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<th>Title</th>
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Mind the drain from strain: effects of strain on the leakage current of Si diodes

Felipe Murphy-Armando\textsuperscript{1,*}, Chang Liu\textsuperscript{2}, Yi Zhao\textsuperscript{3}, Ray Duffy\textsuperscript{1}

\textsuperscript{1}Tyndall National Institute, University College Cork, Ireland
\textsuperscript{2}School of Electronic Science and Engineering, Nanjing University, 22 Hankou Rd, Nanjing 210093, China
\textsuperscript{3}Department of Information Science and Electronic Engineering, Zhejiang University, 38 Zheda Rd, Hangzhou 310027, China

* Email: philip.murphy@tyndall.ie

Abstract
We present a systematic study of the impact of strain on off-state leakage current, using experimental data and ab-initio calculations. We developed new models to account for the impact of strain on band-to-band tunneling and trap-assisted tunneling in silicon. We observe that the strain can dramatically increase the leakage current, depending on the type of tunneling involved. We predict that 1\% compressive strain can increase the band-to-band tunneling and Shockley Read Hall leakage currents by over 5 and 3 times, respectively.

1. Introduction
Strain is nowadays essential to enhance the on-state performance of modern and future CMOS technologies.\cite{1,2} This is achieved by improving the mobility of the device channel. However, most of the strain enhancements have focused on the on-state drive current, and little study has been devoted to the effects of strain on the off-state leakage current. The off-state leakage current originates at the reverse biased drain junction via band-to-band tunneling (BBT), Shockley-Reed-Hall (SRH) and trap-assisted tunneling (TAT).

In this work we explore both theoretically and experimentally the effects of strain on the leakage current of several Si diode samples, selected to isolate the contribution from the different tunneling mechanisms. We find that compressive strain has a dramatic effect on diodes dominated by either BBT or SRH currents, leading to a 2 to over 20 times increase in leakage current per 1\% strain.

2. Diodes and measurements
The diodes used in this study were previously fabricated\cite{3,4} with different doping concentrations in the substrate in order to isolate different leakage mechanisms, including BBT, SRH and TAT. This enabled a closer evaluation of these reverse leakage mechanisms.

The mechanical stresses were applied using a four-point wafer bending system. Using this system, we studied the effects of both uniaxial tensile and compressive strain. Details of the mechanical stress equipment can be found in Refs. 5 and 6.

3. Theory and definitions
Prior to the analysis of the experimental results, a brief review of important theory is now presented. For the sake of this discussion we assume the carriers are electrons. Generation mechanisms that lead to leakage currents are temperature and/or electric field dependent. To extract what mechanisms are dominating we need to analyze (1) the voltage dependence and (2) the temperature dependence of the leakage current. The most relevant to our study are diffusion current, direct transition thermal generation, Shockley Read Hall (SRH) generation, trap assisted tunneling (TAT), and band to band tunneling (BBT).

Diffusion current occurs when carriers, which are at a higher energy than the potential barrier, diffuse across from one side of the junction to the other. Thermal generation occurs when electrons are thermally excited, by light or heat, and make the vertical transition directly into the conduction band. SRH generation is temperature dependent, electric field dependent, and relies on the presence of deep levels in the depletion region. SRH generation occurs when an electron that is trapped in a deep level, gains energy, and climbs out of the Coulombic well. SRH dominated current is proportional to the width of the depletion region and thus V^{0.5}. TAT can be considered as SRH in the presence of an electric field, or as a combination of electron capture and tunneling through the barrier. In this case the tunneling electron uses a deep level trap in the depletion region as a stepping stone to make the transition. BBT occurs when the electric field across the junction is strong enough to propel an electron from the valence band on the p-side through the potential barrier and forbidden band gap, into the conduction band on the n-side. The BBT current $I_{bbt} \propto \exp\left(-\frac{E_g}{2F_m}\right)$, where $E_g$ is the silicon band gap (\approx 1.12 eV), and $F_m$ is the maximum electric field.\cite{7} In other words the probability of BBT increases if the electric field increases or if the tunneling distance decreases. Hurkx et al. reported that BBT...
becomes important above a local electrical field strength of \(7 \times 10^5\) V/cm. [8]

An effective method for determining the different physical components in reverse leakage currents is to perform measurements at elevated temperatures,[9,10] as some generation mechanisms are temperature dependent while others are independent. Ideal diffusion current is proportional to \(n_i^2\), so the temperature dependence behaviour is related to the temperature dependence of \(n_i\), which is

\[ n_i \propto \exp\left(-\frac{E_g}{2kT}\right). \]

Thus \(I_{\text{ideal}} \propto \exp\left(-\frac{E_g}{2kT}\right)\), and the activation energy \(E_i\) is expected to be close to \(E_g\). For direct transition thermal generation \(E_i\) is also expected to be close to \(E_c\). SRH generation is proportional to the intrinsic carrier concentration, \(n_i\). The temperature dependence behaviour is thus related to the temperature dependence of \(n_i\), so

\[ I_{\text{SRH}} \propto \exp\left(-\frac{E_g}{2kT}\right), \]

and \(E_i\) is expected to be \(E_g/2\). TAT is also temperature dependent and the extracted \(E_i\) of the current characteristics will indicate a trap level within the band gap. Usually this value is close to \(E_g/2\). In general the temperature dependence of BBT is related to the temperature dependence of \(E_g/2\). As a rule of thumb, BBT increases approximately \(x2\) for a 100 °C increase above room temperature, so \(E_i\) is quite close to 0 eV.

To compute the leakage current vs. strain, we have modified the models by A. Schenk[11] for BBT and G.A.M. Hurkx for SRH and TAT.[12] The band structure of Si under strain is calculated using the 30-band k.p model of Rideau et al.[13] The electron-phonon coupling necessary for the BBT is calculated using Density Functional Perturbation Theory as in Refs. 14-16, and available in the code Abinit.[17,18] All the parameters required for the calculation of the current have been calculated as a function of strain, where possible (p. eg, effective masses, band structure and electronic distribution). Details of our model will be available in Ref. 19.

4. Discussion

We measured and calculated the reverse bias current percent-change as a function of uniaxial stress in the (100) direction in all the samples. Figures 1 and 2 show these for samples BA2 and BA3 of Ref. 3, respectively. For such small stresses, the change in current density effected by the strain is quite large, up several 10s of percent for sample BA2.

Strain affects BBT and SRH differently, as shown in Figure 3. Notably, BBT is most sensitive to compressive stress. Under enough compressive stress, BBT can become dominant over the other tunneling mechanisms. Figure 3 also shows the predicted calculated leakage current densities at stresses normally used for enhancing the mobility of Si in transistor channels. Worryingly, the leakage current can increase by several hundred percent in both BBT and SRH dominant devices under compressive stress. Conversely, tensile stress may decrease the leakage.
5. Conclusion

We have measured the effect of uniaxial stress on the leakage current of Si diodes. The samples were chosen to elicit the different leakage current mechanisms, i.e. band to band, trap assisted and Shockley-Reed-Hall tunneling. We find that strain strongly affects the leakage current for all types of tunneling. Less than a percent strain can elicit several percent change in the leakage current. The effect is most dramatic for BBT. We have also developed a model partially based on first principles calculations to explain these results, and predict the effect of commonly used strains on the leakage current of devices. We find relatively good agreement between our calculations and the measurements, and are able to explain many of the observed features. Most importantly, we predict that compressive strain can dramatically increase the leakage current, while tensile strain suppresses it.

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References