Electronic Properties and Gap State Defect Passivation of Si/SiO_2 Nanostructures

Bert Stegemann, Daniel Sixtensson, Manfred Schmidt

Hahn Meitner Institute Berlin, Dept. Silicon Photovoltaics, Kekuléstr.5, D-12489 Berlin, Germany

bert.stegemann@hmi.de

A main loss factor in conventional solar cells is the mismatch of solar spectrum and bandgap energy of the absorber material. Thus, photons with energies above the bandgap generate hot carriers which lose their excess energy via thermalization. A concept in 3rd generation photovoltaics that aims to circumvent thermalization losses is to realize appropriate Si based nano- und quantum structures, such as stacked Si/SiO_2 multi quantum wells, that provide bandgap tunability and thus adaptation to the solar spectra via utilization of quantum size effects [1]. However, due to increased interface-to-volume ratios at reduced dimensions, charge carrier recombination at the SiO_2/Si interfaces is facilitated, which lowers the solar cell efficiency. To overcome this drawback, experimental methods are required, that are capable of preparing well-defined Si and SiO_2 layers and of minimizing interface losses. Moreover, adequate analytical tools have to be developed to reveal information about the chemical, structural, and photoelectrical properties at atomic level.

These are the main issues that are addressed in this paper. The focus is on the study of a model system consisting of an ultrathin SiO_2 layer upon a Si(111) wafer representing one of the interfaces as a constituting building block of such a Si/SiO_2 quantum well device. For highest possible purity and control, complete preparation as well as full interface characterization was performed under ultrahigh vacuum (UHV) conditions. Under such conditions plasma oxidation using neutral, thermalized oxygen atoms is found to be superior to conventional thermal oxidation. The transmission electron microscopy image (TEM) in Fig. 1a shows such a homogeneous SiO_2 layer on Si(111) with uniform thickness of about 2 nm and proves the successful formation of an abrupt interface structure. Analysis of the chemical shift by x-ray photoelectron spectroscopy (XPS) revealed dominant contributions of the oxidation states Si^{0+} and Si^{4+}, corresponding to Si and SiO_2, respectively, and extremely low amounts of the intermediate oxidation states Si^{1+}, Si^{2+}, and Si^{3+} (Fig. 1b) [2]. Thus, high quality ultrathin SiO_2/Si interfaces with compositionally abrupt transitions were obtained by UHV plasma oxidation.

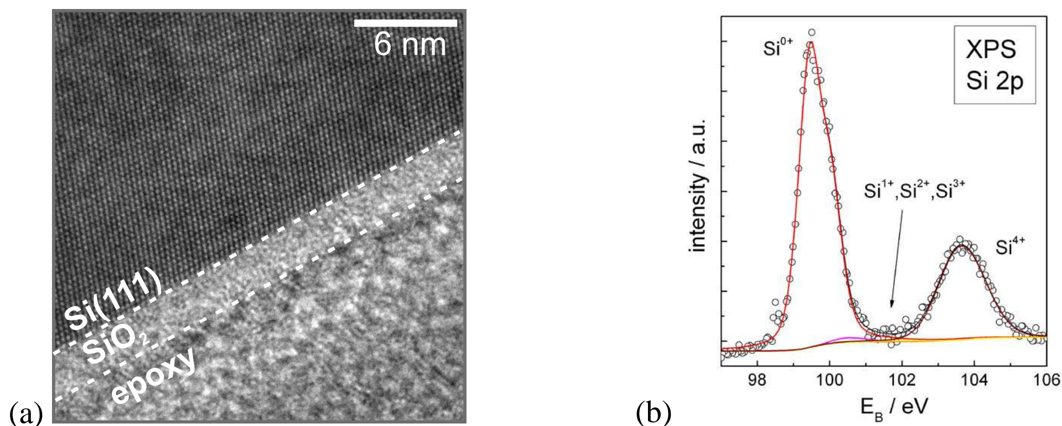

Fig. 1: (a) Cross-sectional TEM image of an ultrathin SiO_2 layer on Si(111) obtained by UHV RF plasma oxidation (P_{RF}=400W, T_{sub}=600°C). (b) Corresponding Si 2p XPS spectrum. Line shape analysis elucidates major contributions from oxidation states Si^{0+} and Si^{4+}, corresponding to Si and SiO_2, respectively.

Recombination losses at the SiO_2/Si interface are mediated by defect states located within the bandgap. Hydrogen is known to passivate such defect states. Therefore, an *in situ* passivation method using low pressure hydrogen plasma up to 10^{-4} mbar with nearly thermalized atoms was established. The decrease of interface gap states upon hydrogen treatment was investigated by near UV-excited photoelectron spectroscopy measurements of the internal yield carried out in constant final state

(CFSYS) mode [3,4]. This technique allows deducing the number of occupied states and was successfully applied to the *in situ* spectroscopy of the density of gap states D_{it} at the SiO_2/Si interface. Comparison of the two curves in Fig. 2a as measured by CFSYS before and after hydrogen plasma treatment reveals a distinct decrease of the gap states around midgap, what can be assigned to a passivation of Si dangling bonds. Contrary, occupied states close to the valence band edge are not influenced by passivation. Thus, these states most likely originate from stress induced tail states rather than from dangling bonds [5].

For comparison, the influence of hydrogen plasma passivation on the SiO_2/Si interface state density was determined from field-dependent SPV measurements (Fig. 2b). It is seen, that as in CFSYS the density of gap states decreases by about one order of magnitude and the width of the measured distribution increases significantly. The former is considered to result from passivation of dangling bonds, while the latter is due to removal of the FERMI level pinning, which results in high defect densities in the band gap and which impedes field induced band bending. Comparison of the D_{it} curves in Figs. 2a/b reveals the striking potential of CFSYS. The measured region is much wider because SPV measurements suffer from the prerequisite that the band bending must be swept over the whole energy range where one wishes to measure the density of interface gap states [6]. Moreover, CFSYS enables a complete *in situ* cycle from preparation and passivation to interface characterization without breaking UHV.

With respect to photovoltaic application this study is extended to Si/SiO_2 single and multi quantum well structures [7]. For these structures it is imperative, not only to prepare high quality interfaces but also highly crystalline Si layers with preferred crystallographic orientation to avoid additional losses due to gain boundary induced defects.

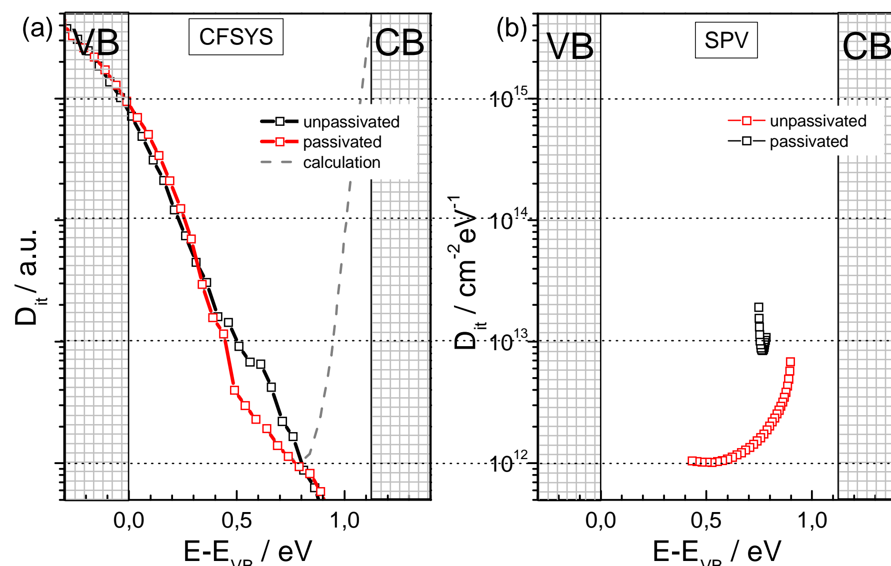

Fig. 2: Influence of UHV hydrogen plasma passivation on the density of states D_{it} at the ultrathin SiO_2/Si(111) interface. (a) *in situ* CFSYS measurement. The valence band edge is chosen as origin of the *x* axis; the *y* axis is scaled in arbitrary units that it matches the minimum of the D_{it} curve in (b). The gray line represents the calculated D_{it} values. (b) Field-dependent SPV measurement.

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