Nondestructive inspection of SiO2/Si interface defect density by nonlinear optics

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1. Introduction

The growing demand for advanced field-effect transistors (FETs) in contemporary technology necessitates ongoing efforts to reduce device dimensions and streamline fabrication procedures.[1] Key developments, such as FinFETs and gate-all-around (GAA) FETs, have been driven by requirements for enhanced portability and improved energy efficiency.[2] As FETs continue to shrink to the nanoscale, surface and interface effects become increasingly significant. The defects arise from broken or imperfect bonds, dangling bonds, or impurities, and they play a critical role in semiconductor device performance. These defects act as centers for charge trapping and scattering, significantly degrading the device's electrical performance by affecting its speed, efficiency, and stability[3]. The interface defect density (Dit) is a crucial parameter for characterizing the quality of semiconductor-dielectric interfaces, and reducing Dit is a key goal in device fabrication processes. While accurately determining Dit are essential for predicting manufacturing yields, traditional electrical measurement methods used in current semiconductor fabrication processes can be destructive and excessively time-consuming, sometimes extending over several months. This significantly delays the optimization of manufacturing parameters. Consequently, there is an urgent need for the development of innovative, real-time methods to ensure precise doping control and accurately measure Dit, thereby facilitating improved transistor fabrication and device performance. This bottleneck underscores the need for a fast, non-destructive alternative for real-time Dit characterization.

In this study, we propose a nonlinear optical technology, second harmonic generation (SHG) as an optical approach for efficient Dit detection. SHG method is a non-destructive optical technique, is highly sensitive to the symmetric structure of surfaces and interfaces, as well as the location of defects therein, making it a useful tool for characterizing doping profiles in semiconductor materials.[4]. Based on analysing time dependent SHG (TD-SHG) signals, we develop a comprehensive model that accounts for the evolution of charge density and corresponding quantum tunnelling effects. Through this framework, we built a simplified equation that accurately fits experimental data. This advancement not only enhances fabrication efficiency but also paves the way for real-time monitoring and optimization of semiconductor devices, facilitating the development of next-generation electronic components.

2. Experimental Procedure

A TD-SHG system with a vacuum chamber is exhibited in Fig.1. This experiment has to perform in a controllable vacuum environment to tune the suitable oxygen pressure for surface charge traps on SiO_2 surface. The light source of this experiment is a femto second laser with the wavelength of 1044 nm and the duration of 100 fs. The detailed system setup and performance refers Ref.4. The sample conditions are listed in Tab.1

3. Results and Discussion

Due to performing in the high-vacuum environment and considering the thickness of the oxide layer, electron transmission and trapping at the SiO_2 surface are obviously hindered.[5] In the TD-SHG experiments, three-photon absorption excites bound electrons to a high-energy state via femto second laser pumping, which then tunnel into defect states in the SiO_2 layer, as the energy band-edge energies of Si/SiO_2, thereby forming a quasi-static DC electric field $(\overrightarrow{E_{DC}})$, as shon in Fig.2. Therefore, the third order susceptibility ($\chi^{(3)}$) dominantly changes the SHG intensity, which is defined as electric-field-induced second harmonic generation (EFISHG). For simplifying, TD-SHG signal can be expressed as Eq.(1)

$$I^{2\omega} = \left| X_2 e^{i(Im)*\frac{\pi}{180}} + E_0\left(1 - e^{-\frac{t}{t_0}}\right) + E_1\left(1 - e^{-\frac{t}{t_1}}\right)\right|^2 \tag{1}$$

Where, $X_2 e^{i(Im)*\frac{\pi}{180}}$ is the complex of $\chi^{(2)}$ and also contains the intrinsic defects in the SiO_2/Si. E_0 and E_1 contain the coefficient $\chi^{(3)}$. The time constant, t_0, is related to the interface traps and The time constant, t_1, is a function of peak power. The value of E_0 is directly related to Dit.

To obtain Dit, we measured the TD-SHG spectra of samples S1–S3 are shown in **Fig.3**. The solid lines in **Fig.3** are the curves simulated using the PINN method. According to **Eq. 1**, the parameter E_0 is expected to be proportional to the total trap density. To further validate this relationship, we performed conductance-voltage (G-V) analysis to extract Dit, with the results summarized in **Tab.1**. These findings support the feasibility of SHG-based techniques as a reliable and non-invasive alternative for interface trap characterization.

Herein, we introduce transfer learning in a physics informed neural network (PINN) to exploit the inherent similarities across datasets [6]. Fig. 4 shows the relationship between the averaged E_0 obtained by TD-SHG and Dit measured by G-V method, that is, $E_0 = \alpha \cdot \log(Dit)$. The increasing trend indicates that there is a correlation between E0 and the interface trap density Dit, suggesting that E_0 can be used as an optical indicator of Dit and is consistent with the results of electrical measurements. This approach improves computational efficiency while ensuring the physical consistency of the model, and is particularly suitable for real-time optical characterization and semiconductor component analysis.

4. Conclusions

This work demonstrates a fast, non-invasive method for Dit extraction, offering a promising alternative to conventional electrical measurements. The integration of SHG-based optical techniques with deep learning provides an efficient approach for real-time semiconductor interface characterization, paving the way for advanced non-destructive Dit measurements in semiconductor manufacturing.

Acknowledgements

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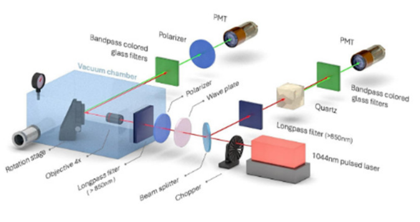

Fig. 1 TD-RSHG experiment system.

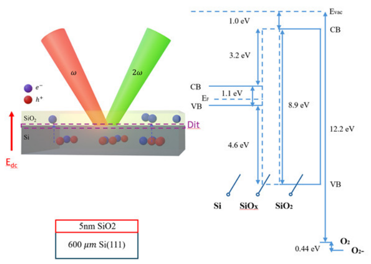

Fig. 2 TD-SHG and band diagram on SiO_2/Si.

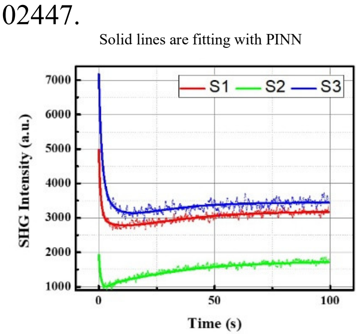

Fig.3 The TD-SHG spectra

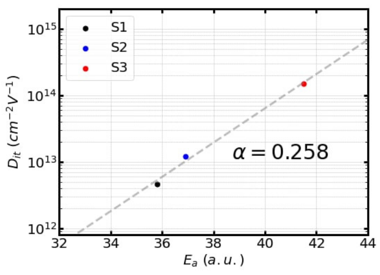

Fig. 4 The relationship between E_0 and Dit.

Sample	Treatment	Dit ($cm^{-2}V^{-1}$)	E_0(a.u.)
S1	As growth	$4.6x10^{12}$	35.8
S2	H_2O 0.5ml+200 atm CO_2, 1hr, 573K	$1.2x10^{13}$	36.9
S3	5 psi NF3+90 atm N_2, 1hr, 573K	$1.5x10^{14}$	41.5

Tab. 1 Sample treatment details, the corresponding Dit and E_0