A novel MOSFET device with TaN/HfAlO gate stacks, silicon-carbide source/drain stressors, strained channel, and silicon-on-insulator (SOI) structures. Various analytical needs are highlighted. The measurements presented here were obtained with an FEI Titan (STEM), equipped with a monochromator and a Gatan Tridiem EELS detector. The microscope was operated in various modes to measure different properties, as will be discussed below.

KEY APPLICATIONS
Ultranan Gate Dielectrics
The ultrathin SiON gate dielectric has been and remains one of the most important materials among semiconductor devices. Its performance, reliability, integrity, leakage, and breakdown behavior have been studied for over 50 years and yet until today, a basic physical and atomic understanding is still missing. Phenomenological models such as percolation path have been successfully applied to explain interface suboxide SO$_2$ layer local k-value monitoring, and thickness monitoring on each layer down to Å-level accuracy.

The silicon channel which is engineered using elevated silicon-carbide source/drain stressors needs to be monitored for its local bandgap, lattice strain, carbon (or germanium in the case of pMOSFETs) interdiffusion, and barrier height (if a Schottky source/drain is used). Ideally, all these analyses need to be done within a device area where the electrical measurement and transistor parameters have been extracted. Such analytical challenges did not exist a few years ago when MOS transistors were composed of only two materials, silicon and silicon dioxide.

With the fast path technology push [2], the analytical requirements for future process technology nodes will only be more challenging. By 2010, we need to be able to measure dimensions of physical features as small as three atomic layers, observing interface roughness of less than one atomic layer, analyzing chemical bonding within two to three atomic layers, characterizing bandgap energies within five atomic layers, and detecting local lattice strain within 10 atomic layers. And all this needs to be done using the real devices instead of large test-key structures.

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most of the electrical breakdown and reliability behavior [3]. Yet, the true nature of a breakdown percolation path has remained to be a mystery for the last 50 years since the invention of MOSFETs.

The holy grail in this study is to pinpoint the breakdown location down to the nm scale and to clearly show its atomic and chemical nature. The challenges are in two different aspects. Firstly, the exact location of breakdown needs to be identified with an accuracy of a few nm, followed by the preparation of a cross-sectional TEM sample from such a location. Percolation paths are invisible in traditional TEM and STEM image modes so there is no simple way to know if the sample prepared contains the percolation path for dielectric breakdown. A clear signature must be identified to navigate the search and to ensure the existence of a percolation path. Secondly, since the true nature of a percolation path is uncertain, there is no clear indication on what are the proper tools that can be used to identify and characterize the percolation path.

Fortunately, the first problem has been resolved recently. Gate dielectric breakdown due to electrical stressing or testing can trigger damages to the physical integrity and microstructures of the device [4,5]. It has been demonstrated that dielectric breakdown induced epitaxy (DBIE) marks an important physical signature where the invisible percolation path can be located unambiguously [6].

Figure 2 shows TEM and STEM images of a 2 nm gate dielectric breakdown location. The DBIE is identified and marked. The percolation path directly on top of DBIE is invisible in ordinary TEM/STEM imaging condition. The next question is how to probe and characterize the percolation path. Here, STEM imaging and high resolution electron energy-loss spectroscopy (EELS) is used to study the percolation path.

Popular gate dielectric breakdown theories predict that Si-O bond breakage and the creation of oxygen vacancies (E’ centers) are possible mechanisms involved in the creation of a percolation path [7,8]. If the theories are correct, the breakdown path should contain signatures potentially detectable using EELS. Figure 3 shows Si-L$_{2,3}$ and O-K core-loss EELS spectra from both a breakdown path and reference locations. It is clear that the breakdown oxide has a different bonding structure from the normal gate dielectric SiON. The results show that the percolation path is a highly oxygen-deficient sub-oxide channel. Local band lowering may have occurred accompanied by the formation of defective bonds and intermediate states [9].

In Figure 3a the background corrected Si-L$_{2,3}$ edge spectra from two different positions are shown. The spectrum for a non-breakdown (normal) gate oxide (dash-dotted blue line) has the Si$^{4+}$ bonding characteristics at 106 and 108 eV with a shoulder peak extended down to 100 eV [10]. The additional energy states appeared below 106 eV are attributed to the delocalized signals from the interface sub-oxide [11,12]. The Si L$_{2,3}$ edge for the breakdown oxide (solid red line) as compared to the non-breakdown oxide (dash-dotted blue line) shows reduced intensities at 108 eV (Si$^{4+}$) but raised intensities between 100 eV and 105 eV (representing Si$^+$ and intermediate oxidation states: Si$^{2+}$, Si$^{3+}$ and Si$^{4+}$).

Our momentum-resolved density of state (DOS) calculations (not shown) using electron density functional theory (DFT) performed on an α-quartz model shows that oxygen vacancies lower the s-states at 108 eV but create more s- and d-states at and below 106 eV, which agrees with the current experimental observations [13]. The obvious increase in the EELS intensities from 100 eV to 105 eV suggests the presence of Si atoms coordinated with less than 4 oxygen atoms (i.e. suboxide) and possible Si nanoscopic clustering [10].

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The O-K edge core-loss from the bulk oxide (solid), the non-breakdown (dashed), and the breakdown (dash-dotted) gate oxide are presented in Figure 3b. The first absorption peak at 537.8 eV as shown for the bulk oxide (solid line) can be directly related to the local conduction band electronic properties [15,16,17]. The spectrum for the non-breakdown gate oxide (dashed line) has the same absorption peak at 537.8 eV. However, the rising portion of the edge onset at ~530 eV is shifted to a lower energy as compared with the bulk oxide. This is likely due to the delocalized scattering from the interface suboxide which lowers the conduction band minimum [16,17].

The reduced edge onset is also observed for the breakdown gate oxide (dash-dotted line). Comparing the first peak position between the non-breakdown and breakdown gate oxide, the peak position shifts from 537.8 eV to 536.3 eV upon breakdown. It is believed such shift is a result of conduction band p-DOS redistribution within the percolation path. Our calculations for oxygen vacancies (VO) 5.6 at% within SiO$_2$ have shown a 0.2 eV DOS peak lowering, confirming that oxygen vacancies are a possible cause for the 537.8 eV peak shift to 536.3 eV. A red shift (to a lower energy of about 4 eV) is observed in the second absorption peak (~560 eV) for both breakdown and non-breakdown gate oxide. This shift originates from the presence of stretched

Figure 3:
Electron energy-loss spectroscopy core-loss on (a) Si-L$_{2,3}$ edge and (b) O-K edge, showing the possible chemical bond changes in a gate dielectric breakdown percolation path.
O-O bonds in the ultrathin gate oxide and was not affected by the breakdown [18-20].

The breakdown gate oxide as compared with the non-breakdown gate oxide shows significantly lower O-K core-loss signals, arising from the missing O atoms at the breakdown site. The deficiency of O atoms within the breakdown SiO₂ can also be quantified using the core-loss signal intensities [21]. The Si/O ratios are calculated using the respective edge intensities for the breakdown oxide while using the non-breakdown oxide calibrated as SiO₂ with Si/O = 0.5. Oxygen deficiency within the breakdown path calculated in this approach is as high as 50-60%.

From the results shown in Figure 3a, the intensity change in Si-L₂,₃ edge is minimal compared with the O-K edge. This suggests that oxygen depletion, instead of silicon accumulation, is the chemical and atomic mechanism for the ultrathin SiO₂ oxide breakdown path formation. This also suggests the possibility of using the O-K and Si-L₂,₃ core-loss signals to evaluate the degree of the breakdown, i.e. the ‘hardness’ of the percolation path.

The above described routine of site-specific chemical analysis using STEM EELS helps to unambiguously locate the breakdown percolation path, even when it is invisible in TEM/STEM images. Si-L₂,₃ and O-K core loss EELS show that oxygen deficiency is the key signature for the structural change in the breakdown path. Chemical bond breakage and the local joule heating due to large current surging through the percolation path are believed to be the main driving forces leading to the oxygen dissociation and wash-out. The creation of oxygen vacancies results in the formation of Si²⁺ while Si³⁺ and Si¹⁺ will be formed when increasingly more oxygen atoms are removed. The presence of Si nanodusting is highly possible within the percolation path.

As discussed by Neaton et al. [17], the variation in oxygen nearest-neighbors results in different local energy gaps. It is believed that the local energy gap at the breakdown path could collapse after the removal of oxygen atoms and the rearrangements of local atomic structures. A nanoscopic conduction path is therefore possible inside the highly oxygen-deficient SiO₂ breakdown location.

STEM-EELS has proven to be an ideal analytical tool for the study of percolation path in very thin dielectrics. The discussed findings will have important implications on our fundamental understanding of gate dielectric breakdown and its reliability. Such understanding forms the foundation for process and technology engineers to push process limitation to the next level and helps to move semiconductor processes into the high-k metal gate domains.

**Silicon Nanowire (SiNW) Devices**

In addition to the above discussed probing of local chemical information, STEM EELS is also unique in providing a technique for measuring nanoscale optical properties of small semiconductor devices. As the relevant energy transitions have values of just a few electron volts, EELS measurements need to be done with high energy resolution. Experiments that combine high spatial and high energy resolution have become possible in the last few years with the development of electron beam monochromators that are incorporated in STEM instruments. In our case, a Wien-type monochromator is present in the electron accelerator and can be excited to disperse the beam electrons in energy. A wedge-shaped energy-selecting slit conveniently allows the selection of electrons with a narrow range of energies. Energy resolutions down to 0.1 eV are possible but in practice, a somewhat less monochromatic electron beam is generally used to maintain enough electrons for doing imaging and analysis.

In this example, we study a silicon nanowire with a triangular cross section, made using a recently developed method for growing CMOS devices [22]. A TEM specimen of the nanowire that is grown with this method uniquely provides a way to do measurements along the axis of the wire, not perpendicular as it is normally done. This orientation opens a route to study materials properties that can be directly related to the shape of the nanowire.

Figure 4 shows measurements that were done with a ~0.25 nm STEM probe and an energy resolution around 0.3 eV. It can be seen that the silicon nanowire is embedded in SiO₂; its cross-section is a somewhat elongated triangle. Through the long axis of the cross-section, an EELS line scan was taken, showing a modulation in the low-loss EEL spectrum, indicated by the dotted ovals. On one side of the nanowire, energy absorption takes place around 4 eV, while on the other side, the absorption is stronger around 8 eV. The energies of these modulations indicate that they result from interface plasmons. It is unlikely that they originate from Čerenkov radiation or guided-light modes, since these effects will only show a strong energy modulation when the specimen thickness varies strongly, which is not the case here. Nevertheless, the interpretation of the peaks in the EEL spectrum is difficult based on just these measurements.

Another factor that adds to the difficulty of interpreting these results is the electron beam damage which visibly occurs at 200 and 300 kV. Any TEM or STEM measurements on silicon or SiO₂ with such high electron beam energies should be treated with extreme care to avoid possible effects of specimen damage such as bond breaking, the creation of vacancies or overall change in morphology or composition.

To avoid misinterpretation, STEM EELS measurements were done on a similar nanowire at 80 kV electron beam energy. The monochromator was set to give energy resolution better than 0.2 eV and to compensate for the drop in beam current, a STEM probe with a diameter around 1 nm was used for the measurements shown in Figure 5. The EEL spectra were acquired in spectrum imaging mode, using the technique of binned gain averaging [23].

Figure 5a shows four points at the silicon-SiO₂ interface from which the four spectra in Figure 5b were taken. The peaks that were only vaguely visible in the data of Figure 4 are much more clearly seen and indicate that the peak modulation also occurs along the edge of the silicon nanowire.

To get a more clear insight in the origin of these energy transitions, EELS mapping provides a powerful visualization technique. Using an EEL spectrum image that was acquired from the same area as Figure 5a, the EELS intensity was plotted at 4.6 eV and 8.4 eV, giving Figures 5c and 5d, respectively. The EELS maps show that the low-energy transition around 4.6 eV is excited more strongly at the corners of the nanowire, while the high-energy transition around 8.4 eV is more localized to the long edges of the wire. The results seem to indicate that surface plasmons on the relatively flat Si-SiO₂ interfaces start to resonate when the distance between the flat surfaces decreases, as is the case near the corners.

A more systematic study is underway to clarify this effect and its consequences for low-loss EELS measurements on nanometer-sized silicon structures.
Specimen preparation has been and still is one of the most important steps in a successful TEM analysis. This is particularly true in semiconductor device and process analysis where the target areas for analysis are often smaller than a few hundred nm. Such samples are now routinely prepared by using focused ion-beam (FIB) technology. However, a well-known problem with FIB-prepared samples is the artifacts introduced by ion-beam damage and ion-beam contamination.

For HREM, HRSTEM and monochromatic EELS analysis, the requirements for sample quality are exceptional. Ultraclean and ultra-flat samples are needed. Sample thickness control is also an issue: a thinner specimen is not necessarily a better sample; the sample thickness needs to be decided based on the analysis requirements. A sample good for core-loss EELS might be too thin for strain measurements. It is thus necessary to determine the optimal sample thickness by testing a few different sample thicknesses for the best results.

Specimen damage by the electron beam is another challenge when TEMs or STEMs are used to study semiconductor devices. As mentioned earlier, beam damage can significantly change the structure and properties of the specimen material and should always be taken into consideration when experiments are planned. In our silicon/SiO₂ nanowire structures, beam damage was clearly observed in both TEM and STEM modes for 200 and 300 keV beam electron energies. This well-known effect is unfortunately not always taken into account when images or EELS data are analyzed. When reliable EELS data are needed from a specimen and cannot be acquired rapidly with a low electron dose, there is no choice but to do these measurements at decreased beam acceleration voltages, in our case at 80 kV. Of course, the ultimate spatial resolution of the measurements degrades when lower beam energies are used. At the same time, the penetration depth of the electron beam is less, so the specimens need to be extra thin to compensate for the decreased electron mean free path.

With the availability of a monochromated, high-resolution STEM, it might be tempting to try doing new types of measurements, such as atomic-resolution band gap measurements. However, expectations should not be too high in this regard as these are two important obstacles for these kinds of measurements. Firstly, there is the well-known effect of electron delocalization: small energy transitions can be excited a large distance away from the actual position of the electron beam. Large electron energy transitions on the other hand, are usually excited over much shorter distances. For low-loss EELS measurements, we therefore have to take into account the effective beam diameter, which will be much larger than the real STEM probe diameter. Even when we do STEM EELS with a very small probe, atomic-resolution measurements are all but impossible below 50 eV, while at even lower energies (equivalent to the visible region of the electromagnetic spectrum), the effective probe size will be several nanometers in diameter. Secondly, now that the very low-energy part of the EELS spectrum can be measured at the nanoscale, we seriously have to think about multi-electron and relativistic effects. A number of recent publications have addressed the challenges of interpreting very low-loss EELS data [24-27] and it was shown that interface or surface plasmons, guided light modes and also Čerenkov radiation can completely obscure any band gap information that might be present in the data. Again, the way in which EELS experiments are done will need to be reconsidered and even modified.

CONCLUSIONS

The scanning transmission electron microscope is more than just an imaging microscope. It has evolved into a platform of analytical technologies where most necessary information can be extracted at near-atomic scale. Basic understandings on nano-electronic devices can be gained including nanoscale physics, chemistry, and processes using a single TEM platform. The knowledge that analytical TEM provides will greatly aid the development of novel structures and devices for nanoelectronic applications.

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