The effects of threading dislocations and tensile strain in Ge/Si photodetector

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Abstract
Purpose – The paper aims to investigate the influences of the tensile strain and the threading dislocations (TDs) in the germanium (Ge) epitaxial layer on the performance of the Ge vertical p-i-n photodetectors on Si substrate.
Design/methodology/approach – The dark current, photo responsivity and time responsivity of detector were calculated using two-dimensional drift-diffusion device modeling and compared with experimental data.
Findings – The incorporation of the tensile strain and the reduction of the TDs in the Ge epilayer can increase the performance of the detector.
Originality/value – An optical design of detector is suggested with lower TD in the Ge buffer layer, which can exhibit superior performance.

Keywords Simulation, Optoelectronic devices, Tensile loading, Signal processing

Paper type Research paper

Introduction

Since the optical communications have been a key technology in high speed and high density signal transmission, photodetectors are important devices in optoelectronic integration technology to convert optical signals into electrical ones. Germanium (Ge) is perceived as the ideal candidate for low cost, high-performance infrared photodetectors because it has large absorption coefficient to near-infrared light $\lambda = 1{,}300\text{-}1{,}550\,\text{nm}$ and is compatible with existing silicon processing (Colace *et al.*, 2002). Additionally, the wavelengths used in the dense wavelength division multiplexing technology have been increased to cover C-band (1,528-1,560 nm) and L-band (1,561-1,620 nm) (Kartalopoulos, 2002). The tensile strained epitaxial Ge films grown on Si (100) substrates have been proposed as the solution for application in L-band telecommunications, because the tensile strain leads to the narrowing in the Ge direct band gap and the extension of the detection range toward the longer wavelength (Cannon *et al.*, 2004).

However, the lattice constant of Ge is 4 percent larger than that of Si, which could generate high densities of threading dislocations (TDs) in the relaxation Ge epilayer. This brings to the high dark currents and difficulties in the process integration of Ge/Si heteroepitaxy. So far, several papers have been devoted to high-quality Ge epilayers on Si with low TDs. One can rely on the use of optimized relaxed graded composition SiGe virtual substrate all the way to pure Ge, with the eventual use of chemical mechanical planarization steps to obtain low TDs densities (Samavedam *et al.*, 1998). Although the dark current in the Ge mesa diode, $J_s = 0.15\,\text{mA/cm}^2$, is close to the theoretical reverse saturation current, the SiGe layer is thicker and to the growth of such a layer is cumbersome and expensive. Another route relies on the deposition of a low-temperature thin Ge buffer layer, followed by the deposition of a high-temperature Ge epilayer, combined with cyclic thermal annealing treatment (Colace *et al.*, 1998). The low-temperature (330-450°C) adopted for the first Ge layer plastically relaxes the strain in the Ge film without the nucleation of any three-dimensional islands. The high temperature (600-850°C) used for the growth of the second, topmost Ge layer lowers the TD density and reduces the overall deposition time. But the dark current densities are at least two orders of magnitude lager than the former, 11 and $15\,\text{mA/cm}^2$ at 0.5 and 1 V, respectively, (Famà *et al.*, 2002).

In this paper, the performances of Ge p-i-n photodetector on Si substrate with a thin Ge buffer layer are investigated in theoretical study and the numerical simulation. The models of the tensile strain and the TDs are added in our simulation based on the 2D drift-diffusion device modeling. The tensile strain model is considering the direct band gap shrinkage according to the deformation potential theory (Van de Walle, 1989) and the absorption coefficient from the experiment (Liu *et al.*, 2005). The TD model is considering the space charge change and recombination and generation of carriers caused by the existence of dislocation center in the forbidden gap (Van *et al.*, 1968). Both of them are described in detail in the next section and the pertinent device parameters are also presented. Then, the simulation results of our simulation to the experimental data are compared, and the behaviors in relation to the tensile strain and the TDs are discussed. The good match of our simulation provides a way to effectively analyze the mechanism of detectors and suggest an optimization method for the device.

Numerical analysis models and parameters

The Ge p-i-n photodetectors on Si substrate presented in this paper are based on the conventional detectors structure with the top n-type doped layer and intrinsic layer made of epitaxial Ge, while the bottom p-type layer is the highly doped ($10^{20}\,\text{cm}^{-3}$) silicon substrate. The schematic cross section of the detector is shown in Figure 1. The thickness of the Ge

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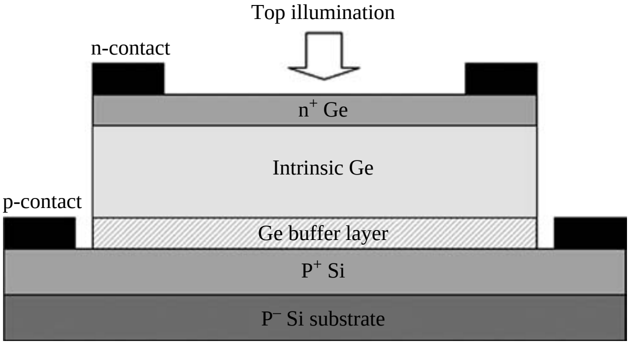
Figure 1 The structural diagram of the Ge p-i-n on Si photodetector



layer is 2.3 μm with a p-type back-ground doping below $10^{16}\,\mathrm{cm}^{-3}$. For realization of the top n contact, $10^{19}\,\mathrm{cm}^{-3}$ phosphorous was doped about 200 nm. A 60 nm relaxed Ge buffer layer is added between Si substrate and intrinsic Ge layer. The photodetector is realized as mesa diodes with diameters about 140 μm. All the device parameters are from Liu *et al.* (2005) in order to compare with the experimental results. Aluminum contact pads are added on the top of the mesa and on the substrate.

A two-dimensional simulation based on drift-diffusion model is used to study the performance of the detector, considering two major effects: the tensile strain and the TDs present in the Ge epilayer.

The tensile strain model is mainly considering the direct band gap shrinkage and the absorption coefficient increase. Experimental measurements have confirmed that the epitaxially Ge layer on Si substrate existence a tensile strain, which is generated during the cooling from the high growth temperature due to the thermal-expansion mismatch between Ge and Si (Tsui and Gershenson, 1980). The strain is dependent on the growth temperature of the Ge film, and 0.34 percent is anticipated the largest value in the case of cooling from the melting point of Ge (937°C) (Sze, 1981). Both theory (Van de Walle, 1989) and experiment (Ishikawa *et al.*, 2003) demonstrate that the tensile stress split the valence band and shrink the direct band gap of Ge. According to deformation potential theory (Van de Walle, 1989), the effect of the strain is quantitatively described as:

$$E_g^\Gamma(lh) = E_g^\Gamma(0) + 2a\left(1-\frac{c_{12}}{c_{11}}\right)\varepsilon + \frac{1}{2}b\left(1+\frac{c_{12}}{c_{11}}\right)\varepsilon + \frac{1}{2}\Delta - \frac{1}{2}\sqrt{\Delta^2 - 2a\Delta\left(1-\frac{c_{12}}{c_{11}}\right)\varepsilon + 9b^2\left(1+\frac{c_{12}}{c_{11})}\right)^2\varepsilon^2} \tag{1a}$$

$$E_g^\Gamma(hh) = E_g^\Gamma(0) + 2a\left(1-\frac{c_{12}}{c_{11}}\right)\varepsilon - b\left(1+\frac{2c_{12}}{c_{11}}\right)\varepsilon \tag{1b}$$

where $E_g^\Gamma(lh)$ and $E_g^\Gamma(hh)$ are the band gaps from the maxima of light hole and heavy hole valence bands to the bottom of the conduction band at $k = 0$ in the band diagram under in-plane strain ε, respectively. $E_g^\Gamma(0) = 0.80$ eV is the direct band gap of unstrained Ge at room temperature; $a = -0.9$ eV and $b = -2.6$ eV are the deformation potential constants and $\Delta = 0.289$ eV is the spin-orbital splitting energy for Ge (Liu *et al.*, 2004). The absorption coefficient, due to the direct transition, is proportional to $\sqrt{\hbar\omega - E_g}$, where $\hbar\omega$ is the photon energy. This means an increase in the absorption coefficient and a shift in the absorption edge towards the lower energy due to the band-gap narrowing. Here, we take the experiment data of absorption coefficient from Liu *et al.* (2005) into the simulation.

For a wide variety of electronic and optoelectronic device applications, particularly for photodetectors, TDs are deleterious for physical performance. Despite there has been a substantial experimental method to reduce TD densities in recent years, there are a great number of TDs exist in Ge epitaxial layer. As we know, the associated energy of the TD lies in the forbidden gap and exchange charge with the conduction and valence bands through the thermal generation and recombination of carriers as the intermediate states. In the Ge material, the TDs act as acceptor-like traps and its energy level is found to be 0.35 eV below the conduction band. In this model, the space charge term caused by TDs $Q_p = qN_pF_p$ is added directly into Poissons' equation in addition to the ionized acceptor impurities. N is the density of dislocation charge; F is the probability of occupation, which is as follows (Simmons and Taylor, 1971):

$$F_p = \frac{v_n\sigma_n n + e_p}{e_n + v_n\sigma_n n + v_p\sigma_p p + e_p} \tag{2}$$

where v_n and v_p are the thermal velocities for electrons and holes, σ_n and σ_p are the carrier capture cross sections for electrons and holes, e_n and e_p are the emission probabilities for electrons and holes. Additionally, the related recombination rate and mobility in the carrier continuity equations also be modified when take into account of the dislocation existence in our simulation.

Results and discussion

Numerical analysis model and fitting material parameter described in above section provide a means for estimating the performance of strained Ge photodetectors on Si substrate with a thin relaxed Ge buffer. In this section, the simulated results and experimental outputs (Liu *et al.*, 2005) are compared in the same parameters and structure as shown in Figure 1, and the effects of the dislocation and strain are discussed in detail. In order to better compare, the parameters are listed in Table I for four detectors with different TD densities and tensile strain. Detector A has the same TD densities as A′ but different tensile strain in the Ge epilayer, and the parameters of both are taken from the literature (Liu *et al.*, 2005). Detectors B and C have the same tensile strain as A, however the TD densities for B is equivalent to the experimental data from without cyclic annealing processing and C is with an optical design of the lower TD density only in buffer layer.

Table I The parameters of detectors

Detectors ID	A	A′	B	C
Tensil strain (percent)	0.25	0.2	0.25	0.25
TD density in active layer (cm^{-2})	1.6×10^7	1.6×10^7	1×10^9	1.6×10^7
TD density in buffer layer (cm^{-2})	2.4×10^{11}	2.4×10^{11}	2.4×10^{12}	2.4×10^{10}

Figure 2 shows the computed dark current densities of detectors as a function of bias, and includes the comparison between our simulated results and experimental data. As the tensile strain heightened the dark current density is increased (compare with A and A′) since the in-build electric field is increased in the Ge region by the narrowing direct band gap, but this effect is not too severe and obvious. For detector A, simulation results of the dark current density are 12 and 19 mA/cm^2 at 0.5 and 2 V, respectively, and well fit the experiment data. The dark current increases with the inverse voltage reveals that the contributions to the dark current come from the bulk effect, carrier generation in the intrinsic-Ge layer, while underlines the negligible contribution of surface leakage at low bias voltage. Therefore, the dark current is mainly attributable to defects exist in the Ge epitaxial layer. The dependence of the dark current on TD densities in the Ge epilayer with same tensile strain is also analyzed by simulation shown in Figure 2. The decreasing TD densities in the Ge epilayer significantly reduce dark current, and influence the forward bias characteristics of the detector as the ideality factor decreases (compare with A and B). The mismatch with the experiment data of the forward currents is due to the neglect of the Ohmic losses. Especially, with only decreasing TD densities in the Ge buffer layer, the current reduces obviously (compare with A and C), because that the $p^- - n^+$ junction is located at the Si/Ge interface and the thin Ge buffer layer is almost positioned inside the depletion region. The contribution of the dark current is dominant from the carriers generated by TDs in Ge buffer layer.

The simulation results of photo responsivities as the function of the bias are shown in Figure 3. The light with optical power of 10 mW at 1,550 nm is incident from the top side of the detector, and the reflectivity is 0.12 in the simulation. A larger improvement was obtained from the 0.25 percent tensile strained detector with responsivity close to 580 mA/W compared to 0.2 percent tensile strained detector (compare of A and A′). With the tensile strain increased the responsivity is increased as expected, and can be explained by the band gap narrowing coupled with the absorption coefficient improvement. The band gap is narrowed from 0.77 eV of detector A′ to 0.76 5eV of detector A, and the absorption coefficient is increased from 3,360 to 4,580/cm in simulation. There is no obviously separation between the responsivities for different TDs in the Ge epilayer due to the recombination current is small compared with the photo generation current carriers. For a better understanding of the effect of tensile strain, the simulated spectra photo responsivities for different tensile strain of the detector are plotted in the wavelength range of 1,500-1,600 nm, as shown in Figure 4. The simulation results are almost similar to the experimental data, and both of them indicate that the strain enhancement increases the responsivity in the C-band and extends the detection range to cover the whole L-band.

Figure 2 Current densities versus the applied voltage

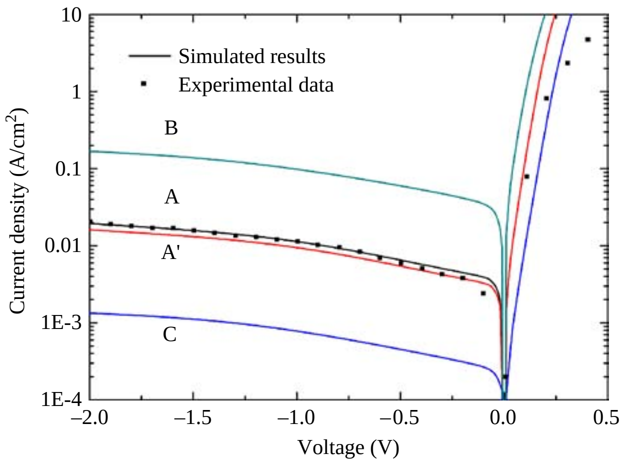
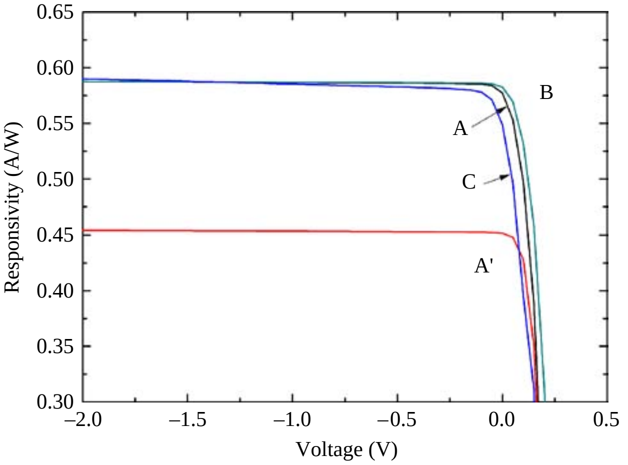


Figure 3 Photo responsivities versus applied voltage at wavelength of 1,550 nm



To properly ponder the influence of the tensile strain and TDs to the transient behavior of the detector, the time responses of detectors under pulse illumination are simulated and shown in Figure 5. A pulsed light of 100 ps full width at half maximum (FWHM) at wavelength of 1,550 nm was illuminate in top side, and the FWHM of the response current is 125 ps calculated at a reverse bias of 1V for detector A. From the figure we can see that the FWHM decreased to 140 ps with the increased TD density in whole Ge epilayer (compare of the A and B). The tensile strain and TD in the buffer layer exerts little influence on the time responsivity.

Figure 4 Spectral responsivities with different tensile strains in the Ge epilayer

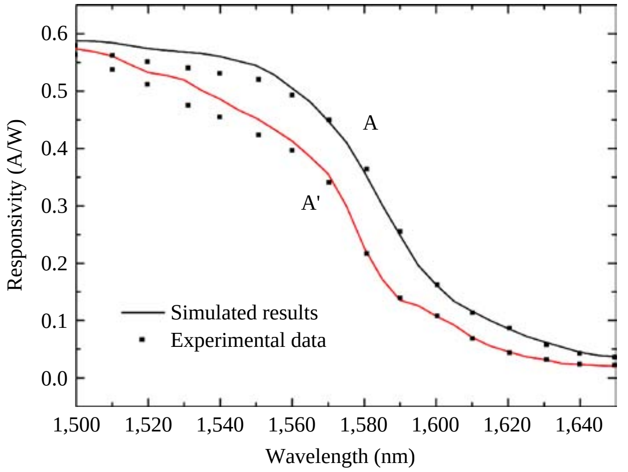
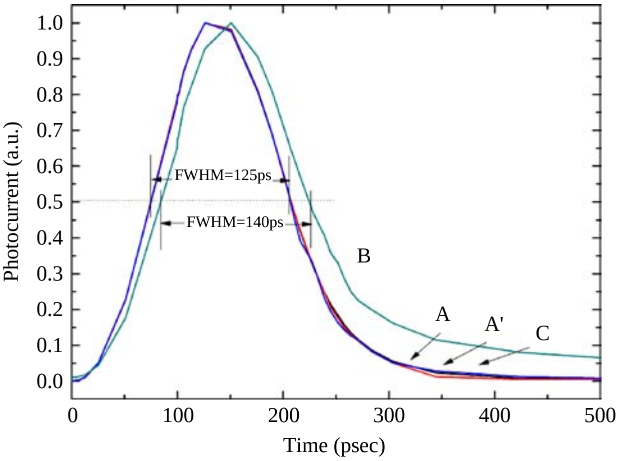


Figure 5 Time responses to 100 ps FWHM optical pulse at 1,550 nm



Because the photogeneration is near the surface region in the Ge layer in this structure, there are two major limitations on the speed of p-i-n photodetectors, the transit time through the depletion region and the diffusion time. The transit time is mainly dependent on the electric field, while the diffusion time is proportional to the intrinsic Ge layer thickness. The TD in the Ge epilayer increases the scatter to the carriers and reduces the electric field, and so delays the response time in case of constant Ge epilayer thickness.

These results show that the high-quality Ge epilayer as well as the larger tensile strain is crucial in improving the Ge p-i-n photodetetors on Si substrate performance from our simulation. Additionally, the TDs present in the Ge buffer are significantly influence the dark current, which is determine the signal-to-noise ratio of the detector. A modified design as detector C is considering a thin low TDs Ge buffer has the superior performance in our simulation, the dark current density of which is 0.001 A/cm^2 at -2V with cutting an order of magnitude of TD density in Ge buffer layer.

Conclusion

In this paper, the performance of the Ge vertical p-i-n photodetectors on Si substrate is investigated considering the influences of the tensile strain and the TDs in the Ge epitaxial layer. The simulated results for the dark currents, photo responsivities and time responsivities of this detector obtained using two-dimensional drift-diffusion device modeling are reported, and the results are good agreement with the reference experimentally data. The tensile strain increases the responsivity of the detector and extends the detective wavelength in L-band as expected. The high density of TDs in Ge epilayer seriously increases the dark current and response time of the detectors. And in our simulation study, the decrease of the TD density in the thin Ge buffer layer can effectively reduce the dark current because they are located in the depletion region of the Ge/Si heterojunction.

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