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Instability mechanism in hydrogenated amorphous silicon thin-film transistors

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The degradation of hydrogenated amorphous silicon under an applied field is studied in an amorphous silicon thin-film transistor. A possible mechanism for metastable defect creation due to trapping of electrons at weak bonds together with a bond-switching event is investigated. The energy for the bond-switching process is assumed to be supplied thermally. The rate equation is set up and it is shown that this new model for defect creation is capable of describing the experimentally observed slow field-effect current transients at various temperatures.

Hydrogenated amorphous silicon (a-Si:H) thin-film transistors (TFT's) exhibit a serious instability problem when these devices are used in a dc mode. Although this problem may be avoided in the application of the TFT's in liquid-crystal displays by a proper addressing scheme, the instability mechanism may be deleterious after long periods of operation.

Therefore, we have investigated in this study the long time current decay phenomena in the dark at an applied gate voltage and several ambient temperatures, in order to reveal the origin of the instability mechanism. The instability of a-Si:H TFT's has also been the subject of a recent paper by Hepburn et al.,[1] and they have attributed the instability to the creation of metastable dangling-bond states close to the dielectric interface.

The purpose of this letter is to present a microscopic model for the defect creation during application of the gate field. We will show that this new model can, in principle, be used to fit the complex current decay curves observed with a straightforward experimental technique. Some interesting parameters can be extracted from the fit. In our view, no bimolecular recombination is required for the creation of metastable defects. Moreover, it will become clear that the phenomena can be described without tunneling of electrons into the gate dielectric.[2]

In the experimental situation we used a single-crystal silicon/thermal oxide/glow-discharge deposited a-Si:H metal/oxide/semiconductor field-effect transistor. Sample preparation has been described elsewhere.[3] Since thermally grown oxide can be considered as essentially trap-free, we can explicitly exclude the influence of trapping in the gate insulator. To this structure a gate voltage and a drain voltage of 10 and 0.25 V respectively were applied. The field-effect current is recorded over a period of about 10^5 s. Between each successive gate field application period the sample was annealed at 430 K for 180 min with no voltage applied. The decay curves could very closely be reproduced, which shows that the degradation is reversible (Fig. 1), as is the case with the Staebler–Wronski effect.[4] By switching off the drain voltage for a certain period of time, while maintaining the applied gate voltage, we observed that current flowing in the channel region is not a necessary condition for degradation

of the device. This can also be seen in Fig. 1. Therefore, the trapping of carriers in the a-Si:H layer due to the applied gate voltage is considered as the dominant degradation inducing mechanism.

In Fig. 2 the decay curves are displayed, recorded at temperatures of 393, 338, and 303 K. It is evident that at higher temperature the initial currents are larger, but the rates of decay are faster. This results in intersection of the curves at different times.

If a voltage is applied to the gate, electrons are drawn from the bulk of the a-Si:H layer and localized deep bandgap states will instantly become filled. Also conduction-band tail states arising from weak Si–Si bonds have a probability of capturing an electron. These bonds are likely to break when occupied by an electron, as suggested by Street and Thompson.[5] The instability of the a-Si:H network therefore depends on the degree of band bending as induced by the gate voltage.

The bond-breaking event can be described by the reaction

$$2T_4^0 + e^- \rightarrow T_4^- + T_4^0 \rightarrow T_3^- + T_3^0, \tag{1}$$
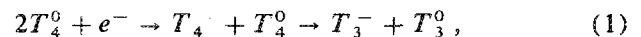
where T_4 is the notation for a fourfold coordinated Si atom and T_3 is a dangling-bond defect. The superscripts denote the charge condition. We assume that the dangling-bond states are created at an energy level below the intrinsic Fermi level, in correspondence with the commonly observed location of these states.[1,6] The additional trapped charge implies a reduction of band bending.

After reaction (1) has taken place, there are two possibilities. The first is re-emission of the electron from the T_3^- site to the conduction band or capture of a hole by that site, resulting into two neighboring neutral dangling bonds that can easily recombine. Alternatively, the T_3^0 site may capture a second electron. This is, however, not easily done, because of the neighboring negatively charged dangling bond T_3^-. As has been suggested[7] in the context of dangling-bond creation due to illumination, an essential process could be the switching of a back-bonded hydrogen atom into the position of one of the dangling-bond sites. The two dangling bonds will then become spatially isolated and a second electron can
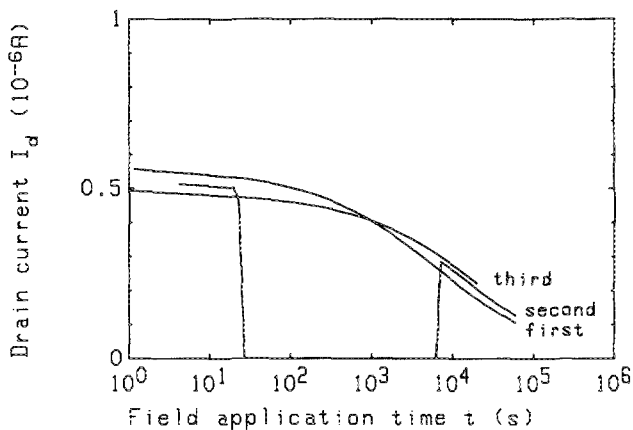
FIG. 1. Field-effect current I_d as a function of gate voltage application time t at 338 K for three successive gate voltage ($V_g = 10$ V) applications. Between individual measurements the sample was annealed at 430 K. During the second cycle, the source-drain voltage was set equal to zero for a certain period of time, showing that the degradation is independent of current flowing in the channel.

be trapped. The second trapping event further reduces the band bending.

$$T_3^0 + e^- \rightarrow T_3^- \ . \tag{2}$$
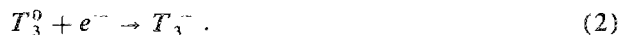
The bond-switching process requires additional energy. According to Stutzmann et al.,[7] this energy is supplied by a bimolecular recombination event. We propose that the required energy is supplied thermally, so that metastable dangling bonds can be created in the dark without recombination, as is observed here and in Ref. 1. The activation energy for this bond-switching process will be much lower than the Si–H bond energy of 3 eV and also some energy will be gained by structural relaxation. The mechanism may be similar to that existing in chalcogenide glasses.[8,9] The energy required for such a local rearrangement is determined by a potential barrier. The height of the barrier can be extracted from our experiments.

We do not want to speculate on the sequential order of the two latter steps in the process (i.e., electron capture and bond switching), but it is clear that the probabilities have to
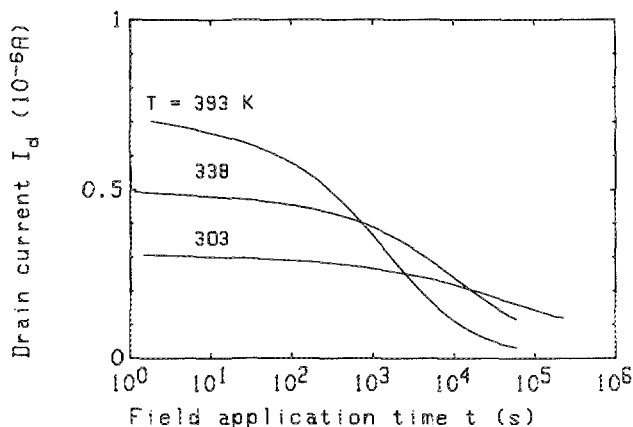

FIG. 2. Field-effect current decay curves at various temperatures T as indicated. The sample was stressed with a gate voltage of 10 V, and re-annealed after each measurement.

be multiplied. Considering the trapping of a pair of electrons at a single weak bond, and the energy barrier E_b to be overcome, the rate equation may be written as

$$\frac{dn_{\text{tr}}}{dt} = \left(\frac{n_s}{\tau}\right)^2 c_{\text{sw}} \exp\left(-\frac{E_b}{kT}\right), \tag{3}$$

where n_{tr} is the concentration of electron occupied dangling-bond states, n_s is the density of free electrons to become trapped in the interface region, τ is the lifetime of the free electrons, and c_{sw} is a constant expressing the efficiency of the bond switching. The lifetime τ is determined by the capture cross section of the traps established by the weak bonds, the thermal velocity of the electrons in the channel, and the concentration of weak bonds that are not already broken at a time t. This concentration will be denoted by $N_{\text{pot}} - 2n_{\text{tr}}$, since it takes two trapped electrons for a bond to be metastably broken, so that

$$\tau = 1/b(N_{\text{pot}} - 2n_{\text{tr}}) \ , \tag{4}$$

where N_{pot} is the concentration of the weak Si–Si bonds that can potentially be broken, and b is a constant. The concentration of weak bonds with at least one H atom at the three remaining back bonds has earlier been estimated to be 10^{18} cm^{-3}.[7] The constant b for electron trapping in Eq. (4) is expected to be extremely small, because conduction-band tail states are less localized than valence-band tail states. The small value of b can also be understood from the experimental fact that the degradation of a-Si:H in n-i-n diodes is of a much lower degree than in p-i-p samples.[10,11]

Notice that the rate equation [Eq. (3)] is of almost the same form as the one proposed by Stutzmann et al.[7] Here, a self-limiting character is established by the fact that $(N_{\text{pot}} - 2n_{\text{tr}})$ decreases continuously and τ consequently increases.

A word has to be said about possible simultaneous thermally activated annealing of dangling bonds. The resulting electron detrapping can be described by

$$\frac{dn_{\text{tr}}}{dt} = -\nu \exp\left(-\frac{E_A}{kT}\right) n_{\text{tr}} \ , \tag{5}$$

where we have assumed that all dangling bonds have an equal activation energy of $E_A = 1.5$ eV for annealing and that $\nu = 10^{-12}$ s. This annealing effect can be neglected in the range of temperatures investigated.

We have numerically integrated Eq. (3) in order to find the total number of occupied dangling bonds. The interface band bending is calculated using Poisson's equation with the usual boundary conditions. For the purpose of this paper it is not necessary to assume a specific state distribution, so that we take a uniform density of states N_{tr} throughout the band gap. The interface band bending y_s at a time t is then expressed by

$$y_s(t) = \frac{\kappa_{\text{ins}}}{d_{\text{ins}}} V_F \left(\frac{\kappa_{\text{si}}}{\epsilon_0} n_{\text{tr}}(t)\right)^{-1/2} , \tag{6}$$

where V_F is the applied gate voltage, d_{ins} is the thickness of the insulator layer, and the other symbols have their usual meaning. The resulting free-electron concentration $n_s(t)$ at the interface is approximated by

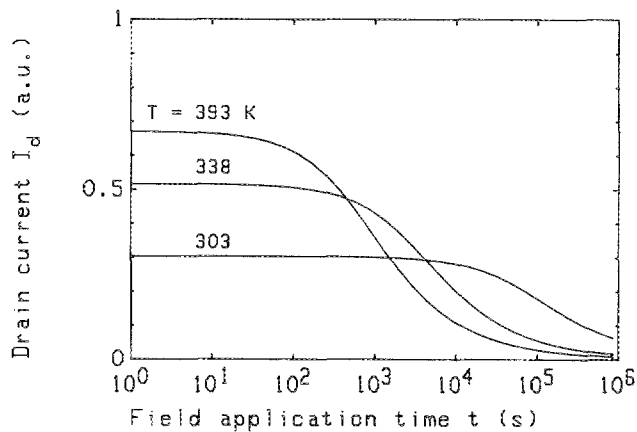$$n_s(t) = n_b \exp[y_s(t)/kT] \ , \tag{7}$$

FIG. 3. Calculated field-effect current decay curves at the same temperatures as in Fig. 2, using the trapping induced bond-breaking model. Notice the striking resemblance to the curves displayed on Fig. 2.

where n_b is the flatband intrinsic free-electron density.

The source-drain currents are proportional to $n_s(t)$ via a scaling factor containing the device geometry and the electron mobility. The calculated decay curves are shown in Fig. 3. Considering the preliminary character of this calculation, we did not attempt to fit these curves to the experimental results. The calculated set of curves closely matches the complexity of the experimentally observed temperature dependence of the decay curves. The nonadjustable parameters used here are $\kappa_{ins} = 3.9, \kappa_{si} = 11.7, d_{ins} = 110\,nm, V_F = 10$ V, and $n_b = 10^9\,cm^{-3}$. The concentration of weak bonds is assumed to be $N_{pot} = 1.5 \times 10^{18}\,cm^{-3}$. The relatively long decay times are reflected by the low value for the product $b^2 c_{sw}$ in Eq. (3) of $5 \times 10^{-54}\,cm^3\,s^{-1}$. Another interesting

parameter is the energy barrier E_b, which was found to be 0.4 eV in order to get the correct placement of intersection of decay curves. This energy may be related to the positive effective correlation energy of dangling-bond complexes in the tail states, $U_{eff} = 0.3–0.5\,eV$.[12,13]

In conclusion, we have shown that trapping of a pair of electrons at weak bond sites in the amorphous silicon network together with Si–H bond switching may be the mechanism for creation of dangling-bond states. The energy required for the bond switching is supplied thermally and amounts to 0.4 eV. The observed decay of the field-effect current is accurately described by this model.

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