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Ellipsometric Characterization of Very Thin Gate Oxides and Correlation with Electrical Properties

Y.Z. Yu
Department of Physics, Zhongshan University, Guangzhou, China

K.K. Hung, Y.C. Cheng
Department of Electrical Engineering,
University of Hong Kong, Hong Kong

Spectroscopic Ellipsometry is used to investigate the microscopic structure of the interface between Si and its thin thermal oxide. Analysis of the measured spectra reveals the presence of an interlayer between the substrate and the oxide layer. The interlayer is found to have an average composition of $SiO_{0.8}$ and the width varies inversely with the oxide overlayer thickness. Moreover, direct correlation is observed between the interfacial structure and the electrical characteristics of the resulting metal-oxide-semiconductor devices.

§1. Introduction

The interface between Si and its thermal oxide has been a subject of intensive study for many years due to its overwhelming importance. Numerous research efforts have confirmed the existence of a transition region at the interface which shows a rather different nature comparing to that of bulk oxide.[1] Recently, the interest has been extended to thin oxides due to their increasing applications in VLSI technology. As the $Si-SiO_2$ interface plays a dominant role in determining the electrical performance of the metal-oxide-semiconductor (MOS) devices, obviously a systematic investigation of the interfacial structure of thin oxides will be highly informative.

In this summary, we report our attempt to study the interfacial structure of thin gate-oxides using the technique of spectroscopic ellipsometry.[2] It has been recognised that ellipsometry is particularly suitable to study such a system jointly due to its non-perturbing manner and high sensitivity to surface structure.[3,4] By varying the wavelength of the incident beam, a wealth of information on both the chemical composition and geometry of the structure can be extracted. In order to investigate the effect of the interface on the electrical properties of the resulting devices, MOS transistors were fabricated on the same substrate, for which the channel mobility was accurately measured. Direct correlation is observed between the electrical properties and the interfacial structure.

§2. Experimental

The ellipsometric parameters $\psi(\lambda)$ and $\Delta(\lambda)$ of the oxide films were measured at an incident angle of 70° by photometric method,[2] with the wavelength λ varying from 4800Å to 7400Å. The samples are bare gate-oxide films grown on the same substrate on which active MOS devices were fabricated. The Si wafers are p-type, with 12-22 Ωcm resistivity and (100) surface orientation. The oxidation process was carried out in an ambient of diluted O_2 at 1050°C, and followed by in-situ N_2 annealing at the same temperature. The oxidation time was varied to obtain four different oxide thicknesses, ranging from 150Å to 450Å. As a control experiment, another series of etched-back oxides were also characterized. For these samples, the oxide films were first grown to about 450Å and annealed as usual. Then they were etched in diluted HF solution to different thickness at a rate of 1Å/sec. As there is no high temperature process following the etching step, it is expected that the etched-back samples have identical $Si-SiO_2$ interface despite the variation of oxide thickness.

MOS capacitors and transistors were fabricated using a standard metal-gate technology. The fixed oxide charge density was

determined from high frequency C-V measurement with the MOS capacitors and the channel mobility from drain conductance of the MOS transistors. The details of electrical characterization have been published elsewhere.[5)]

§3. Analysis and Results

The experimental spectra of ψ and Δ are analyzed based on different hypothetical models of the $Si\text{-}SiO_2$ system. The system configuration consists of a crystalline-Si substrate, an interlayer, an oxide overlayer, and the air-ambient. The model parameters are optimized objectively by minimizing the root-mean-square deviation σ between the experimental and theoretical spectra,

$$\sigma = \frac{1}{N}\{\Sigma_N[(\psi_{exp}-\psi_{cal})^2 + (\Delta_{exp}-\Delta_{cal})^2]\}^{\frac{1}{2}},$$

where N is the number of data points in each spectrum. Different microscopic models to simulate the interlayer have been tried and the validity is judged by how well it fits the experimental data. It is found that a model involving pyramids of Si buried in SiO_x ($0<x<2$), as shown in fig. 1, can generally produce the best results. A similar model has been proposed by Smith and Ghidini[6)] in studying the oxidation mechanism of Si.

To compute the model spectra we have to know the effective dielectric function of the interlayer as a function of its chemical composition. According to Webman's effective medium theory,[7)] the complex effective dielectric function $\varepsilon(\lambda)$ for a medium of microscopic mixture of Si and SiO_x is given by,

$$(1-\nu_{Si})\frac{\varepsilon_{SiOx}(\lambda)-\varepsilon(\lambda)}{\varepsilon_{SiOx}(\lambda)+2\varepsilon(\lambda)} + \nu_{Si}\frac{\varepsilon_{Si}(\lambda)-\varepsilon(\lambda)}{\varepsilon_{Si}(\lambda)+2\varepsilon(\lambda)} = 0 ,$$

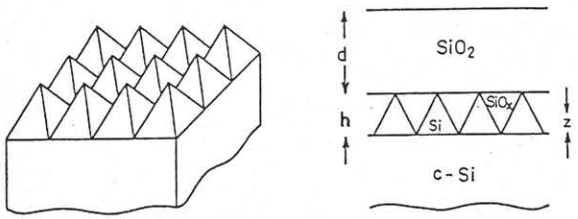


Fig. 1 A hypothetical model of $Si\text{-}SiO_2$ system

where ν_{Si} is the volume fraction of Si in the mixture, $\varepsilon_{SiOx}(\lambda)$ and $\varepsilon_{Si}(\lambda)$ are the complex dielectric functions of SiO_x and Si, respectively. For given x, $\varepsilon_{SiOx}(\lambda)$ can be determined from the experimental spectra of $\varepsilon_{Si}(\lambda)$ and $\varepsilon_{SiO2}(\lambda)$ following the scheme suggested by Zuther.[8)]

For the pyramidal model, the average volume fraction of Si over a plane is a function of its location. For numerical reasons, the interlayer is further partitioned into a number of sublayers parallel to the interface, such that ν_{Si} of each sublayer is approximately constant. For the sublayer confined by the two planes at distances z_1, z_2 from the basal plane of the pyramid, one has

$$\nu_{Si} = 1 - \frac{z_1+z_2}{h} + \frac{z_1^2+z_1z_2+z_2^2}{3h^2},$$

where h is the height of the pyramid. The ellipsometric parameters of the entire structure can readily be calculated using the standard equation of reflection for a multi-film planar structure.[2)]

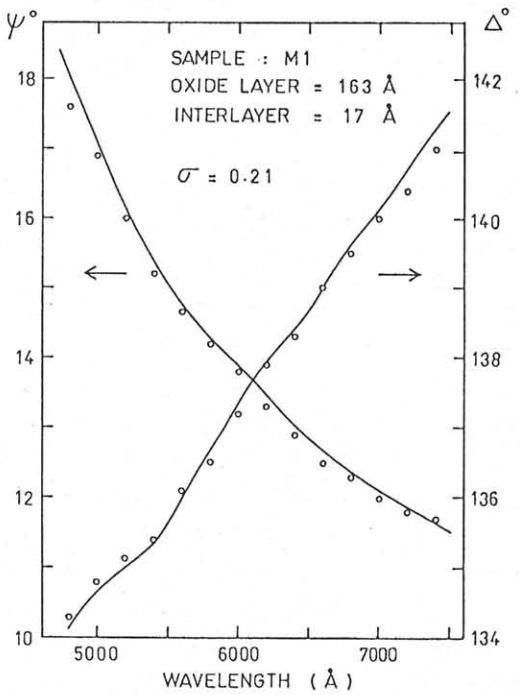


Fig. 2 Comparison between the experimental spectra of ψ, Δ(circles) and the calculated spectra (solid line) based on the model of Fig. 1.

The adjustable model parameters are the thicknesses of the interlayer (h) and the oxide overlayer (d). In the present model, the stoichiometry (x) of SiO_x is assumed to be independent of the oxidation conditions, and obtained by fitting over all the samples.

The experimental and calculated spectra for a typical sample are shown in fig. 2, with the numerical results for all the samples summarized in table I. For the as-grown oxides, it is found that the interlayer width increases inversely with the oxide thickness. The interlayer thickness of the 451Å oxide is 6Å which is consistent with the results reported for thick oxides.[3,4] For the etched-back oxides, the interlayer thickness is constant within the experimental error. The control experiment clearly demonstrates that the observed thickness dependence of the optical properties of the as-grown oxides is due to their interfacial structure rather than to any possible systematic error inherent with the geometry of the oxides. Our finding is not inconsistent with the recent experimental results of Carim and Bhattacharyya.[9] By high-resolution transmission electron microscopy (HRTEM), they observed that thin oxides may possess very rough interfaces comparing to that of conventional thick oxides.

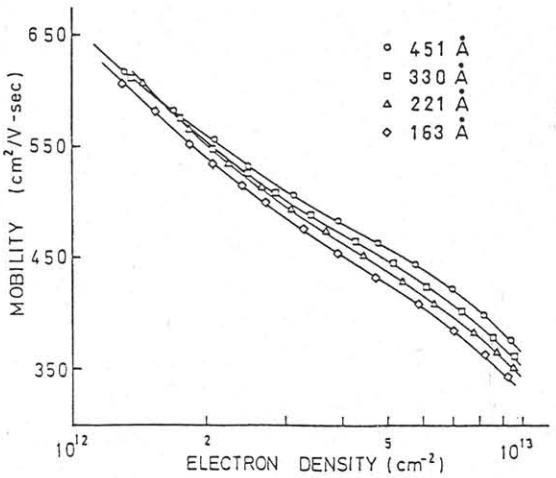
For the pyramidal model, the average chemical composition of the interlayer is roughly equal to 1/3Si + 2/3 SiO_x. The optimal stoichiometry of SiO_x is found to be x = 1.25. therefore the average composition of the interlayer is $SiO_{0.83}$ or SiO_2 + 1.4Si, implying the presence of excess Si. The result is in qualitative agreemet with the interlayer composition obtained for thick oxides.[4]

TABLE I. Results of ellipsometric characterization

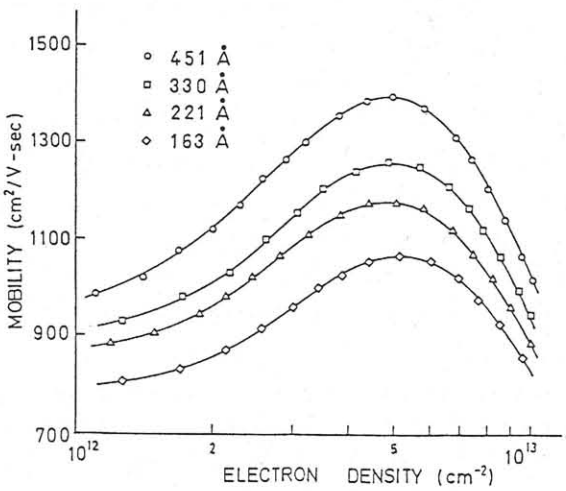
As-grown oxide			Etched-back oxide		
d(Å)	h(Å)	σ	d(Å)	h(Å)	σ
163	17	0.21	199	6	0.18
221	11	0.17	247	6	0.20
330	8	0.47	360	5	0.21
451	6	0.24	459	7	0.22
Stoichiometry of SiO_x : x = 1.25					

§4. Correlation of Interfacial Structure and Electrical Properties

The channel mobility of the MOS transistors were measured at 300K and 77K. The results for the as-grown samples are shown in fig. 3. Even at room temperature, the mobility of the as-grown samples clearly shows degradation with the reduction of oxide thickness. The thickness dependence can be partially explained



(a)



(b)

Fig. 3 Channel mobility versus induced electron density for the as-grown samples with different oxide thickness. (a) 300K, and (b) 77K.

by the role of coulomb scattering due to the higher fixed charge density inherent with thin oxides, which has been confirmed by high frequency C-V measurement. At strong inversion, the contribution of coulomb scattering is weakened due to enhanced carrier screening. On the contrary, the thickness dependence of mobility increases monotonically with the surface electric field. It suggests that the dependence may arise from different degree of roughness scattering.[10] The channel mobility of the etched-back samples has also been measured. No systematic dependence of the mobility on the oxide thickness is observed,[5] as expected.

The observed correlation between electrical properties and ellipsometric results provides evidence that the thickness dependence of mobility is partly due to the interfacial structure. The interlayer thickness reflects the degree of departure from an ideal interface, and may be loosely interpreted as the asperity height of the interface roughness.[10] In other words, the graded composition of the interface allows penetration of the wavefunction of the channel carriers into the transition region, resulting in additional scattering.[11] Both pictures can equally describe the effect of interlayer on the channel mobility.

For thick oxides, Hahn and Henzler found a strong correlation between channel mobility, oxide charge density, and the interface roughness revealed by the technique of low-energy electron diffraction.[12] In their HRTEM study on thin oxides, Carim and Bhattacharyya observed a direct correlation between the interface roughness and the undesirable electrical characteristics.[9] Our results are in agreement with their observation and may be regarded as a natural extension of the findings of Hahn and Henzler to thin oxides.

§5. Conclusions

The transition region at the Si-SiO_2 interfaces of thin gate oxides is characterized by spectroscopic ellipsometry. A microscopic structural model has been proposed to simulate the effect of the interlayer. It is found that the width of the interlayer increases inversely with the oxide thickness which may have a very significant implication when dealing with submicron devices. Direct correlation is observed between the interfacial structure and the electrical properties of the resulting MOS devices, which provides evidence that interface roughness may play an important role in the observed mobility degradation with oxide thickness for thin-oxides.

Acknowledgments

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