

10.0 Reaction Diffusion Model: Review

Negative Bias Temperature Instability (NBTI) leads to generation of interface traps in PMOS transistors that are subjected to negative gate biases. The time evolution of interface traps follows a power law ($\Delta N_{IT} = At^n$), with a robust time exponent n in the range 0.16-0.25. The degradation mechanism has been successfully explained by Reaction-Diffusion (R-D) model, which attributes the generation of interface traps to hole assisted electro-chemical reaction. Based on the R-D model, the following equations can be used to model the time evolution of interface traps during NBTI stress:

$$\frac{dN_{IT}(t)}{dt} = k_f(N_0 - N_{IT}(t)) - k_r N_{IT}(t) N_H^0(t) \quad (1)$$

$$\frac{dN_{IT}}{dt} = D_H \left. \frac{dN_H(x,t)}{dx} \right|_{x=0} \quad (2)$$

where N_0 is the initial number of Si-H bonds, k_f and k_r are the forward and reverse reaction rates, N_H^0 is the concentration of hydrogen at Si/SiO₂ interface and D_H is the diffusion coefficient of hydrogen species (H). The reversible nature of the rate equation is critical to explain the robust power law dependence of NBTI over several orders of magnitude in time and the recovery of NBTI degradation on removal of the stress conditions.

In general, the forward and reverse rate constants k_f and k_r are large so that the forward dissociation ($k_f[N_0 - N_{IT}]$) and reverse recombination ($k_r N_{IT} N_H^0$) fluxes are much larger than the interface trap generation rate (dN_{IT}/dt). Under this condition of detailed balance, the left hand side of the rate equation can be neglected and approximated to zero. This leads to the following simple relation between the generated interface trap density and hydrogen concentration at the Si/SiO₂ interface:

$$N_{IT}(t) N_H^0(t) = k_f(N_0 - N_{IT}(t)) / k_r \approx k_f N_0 / k_r \quad (3)$$

An integral form of the R-D model can also be developed to compute the time evolution of interface traps by integrating the total hydrogen species released from broken Si-H bonds. This leads to the following equation:

$$N_{IT}(t) = \int_0^{f(t)} N_H(x,t) dx \quad (4)$$

Where $N_H(x, t)$ is the hydrogen profile and $f(t)$ is the extend of the profile at time t . For neutral hydrogen species, where the transport is dominated by diffusion, the hydrogen profile can approximated to be triangular with $f(t) \approx (2D_{HT})^{1/2}$ (see Figure 1). Integration of the profile gives the area under the curve and is given by:

$$N_{IT}(t) = (1/2)N_H^0 \sqrt{2D_{HT}t} \quad (5)$$

Substituting for N_H^0 in equation 3 and solving for N_{IT} gives the following power law relation:

$$N_{IT}(t) = (0.5 * k_f N_0 / k_r)^{1/2} (2D_{HT}t)^{1/4} \quad (6)$$

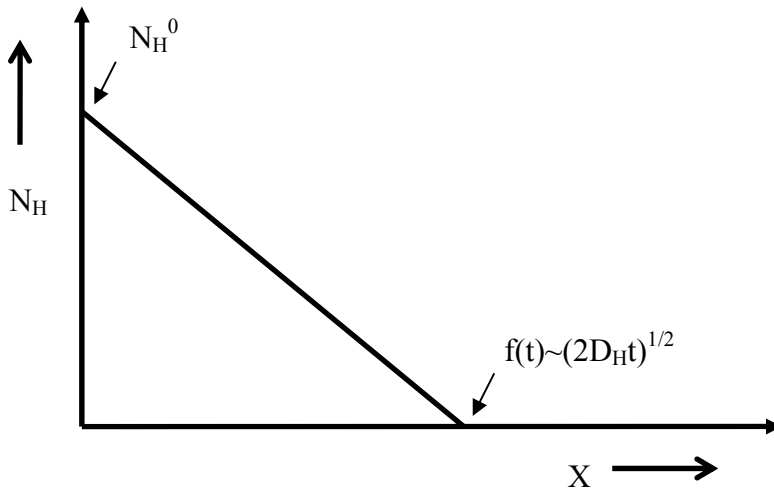


Figure 1. Profile of hydrogen diffusing species

10.1 AC Degradation

10.1.1 Motivation

Experiments carried out to monitor NBTI degradation in PMOS transistors reveal a unique feature of NBTI; that the degradation in device parameters recovers on removal of the stress conditions! Due to this recovery of degradation during the “stress off” phase, a device subjected to alternate stress/relax cycles (AC) shows lower degradation compared to a device subjected to continuous (DC) stress.

This is certainly good news, as the transistors in digital IC designs seldom undergo a continuous NBTI stress. The dynamic nature of NBTI can lead to longer device lifetimes compared to predictions based on continuous DC stress. Figure 2 shows a typical

stress/relax cycle that a transistor might undergo during its operation and the corresponding evolution of interface trap density.

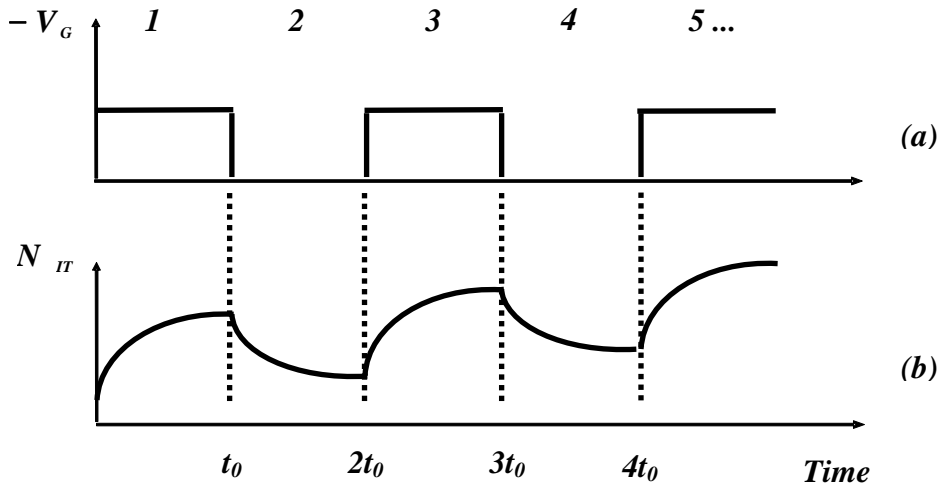


Figure 2. Transistor subjected to alternate stress and relaxation cycles. (a) Stress waveform (b) Time evolution of interface trap density

An exact expression for the time evolution of interface trap density under AC operating conditions can be obtained by solving the Reaction-Diffusion equations (Eq. 1 & 2). However this can be quite costly in terms of time and resources, given the wide range of operating conditions that the transistors might undergo (the stress waveform can be different for different transistors) and the extremely large number of transistors present in modern IC designs. To overcome this issue, an approximate analytical solution based on the Reaction-Diffusion model has been developed and is discussed in the following section.

10.1.2 Analytical Solution

Under AC operating conditions, the device undergo alternate stress/relax cycles as shown in figure 2. Each cycle is analyzed separately to derive an approximate expression for the time evolution of interface traps.

(A) Cycle 1:

The device is subjected to NBTI stress during cycle 1. The hydrogen profile during this cycle is shown in Figure 1. Equation 6 provides an analytical expression for interface trap generation during this cycle. Net interface trap density at the end of cycle 1 can be obtained by evaluating the above equation at time t_0 .

$$N_{IT}(t_0) = \left(0.5 * k_f N_0 / k_r\right)^{1/2} (2D_H t_0)^{1/4} = A t_0^{1/4} \quad (7)$$

The residue R_N after N cycles of operation is defined as fraction of net interface trap density at the end of N cycles to the interface traps generated during the first cycle. R_1 by definition is equal to 1.

(B) Cycle 2:

The device is subjected to relaxation during this cycle. The forward reaction term in Eq. 1 become zero, and no net generation of interface trap take place during this phase. The hydrogen species that were generated during cycle 1 and that are away from the interface continue to diffuse and the profile of hydrogen species spreads further to the right as shown in Figure 3.

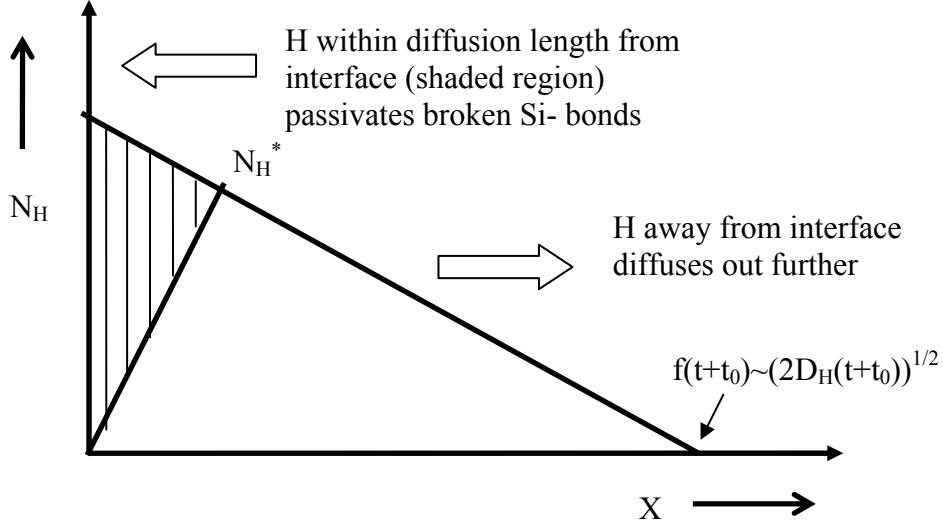


Figure 3. Hydrogen profile during cycle 2. Hydrogen that are away from the interface diffuses out further, while that are close to the interface diffuse back and re-passivate broken Si- bonds. Time t is measured from start of cycle 2

However the reverse reaction term remains non-zero during the relaxation phase. As a result, some of the hydrogen species that are closer to the Si/SiO₂ interface diffuse back to the interface and re-passivate the broken Si- bonds. This results in the reduction of interface trap density as shown in Figure 2. The number of interface traps that get annealed during the relaxation phase must be equal to the area of the shaded region and can be approximated as:

$$N_{IT}^*(t+t_0) = (1/2)\sqrt{2\xi D_H t} N_H^*(t) \quad (8)$$

Where N_H^* is the hydrogen concentration at the top edge of the profile. The factor ξ is used to differentiate between free diffusion ($\xi = 1$) and diffusion with capture ($\xi = 1/2$). A single-sided diffusion with capture is assumed in the present analysis.

Similarly, the number of un-passivated bonds should be equal to the area of the un-shaded region and is given by:

$$N_{IT}(t+t_0) = (1/2)\sqrt{2D_H(t+t_0)} N_H^*(t) \quad (9)$$

The unknown N_H^* can be eliminated by taking a ratio of the above equations.

$$\frac{N_{IT}^*(t+t_0)}{N_{IT}(t+t_0)} = \sqrt{\frac{\xi t}{t+t_0}} \quad (10)$$

As the sum of passivated and un-passivated traps at any time t should be equal to the number of interface traps generated at the end of cycle 1, we get the following expression:

$$N_{IT}(t+t_0) + N_{IT}^*(t+t_0) = N_{IT}(t_0) \quad (11)$$

Solving for $N_{IT}(t+t_0)$:

$$N_{IT}(t+t_0) = \frac{N_{IT}(t_0)}{\left(1 + \sqrt{\frac{\xi t}{t+t_0}}\right)} \quad (12)$$

The residue R_2 at the end of second cycle can be obtained as:

$$R_2 = \frac{N_{IT}(2t_0)}{N_{IT}(t_0)} = \frac{1}{\left(1 + \sqrt{\frac{(1/2)t_0}{2t_0}}\right)} = (2/3)R_1 \quad (13)$$

So roughly 1/3rd of the degradation during the first cycle has been recovered during the relaxation phase.

(C) Cycle 3:

The device is again subjected to NBTI stress during this cycle. However unlike the first cycle, the device already has some interface traps generated during the previous cycles, which needs to be accounted for. This can be done by computing the effective time t_e that the device would have taken to reach the residual degradation present at the beginning of cycle 3, starting from zero degradation (see Figure 4).

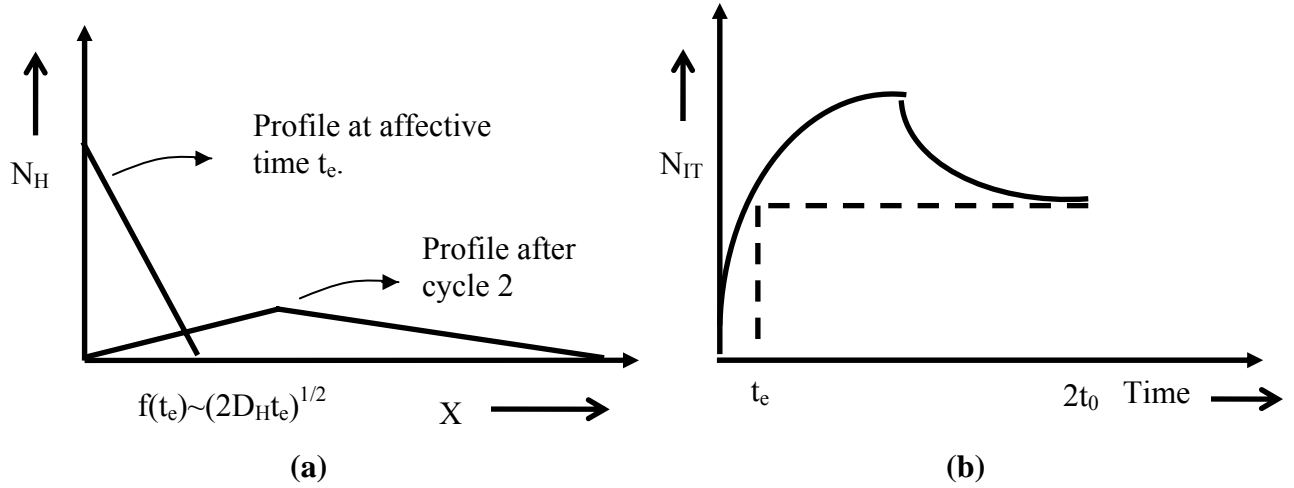


Figure 4. (a) Hydrogen profile at the end of cycle 2 and at effective time t_e . t_e is computed such that area under both profiles are same. (b) t_e can also be computed from N_{IT} by projecting the residual trap density to degradation curve in cycle 1 and finding the corresponding degradation time.

Equating the residual degradation to the degradation at a hypothetical effective time t_e , we get the following equation:

$$R_2 A t_0^n = A t_e^n \quad (14a)$$

$$t_e = (R_2)^{1/n} t_0 \quad (14b)$$

Now we can compute the net interface trap density in cycle 3 as:

$$N_{IT}(2t_0 + t) = N_{IT}(t_e + t) = A(t_e + t)^n \quad (15)$$

The residue at the end of cycle 3 can be computed by evaluating the above equation at $t=t_0$ (time t is measured from the beginning of the 3rd cycle) and taking the ratio against degradation at the end of first cycle.

$$R_3 = \frac{N_{IT}(3t_0)}{N_{IT}(t_0)} = \frac{A(t_e + t_0)^n}{A t_0^n} = \left(1 + (R_2)^{1/n}\right)^n \quad (16a)$$

$$(R_3)^{1/n} = 1 + (R_2)^{1/n} \quad (16b)$$

A similar argument can be made to compute residue at end of any odd numbered cycle and hence the above equation can be easily generalized as:

$$(R_{2k-1})^{1/n} = 1 + (R_{2k-2})^{1/n} \quad (17)$$

(D) Cycle 4:

The device is subjected to relaxation during this phase. The hydrogen profile at the beginning of this cycle has two components; one from the stress phase that immediately preceded the present cycle and another from stress phases before the immediately preceding one (see Figure 5). It is clear from Figure 5 that the hydrogen profile from stress phases other than the immediately preceding one has diffused far away from the interface and hence cannot take part in re-passivation.

Under the above conditions, Eq. 8 remains basically the same, while Eq. 9 has to be modified to account for the additional hydrogen that does not take part in passivation. The corresponding equations can be written as:

$$N_{IT}^*(3t_0 + t) = (1/2)\sqrt{2\xi D_H t} N_H^*(t) \quad (18)$$

$$N_{IT}(3t_0 + t) - N_{IT}(2t_0) = (1/2)\sqrt{2D_H(t_0 + t)} N_H^*(t) \quad (19)$$

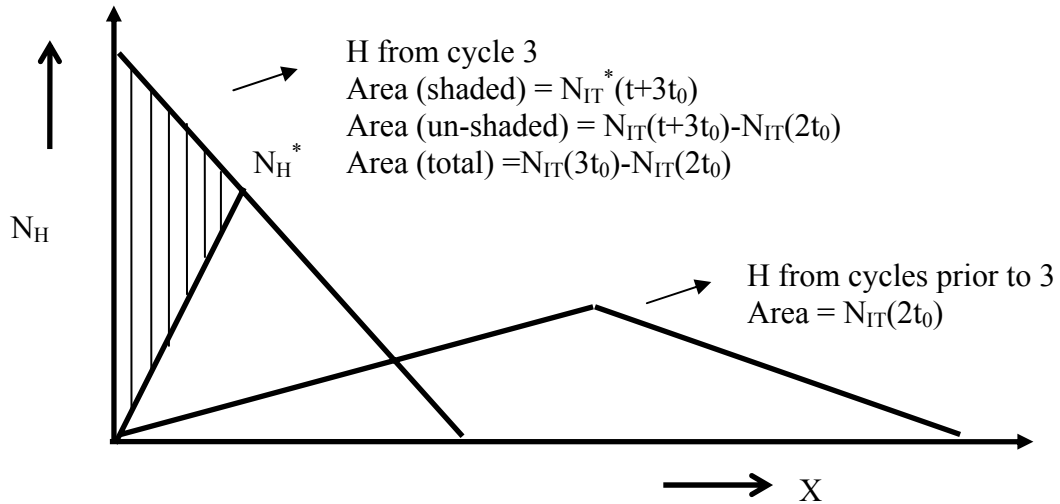


Figure 5. Two components of hydrogen during cycle 4. First component, which is from the stress phase immediately preceding present cycle, can take part in passivation. Second component, which is from cycles prior to that, has diffused away from interface and cannot contribute to passivation.

$N_H^*(t)$ can be eliminated by taking the ratio of the above equations.

$$N_{IT}^*(3t_0 + t) = \sqrt{\frac{\xi t}{t + t_0}} (N_{IT}(3t_0 + t) - N_{IT}(2t_0)) \quad (20)$$

Finally, the number of passivated and un-passivated interface traps during this cycle should be equal to the total number of traps at the beginning of the cycle.

$$N_{IT}(3t_0 + t) = N_{IT}(3t_0) - N_{IT}^*(3t_0 + t) \quad (21)$$

Substituting for $N_{IT}^*(3t_0+t)$ from equation 20 and solving for N_{IT} , we get:

$$N_{IT}(3t_0 + t) = \frac{N_{IT}(3t_0)}{1 + \sqrt{\frac{\xi t}{t + t_0}}} - \frac{\sqrt{\frac{\xi t}{t + t_0}}}{1 + \sqrt{\frac{\xi t}{t + t_0}}} N_{IT}(2t_0) \quad (22)$$

The residue at end of fourth cycle can be computed by evaluating the above expression at time t_0 (time t is measured from beginning of 4th cycle).

$$R_4 = \frac{N_{IT}(4t_0)}{N_{IT}(t_0)} = (2/3) \frac{N_{IT}(3t_0)}{N_{IT}(t_0)} + (1/3) \frac{N_{IT}(2t_0)}{N_{IT}(t_0)} = (2/3)R_3 + (1/3)R_2 \quad (23)$$

A similar argument can be applied for any even numbered cycle and hence the above equation can be easily generalized as:

$$R_{2k} = (2/3)R_{2k-1} + (1/3)R_{2k-2} \quad (24)$$

10.1.3 Discussion of analytical solution

The analytical solution described in the previous section clearly results in a series (Eq. 17 and 24), which can be solved to find out the degradation at the end of N cycles of operation. For example, the degradation at the end of 2k-1 cycles can be expanded in the form of a series as shown below:

$$R_{2k-1}^4 = 1 + R_{2k-2}^4 \quad (25a)$$

$$R_{2k-2} = (2/3)R_{2k-3} + (1/3)R_{2k-4} \quad (25b)$$

$$R_{2k-3}^4 = 1 + R_{2k-4}^4 \quad (25c)$$

The terms R_{2k-2} and R_{2k-4} can be eliminated to get the following expression between R_{2k-1} and R_{2k-3} :

$$R_{2k-1}^4 = 1 + \left[(2/3)R_{2k-3} + (1/3)(R_{2k-3}^4 - 1)^{1/4} \right]^4 = 1 + R_{2k-3}^4 \left[(2/3) + (1/3) \left(1 - \frac{1}{R_{2k-3}^4} \right)^{1/4} \right]^4 \quad (26)$$

For large number of cycles, R_{2k-3} will be much greater than unity and hence the above equation can be reduced by doing a power series expansion and collecting the first order terms.

$$R_{2k-1}^4 \approx 1 + R_{2k-3}^4 \left[1 - \frac{1}{12} \frac{1}{R_{2k-3}^4} \right]^4 \approx 2/3 + R_{2k-3}^4 \quad (27)$$

The above equation can be used recursively to express R_{2k-3} in terms of R_{2k-5} , R_{2k-5} in terms of R_{2k-7} etc., till R_1 term is reached. Summing up all such equations, we get:

$$R_{2k-1}^4 \approx \frac{2}{3}(k-1) + R_1^4 \approx \frac{2}{3}(k-1) \quad (28)$$

The above equation predicts that the AC NBTI degradation should be frequency independent. To prove this, consider two AC waveforms with different cycle times T_1 , and T_2 as shown in figure 6. The number of cycles at any given time t for these waveforms are k_1 and k_2 respectively, such that $t = k_1 T_1 = k_2 T_2$.

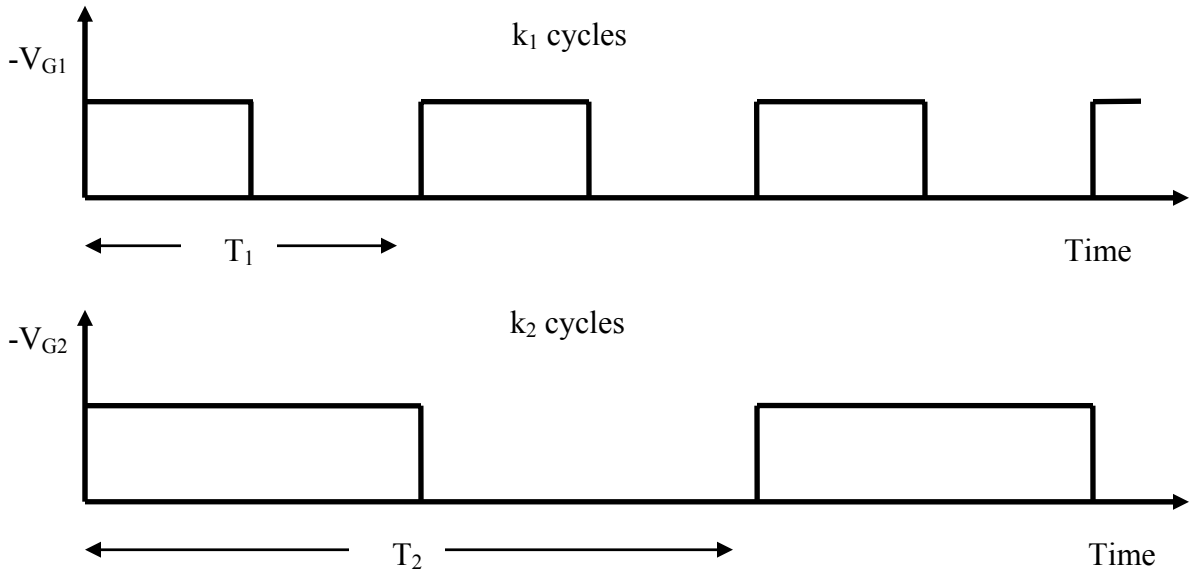


Figure 6. AC stress waveform with two different time periods T_1 and T_2 . k_1 and k_2 are number of cycles at any given time t for each waveform. $t = k_1 T_1 = k_2 T_2$

At long degradation time (*i.e.*, large k_1 , k_2), the ratio of net degradation for two waveforms is give by:

$$\frac{N_{IT1}(t)}{N_{IT2}(t)} = \frac{N_{IT1}(k_1 T_1)}{N_{IT2}(k_2 T_2)} = \frac{R_{k_1} N_{IT}(t_1)}{R_{k_2} N_{IT}(t_2)} \approx \left(\frac{k_1}{k_2}\right)^{1/4} \left(\frac{t_1}{t_2}\right)^{1/4} = 1 \quad (29)$$

Figure 7a shows the time evolution of interface traps for DC stress and for AC stress at two different frequencies. The AC degradation is found to be lower compared to DC due to recovery effects. However it can be observed that, two AC waveforms with different time periods lead to roughly the same degradation at long stress times, demonstrating the frequency independence of AC degradation. Figure 7b shows the measured interface trap density at long stress times, under DC and AC stress conditions. A similar trend is again observed in this figure, where the AC degradation is lower compared to DC, but shows no change with frequency up to the measured GHz range! The fact that the recovery effects reduces NBTI degradation when moving from DC to AC stress, but no further reduction in degradation is possible with increasing frequencies is very interesting. This is also an important result which impacts device lifetime estimation due to NBTI under actual operating conditions.

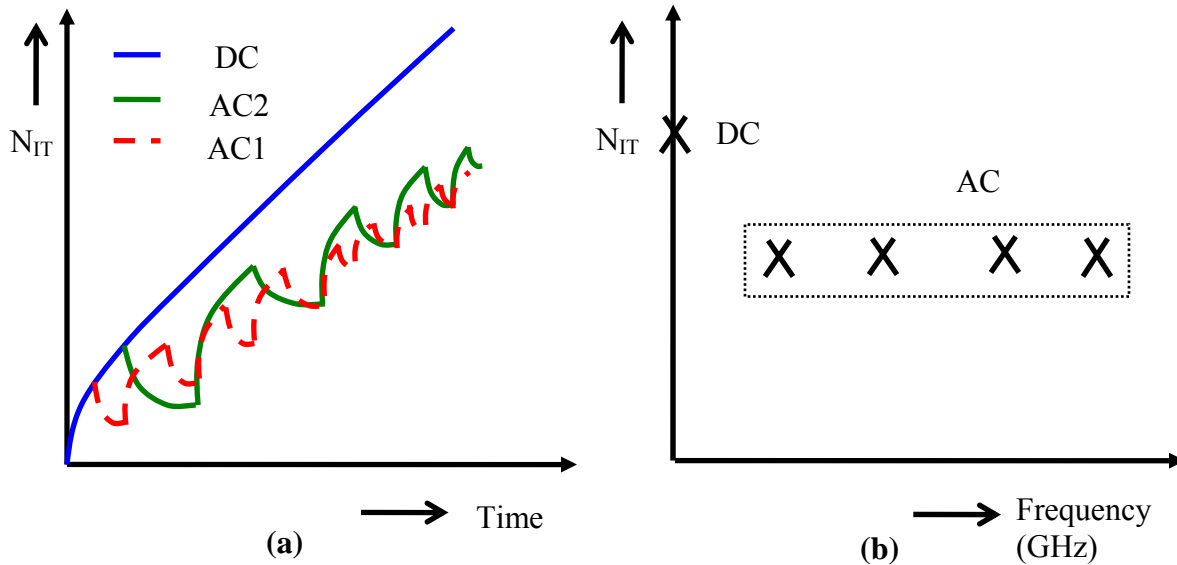


Figure 7. (a) Time evolution of interface traps under DC and AC stress conditions. (b) NBTI degradation measured at long stress times for DC and AC stress conditions.

The frequency independence of AC NBTI degradation is a non-trivial result that the analytical formulation based on the Reaction-Diffusion model predicted to happen. The success of such a prediction acts as a strong and independent validation for the model.