Novel Mechanism for Tunneling and Breakdown of Thin SiO_2 Films

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It is suggested that resonant tunneling via defect-related states is an important mechanism for high-field carrier injection into thin SiO_2 films of metal-oxide-semiconductor structures. A model is also proposed for high-field insulator breakdown which cannot be explained by available theories.

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The use in metal-oxide-semiconductor (MOS) technology of ever thinner SiO_2 films subject to high electric fields has increased the interest in carrier transport within the insulator. Fundamental questions are still open; in particular, the mechanism causing oxide breakdown is not yet really understood since when film thicknesses t_{ox} are $\lesssim 100$ Å, it occurs at voltages too low for the available models to be applicable. In this work we address the problem of tunneling carrier injection, trapping, and breakdown from a new point of view. We suggest that resonance effects due to defect-related states in the insulator energy gap should be observed in tunneling through a thin SiO_2 film. Specifically, we point out that, since all the conditions required for resonant tunneling to occur are common to MOS structures and since it can give rise to extremely large effects, it should be an important mechanism for carrier injection at high fields. This has been generally neglected in the literature. For example, trap-assisted tunneling has been treated overlooking its intrinsic resonant nature.[1] On the other hand, resonant tunneling in SiO_2 has been experimentally realized[2] with use of a double-barrier structure. The case of resonant tunneling via defect states, which we consider here, differs in many respects from that of Ref. 2.

We also show how resonant tunneling produces carrier trapping near the injecting interface, i.e., within the tunneling distance. This implies a self-accelerating mechanism for current runaway due to positive feedback from space-charge build-up on the defect state. A rapid increase of (local) current then takes place with strong thermal effects eventually leading to irreversible failure. We suggest this as the most likely mechanism for high-field breakdown in thin insulators, $\lesssim 100$ Å, at applied voltages $V_a \lesssim 10$ V.

In this range the available models are inapplicable.[3] Impact ionization[4] is inadequate because the maximum energy gain available for tunneling carriers injected into the insulator conduction band (ΔE in Fig. 1) is not enough to impact ionize bonds regardless of the shape of the potential energy barrier (Fig. 1). For ionization V_a must exceed about 12 V since ΔE must be greater than the SiO_2 energy gap (~ 9 eV) and 3 eV are lost because of the cathode energy barrier. Another category of models relies on local intensification of the oxide field (E_{ox}) due to the buildup of space charge caused by carrier trapping within the insulator (Fig. 1). These theories, however, ultimately fail because the field never approaches the limit (roughly 100 MV/cm)

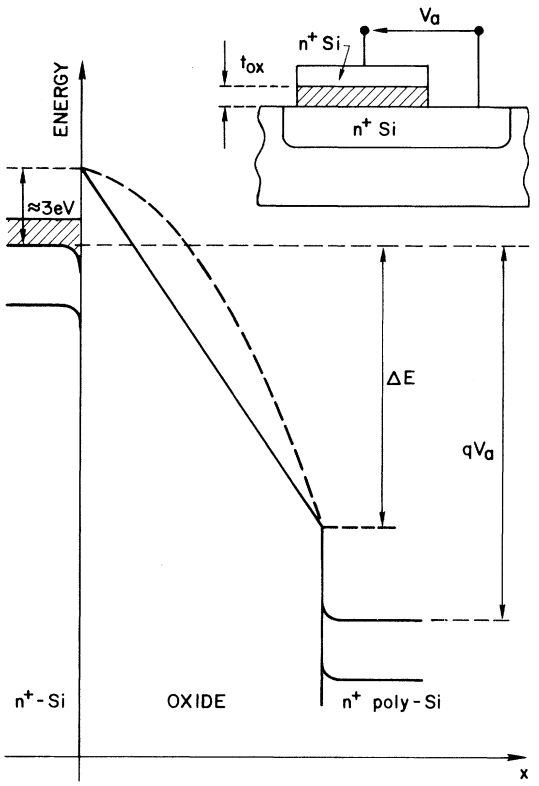

FIG. 1. Schematic representation (not drawn to scale) of the electron potential energy with (dashed line) and without (full line) electrons trapped within the insulator.

required to disrupt the material bonds by field effects.[5] Furthermore, thermal positive feedback for current runaway does not occur experimentally,[3] though the final stages of destructive breakdown involve extremely large thermal effects. Other proposed theories[6] can also be ruled out: Hole injection fails because breakdown occurs under conditions where there are no holes to be injected[3]; ionic effects imply the wrong temperature and time dependences[6]; other theories, for instance, that of gas discharge,[6] are only phenomenological and offer no microscopic picture.

We present here a model whose only requirement is the presence of localized electron states in the insulator energy gap. This condition is always observed in MOS structures as well as other electrode-insulator systems. For this reason, our discussion will be kept at a rather general level with the Si-SiO_2 system treated in more detail elsewhere. We do not discuss the origin of the localized states which we simply treat as wells in the potential-energy barrier (see Fig. 2). These states are assumed to be strongly localized; namely, enclosed by barriers of transmission coefficient $\ll 1$; hence they behave as eigenstates of their energy wells. For simplicity, we only consider one dimension.

Let us denote the transmission coefficient of the total barrier by T_g and those of the left- and right-hand barriers (see Fig. 2) by T_l and T_r, respectively. T_{min} and T_{max} indicate the smaller and larger of T_l and T_r, respectively. Each (eigen-)state then has an energy width proportional to T_{max} (and hence a lifetime inversely proportional to it) and the condition for strong localization implies that they are "exponentially narrow."[7] Nevertheless, because T_{max} is finite, if the defect is part of a virtually unbounded system it contains an unlimited number of electron states.

We first consider the ideal case of a flux of noncharged, monoenergetic carriers with energy E incident from the left of the barrier of Fig. 2 assumed to contain only one localized state of energy E_s. If E does not match the energy of the eigenstate the only effect due to the well is a (small) reduction of the barrier phase area and T_g is given by T_lT_r ($= T_{min}T_{max}$). The carrier wave function decreases exponentially and monotonically within the classically forbidden region. If the carrier energy matches that of the eigenstate, resonant tunneling occurs and the picture changes completely.[7] The wave function is now exponentially peaked at the eigenstate (Fig. 2) and there is an accumulation of probability density in the well. This implies $T_g = T_{min}/T_{max}$.

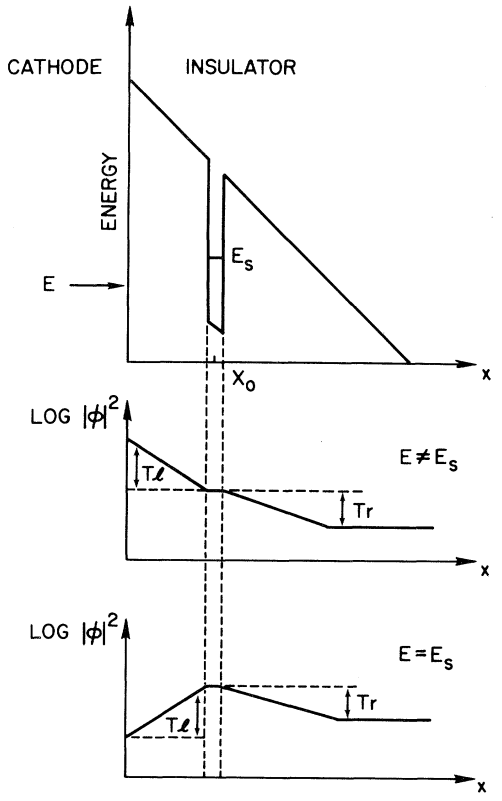

FIG. 2. Schematic representation (not drawn to scale) of the potential energy including a defect-related eigenstate and of the wave function at an energy different from and equal to that of the eigenstate.

Two straightforward consequences can then be drawn. First, for T_g to be of order of 1 it is only required that T_l and T_r are almost equal. If this is the case the barrier normally opposing carrier transport no longer does so and a short is effectively created between the electrodes. More precisely, with the current density denoted by J_s, then $J_s^{off} \propto T_{min}T_{max}$ and $J_s^{res} \propto T_{min}/T_{max}$, "off" and "at" resonance, respectively, so that the current ratio between the two cases is $J_s^{res}/J_s^{off} = 1/T_{max}^2$. When at resonance T_{min} approaches T_{max}, the local current increases dramatically thus giving rise to very large thermal effects ultimately responsible for the material failure. Second, because of the resonant probability accumulation, the eigenstate essentially behaves as a trap for tunneling carriers.

We point out three experimental difficulties that may limit the observation of these strong resonance effects: (i) Although high conductivity

can be achieved even with thick and high barriers so long as $T_l = T_r$, smaller transmission coefficients lead to longer times to accumulate the charge required for the (resonant) high-conductivity regime; (ii) if at resonance T_l and T_r are substantially different, the local current increase, though large (T_{min}/T_{max} compared to $T_{min}T_{max}$), can be too small to be noticed when measuring the total current (I_{meas}) in experimental structures; (iii) three-dimensional effects might be important. Since the eigenstate area can be roughly estimated to be of the order of a molecular defect $\sim 10^{-15}$ cm^2, while the area of experimental structures is normally $\sim 10^{-3}$ to 10^{-4} cm^2, strong resonance or a minimal number of resonant parallel paths (i.e., a sufficient concentration of defects) are required for J_s not to be negligible compared with I_{meas}.

Since the concentration of defects is expected to be strongly peaked at the interface,[8] at low fields $T_l \gg T_r$ and the eigenstates simply behave as fast carrier traps. As the field increases, however, T_l and T_r become more nearly equal (Fig. 3) until eventually the condition for breakdown (i.e., $T_g = 1$) is reached. As shown in Fig. 3, for realistic cases this requires E_{ox} in excess of 10 MV/cm in good agreement with experiments. (An anomalous current increase such as that implied by the rise in T_g to the right of the peak in Fig. 3 has been experimentally found just before breakdown.[9-11]) The possibility of insulator failures at lower fields due to eigenstates deep inside the oxide bulk exists though the time required for carrier accumulation increases exponentially with distance from the interface.

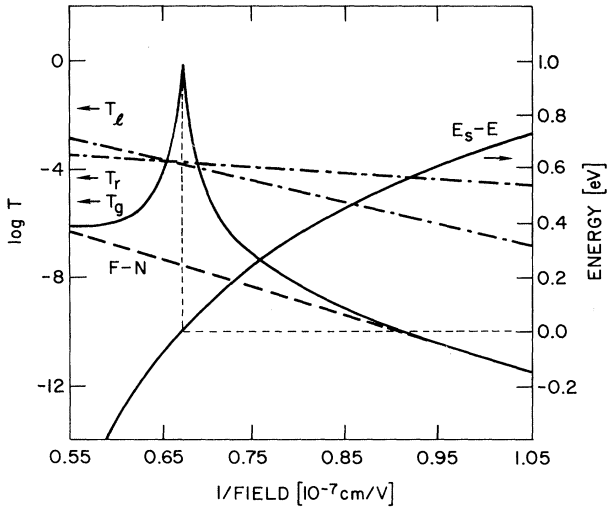

FIG. 3. Calculated transmission coefficients and energy difference for the barrier of Fig. 2 with the energy well replaced by a δ function located at 7 Å from the cathode and of strength chosen of have E_s at 2 eV below the insulator conduction band. The thick dashed line represents Fowler-Nordheim tunneling.

Because, as already mentioned, tunneling carriers are progressively trapped at the resonant states, space charge is accumulating within the oxide and a self-consistent potential must be used to describe the system time evolution. The buildup of a negative space charge raises the potential energy, and hence E_s, so that, to be maintained, the resonance condition requires carriers at a higher energy than normally available because of thermal and band-banding effects (shaded area in Fig. 1). Since the charge accumulation makes T_l and T_r larger, and for defects near the cathode more nearly equal, it increases the tunneling rate and gives rise to a self-accelerating mechanism. The finite time to reach breakdown is expected to decrease with increasing tunneling rate (and hence current) in good agreement with experiments.[3]

Because the cathode electrons are not monochromatic all the carriers lying within the energy width of a resonant state are affected. Under these conditions $J_s \propto T_{max}(T_{min}/T_{max})$, where the first factor simply represents the incoming particles within the state width: The current is then essentially proportional to T_{min} which reaches its maximum when $T_{min} = T_{max}$.

If a whole set of eigenstates is available with a distribution in both energy and space, the model still essentially holds. In particular, if the conditions for strong localization apply and the carriers do not lose energy during tunneling, we deal with an ensemble of similar single-state situations and the net result is to increase the probability of breakdown. In general, only very few eigenstates (and only one at the time) will be in the right position to fulfill the condition $T_l = T_r$, while the overwhelming majority of them must be expected to simply contribute to electron trapping.

Our final point concerns temperature effects. In this regard, the model suggests that breakdown should be accelerated by increasing temperature (T), in agreement with experimental data,[3] because as the carrier energy distribution spreads the probability of finding the right eigenstate increases. It is also worth pointing out that for any single eigenstate, J_s should decrease (slightly) with increasing T as the concentration of available carriers at a given energy decreases

as the Fermi distribution spreads out. This, actually, implies a metallic type of behavior for I_{meas} near breakdown (i.e., when it is dominated by the localized J_s). The experimental observation of such a metallic behavior and of transient resonant peaks in the oxide I-V characteristics would provide convincing support for our proposed breakdown model.

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[5]With the assumption of a trapped charge of 5 $\times 10^{-12}$ cm^{-2}, the field enhancement is ≤ 2 MV/cm. As for the estimate of the field F required to ionize a bond, extrapolating the result of D. F. Blossey [Phys. Rev. B 2, 3976 (1970)] yields $F = c^* F_i$, where $c \simeq 0.7$ and $F_i = E_b/q^* l$. Here E_b and l represent the state bonding energy and spatial extension, respectively.

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[11]The current increase is also found in experiments where short voltage pulses (≈ 1 μsec) are used to avoid substantial generation of positive charge and electron trapping.