Thick gate oxide extrinsic breakdown – the potential role of neutral hydrogen atom

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Abstract – Power electronics is currently a hot topic due to its important role in fighting climate change. Gate oxide breakdown is the Achilles heel of power devices, and it is well known that extrinsic breakdown is the chief concern. However, the root cause of extrinsic breakdown is poorly understood. Recently, a "lucky defect" model was introduced to explain extrinsic breakdown beyond the traditional "local thinning" model. In this work, the "lucky defect" model is further developed to allow it to examine the responsible defect's energy distribution. It is found that only defects with energy 1.5 eV ± 0.3 eV above the substrate conduction band can produce the breakdown distributions commonly reported. Few studied defects can satisfy this requirement. An exception is the neutral hydrogen atom, and its known properties are consistent with experimental results in the literature. If confirmed, this has important implication on how to remedy extrinsic breakdown.

Index Terms: thick oxide; extrinsic breakdown, atomic hydrogen, trap-assisted-tunneling

Introduction

Wide bandgap semiconductor-based power electronics are rapidly making commercial inroads in old and new applications, generating excitements about the dawn of all electric transportations. However, reliability remains a concern of many engineers. Gate oxide breakdown is one of the reliability issues, particularly extrinsic breakdown failures [1]. Extrinsic breakdown of thick gate oxide is surprisingly not a problem unique to wide bandgap semiconductor-based power devices. It is a persistent problem in power electronics employing "thick" gate oxides [2-4]. Indeed, there is strong similarity between breakdown distributions in thick oxide grown on SiC and those on silicon, hinting at a common origin.

Most literature reports link extrinsic breakdown to weak points (thin spots or defects) in the oxide film due to contaminants. The local thinning or its equivalent idea was formulated by Lee et al. [5]. The local thinning being an actual physical reduction of oxide thickness was reenforced by the same group later [6]. The non-thinning weak points' (defects) contribution are largely ignored since then as a cause for extrinsic breakdowns. The local thinning model suggests that the way to minimize/eliminate oxide extrinsic breakdowns is by relentlessly improving the cleanliness of the processes leading up to the oxide growth step. However, this approach reduces extrinsic breakdown only to a certain extent, beyond which cleaning efforts cannot further improve the breakdown distribution, leading to the persistent extrinsic failure problem mentioned above.

Clearly, there is a need to go beyond the local thinning model to address the persistent extrinsic breakdown problem. An obvious choice is to bring back the defect related weak points even though how does a defect becomes a weak point has never been clarified. To that end, a "lucky" defect model was introduced [7,8]. In this model, oxide point defects with the appropriate energy and distance from the interface can increase the local current flow under electric stress and therefore shorten the lifetime. The model produces extrinsic breakdown without the physical reduction of oxide thickness. It was able to reproduce the observed, post-cleaning extrinsic breakdown distributions. The important consequence of the lucky defect model is that it is possible to *further* minimize/eliminate extrinsic breakdowns by improving the oxide growth process. While no specifics are given, several recent reports in the literature hinted at improving the growth process did have an impact on extrinsic breakdowns [9,10].

The "lucky' defect model did not specify the details of these lucky defects, rather just relying on the assumption of their presence. In this work, the "luck" defect model is further developed to examine what candidates that could serve as "lucky" defects.

Trap-Assisted-Tunneling (TAT) with two defect types

The "lucky" defect model leverages four well accepted ideas about gate oxide breakdown: (1) current flow through the oxide during stress drives new defect creation; (2) breakdown occurs when defect density reaches a critical level; (3) the critical defect density is area and oxide thickness dependent and (4) Trap-assisted-tunneling (TAT) enhances current flow locally. No other assumptions are required.

There are many defects exist in thermally grown SiO_2 films, regardless of the film quality. While many defects affect the performance of the metal-oxide-semiconductor-field-effect-transistor (MOSFET) in varied ways, only defects with the appropriate energy and spatial location can affect the breakdown distribution by increasing the tunneling current through the TAT mechanism. These are the "lucky" defects. The aim of this work is to further explore the characteristic of the "lucky" defects. Specifically, under the uniform spatial distribution assumption, the energy constraints of the defects. More details of the simulation procedure have been given in a recent publication [11].

Fig. 1a is a typical breakdown distribution for a thick gate oxide capacitor structure [1]. These capacitors are thermal oxide on SiC. Many similar distributions are found in the literature for thermal oxide on Silicon [2-4]. Three regions are commonly identified: dead-on-arrival (mode A); extrinsic breakdowns (mode B) and intrinsic breakdowns (mode C). It is believed that mode C and mode B are distinct distributions [4].

Fig. 1b shows, under the "lucky' defect framework, the band diagram of TAT with two defect bands at different energies that could lead to the observed dual breakdown distributions. The question to address is that, starting with a Weibull breakdown distribution from a defect-free oxide film of a given thickness under a given electrical stress field (assuming the percolation model works), what kind of defect distribution can produce the experimentally observed mode B breakdown distribution (under the same electrical stress field)? Similar

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question was addressed for the mode C distribution in a previous work [11], and it was found that the narrow defect band (close to the electron injection Fermi level) is required. Mode B being a distinctly different distribution, a different type of defects will be needed to produce it. In this work, the same simulation approach is used, with an additional defect distribution added to produce the extrinsic failure distribution (mode B).

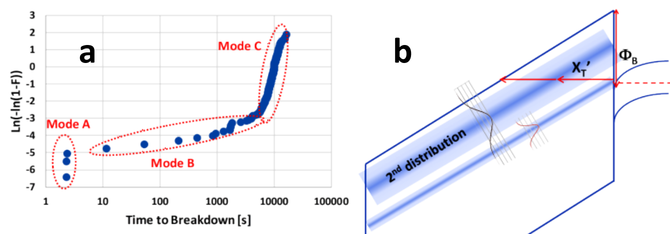

Fig. 1. a: typical breakdown distribution for thick oxide in Weibull scale. 3 modes are commonly identified. b: the band diagram for tarp-assisted-tunneling with two uniformly distributed (spatial) defect bands each has a Gaussian energy distribution as shown. The defect is located at X_T'.

Results and discussion

The mode B distribution represents much more severe lifetime degradation than mode C, the defects responsible must have an energy distribution center around or at least close to the "sweet spot" where the TAT is peak. Referring to fig. 1b, the defect distribution responsible for extrinsic (mode B) breakdown must be at energy substantially higher than the electron injection Fermi level. The question is how high? The simulation framework can vary the mean energy and the energetic distribution of the defects to help determine the characteristic of the second defect band. Fig. 2a shows a simulated breakdown distribution that bears great similarity with fig. 1a. The parameters were, for 1st (low energy) distribution, defect density was $1 \times 10^{10}/cm^3$; mean energy = 0.1 eV (above the electron injection Fermi level) and standard deviation = 0.025 eV [11]. For the 2nd (higher energy) distribution, defect density was $1 \times 10^8/cm^3$; mean energy = 1.7 eV and standard deviation = 0.6 eV. The starting defect-free breakdown distribution was β=40, and τ_{63}=100,000 s for 9 MV/cm field.

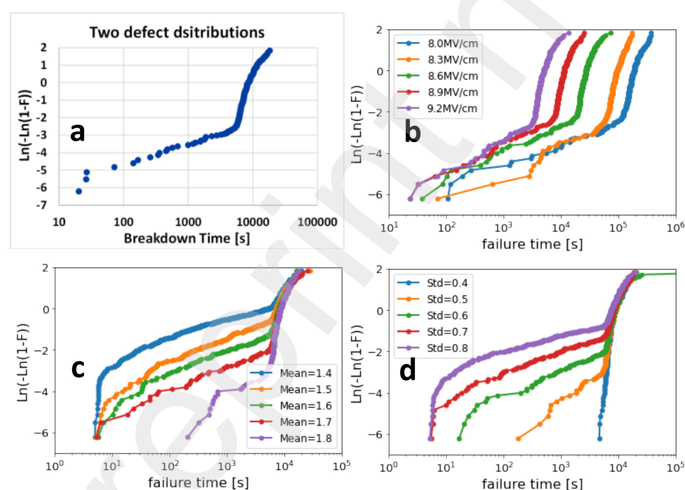

Fig. 2. a: a simulated breakdown distribution that looks very similar to the one in fig. 1a. b: the breakdown distributions when the stress field is varied. c: the breakdown distributions (at 9 MV/cm) when the mean defect energy in eV is varied. d: the breakdown distribution (at 9 MV/cm) when the defect energy in eV spread is varied.

For a given distribution with known βs for mode B and mode C, and the point at which mode B meets mode C, the simulation parameters to produce the distribution are quite tightly bounded. This provides confident in the simulation results.

Fig. 2b shows how the distribution in fig. 2a varies with stress field, similar to those reported in [12]. The β value for these extrinsic distributions is quite low. The reported β in the literature varies from close to 0.1 to over 1 [2, 12]. It is therefore important to use the simulation framework to check which variables control the observed β. Fig. 2c shows the result of varying the mean energy of the defect distribution. The results suggest that the mean energy does not change β for extrinsic distributions. The highest mean energy case, where β is larger, is likely due to a statistical artifact from the small numbers of extrinsic breakdowns.

Fig. 2d varies the standard deviation of the defect distribution. Here, a clear effect on the β values of the extrinsic distributions is evident - smaller energy spread leads to steeper Weibull slope. Conversely, those extrinsic distributions with high β in the literature signify a tighter defect energy spread, not lower defect density.

The transition from mode B to mode C is, intuitively, linked to the defect density which is borne out in additional simulations (not shown). However, fig. 2c suggests that the mean defect energy plays a strong role as well. One can understand this feature from the band diagram shown in fig. 1b. Note that TAT is sharply peaked at the optimal distance from the interface where the two tunneling steps have equal probability. This feature can be used to set a boundary for the defect's energy band (assume uniform distribution spatially).

With the standard deviation of the defect energy distribution as the main factor influencing β, and the mean defect energy as the main factor affecting where mode B meets mode C, one can, in principle find the mean defect energy and standard deviation for defects responsible for the extrinsic failures reported in the literature. As mentioned in the introduction, there is a strong similarity between the SiO_2/Si and SiO_2/SiC systems in the persistent extrinsic breakdown phenomena. It makes sense to include data from both systems in the literature [1-4, 12-21] for this analysis to find a common cause.

Unfortunately, most reports do not extract β from data so one can only perform an estimation from plotted data in the reports. With the reported breakdown distributions as constraints the defect energy is found to be 1.5 eV ± 0.3 eV for mean energy and 0.65 eV ± 0.15 eV for standard deviation. It should be emphasized that the uncertainties are chosen to accommodate all the known data in the literature, not from statistical analysis. Note that SiO_2/SiC system has conduction band offset 0.34 eV smaller than the SiO_2/Si system [10], so, having the same mean energy (above the injection Fermi level) means that, for the SiO_2/SiC system, the defect energy band is 0.34 eV closer to the SiO_2 conduction band. The SiO_2 film on SiC is expected to have higher compressive stress due to SiC's larger linear thermal expansion coefficient). If the defect energy is sensitive to compressive stress as discussed later, this could explain the higher defect mean energy.

Most studies of defects in the oxide focus on those with energies close to the substrate conduction band and valence band. This emphasis is because those defects are electrically accessible and therefore impact the performance/reliability of the MOSFET. Theoretical calculations rarely report defects with energies that extend outside of the range between the substrate valence band and conduction band. However, one exception is the neutral hydrogen atom [22-25]. While the calculated energy levels for the neutral hydrogen atom defect in SiO_2 do vary in the literature, the energy range matches the 1.5 eV ± 0.3 eV value reasonably well.

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Could trapped neutral hydrogen atom be the culprit for the persistent extrinsic breakdown problem in thick oxide? A closer examination is required. A common last step of processing is a forming gas anneal. This process ensures that hydrogen in various form exists in the oxide in high concentrations, and these hydrogen species interacts with defects through a series of complicated reactions [26-28]. Neutral hydrogen atoms are created and annihilated by these reactions. Compared to other hydrogen moieties, the neutral atom is energetically unfavorable and can easily be converted to charged states with lower energies [22-25]. It is therefore expected to be present in low concentrations and that these concentrations are controlled by kinetics rather than energetics [28]. Furthermore, neutral hydrogen atoms are known to interact with the passivate interfacial silicon dangling bonds exothermically to produce interface defects [28]. Thus, the neutral hydrogen atom can be expected to have even lower concentration near the interface.

From our simulations based on the "lucky" defect model, the neutral hydrogen atom density required to generate the extrinsic breakdown distribution is only $1 \times 10^8/cm^3$. The range of concentration that can produce the distributions reported in the literature is $1 \times 10^7/cm^3$ to $1 \times 10^9/cm^3$. These are very low concentrations. If these defects are indeed neutral atomic hydrogens, it is reasonable to expect such concentrations exists in all the thick oxides. That may explain why there is a persistent extrinsic breakdown problem in thick oxides.

The persistent extrinsic breakdown problem seems to only plague thick oxides. Ultra-thin oxides seem largely unaffected even though it too must have a lot of hydrogens. Indeed, nearly extrinsic-free breakdown distribution is commonly reported [29,30]. Fig. 3a shows that if the defect consistent with neutral hydrogen atom is present in similar concentrations, extrinsic failure should be observed in ultra-thin oxide (β=4), albeit less severe due to the benefit of strong area scaling [11]. How can this conflict be resolved?

As mentioned above, the neutral hydrogen atom concentration is expected to be lower near the interface, and that concentration is controlled by kinetics rather than energetics. For simulated ultra-thin oxide with β of 4, the thickness is about 5nm [31]. The effect of both interfaces will lower the neutral hydrogen atom concentrations. In addition, for an interface dominated film, the compressive strain level is higher which can lead to higher energy for the neutral hydrogen atom (neutral hydrogen atom does not form bond in the oxide, it merely exists interstitially [22-25]. Fig. 3b shows when the mean defect energy is shifted to 1.9 eV, extrinsic failures largely disappear.

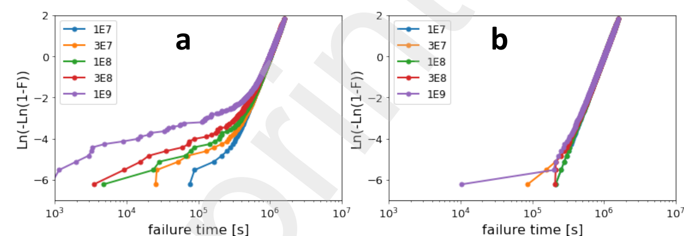

Fig. 3. a: extrinsic breakdown distributions for thin oxide (β=4) as a function of neutral hydrogen atom concentration (cm^{-3}) (9MV/cm). b: the thin oxide breakdown distributions when the defect mean energy is increased to 1.9eV.

While these simulation results are promising, the analysis can only identify the importance of defects exist in specific energy range centered at 1.5 eV ± 0.3 eV above the injection Fermi level. This is consistent with the neutral hydrogen atom trapped in SiO_2 and may be the defect responsible for the persistent extrinsic breakdowns in thick oxides. It does not rule out other defect candidates if they too have the identified energy and spread.

Conclusion

By using a simple model based on well established, widely accepted facts about oxide breakdown, the defect energy and standard deviation needed to reproduce extrinsic breakdown distribution is examined. The result is a well-defined defect mean energy and spread which is consistent with the theoretical energy of neutral hydrogen atoms. The known/expected nature of the neutral hydrogen behavior in oxide films is consistent with the model explanation of measured results in the literature. While not conclusive, it strongly indicates a strong role for neutral hydrogen atoms in extrinsic breakdown in thick gate oxide

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