in MD simulations.⁸ Here, we have investigated the creation of the amorphous silicon layer on a H:Si(100) sample as a result of ion bombardment.

Figure 7 shows how the amorphous layer develops for

70 eV Ar^+ -ion bombardment with an ion flux $\Phi_{\text{ion}} = 0.07 \text{ ML s}^{-1}$ as a function of time t and ion-dose $D = \Phi_{\text{ion}} \cdot t$. The amorphous fraction $f_a = d_{\text{eff}}(t) / d_{\text{eff}}(t_{\text{sat}})$ shows an initially very rapid increase, followed by a slower increase towards saturation after $t = t_{\text{sat}} = 400 \text{ s}$, which corresponds to a total of $\sim 30 \text{ ML}$ Ar^+ dose. Despite the fact that the MD simulation for 100 eV Ar^+ ions shows a much more rapid creation of the amorphous layer,⁸ the SE measurement shows the same initially fast followed by a slower amorphization process. Curve fitting the measurement with single exponential growth function failed, which suggests that at least two processes occur during the creation of the amorphous layer. Hence, the measurements have been curve fitted with a double exponential growth function of time,

$$f_a(t) = f_1[1 - \exp(-t/\tau_1)] + f_2[1 - \exp(-t/\tau_2)], \quad (2)$$

which has been used to derive characteristic $1/e$ constants for the creation processes. The curve-fit results in $1/e$ time constants for amorphization $\tau_1 = 28 \pm 2 \text{ s}$ corresponding to a $1/e$ ion-dose constant $\Delta_{\tau_1} = 2 \text{ ML}$ Ar^+ dose ($f_2 = 0.43$) and $\tau_2 = 124 \pm 5 \text{ s}$ corresponding to $\Delta_{\tau_2} = 9 \text{ ML}$ Ar^+ dose ($f_2 = 0.57$). We believe that the observation of two $1/e$ constants for amorphization is related to a fast initial damage creation throughout the whole layer, followed by a slower process during which subsequent ion impacts fully modify the crystalline matrix into an amorphous matrix. A full SE study of the ion energy and ion flux dependence has not yet been undertaken, but could give more insight into the two observed processes. Here, it has been demonstrated that real-time SE can resolve the details of the amorphous layer creation process.

B. Relaxation dynamics

When the ion bombardment is terminated, a relaxation of the amorphous matrix has been observed. The change in the effective *a*-Si layer thickness $\Delta d_{\text{eff}}(t) = d_{\text{eff}}(t) - d_{\text{eff}}(t_{\text{sat}})$ from the saturation thickness $d_{\text{eff}}(t_{\text{sat}})$ measured during ion bombardment has been studied as a function of ion energy. It should be noted that the true physical process governing the relaxation is probably not a physical change in the effective layer thickness, but more likely a change in optical properties of the thin film as a result of changes in the amorphous matrix due to bulk reconstruction and relaxation of defects such as dangling bonds and highly strained (stretched and compressed) Si-Si bonds. A full modeling of the measured relaxation should include the analysis of the changes in the dielectric properties, i.e., the Tauc-Lorentz model of the *a*-Si. This extended analysis is more complex, since more parameters are involved in the description of the relaxation process. However, preliminary tests of such an extended analysis yielded no difference in the observed time dependence of the relaxation. Hence, here we show that a first order analysis based on the change of the *a*-Si layer thickness can be used to elucidate the relaxation process.

Figure 8 shows the change in the effective layer thickness $\Delta d_{\text{eff}}(t)$ as a function of time for the relaxation measured after various ion energy and ion flux bombardment condi-

FIG. 8. Relaxation of *a*-Si, modeled as the total change in effective *a*-Si layer thickness Δd_{eff} , as a function of time after termination of the ion bombardment at $t=0$ with various ion energies E_{ion} (eV) and ion fluxes Φ_{ion} (ML s^{-1}). The lines are fits to the data using a stretched-exponential decay typically used to describe defect-controlled relaxation. Note that the true physical process governing the relaxation is probably not a physical change in the effective layer thickness, but more likely a change in optical properties of the thin film.

tions. The lines in Fig. 8 are curve fits to the measurements using the stretched-exponential time dependence as commonly used and observed in defect relaxation/annealing in amorphous materials,^{28,29}

$$\Delta d_{\text{eff}}(t) = d_{\infty} \{ \exp[-(t/\tau)^{\alpha}] - 1 \}, \quad (3)$$

where d_{∞} is the fully relaxed (in static equilibrium) amorphous layer thickness, τ is the $1/e$ time constant for the relaxation process, and α is a dispersion parameter related to the fact that with increasing time the relaxation becomes more difficult due to an increase in the activation energy for defect relaxation. This model is called defect controlled relaxation in which an ensemble of local defects relax without the aid of diffusing atoms.²⁸

The first observation that can be made is that $\Delta d_{\text{eff}}(t)$ becomes larger with ion energy. This can be understood from the fact that with increasing ion energy the thickness of the amorphous layer increases and, thus, the number density of defects. The total change in effective layer thickness d_{∞} from the fit also showed a linear dependence on the starting thickness of the amorphous layer $d_{\text{eff}}(t_{\text{sat}})$. This observation is indicative for the fact that a bulk process is being observed and *not* a modification of the surface by molecular background gases [background pressure high voltage (HV) chamber $p_{\text{HV}}=10^{-8}$ Torr]. All measurements have been fitted simultaneously with the same time constant $\tau=360$ s and $\alpha=0.32$. The parameter α is close to the value of $1/3$, as observed for relaxation in hydrogenated amorphous silicon.^{28–30} The time constant $\tau=360$ s is on the order of previously observed time constants for relaxation in ion implanted *a*-Si.¹¹ Holtslag and van Silfhout also observed a substrate temperature dependence in the relaxation process, which was used to determine the activation energy for relaxation.

VI. CONCLUSIONS

Spectroscopic ellipsometry has been applied to study the ion-induced damage of crystalline silicon. Dielectric functions for the amorphous, ion-induced damaged silicon have been established using a Tauc-Lorentz parametrization. The dielectric functions resemble dielectric functions found for other *a*-Si-like materials in literature. Using these dielectric functions of *a*-Si, the layer thickness has been derived as a function of ion energy. The *a*-Si layer thickness shows an increase with ion energy. Good agreement with predictions for the amorphous layer thickness as a function of ion energy from SRIM and MD calculations has been found. The steady-state surface roughness during ion bombardment is shown to be extremely low. The rough layer thickness measured by spectroscopic ellipsometry yields typically $\approx 5\text{--}15$ Å. The surface roughness shows a minimum roughness at approximately 250 eV and increases for both higher and lower ion energies.

Spectroscopic ellipsometry has proven to be able to resolve the dynamics of amorphization of the crystalline silicon and self-annealing/relaxation of damaged, amorphous silicon layers. The creation of the *a*-Si layer is shown to be a very rapid process. The creation dynamics for 70 eV Ar^+ ions with an ion flux of 0.07 ML s^{-1} can be described by two $1/e$ ion-dose constants: an initially fast process with $\Delta\tau_1=2$ ML Ar^+ dose, the initial damage creation, followed by a slower process with $\Delta\tau_1=9$ ML, in which the damaged layer is fully amorphized. Well within about 30 ML of ion dose the damaged layer is fully amorphous. An ion energy and dose dependence study has not yet been undertaken, which could shed a light on the origin of the two processes. A relaxation process of the amorphous layer has been observed and has been ascribed to self-annealing of bulk defects. The relaxation process shows a stretched-exponential time dependence, fully in accordance with a literature model for defect-controlled relaxation. The time scale of $\tau=360$ s correspond with literature reports for relaxation dynamics in amorphous silicon.

Hence, it has been established that the dielectric functions and the thickness of the *a*-Si layer are in good agreement with literature and model predictions and, furthermore, surface roughness and dynamic aspects of ion bombardment can be resolved with spectroscopic ellipsometry, which is important for future studies of Ar^+/XeF_2 etching of Si(100).

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APPENDIX: TAUC-LORENTZ MODEL OF *a*-Si

To obtain dielectric functions of *a*-Si the Tauc-Lorentz (TL) model has been used. The model is a combination of a classical Lorentz oscillator and an expression for the imaginary part of the dielectric function above the band edge given by³¹

$$\epsilon_2(E) = \begin{cases} A_T(E - E_g)^2/E^2 & \text{for } E \geq E_g \\ 0 & \text{for } E < E_g, \end{cases} \quad (\text{A1})$$

where A_T is a strength parameter (dimensionless). The expression given by Tauc *et al.* in Eq. (A1) is based on the assumption that, due to a broad distribution of bonding configurations in amorphous media in contrast to crystalline media, the density of states above the band edge E_g can be decreased with the energy E . As a consequence the interband absorption can be described by a quadratic decrease, which is captured by $\epsilon_2(E)$ in Eq. (A1). The Tauc expression combined with a classical Lorentz oscillator leads to the Tauc-Lorentz oscillator model, for which $\epsilon_2(E)$ is given by

$$\epsilon_2(E) = \frac{AE_0C(E - E_g)^2}{(E^2 - E_0^2)^2 + C^2E^2E}, \quad (\text{A2})$$

where A is the oscillator amplitude, E_0 is the central oscillator energy, C is the broadening of the oscillator, and E_g is the optical band gap, all in units of energy (eV). The real part of the dielectric function $\epsilon_1(E)$ is obtained by Kramers-Kronig integration of $\epsilon_2(E)$, which leads to an additional parameter $\epsilon_1(\infty)$. The additional fit variable $\epsilon_1(\infty)$ is often used to improve fits but has been kept equal to 1 in this case.

Three multilayer models have been evaluated on the SE measurements. There are basically three reasons for testing various multilayer models. (1) The optical properties of amorphous silicon are not unique and are subject to specific processing/production methods, whether ion bombardment (relaxed/unrelaxed) or chemical-vapor deposition has been used.^{3,15} The optical properties may depend on the ion energy used. (2) Ions are known for their polishing behavior, which means that the roughness can be expected to be extremely low. The question is therefore whether or not roughness can be derived from the measurements presented here. (3) Fitting both layer thicknesses and dielectric function models results in a large number (up to 7) fit variables P . A large number of fit variables will almost certainly result in extremely good fits. However, correlations may exist between fit variables and, consequently, fit results may not be very reliable for interpretation in terms of physical problems.

The three multilayer models that have been used are defined as follows. Model (a) consists of an *a*-Si layer with thickness $d_{a\text{-Si}}$ on top of a semi-infinite *c*-Si substrate. The fit variables in this model are the TL-model parameters for the dielectric functions of *a*-Si and the *a*-Si layer thickness $d_{a\text{-Si}}$, which is a total number of five fit variables. Model (b) includes, with respect to model (a), a surface roughness layer with thickness d_r , which is modeled by a Bruggemann effective medium approximation.³² Here, we have used a mixture for the surface roughness layer of 50% *a*-Si and 50% voids.

FIG. 9. Tauc-Lorentz parameters and the χ^2 of fits as a function of ion energy as determined using multilayer models (1) and (2). The Tauc-Lorentz parameters have been fixed for multilayer model (3) at the shown values (lines). The variance in the TL parameters at a specific ion energy are caused by differences in ion flux and sample-to-sample fluctuations.

Thus, model (b) has a total of six fit variables. Model (c) uses fixed dielectric functions for *a*-Si, which are derived from the modeling with models (a) and (b). The latter one allows us to reduce the number of fit variables to two, only if the dielectric function model for *a*-Si is not extremely sensitive to the Ar^+ ion energy or flux.

Figure 9 shows the Tauc-Lorentz (TL) parameters for models (a) and (b) as a function of ion energy, including the absolute values of χ^2 . As can be seen, both A and E_g decrease with increasing ion energy up to 500 eV, whereas E_0 and C increase. The absolute values of χ^2 for these models are typically 2.5 and independent of ion energy. The multiple data points at a specific ion energy are the result of different ion fluxes and sample-to-sample reproducibility. These two variables are of minor importance and are therefore ignored. The TL-model parameters seem to depend on ion energy. The reason for the observed trends in the TL parameters is believed to result from correlations between the TL parameters, but a minor dependence on the ion energy cannot be fully excluded.

Therefore, model (c) has been tested on the measured spectra, i.e., fixed TL-model parameters. The lines and numbers mentioned in Fig. 9 correspond to the values at which the TL parameters have been fixed, thus $A=120$ eV, $E_0=3.58$ eV, $C=2.30$ eV, and $E_g=0.86$ eV. The reasons for fixing the TL parameters at these values are (1) it is more reliable to determine TL parameters from thick films, thus for *a*-Si layers generated by higher ion energy bombardment, and (2) the absolute values of χ^2 for model (c) show again

FIG. 10. (a) Amorphous layer thickness d_{a-Si} and (b) roughness layer thickness d_r as a function of ion energy, resulting from the Tauc-Lorentz parameters for multilayer model (a) open squares, (b) open circles, and (c) closed circles. The variance in layer thickness at a specific ion energy are caused by differences in ion flux and sample-to-sample fluctuations.

almost no dependence on the ion energy, whereas fixing the TL parameters at values obtained for 70 eV ion bombardment resulted in significantly increasing absolute values of χ^2 when going to higher ion energies.

In Fig. 10 the layer thickness obtained for all three models is shown. Above an ion energy of 300 eV the amorphous layer thickness d_{a-Si} is independent of model choice, whereas below 300 eV the models show small variations. The surface roughness d_r is equal to zero for model (a), since no roughness layer is included in the model. For model (b) the roughness shows a minimum at 500 eV and an increasing trend towards both lower and higher ion energies. Model (c) shows a similar trend but with the minimum at 250 eV ion bombardment and a less pronounced increase towards lower ion energies. Since the TL parameters were found to be constant above 300 eV the trend at higher energies is believed to be genuine. At ion energies $E_{ion} \geq 300$ eV no difference in absolute values of $d_{a-Si}(E_{ion})$ and $d_r(E_{ion})$ are observed for the three multilayer models. Below 300 eV the variations in $d_{a-Si}(E_{ion})$ are within a factor of 2, that is because the amorphous material in rough layer is not accounted for. This can be taken care of by introducing the effective amorphous layer thickness $d_{eff} = d_{a-Si} + 0.5 \cdot d_r$, which varies only by a factor of 1.3 between the various multilayer models at a specific ion energy. It seems that at lower ion energies the modeling results become slightly less accurate. The main reason

is of course that the penetration depth of the Ar^+ ions is low, thus, the thickness of the amorphous layer will be rather small.

All these aspects and the fact that the absolute values of χ^2 are only slightly higher for model (c) ($\chi^2 = 3-4$) than for models (a) and (b) ($\chi^2 = 2.5$) have resulted in a choice for the use of model (c) in the analysis of all SE measurements discussed in this article, which means fixed dielectric functions for the $a-Si$ and only two fit variables: the amorphous layer thickness d_{a-Si} and the surface roughness layer thickness d_r .

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